Attentive Graph Neural Networks
for Few-Shot Learning

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Abstract

Graph Neural Networks (GNN) has demonstrated the superior performance in many challenging applications, including the few-shot learning tasks. Despite its powerful capacity to learn and generalize from few samples, GNN usually suffers from severe over-fitting and over-smoothing as the model becomes deep, which limit the model scalability. In this work, we propose a novel Attentive GNN to tackle these challenges, by incorporating a triple-attention mechanism, i.e., node self-attention, neighborhood attention, and layer memory attention. We explain why the proposed attentive modules can improve GNN for few-shot learning with theoretical analysis and illustrations. Extensive experiments show that the proposed Attentive GNN outperforms the state-of-the-art GNN-based methods for few-shot learning over the mini-ImageNet and Tiered-ImageNet datasets, with both inductive and transductive settings.

1 Introduction

Deep neural networks, e.g., Convolutional Neural Networks (CNNs), have been widely applied and achieve superior results on computer vision tasks such as image classification, segmentation, etc. The conventional approach is by supervised learning over a large-scale labeled dataset for the task, thanks to the scalability of CNNs. However, for some tasks with only a few samples available, training a generic and highly-flexible deep model may result in over-fitting and thus fail to generalize. Such a challenge presents in few-shot learning [4], in which a classifier is learned to predict the labels of the query samples using only a few labeled support samples of each class. The training set contains only data of classes different from the test. Various methods have been recently proposed for few-shot learning [31, 26, 28, 6], including the popular meta-learning framework [31] based on episodic training. Meta-learning splits the training set into a large number of sub-tasks to simulate the testing task, which are used to train a meta-learner to generalize knowledge for unseen classes. Another approach for few-shot learning is by metric learning [31, 26, 28], which aim to learn a generalizable feature embedding to fully exploit correlation between samples and classes.

Most of the proposed few-shot learning methods are based on CNNs, which are effective at modeling local and Euclidean-structure data properties. However, in few-shot learning tasks, CNNs have limitations in exploiting the intra- and inter-class relationships that are typically non-local and non-Euclidean structured. Therefore, more recent works focused on the Graph Neural Network (GNN) or Graph Convolutional Networks (GCN). The paper [6] first applied the dense-GNN for few-shot learning. Transductive Propagation Network (TPN) [18] introduced transductive mechanism to utilize

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entire query set for transductive inference. Moreover, Edge-GNN \cite{12} considered propagation of edge label information to model the intra-class similarity and the inter-class dissimilarity. AdarGCN \cite{34} proposed a new few-shot setting called FSFSL and proposed an adaptive aggregation GCN to remove the noise from support images crawled from the web. However, several works \cite{16, 25} reported the over-fitting and over-smoothing issues when learning GNN models that become deep (i.e., poor scalability), as applying GCN or GNN is a special form of Laplacian smoothing, which averages the neighbors of the target nodes. Very recent work \cite{25} attempted to alleviate these obstacles via randomly dropping graph edges in training, showing promising improvement for node classification. To the best of our knowledge, no work to date has addressed these issues on GNN-based methods for few-shot learning using graph attention mechanism.

In this work, we propose a novel Attentive GNN for highly-scalable and effective few-shot learning. We incorporate a novel triple-attention mechanism, i.e., node self-attention, neighborhood attention, and layer memory attention, to tackle the over-fitting and over-smoothing challenges towards more effective few-shot image classification. Specifically, the node self-attention exploits inter-node and inter-class correlation beyond CNN-based features. Neighborhood attention modules impose sparsity on the adjacency matrices, to attend to the most related neighbor nodes. Layer memory attention applies dense connection to earlier-layer “memory” of node features. Furthermore, we explain how the proposed attentive modules help GNN generate discriminative features, and alleviate over-smoothing and over-fitting, with feature visualization and theoretical analysis. We conduct extensive experiments showing that the proposed Attentive GNN outperforms the state-of-the-art GNN-based methods for few-shot image classification over the mini-ImageNet and Tiered-ImageNet datasets, under both inductive and transductive settings.

2 Related Work

GNN for Few-shot Learning. GNN \cite{1, 3} was first proposed for learning with graph-structured data and has proved to be a powerful technique for aggregating information from neighboring vertices. GNN was first used for few-shot learning \cite{6}, which aims to learn a complete graph network of nodes with both feature and class information. Based on episodic training mechanism, meta-graph parameters were trained to predict the label of a query node on the graph. Then TPN \cite{18} introduced transductive setting into few-shot learning. Based on relation information between nodes, TPN constructs a top-k graph with a close-form label propagation. In addition to utilizing node label information, EGNN \cite{12} considers edge information for directed graph by defining both class and edge labels for fully exploring the internal information of the graph.

Attention Mechanism. Attention Mechanism \cite{29} aims to focus more on regions which are more related for tasks and less on unrelated regions by learning a mask matrix or a weighted matrix. In particular, self-attention \cite{2, 22} considers the inherent correlation (attention) of the input features itself, which is mostly applied in graph model. For node classification, Graph Attention Network (GAT) \cite{30} uses a graph attention layer to learn a weighted parameter vector based on entire neighborhoods to update node representation. By utilizing graph convolution, SAGPool \cite{14} selected the top \( kN \) nodes to generate mask matrix for graph pooling. Moreover, attention mechanism is also utilized for few-shot learning \cite{8, 11, 35}. Cross Attention Module (CAM) \cite{8} generated cross attention maps for each pair of nodes to highlight the object regions for classification. Considering the attention between query sample with each support class, Category Traversal Module (CTM) \cite{15} finds task-relevant features based on both intra-class commonality and inter-class uniqueness in the feature space. Inspired by non-local block, Binary Attention Network \cite{11} considered a non-local attention module to learn the similarity globally. For few-shot fine-grained image recognition, MattML \cite{35} uses attention mechanisms of the base learner and task learner to capture discriminative parts of images.

3 Attentive Graph Neural Networks

3.1 Preliminaries

GNN \cite{27, 1, 3} are the neural networks based on a graph structure \( G = (V, E) \) with nodes \( V \) and edges \( E \). Different from the classic CNNs that mainly exploit the local features (e.g., image patch textures, sparsity) for representation, GNN regards each sample (e.g., image) as a vertex on the graph,
and focuses on mining the important neighborhood information of each node, which are critical to construct discriminative and generalizable features for many tasks, e.g., node classification, few-shot learning, etc. To be specific, considering a multi-stage GNN model, the output of the \(k\)-th GNN layer can be represented as

\[
X^{(k+1)} = F_k(X^{(k)}, W^{(k)}) = \rho \left( \hat{A}^{(k)} X^{(k)} W^{(k)} \right)
\]

where \(X^{(k)} \in \mathbb{R}^{V \times d_k}\) denotes the input feature and \(x_i^{(k)}\) denotes the feature of node \(i\) in the \(k\)-th layer, with \(V\) and \(d_k\) being the number of nodes and feature dimension at the \(k\)-th layer. Besides, \(\hat{A}^{(k)} \in \mathbb{R}^{V \times V}\) is the weighted adjacency matrix, \(W^{(k)} \in \mathbb{R}^{d_k \times d_{k+1}}\) is the trainable linear transformation, and \(\rho\) denotes a non-linear function, e.g., ReLU or Leaky-ReLU.

There are different ways to construct the adjacency matrix \(A^{(k)}\), e.g., \(A_{i,j}^{(k)}\) indicates whether node \(i\) and \(j\) are directly connected in the classic GCN \(\Pi\). Besides, \(A_{i,j}^{(k)}\) can be the similarity or distance between node \(i\) and \(j\), i.e., \(A_{i,j}^{(k)} = f_\theta(\phi(x_i^{(k)}), \phi(x_j^{(k)}))\), where \(\phi\) denotes the node feature embedding, and the parameter \(\theta\) can be fixed or learned. One popular example is to apply cosine similarity as the similarity metric, while a more flexible method is to learn a multi-layer perceptron (MLP) as the metric, i.e., \(f_\theta(x_i^{(k)}, x_j^{(k)}) = \text{MLP} \left( \|x_i^{(k)} - x_j^{(k)}\|, \sigma_j \right)\), where \(|\cdot|\) denotes the absolute function. More recent works applied Gaussian similarity function to construct the adjacency, e.g., TPN \(\Pi\) proposed the similarity function as \(A_{i,j} = \exp(-0.5d(\phi(x_i)/\sigma_i, \phi(x_j)/\sigma_j))\), with \(\sigma\) being an example-wise length-scale parameter learned by a relation network of nodes used for normalization.

Different from the classic GNNs, the recently proposed GAT \(\Pi\) exploited attention mechanism amongst all neighbor nodes in the feature domain, after the linear transformation \(W^{(k)}\) and computes the weighted parameter \(\alpha\) based on attention coefficients for graph update as

\[
x_i^{(k+1)} = \rho \left( \sum_{j \in \mathcal{N}_i} \alpha_{ij} x_j^{(k)} W^{(k)} \right)
\]

where \(\mathcal{N}_i\) denotes the set of the neighbor (i.e., connected) nodes of \(x_i\). GAT considers self-attention on the nodes after the linear transformation \(W\). With a shared attention mechanism, GAT allows all neighbor nodes to attend on the target node. Moreover, GAT can generate a more powerful feature representation with an extension of multi-head attention. However, GAT only considers the relationship among neighbors in the same layer while it fails to utilize the layer-wise information, which may lead to over-smoothing. Furthermore, GAT just applies self-attention based on node features, while ignoring label information.

### 3.2 What We Propose: Attentive GNN

We propose an Attentive GNN model which contains three attentive mechanisms, i.e., node self-attention, neighborhood attention, and layer memory attention. Fig.\(\Pi\) shows the end-to-end pipeline of Attentive GNN for the few-shot learning problem. We discuss each of the attention mechanisms, followed by how Attentive GNN is applied for few-shot learning.

#### 3.2.1 Node Self-Attention

Denote the feature of each sample \(i\) (i.e., node) as \(x_i \in \mathbb{R}^d\), and the one-hot vector of its corresponding label as \(y_i \in \mathbb{R}^N\), where \(d\) is the feature dimension, \(N\) is the total number of classes, and \(1 \leq i \leq V\). The one-hot vector sets only the element corresponding to the ground-truth category to be 1, while the others are all set to 0. We propose the node self-attention to exploit the inter-class and inter-sample correlation at the initial stage. Denote the sample matrices and label matrices as

\[
X = [x_1, x_2, \ldots, x_V]^T \in \mathbb{R}^{V \times d}, \quad Y = [y_1, y_2, \ldots, y_V]^T \in \mathbb{R}^{V \times N}.
\]

The first step is to calculate the sample and label correlation matrices as

\[
C_X = \text{softmax}(XX^T \odot M), \quad C_Y = \text{softmax}(YY^T).
\]

Here, \(M\) is the normalization matrix defined as \(M(i,j) = \left(\|x_i\|_2 \|x_j\|_2\right)^{-1}\), \((\odot)\) denotes a point-wise product operator, and \(\text{softmax}(-)\) denotes a row-wise softmax operator for the sample and label.
correlation matrices. Take the sample correlation as an example, and let $P = XX^T \in \mathbb{R}^{V \times V}$. The row-wise softmax operator is defined as

$$C^X(i, j) = \frac{\exp \{P(i, j)\}}{\sum_{k \in \mathcal{N}_i} \exp \{P(i, k)\}}$$  \hspace{1cm} (5)$$

where $\mathcal{N}_i$ denotes the set of nodes that are connected to the $i$-th node.

The proposed node self-attention module exploits the correlation amongst both sample features and label vectors, which should share the information from different perspectives for the same node. Thus, the next step is to fuse $C^X$ and $C^Y$ using trainable $1 \times 1$ kernels as

$$C^f = \text{fusion}_\tau \left( (C^X, C^Y) \right) \in \mathbb{R}^{V \times V}$$  \hspace{1cm} (6)$$

where $[C^X, C^Y]$ denotes the attention map concatenation, and $\tau$ is the kernel coefficients. With the fused self-attention map, both the feature and the label vectors are updated on the nodes:

$$\tilde{X}^{(1)} = C^f X, \quad Y^{(1)} = \alpha Y + (1 - \alpha) C^f Y$$  \hspace{1cm} (7)$$

where $\alpha \in [0, 1]$ is a weighting parameter. Different from the feature update, the label update preserves the initial labels, which are the ground truth, in the support set, using the weighting parameter $\alpha$ to regularize the label update. The updated sample features $\tilde{X}^{(1)}$ and labels $Y^{(1)}$ are concatenated to form the node features $X^{(1)}$.

### 3.2.2 Graph Neighbor Attention via Sparsity

Similar to various successful GNN framework, the proposed Attentive GNN applies a MLP to learn the adjacency matrix $A_{ij}$ for feature updates. When the GNN model becomes deeper, the risk of over-smoothing increases as GNN tends to mix information from all neighbor nodes and eventually converge to a stationary point in training. To tackle this challenge, we propose a novel graph neighbor attention via sparsity constraint to attend to the most related nodes:

$$\hat{A}^{(k)} = \arg \min_{A^{(k)}} \left\| A^{(k)} - U^{(k)} \right\|_F$$

$$\text{s.t. } U^{(k)}(i, j) = \text{MLP}^{(k)} \left( \left| x_i^{(k)} - x_j^{(k)} \right| \right), \quad \left\| A_i^{(k)} \right\|_0 \leq \beta V \forall i, j.$$  \hspace{1cm} (8)$$

Here, $A_i^{(k)} \in \mathbb{R}^{1 \times V}$ denotes the $i$-th row of $A^{(k)}$, $\beta \in (0, 1]$ denotes the ratio of nodes maintained for feature update, and $V$ is the number of graph nodes. With the $\ell_0$ constraint, the adjacency matrix $\hat{A}^{(k)}$ has up to $\beta V$ non-zeros in each row, corresponding to the attended neighbor nodes. The solution to (8) is achieved using the projection onto a $\ell_0$ unit ball, i.e., keeping the $\beta V$ elements of each $U_i^{(k)}$ with the largest magnitudes. Since the solution to (8) is non-differentiable, we apply alternating projection for training, i.e., in each epoch $U^{(k)}$'s are first updated using back-propagation, followed by applying (8) to update $\hat{A}^{(k)}$ which is constrained to be sparse.

### 3.2.3 Layer Memory Attention

To avoid the over-smoothing and over-fitting issues due to “over-mixing” neighboring nodes information, another approach is to attend to the “earlier memory” of intermediate features at previous layers. Inspired by DenseNet [9], JKNet [33], GFCN [10] and few-shot GNN [6], we densely connect the
output of each GNN layer, as the intermediate GNN-node features maintain the consistent and more general representation across different GNN layers.

The proposed attentive GNN applies the transition function based on [1]. In addition, we utilize graph self-loop i.e., identity matrix $I$ to utilize self information as

$$F_k(X^{(k)}, W^{(k)}) = \rho ([A^{(k)} X^{(k)} \parallel I X^{(k)}] W^{(k)})$$  
(9)

where $\parallel$ means row-wise feature concatenation and $W^{(k)} \in \mathbb{R}^{d_k \times m}$. Furthermore, instead of using $F_k(X^{(k)}, W^{(k)}) \in \mathbb{R}^{V \times m}$ directly as the input node feature at the $(k+1)$-th layer, we propose to attend to the “early memory” by concatenating the node feature at the $k$-th layer as

$$X^{(k+1)} = [X^{(k)}, F_k(X^{(k)}, W^{(k)})] \in \mathbb{R}^{V \times (d + N \times km)}.$$  
(10)

With the proposed layer memory attention module, though the node feature increases as the mode becomes deep, there is only $V \times m$ new features introduced in a new layer, while the other features are attended to the early memory.

3.3 Application: Few-Shot Learning Task

**Problem Definition** We apply the proposed Attentive GNN for the few-shot image classification tasks: Given a large-scale and labeled training set with classes $C_{\text{train}}$, and a few-shot testing set with classes $C_{\text{test}}$ which are mutually exclusive, i.e., $C_{\text{train}} \cap C_{\text{test}} = \emptyset$, we aim to train a classification model over the training set, which could be applied to the test set with only few labeled information. Such test is called the $N$-way $K$-shot task $T$, where $K$ is the number of labeled samples which is often set from 1 to 5, i.e., the testing set contains a support set $S$ which is labeled, and a query set $Q$ to be predicted, denoted as $T = S \cup Q$. The $N$ and $K$ are both very small for few-shot learning.

**Attentive Model for Few-Shot Learning** Following the same strategy of episodic training [31] and meta-learning framework, we simulate $N$-way $K$-shot tasks which are randomly sampled from the training set, in which the support set includes $K$ labeled samples (e.g., images) from each of the $N$ classes and the query set includes unlabeled samples from the same $N$ classes. Each task is modeled as a complete graph [6], in which each node represents an image sample and its label. The objective is to learn the parameters of Attentive GNN using the simulated tasks, which is generalizable for an unseen few-shot task.

**Loss Function** For each simulated few-shot task $T_{\text{train}}$ with its query set $Q = \{(x_i, y_i)\}_{i=1}^Q$, the parameters of the backbone feature extractor, self-attention block $\tau$, and GNNs $\{\text{MLP}^{(k)}, W^{(k)}\}$ are trained by minimizing the cross-entropy loss function of classes over all query samples as:

$$L_{T_{\text{train}}} = - \sum_{i=1}^Q y_i \log P(\hat{y}_i = y_i | T)$$  
(11)

where $\hat{y}_i$ and $y_i$ denote the predicted and ground-truth labels of the query sample $x_i$, respectively. We evaluate the proposed Attentive GNN for few-shot task using both inductive and transductive settings, which correspond to $Q = 1$, and $Q = Nq$ with $q > 1$, respectively.

4 Why it works

**Discriminative Sample Representation.** It is critical to obtain the initial feature representation of the samples that are sufficiently discriminative (i.e., samples of different classes are separated) for the GNN models in few-shot tasks. However, most of the existing GNN models work with generic features using CNN-based backbone, and fail to capture the task-specific structure. The proposed node self-attention module exploits the cross-sample correlation, and can thus effectively guide the feature representation for each few-shot task. Fig [2] compares two examples of the graph features for 5-way 1-shot transductive learning using t-SNE visualization [19], using the vanilla GNN and the proposed Attentive GNN. The vanilla GNN generates node representation that are “over-smoothed” due to bad initial feature using CNN-based backbone. On the contrary, the node self-attention module can effectively generate the discriminative features, which lead to the more promising results using the Attentive GNN.
Alleviation of Over-Smoothing and Over-Fitting. Over-fitting arises when learning an over-parametric model from the limited training data, and it is extremely severe as the objective of few-shot learning is to generalize the knowledge from training set for few-shot tasks. On the other hand, over-smoothing phenomenon refers to the case where the features of all (connected) nodes converge to similar values as the model depth increases. We provide theoretical analysis to show that the proposed triple-attention mechanism can alleviate both over-fitting and over-smoothing in GNN training. For each of the result, the proof sketch is presented, while the corresponding full proofs are included in the Appendix.

Lemma 1. The node self-attention module is equivalent to a GNN layer if \( \alpha = 0 \) as

\[
X^{(k)} = \left[ X, Y \right], \quad A^{(k)} = C^f, \quad W^{(k)} = I,
\]

(12)

Proof Sketch. The feature and label vector updates using (7) is similar to multiplying with an adjacency matrix in (1), while such matrix is obtained in a self-supervised way.

Proposition 1. Applying the node self-attention module to replace a GNN layer in Attentive GNN, reduces the trainable-parameter complexity from \( \mathcal{O}\{d(d + L)\} \) to \( \mathcal{O}\{1\} \), where \( L \) denotes the depth of MLP for generating the adjacency metric.

Proof Sketch. The trainable parameters in a GNN layer (1) are mainly the linear transformation \( W^{(k)} \) and the MLP \( (k) \), which scale as \( \mathcal{O}\{d^2\} \) and \( \mathcal{O}\{dL\} \), respectively. On the contrary, the graph self-attention only involve the \( 1 \times 1 \) kernels that are trainable.

Lemma 1 and Proposition 1 prove that the node self-attention module involves much fewer trainable parameters than a normal GNN layer. Thus, applying node self-attention instead of another GNN layer will reduce the model complexity, thus lowering the risk of over-fitting.

Next we show that using graph neighbor attention can help alleviate over-smoothing for training GNN. The analysis is based on the recent works on dropEdge [25] and GNN information loss [21]. They proved that a sufficiently deep GNN model will always suffer from “\( \epsilon \)-smoothing” [21], where \( \epsilon \) is defined as the error bound of the maximum distance among node features. Another concept is the “information loss” [21] of a graph model \( G \), i.e., the dimensionality reduction of the node feature-space after \( T \) layers of GNNs, denoted as \( \Theta_{T,G} \). We use these two concepts to quantify the over-smoothing issue in our analysis.

Theorem 1. Denote the same multi-layer GNN model with and without neighbor attention as \( \hat{G} \) and \( G \), respectively. Besides, denote the number of GNN layers for them to encounter the \( \epsilon \)-smoothing [27] as \( T(G, \epsilon) \) and \( T(\hat{G}, \epsilon) \), respectively. With sufficiently small \( \beta \) in the node self-attention module, either (i) \( T(\hat{G}, \epsilon) \leq T(G, \epsilon) \), or (ii) \( \Theta_{T(G,\epsilon),\hat{G}} > \Theta_{T(\hat{G},\epsilon),\hat{G}} \), will hold.

Remarks. The result shows that the GNN model with graph neighbor attention (i) increases the maximum number of layers to encounter over-smoothing, or if the number of layers remains, (ii) the over-smoothing phenomenon is alleviated.
Table 1: Few-shot classification accuracy averaged over mini-ImageNet and tiered-ImageNet. The best and second best results under each setting and dataset are highlighted as Red and blue, respectively. “BN” denotes that the batch normalization where query statistical information is used instead of global batch normalization.

| Model           | Trans | mini-ImageNet | 5-way 1-shot | 5-way 5-shot | tiered-ImageNet | 5-way 1-shot | 5-way 5-shot |
|-----------------|-------|---------------|--------------|--------------|----------------|--------------|--------------|
| Matching-Net    | ✗     | 46.60         | 55.30        | -            | -              | -            | -            |
| Proto-Net       | ✗     | 46.14         | 65.77        | 48.58        | 69.57          | -            | -            |
| Reptile         | ✗     | 47.07         | 62.74        | -            | -              | -            | -            |
| Relation-Net    | ✗     | 50.44         | 65.32        | -            | -              | -            | -            |
| GNN             | ✗     | 50.33         | 66.41        | -            | 54.97          | 70.92        |              |
| SAML            | ✗     | 52.22         | 66.49        | -            | -              | -            | -            |
| EGNN            | ✗     | 52.86         | 66.85        | -            | 70.98          |              |              |
| Ours            | ✗     | 54.81         | 69.85        | -            | 57.47          | 72.29        |              |
| Reptile         | BN    | 49.97         | 65.99        | 52.36        | 71.03          |              |              |
| MAML            |       | 48.70         | 63.11        | 51.67        | 70.30          |              |              |
| Relation-Net    | ✓     | 50.83         | 66.19        | 53.23        | 70.83          |              |              |
| GNN             | ✓     | 51.38         | 67.07        | 54.48        | 71.31          |              |              |
| EGNN            | ✓     | 54.14         | 70.38        | 65.11        | 76.40          |              |              |
| TPN             | ✓     | 59.18         | 76.37        | 63.52        | 80.15          |              |              |
| TPN             | ✓     | 53.75         | 69.43        | 57.53        | 72.85          |              |              |
| DN4             | ✓     | 51.24         | 71.02        |              |                |              |              |
| Ours (Normalized)| ✓    | 59.87         | 74.46        | 66.87        | 79.26          |              |              |
| Ours (Fusion)   | ✓     | 60.14         | 72.41        | 67.23        | 79.55          |              |              |

5 Experiments

Datasets. We conducted extensive experiments to evaluate the effectiveness of the proposed Attentive GNN model for few-shot learning, over two widely-used few-shot image classification benchmarks, i.e., mini-ImageNet [31] and tiered-ImageNet [24]. Mini-ImageNet contains around 60000 images of 100 different classes extracted from the ILSVRC-12 challenge [13]. We used the proposed splits by [23], i.e., 64, 16 and 20 classes for training, validation and testing, respectively. Tiered-ImageNet dataset is a more challenging data subset from the ILSVRC-12 challenge [13], which contains more classes that are organized in a hierarchical structure, i.e., 608 classes from 34 top categories. We follow the setups proposed by [24], and split 34 top categories into 20 (resp. 351 classes), 6 (resp. 97 classes), and 8 (resp. 160 classes), for training, validation, and testing, respectively. For both datasets, all images are resized to $84 \times 84$.

Implementation Details. We follow most of the DNN-based few-shot learning schemes [26, 31, 6, 18], and apply the popular ConvNet-4 as the backbone feature extractor, with $3 \times 3$ convolution kernels, numbers of channels as $[64, 96, 128, 256]$ at corresponding layers, a batch normalization layer, a max pooling layer, and a LeakyReLU activation layer. Besides, two dropout layers are adapted to the last two convolution blocks to alleviate over-fitting [6].

We conducted both 5-way 1-shot, and 5-way 5-shot experiments, under both inductive and transductive settings [18]. We use only one query sample for the inductive, and 5 query samples per class for the transductive experiments. Our models are all trained using Adam optimizer with an initial learning rate of $1 \times 10^{-3}$ and a weight decay of $1 \times 10^{-6}$. The mini-batch sizes are set to 100 / 40 and 30 / 20, for 1-shot / 5-shot inductive and transductive settings, respectively. We cut the learning rate in half every 15K and 30K epochs, for experiments over mini-ImageNet and tiered-ImageNet, respectively.

Results. We compare the proposed Attentive GNN to the state-of-the-art GNN-based approaches, which are all using the same backbone, i.e., ConvNet-4. Table 1 lists the average accuracies of the few-shot image classification. In general, results under the transductive setting improve from the inductive results, as the algorithm can further exploit the correlation amongst support and multiple query samples. Note that the transductive setting by EGNN [12] is different from the other methods, i.e., 15 query samples are used rather than 5 in Attentive GNN. For all datasets and settings, Attentive GNN outperforms all the competing methods, except for transductive EGNN. Even under an “unfair” transductive setting, the proposed Attentive GNN performs comparably to EGNN in average.

Ablation Study. We investigate the effectiveness of each proposed attention module by conducting an ablation study. Fig. 3 plots the image classification accuracy over the mini-ImageNet dataset, with
different variations of the proposed Attentive GNN, by removing the node self-attention (self att) and layer memory attention (memory att) modules. Besides, instead of applying layer memory attention which attends to the concatenated early feature, we try another variation by concatenating only the label vectors (label concat). It is clear that all variations generate degraded results, and suffers from more severe over-smoothing, i.e., accuracy drops quickly as the number of GNN layers increases. We show that the label concatenation is a reasonable alternative (i.e., red curve) to replace layer memory attention which requires less memory complexity. Furthermore, we study the influence of the graph neighbor attention for few-shot learning by varying the hyper-parameter $\beta$. Fig. 4 plots the inductive image classification accuracy by applying Attentive GNN with varying $1 - \beta$ (i.e., ratio of elements in $A$ being zero) in the graph neighbor attention module. When $1 - \beta = 0$, it is equivalent to removing the graph neighbor attention at all. By choosing the optimal $\beta \in (0, 1)$’s for 5-way 1-shot and 5-way 5-shot settings, respectively, the graph neighbor attention can further boost the classification results.

Hyper-Parameters. There are two hyper-parameters in the proposed Attentive GNN, namely $\alpha$ and $\beta$, corresponding to the ratio for label fusion, and the sparsity ratio in the neighbor attention module. Table 2 shows how varying these two parameters affects the inductive learning for image classification averaged over tiered-ImageNet. Both $\alpha$ and $\beta$ range between 0 and 1. Besides, we also test the model when then label fusion mechanism is totally removed, denoted as “-” in the table. The empirical results demonstrate the effectiveness of label fusion with $\alpha = 0.5$ to be a reasonable ratio. Besides, for 5-way 1-shot learning, the best result is generated when $\beta = 1$, which is equivalent to remove the graph neighbor attention. It is because the total number of nodes is small for 5-way 1-shot learning, thus imposing sparsity leads to too restrictive model.

Robustness in Transductive Learning. While the query samples are always uniformly distributed for each class in the conventional transductive learning setting [18], such assumption may not hold in practice, e.g., query set contain samples with random labels. We study how robust the proposed Attentive GNN is for such setting by comparing to the baseline GNN method [6] and GNN with only neighbor attention (e.g., w/ Neighbor Att.). In the training, we simulate the query set with samples with random labels correspondingly for Attentive GNN and all competing methods under such setting. Table 3 shows the image classification accuracy with 5-way 1-shot transductive learning, averaged over tiered-ImageNet. With the query-set samples of “random” labels, the proposed Attentive GNN can still generate significantly better results comparing to the vanilla GNN. Table 3 shows that the proposed graph neighbor attention module contributes to the robustness. As the sparse adjacency matrix can attend to the related nodes (i.e., nodes with the same class) in an adaptive way, preventing “over-mixing” with all nodes.

Table 2: Inductive accuracy on tiered-ImageNet dataset with different graph settings. Here “-” means not applying node self-attention.

| Hyper-Parameter Setting | Accuracy | 5-way 1-shot | 5-way 5-shot |
|-------------------------|----------|--------------|--------------|
| $\beta$ | $\alpha$ | 1-shot | 5-shot | 1-shot | 5-shot |
| 1.0 | - | 54.97 | 70.92 | 57.18 | 70.58 |
| 0.7 | - | 57.18 | 70.58 | 57.41 | 72.03 |
| 1.0 | 0.5 | 57.68 | 71.03 | 57.18 | 70.58 |
| 0.7 | 0.5 | 57.47 | 72.29 | 57.18 | 70.58 |

Table 3: Effect of query samples distribution on tiered-ImageNet dataset of 5-way 1-shot task based on transductive setting. Here the total number of query samples for two settings is fixed.

| Model | Random | Uniform |
|-------|--------|---------|
| Vanilla GNN [6] | 59.77 | 65.11 |
| GNN w/ Neighbor Att. | 60.18 | 65.49 |
| Attentive GNN | 61.39 | 67.23 |
6 Conclusion

In this paper, we proposed a novel Attentive GNN model for few-shot learning. The proposed Attentive GNN makes full use of the relationships between image samples for knowledge modeling and generalization. By introducing a triple-attention mechanism, Attentive GNN model can effectively alleviate over-smoothing and over-fitting issues when applying deep GNN models. Extensive experiments are conducted over popular mini-ImageNet and tiered-ImageNet, showing that our proposed Attentive GNN outperforms the state-of-the-art GNN-based few-shot learning methods. We plan to apply Attentive GNN for other challenging applications in future work.

7 Appendix

Here we present (1) the detailed proofs of the results for the proposed Attentive GNN, i.e., Lemma 1 and Theorem 1; (2) additional experimental results applying the proposed Attentive GNN scheme for the study of the number of graph layers;

7.1 Proofs of the results for Attentive GNN

We prove the main results regarding the proposed attentive GNN. First of all, we analyze the proposed node self-attention, whose feature and label vector updates are

\[ \tilde{X}^{(1)} = C^f X, \quad \tilde{Y}^{(1)} = \alpha Y + (1 - \alpha) C^f Y, \]

where \( C^f \) denotes the attention map, \( X \) and \( Y \) (resp. \( X^{(1)} \) and \( Y^{(1)} \)) denote the input (resp. output) feature and label vectors, respectively.

We prove Lemma 1 which shows that the proposed node self-attention can alleviate Over-fitting by reducing the model complexity comparing to adding more GNN layer. The output of the \( k \)-th GNN layer can be represented as

\[ X^{(k+1)} = F_k(X^{(k)}, W^{(k)}) = \rho(\hat{A}^{(k)} X^{(k)} W^{(k)}) \]

Lemma 1. The node self-attention module is equivalent to a GNN layer if \( \alpha = 0 \) as \( X^{(k)} = [X, Y] \), \( \hat{A}^{(k)} = C^f \), \( W^{(k)} = I \).

**Proof of Lemma 1.** With the condition for equivalence, the output of the \( k \)-th GNN layer becomes

\[ X^{(k+1)} = F_k(X^{(k)}, I) = C^f X^{(k)} I = C^f X^{(k)}. \]

Thus, (16) is equivalent to putting the node self-attention to replace the \( k \)-th GNN layer, with \( X^{(k+1)} = X^{(1)} \) and \( X^{(k)} = [X, Y] \). \( \square \)

Next, we prove Proposition 1 which shows the model complexity decrease from a trainable GNN layer to the proposed node self-attention module.

**Proposition 1.** Applying the node self-attention module to replace a GNN layer in Attentive GNN, reduces the trainable-parameter complexity from \( O\{d(d + L)\} \) to \( O\{1\} \), where \( L \) denotes the depth of MLP for generating the adjacency metric.

**Proof of Proposition 1.** For a GNN layer following (1), both \( W^{(k)} \) and the MLP\(^{(k)} \) are trainable, corresponding to free parameters scale as \( O\{d^2\} \) and \( O\{dL\} \), respectively. On the contrary, based on Lemma 1, the proposed node self-attention is equivalent to a GNN layer, with the \( W^{(k)} \) and the MLP\(^{(k)} \) fixed. The only trainable parameters are the \( 1 \times 1 \) kernels to fuse the \( C^X \) and \( C^Y \), with the complexity scales as \( O\{1\} \). \( \square \)

Next we show that using graph neighbor attention can help alleviate over-smoothing for training GNN. We first quantify the degree of over-smoothing using the definitions from [25] and [21].

**Definition 1 (Feature Subspace).** Denote the \( M \)-dimensional subspace \( M = \{U \Sigma | U \in \mathbb{R}^{V \times M}, U^T U = I_M, \Sigma \in \mathbb{R}^{M \times d}\} \) as the feature space, with \( M \leq V \).
With these definitions from \[25\] and \[21\], we can now prove Theorem 1 for the graph neighbor attention. Denote the projection loss as

\[
P_M(X) = \arg \min_{Z \in M} \|X - Z\|_F. \tag{17}
\]

Denote the projection loss \(\theta_M(X)\) as

\[
\theta_M(X) = \|X - P_M(X)\|_F = \min_{Z \in M} \|X - Z\|_F. \tag{18}
\]

Definition 3 (\(e\)-smoothing). The GNN layer that suffers from \(e\)-smoothing if \(\theta_M(X) < \epsilon\). Given a multi-layer GNN \(G\) with each the feature output of each layer as \(X^{(k)}\), we define the \(e\)-smoothing layer as the minimal value \(k\) that encounters \(e\)-smoothing, i.e.,

\[
T(G, \epsilon) = \min_k \{\theta_M(X) < \epsilon\} \tag{19}
\]

Definition 4 (Dimensionality Reduction). Suppose at the The dimensionality reduction of the node feature-space after \(T\) layers of GNNs is denoted as \(\Theta_{T,G} = d - \|
\]

\[
T(G, \epsilon) = \min_k \{\theta_M(X) < \epsilon\} \tag{20}
\]

With these definitions from \[25\] and \[21\], we can now prove Theorem 1 for the graph neighbor attention as

\[
\hat{A}^{(k)} = \arg \min_{A^{(k)}} \|A^{(k)} - U^{(k)}\|_F \quad \text{s.t.} \quad U^{(k)}(i, j) = \text{MLP}^{(k)}(x_i^{(k)} - x_j^{(k)}) \quad \text{and} \quad \|A^{(k)}\|_0 \leq \beta V \quad \forall i, j \tag{21}
\]

Here, \(A^{(k)}_i \in \mathbb{R}^{1 \times V}\) denotes the \(i\)-th row of \(A^{(k)}\), \(\beta \in (0, 1]\) denotes the ratio of nodes maintained for feature update, and \(V\) is the number of graph nodes. Besides, \(U^{(k)}\) is the original adjacency matrix with the graph neighbor attention.

**Theorem 1.** Denote the same multi-layer GNN model with and without neighbor attention as \(\tilde{G}\) and \(G\), respectively. Besides, denote the number of GNN layers for them to encounter the \(e\)-smoothing \[27\] as \(T(G, \epsilon)\) and \(T(G, \epsilon)\), respectively. With sufficiently small \(\beta\) in the node self-attention module, either (i) \(T(\tilde{G}, \epsilon) \leq T(G, \epsilon)\), or (ii) \(\Theta_{T(G, \epsilon), \tilde{G}} > \Theta_{T(G, \epsilon), G}\), will hold.

**Proof of Theorem 1** Given the original \(U^{(k)}\), the solution to (21) is achieved using the projection onto a \(\ell_0\) unit ball, i.e., keeping the \(\beta\) elements of each \(U_i^{(k)}\) with the largest magnitudes \[32\], i.e.,

\[
\hat{A}^{(k)}_i(j) = \begin{cases} 
U_i^{(k)}(j), & j \in \Omega_i^{\beta V} \\
0, & j \in \bar{\Omega}_i^{\beta V} 
\end{cases} \tag{22}
\]

Here, the set \(\Omega_i^{\beta V} = \text{supp}(\hat{A}^{(k)}_i)\) indexes the top-\(\beta\) elements of largest magnitude in \(U_i^{(k)}\), and \(\bar{\Omega}_i^{\beta V}\) denotes the complement set of \(\Omega_i^{\beta V}\). When \(\hat{A}^{(k)}_i(j) = 0\), it is equivalent to remove the edge connecting the \(i\)-th node and \(j\)-th node. Thus, \(|\Omega_i^{\beta V}|\) equals to the number of edges been dropped by the node self-attention, and \(|\bar{\Omega}_i^{\beta V}| \rightarrow V\) as \(\beta \rightarrow 0\).

Therefore, when \(\beta\) is sufficiently small, there are sufficient number of edges been dropped by the node self-attention. Based on the Theorem 1 in \[25\], we have either of the two to alleviate over-smoothing phenomenon:

- The number of layers without \(e\)-smoothing increases by node self-attention, i.e., \(T(\tilde{G}, \epsilon) \leq T(G, \epsilon)\).
- The information loss (i.e., dimensionality reduction by feature embedding) decreases by node self-attention, i.e., \(\Theta_{T(G, \epsilon), \tilde{G}} > \Theta_{T(G, \epsilon), G}\).
7.2 Study on the effectiveness of different Attentive GNN Layers

Here we investigate the effectiveness of the number of GNN layers for our proposed Attentive GNN. Fig. 5 plots the classification accuracy of 5-way 5-shot task over the tiered-ImageNet under transductive setting with different Attentive GNN layers. When the number of Attentive GNN layer is set to 0, it means that we only adapt node self-attention module following with a fully-connected layer for classification. It is clear that the test accuracy has a significant increase as the number of GNN layers increases, which is due to the powerful ability of GNN to integrate neighbor information. However, as the number of GNN layers increases, test accuracy starts to drop and our Attentive GNN model is more likely to suffer from over-smoothing when the number of GNN layers continues to increase. In conclusion, we decide to adopt a 3-layer Attentive GNN model.

Figure 5: Accuracy on tiered against different numbers of GNN layers with transductive setting for 5-way 5-shot task.
References

[1] Bruna, J., Zaremba, W., Szlam, A., LeCun, Y.: Spectral networks and locally connected networks on graphs. arXiv preprint arXiv:1312.6203 (2013)

[2] Cheng, J., Dong, L., Lapata, M.: Long short-term memory-networks for machine reading. arXiv preprint arXiv:1601.06733 (2016)

[3] Defferrard, M., Bresson, X., Vandergheynst, P.: Convolutional neural networks on graphs with fast localized spectral filtering. In: Advances in neural information processing systems. pp. 3844–3852 (2016)

[4] Fei-Fei, L., Fergus, R., Perona, P.: One-shot learning of object categories. IEEE transactions on pattern analysis and machine intelligence 28(4), 594–611 (2006)

[5] Finn, C., Abbeel, P., Levine, S.: Model-agnostic meta-learning for fast adaptation of deep networks. In: Proceedings of the 34th International Conference on Machine Learning-Volume 70. pp. 1126–1135. JMLR. org (2017)

[6] Garcia, V., Bruna, J.: Few-shot learning with graph neural networks. arXiv preprint arXiv:1711.04043 (2017)

[7] Hao, F., He, F., Cheng, J., Wang, L., Cao, J., Tao, D.: Collect and select: Semantic alignment metric learning for few-shot learning. In: Proceedings of the IEEE International Conference on Computer Vision. pp. 8460–8469 (2019)

[8] Ji, F., Yang, J., Zhang, Q., Tay, W.P.: Gfcn: A new graph convolutional network based on parallel flows. In: ICASSP 2020-2020 IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP). pp. 3332–3336. IEEE (2020)

[9] Krizhevsky, A., Sutskever, I., Hinton, G.E.: Imagenet classification with deep convolutional neural networks. In: Advances in neural information processing systems. pp. 1097–1105 (2012)

[10] Lee, J., Lee, I., Kang, J.: Self-attention graph pooling. arXiv preprint arXiv:1904.08082 (2019)

[11] Li, W., Wang, L., Xu, J., Huo, J., Gao, Y., Luo, J.: Revisiting local descriptor based image-to-class measure for few-shot learning. In: Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition. pp. 7260–7268 (2019)

[12] Maaten, L.v.d., Hinton, G.: Visualizing data using t-sne. Journal of machine learning research 9(Nov), 2579–2605 (2008)

[13] Nichol, A., Achiam, J., Schulman, J.: On first-order meta-learning algorithms. arXiv preprint arXiv:1803.02999 (2018)

[14] Oono, K., Suzuki, T.: Graph neural networks exponentially lose expressive power for node classification. In: International Conference on Learning Representations (2020)

[15] Parikh, A.P., Täckström, O., Das, D., Uszkoreit, J.: A decomposable attention model for natural language inference. arXiv preprint arXiv:1606.01933 (2016)

[16] Ren, M., Triantafillou, E., Ravi, S., Snell, J., Swersky, K., Tenenbaum, J.B., Larochelle, H., Zemel, R.S.: Meta-learning for semi-supervised few-shot classification. arXiv preprint arXiv:1803.00676 (2018)
[25] Rong, Y., Huang, W., Xu, T., Huang, J.: Dropedge: Towards deep graph convolutional networks on node classification. In: International Conference on Learning Representations (2019)

[26] Snell, J., Swersky, K., Zemel, R.: Prototypical networks for few-shot learning. In: Advances in neural information processing systems. pp. 4077–4087 (2017)

[27] Sperduti, A., Starita, A.: Supervised neural networks for the classification of structures. IEEE Transactions on Neural Networks 8(3), 714–735 (1997)

[28] Sung, F., Yang, Y., Zhang, L., Xiang, T., Torr, P.H., Hospedales, T.M.: Learning to compare: Relation network for few-shot learning. In: Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition. pp. 1199–1208 (2018)

[29] Vaswani, A., Shazeer, N., Parmar, N., Uszkoreit, J., Jones, L., Gomez, A.N., Kaiser, Ł., Polosukhin, I.: Attention is all you need. In: Advances in neural information processing systems. pp. 5998–6008 (2017)

[30] Veličković, P., Cucurull, G., Casanova, A., Romero, A., Lio, P., Bengio, Y.: Graph attention networks. arXiv preprint arXiv:1710.10903 (2017)

[31] Vinyals, O., Blundell, C., Lillicrap, T., Wierstra, D., et al.: Matching networks for one shot learning. In: Advances in neural information processing systems. pp. 3630–3638 (2016)

[32] Wen, B., Ravishankar, S., Bresler, Y.: Structured overcomplete sparsifying transform learning with convergence guarantees and applications. International Journal of Computer Vision 114(2-3), 137–167 (2015)

[33] Xu, K., Li, C., Tian, Y., Sonobe, T., Kawarabayashi, K.i., Jegelka, S.: Representation learning on graphs with jumping knowledge networks. arXiv preprint arXiv:1806.03536 (2018)

[34] Zhang, J., Zhang, M., Lu, Z., Xiang, T., Wen, J.: Adargcn: Adaptive aggregation gcn for few-shot learning. arXiv preprint arXiv:2002.12641 (2020)

[35] Zhu, Y., Liu, C., Jiang, S.: Multi-attention meta learning for few-shot fine-grained image recognition. In: Twenty-Ninth International Joint Conference on Artificial Intelligence and Seventeenth Pacific Rim International Conference on Artificial Intelligence. pp. 1090–1096 (07 2020). https://doi.org/10.24963/ijcai.2020/152