Few-Shot Graph Classification with Model Agnostic Meta-Learning

Ning Ma
College of Computer Science, Zhejiang University
ma_ning@zju.edu.cn

Abstract
Graph classification aims to perform accurate information extraction and classification over graph-structured data. In the past few years, Graph Neural Networks (GNNs) have achieved satisfactory performance on graph classification tasks. However, most GNNs based methods focus on designing graph convolutional operations and graph pooling operations, overlooking that collecting or labeling graph-structured data is more difficult than grid-based data. We utilize meta-learning for few-shot graph classification to alleviate the scarce of labeled graph samples when training new tasks. More specifically, to boost the learning of graph classification tasks, we leverage GNNs as graph embedding backbone and meta-learning as training paradigm to capture task-specific knowledge rapidly in graph classification tasks and transfer them to new tasks. To enhance the robustness of meta-learner, we designed a novel step controller driven by Reinforcement Learning. The experiments demonstrate that our framework works well compared to baselines.

1 Introduction
In many real-world scenarios, such as modelling social networks, chemical molecule structures and citation networks, it’s a better way to formulate these data as graphs into the non-Euclidean domain. Recently, there have been various attempts to extend CNNs and pooling methods to graph-based data. These methods are named as Graph Neural Networks (GNNs) and have been successfully applied to different graph related tasks containing graph classification, node classification and link prediction [Zhang et al., 2018]. However, most existing GNNs based graph classification methods focus on designing graph convolutional operations and graph pooling operations, while overlooking that it’s complicated and time consuming to collect or label graph data. To alleviate the scarce of labeled graph samples, few-shot learning on graphs is challenging but meaningful work.

There have been several methods for few-shot node classification [Satorras and Estrach, 2018; Kim et al., 2019] and few-shot link prediction [Du et al., 2019], but they are not customized for few-shot graph classification. [Chauhan et al., 2020] proposed few-shot graph classification based on graph spectral measures. We consider few-shot knowledge transfer or fast adaptation from learned graph classification tasks to new tasks. While unlike images, graphs have arbitrary node size and sub-structure, which brings more uncertainty for knowledge transfer. To alleviate the problem in few-shot learning and inspired by meta-learning [Finn et al., 2017], we proposed a GNNs and meta-learning based framework to facilitate few-shot graph classification tasks. More specifically, when given only a few graph data, we leverage GNNs as graph embedding backbone and meta-learning as training paradigm to rapidly capture task-specific knowledge in graph classification tasks and transfer them to new tasks. Model Agnostic Meta-Learning (MAML, proposed by [Finn et al., 2017]) attracted great attention because of its fast adaptation and knowledge transferability. So we use MAML to implement fast adaptation mechanism when performing new graph classification tasks.

However, MAML requires arduous hyperparameter searches to stabilize training and achieve high generalization [Antoniou et al., 2019], so it’s difficult to optimize a MAML based meta-learner for graph classification. To improve learning performance and inspired by [Du et al., 2019], we designed an adaptive step controller to learn optimal adaptation step for meta-learner. The controller evaluates the meta-learner and decides when to stop adaptation by graphs’ embedding quality and meta-learner’s training state. The embedding quality is viewed as a meta-feature and indicated with Average Node Information (ANI, the average amount of node information in a batch of graphs). Besides, the meta-learner’s training state is indicated with training loss.

We formulate our framework as Adaptive Step MAML (AS-MAML). To the best of our knowledge, we are the first to leverage MAML to alleviate the scarce of labeled graph samples for graph classification. Our contributions are summarized as follows:

- To accelerate the learning of graph classification tasks, we proposed a framework integrating GNNs and MAML for few-shot graph classification.
- To enhance the robustness and compatibility of MAML based meta-learner, we designed a novel step controller, which is driven by Reinforcement Learning (RL, [J.,
2 Related Works

2.1 Graph Classification

There exist several branches for graph classification. The first is graph kernel methods which design kernels for the substructures exploration and exploitation of graph data. The typical kernels include Shortest-path Kernel [Borgwardt and Kriegel, 2005], Graphlet Kernel [Shervashidze et al., 2009] and Weisfeiler-Lehman Kernel [Shervashidze et al., 2011].

As the main branch in recent years, GNNs have been successfully applied to graph classification. GNNs focus on node representations, which are iteratively computed by message passing from the features of their neighbor nodes using a differentiable aggregation operation. [Kipf and Welling, 2017] proposed Graph Convolutional Neural Network (termed as GCN) and got satisfying results based on directly feature aggregation from neighborhood nodes. [Veličković et al., 2018] imported attention mechanism for graph convolutional operations (GAT). [Hamilton et al., 2017] proposed an inductive framework called GraphSAGE which leverages node features to generate node embeddings efficiently for unseen graphs. In our framework, we use GraphSAGE to generate node embeddings for unseen graphs of new classes.

In the meantime, a bunch of researchers concentrate on efficient pooling methods [Lee et al., 2019; Diehl, 2019; Gao and Ji, 2019] for accurate graph representation summary and computation efficiency.

2.2 Meta-Learning/Few-Shot Learning

Few-shot classification is usually powered by meta-learning. Meta-learning was also known as learning to learn, with a meta-learner observing various task learning processes and summarizing meta-knowledge to accelerate the learning efficiency of new tasks. [Baxter, 2000] proposed a model to learn inductive bias from the perspective of bias learning automatically, and they analytically showed that the number of examples required of each task decrease as the number of task rises.

Recent meta-learning related works can be classified into three categories: optimization (or gradients) based methods, metric learning based methods and memory networks based methods. Optimization based methods aim to train a model to learn optimization [Ravi and Larochelle, 2017; Li et al., 2018], learn a good initialization [Finn et al., 2017] for rapid adaptation, or train parameter generator for task-specific classifier [Rusu et al., 2019]. Metric learning based methods aim to learn a feature space shared with new tasks [Vinyals et al., 2016; Snell et al., 2017]. Moreover, memory networks based methods learn new tasks by reminiscence mechanism in virtue of physical memory [Santoro et al., 2016].

2.3 Graph Neural Networks with Transfer Methods

We have seen several few-shot node classification works boosting transferability via GNNs [Satorras and Estrach, 2018; Kim et al., 2019; Liu et al., 2019; Yao et al., 2020]. For the graph classification task, [Knyazev et al., 2019] focus on the ability of attention GNNs to generalize to larger, more complex or noisy graphs. [Lee et al., 2017] imported domain transfer method by transferring the intrinsic geometric information learned in the source domain to the target. Based on graph spectral measures, [Chauhan et al., 2020] proposed few-shot graph classification using Graph Isomorphism Network [Xu et al., 2019] and GAT, but they assume that the test classes belong to the same set of super-classes built from the training classes. We loosen the assumption and emphasize fast adaptation to boost few-shot graph classification.

3 Problem Setup

We form the few-shot problem as N-way-K-shot graph classification. Firstly, given graph data $G = \{(G_1, y_1), (G_2, y_2), \ldots, (G_n, y_n)\}$, where $G_i = (V_i, E_i, X_i)$. We use $n_i$ to denote the number of node set $V_i$. Each graph $G_i$ has a adjacent matrix $A_{i} \in \mathbb{R}^{n_i \times n_i}$ and a node attribute matrix $X_i \in \mathbb{R}^{n_i \times d}$, where $d$ is the dimension of node attribute. Secondly, according to label $y$, we split $G$ into $\{(G^{\text{train}}_i, y_i^{\text{train}})\}$ and $\{(G^{\text{test}}_i, y_i^{\text{test}})\}$ as training set and test set respectively. Notice that $y_i^{\text{train}}$ and $y_i^{\text{test}}$ must have no common classes. We use episodic training method, which means that at the training stage we sample a task $T$ each time, and each task contains support data $D_{\text{sup}} = \{(G_i^{\text{train}}, y_i^{\text{train}})\}_{i=1}^{s}$ and query data $D_{\text{que}} = \{(G_i^{\text{test}}, y_i^{\text{test}})\}_{i=1}^{q}$, where $s$ and $q$ are the number of support data and query data respectively. Given labeled support data, our goal is predicting the labels of query data. Please note that in a single task, support data and query data share the same class space. If $s = N \times K$, which means that support data contain $N$ classes and $K$ labeled samples per class, we name the problem as N-way-K-shot graph classification.

4 Proposed Framework

Our few-shot graph classification framework consists of GNNs based meta-learner and a step controller to decide the adaptation steps of meta-learner. We use typical graph convolutional modules and pooling modules as the backbone. Besides, MAML drew great attention because of its model agnostic property for meta-learning models. We use MAML to implement fast adaptation mechanism for meta-learner. [Du et al., 2019] proposed a RL based step controller to conduct meta-learner for link prediction. We argue that classification loss is suboptimal to be viewed as reward for overcoming overfitting. Therefore, we adopt a novel step controller to accelerate training and overcome overfitting. Our step controller is also driven by RL but learns optimal adaptation step by using ANI and loss as inputs and classification accuracy as reward. Figure 1 demonstrates the training process of our framework.
4.1 Graph Embedding Backbone
For few-shot learning scenario which emphasizes the model's transferability, inductive learning methods (e.g., GraphSAGE [Hamilton et al., 2017]) are more flexible compared with transductive methods (e.g., GCN [Kipf and Welling, 2017]). For the clarity of the framework, we use mean aggregator of GraphSAGE as follows:

\[
    h^l_v = \sigma(W \cdot \text{mean}(\{h^{l-1}_u \cup \{h^{l-1}_u, \forall u \in \mathcal{N}(v)\}))
\]

where \( h^l_v \) is the \( l \)-th layer representation of node \( v \), \( \sigma \) is sigmoid function, \( W \) is the parameters of aggregator, and \( \mathcal{N}(v) \) contains the neighborhoods of \( v \).

After that, we choose self-attention pooling (SAGPool) [Lee et al., 2019] as our pooling layer:

\[
    Z_i = \sigma(\tilde{D}_i^{-\frac{1}{2}} \tilde{A}_i \tilde{D}_i^{-\frac{1}{2}} X_i \Theta_{att})
\]

where the \( Z_i \in \mathbb{R}^{n \times 1} \) indicates the self-attention score, \( n \) is node number of graph, \( \sigma \) is the activation function (e.g., tanh), \( \tilde{A}_i \in \mathbb{R}^{n \times n} \) is the adjacency matrix with self-connections, \( \tilde{D}_i \in \mathbb{R}^{n \times n} \) is the diagonal degree matrix of \( \tilde{A}_i \), \( X_i \in \mathbb{R}^{n \times d} \) is \( n \) input features with dimension \( d \), and \( \Theta_{att} \in \mathbb{R}^{d \times 1} \) is the parameters of pooling layer.

Following [Zhang et al., 2019], we use the concatenation of mean-pooling and max-pooling for each level of graph embeddings as follows:

\[
    r^l_i = \mathcal{R}(H^l_i) = \sigma\left(\frac{1}{n^l_i} \sum_{p=1}^{n^l_i} H^l_i(p, :) \| \max_{q=1}^{d} H^l_i(:, q)\right)
\]

where \( r^l_i \in \mathbb{R}^{2d} \) is the \( l \)-th layer embedding of \( G_i \), \( n^l_i \) is the node number of \( G_i \) in \( l \)-th layer, \( H^l_i \) denotes \( l \)-th layer hidden representation matrix of \( G_i \), \( \| \) is concatenation operation, \( p \) and \( q \) are row number and column number respectively, \( d \) is feature dimension, and \( \sigma \) is the activation function.

Following the graph embedding backbone, we put the final graph embedding \((r^1_i + r^2_i + \cdots + r^T_i)\) into MLP layers to perform classification.

4.2 Meta-Learner for Fast Adaptation
We use \( \theta_e \) and \( \theta_c \) to denote the parameters of graph embedding modules and MLP classifier respectively. To achieve the fast adaptation of \( \theta_e \) and \( \theta_c \), we put them into MAML framework to create a GNNs based meta-learner. First, we sample support data \( D_{sup} \) and query data \( D_{que} \) in an episode. Then we perform adaptation operation by updating \( \theta_e \) and \( \theta_c \) for \( T \) steps on \( D_{sup} \). Lines 6 to 8 in Algorithm 1 demonstrate the adaptation of meta-learner. After adaptation, demonstrated by line 10, we use the loss on \( D_{que} \) to perform backpropagation and update \( \theta_e \) as well as \( \theta_c \). On the test stage, the meta-learner will perform adaptation on labeled support graphs and predict the label of query graphs.

4.3 Adaptation Controller
Finding available combinations of learning rates and step size is difficult for MAML [Antoniou et al., 2019]. Besides, arbitrary graph size and structure bring difficulty for finding optimal step size. As a feasible solution to alleviate these problems, we designed a RL based controller to decide optimal step size when given other parameters. To make it work, our controller must roughly know when to stop adaptation according to the embedding quality and training state (denoted by loss). We mainly focus on Average Node Information (ANI) to indicate the embedding quality. Intuitively, if a node can be well reconstructed by its neighborhoods, it has less information for the graph classification. Conversely, the
rising of batch graphs’ ANI indicates that the pooling module has learned to select the most informative nodes. [Zhang et al., 2019] defined the node information as the Manhattan distance between the node representation itself and the one constructed from its neighbors. Inspired by their work, we define the ANI of a single graph $G$, as follows:

$$ANI_i = \frac{1}{n^l_i} \sum_{j=1}^{n^l_i} \left\| \left[ \left( I^l_t - (D^l_t)^{-1} A^l_t \right) H^l_t \right]_{j} \right\|_1$$  \hspace{1cm} (4)

where $l$ denotes the embedding layer of graph, $n^l_i$ denotes the number of node, $j$ denotes the row index of matrix or $j$-th node, $\| \cdot \|_1$ denotes the L1 norm of row vector, $A^l_t$ denotes the adjacency matrix, $D^l_t$ is the degree matrix of $A^l_t$, $H^l_t$ denotes $l$-th layer hidden representation matrix. In our work, we only use the last layer of graph embedding (e.g., $H^l_1$). And unless specifically stated, we use ANI to denote the average node information of the batch graphs in a task (e.g., The ANI of the support graphs is 100).

We set the ANIs in $T$ steps as $M \in \mathbb{R}^{T \times 1}$ and denote classification losses on support graphs as $L \in \mathbb{R}^{T \times 1}$. Then we update $T$ as following:

$$T = \left\lfloor \frac{1}{\sigma(f(M, L; \theta_s))} \right\rfloor$$  \hspace{1cm} (5)

where $f$ is the MLP based controller with parameters $\theta_s$, $\lfloor \cdot \rfloor$ is round down operation, and $\sigma$ is sigmoid function.

Besides, we get controller’s total reward as following:

$$Q = \sum_{t=1}^{T} r^{(t)} = \sum_{t=1}^{T} (acc_T - acc_t - \eta \times t)$$  \hspace{1cm} (6)

where $T$ is total steps and $acc_t$ is the classification accuracy on query data at step $t$, and $\eta \times t$ denotes the penalty item.

We select four public graph datasets including COIL-DEL, R52, Letter-High and TRIANGLES. These datasets can be downloaded here (https://www.cs.umb.edu/smimarog/textmining/datasets) except R52 (https://ls11-www.cs.tu-dortmund.de/staff/morris/graphkerneldatasets). The statistics are summarized in Table 1.

**COIL-DEL.** COIL-DEL is built on images, and each graph is constructed by applying corner detection and Delaunay triangulation to corresponding image [Riesen and Bunke, 2008].

**R52.** R52 is a text dataset in which each text is viewed as a graph. We transformed it into a graph dataset as follows: if two words appear together in a specified sliding window, they have an undirected edge in the graph. We keep classes with more than 20 samples and get 28 classes. We named the new dataset as Graph-R52.

**Letter-High.** Each graph represents distorted letter prototype drawings with representing lines by undirected edges and ending points of lines by nodes [Riesen and Bunke, 2008].

**TRIANGLES.** The dataset contains 10 different graph classes numbered from 1 to 10 corresponding to the number of triangles in each graph of the dataset [Knyazev et al., 2019].

### 5.2 Baselines

We adopt four groups of baselines made up of Graph Kernel, Finetuning, GNNs-Prototypical-Classifier (GNNs-Pro) and Graph Spectral Measures (GSM) [Chauhan et al., 2020]. For Graph Kernel baselines, we perform N-way-K-shot graph classification over the test set directly, because there are no datasets.

---

1. https://ls11-www.cs.tu-dortmund.de/staff/morris/graphkerneldatasets
2. https://www.cs.umb.edu/smimarog/textmining/datasets/
parameters to transfer. The baselines of the last three groups train a GNNs based graph classifier by performing classification over $C_0$ training classes (see Table 1). On the test stage, they perform N-way-K-Shot classification.

**Graph Kernel.** This group of methods firstly measure the similarity between labeled support data and query data on the test stage. After that, the similarity matrix was put into a Prototypical Classifier, which has none of parameters [Snell et al., 2017], to get predicted labels of query data. We choose typical graph kernel algorithms including Shortest-path Kernel (SP) [Borgwardt and Kriegel, 2005], Graphlet Kernel [Shervashidze et al., 2009] and Weisfeiler-Lehman Kernel (WL) [Shervashidze et al., 2011].

**Finetuning.** In this baseline, we train a naive graph classifier consisting of GraphSAGE, SAGPool and MLP classifier. On the test stage, we change the output dimension of the last layer of the classifier and fine tuning the layer’s parameters, while keeping other modules unchanged.

**GNNs-Pro.** We train a graph classifier following Finetuning. On the test stage, we replace the MLP classifier with Prototypical Classifier. We choose GCN [Kipf and Welling, 2017], GraphSAGE [Hamilton et al., 2017] and GAT [Veličković et al., 2018] as graph convolutional modules, and Self-attention Pooling (SAGPool) [Lee et al., 2019], TopK Pooling (TopKPool) [Gao and Ji, 2019] and Edge Pooling (EdgePool) [Dielh, 2019] as graph pooling modules.

**GSM.** [Chauhan et al., 2020] proposed the GSM based method customized for few-shot graph classification. On the training stage, they compute prototype graphs from each class, then they cluster the prototype graphs to produce superclasses. After that, they predict the origin class and superclass of each graph. On the test stage, they only update the classifier based on the classification of origin classes.

### 5.3 Experimental Details

To ensure a fair comparison, we use three convolutional layers followed by corresponding pooling layers for the GNNs based baselines and our proposed framework. We set the same node dimension as 128 for all GNNs based baselines. For the adaptation step, we set the minimum and maximum step by 4 and 15. We implement GNNs based baselines and our framework with PyTorch Geometric (PyG) and graph kernel baselines based on GraKeL. We use SGD optimizer with 1e-5 for weight decay and versatile learning rates 0.0001, 0.001, 0.0001 for $\alpha$, $\beta$ and $\gamma$, respectively.

### 5.4 Comparison with Graph Kernel, Finetuning and GNNs-Pro

To evaluate the performance of our framework, we performed 5-way-5-shot and 5-way-10-shot graph classification on COIL-DEL dataset. On Graph-R52 dataset, we performed 2-way-5-shot and 2-way-10-shot graph classification. The results are reported in Table 2. Our framework utilizes GraphSAGE and SAGPool as graph embedding backbone. So firstly we compare our framework with finetuning baseline built on GraphSAGE and SAGPool. We found our framework is superior to the finetuning baseline with a large margin, which indicates that the meta-learner works well with fast adaptation mechanism. Moreover, under 5-way-10-shot setting in GraphSAGE-SAGPool baseline, our framework achieves about 3.84% improvement on the COIL-DEL dataset.

#### Table 2: Accuracies with a standard deviation of baseline methods and our framework. We tested 200 and 500 N-way-K-shot tasks on COIL-DEL and Graph-R52, respectively. The **bold** numbers denote the best results we get, and the **blue** numbers denote the second best results. AS-MAML (wo/AS) denotes our framework without Adaptive Step (AS) which is controlled by our step controller, and AS-MAML (w/AS) denotes the whole framework we proposed.

| Categories | Baselines | COIL-DEL | Graph-R52 |
|------------|-----------|---------|-----------|
|            |           | 5-way-5-shot | 5-way-10-shot | 5-way-5-shot | 5-way-10-shot |
|            |           | 2-way-5-shot | 2-way-10-shot | 2-way-5-shot | 2-way-10-shot |
| Kernels    | GRAPHLET  | 47.47 ± 1.06 | 49.04 ± 0.98 | 56.52 ± 1.46 | 57.16 ± 1.47 |
|            | SP         | 38.33 ± 0.62 | 42.18 ± 0.69 | 74.38 ± 1.50 | **76.96 ± 1.34** |
|            | WL         | 43.05 ± 1.25 | 52.28 ± 1.47 | **76.90 ± 1.48** | 75.91 ± 1.46 |
| Finetuning | finetuning | 68.21 ± 1.29 | 72.38 ± 1.40 | 71.87 ± 2.04 | 72.39 ± 1.88 |
|            | GCN, TopKPool | 78.01 ± 1.83 | 78.98 ± 1.53 | 69.98 ± 1.53 | 70.19 ± 1.37 |
|            | GCN, EdgePool | 76.21 ± 1.54 | 79.43 ± 1.58 | 67.24 ± 1.34 | 67.72 ± 1.59 |
|            | GCN, SAGPool | 76.58 ± 1.19 | 79.16 ± 1.06 | 69.88 ± 1.40 | 70.46 ± 1.47 |
|            | GraphSAGE, TopKPool | 69.80 ± 1.25 | 74.18 ± 1.73 | 70.43 ± 1.76 | 70.52 ± 1.83 |
|            | GraphSAGE, EdgePool | 80.08 ± 1.26 | 80.96 ± 1.26 | 68.13 ± 1.59 | 70.72 ± 1.58 |
|            | GraphSAGE, SAGPool | 79.30 ± 1.12 | 80.91 ± 1.62 | 68.10 ± 1.40 | 70.49 ± 1.32 |
|            | GAT, TopKPool | 76.37 ± 1.10 | 77.29 ± 1.40 | 71.99 ± 1.51 | 73.31 ± 1.44 |
|            | GAT, EdgePool | 81.00 ± 1.22 | 83.57 ± 0.99 | 66.49 ± 1.32 | 70.49 ± 1.17 |
|            | GAT, SAGPool | 72.54 ± 1.07 | 73.99 ± 1.00 | 67.78 ± 1.52 | 74.10 ± 1.57 |
| Ours       | AS-MAML (wo/AS) | 79.54 ± 1.48 | 81.24 ± 1.27 | 74.12 ± 1.39 | 76.05 ± 1.17 |
|            | AS-MAML (w/AS) | **81.55 ± 1.39** | **84.75 ± 1.30** | **75.33 ± 1.19** | **78.33 ± 1.17** |

---

1. https://github.com/rusty1s/pytorch_geometric
2. https://github.com/ysig/GraKeL
5.5 Comparison with GSM Based Method

The GSM based method proposed by [Chauhan et al., 2020] did not adopt the episodic training paradigm utilized by our paper, so the method is inappropriate to be trained by N-way-K-shot graph classification on COIL-DEL and Graph-R52 dataset. For a fair comparison, we evaluate our framework on TRIANGLES and Letter-High, which are typical datasets used in their paper. Note that the total sample size of TRIANGLES is reduced from 45000 to 2000. Just like their partition, we randomly split out 20% examples from the training set to perform validation. Following their test configuration, we perform 3-way-K-shot and 4-way-K-shot classification on TRIANGLES and Letter-High respectively. The comparison of performances can be seen in Table 3. From the table, we concluded that our framework outperforms GSM with a large margin. The reason behind it is that they assume the test classes belong to the same set of super-classes built from the training classes. However, the label spaces of training classes and test classes usually do not overlap in few-shot settings. We believe that the graphs of training classes and test classes have similar sub-structures, which can be discovered by a well initialized meta-learner within a few adaptation steps.

| Methods | Shots | Datasets       | TRIANGLES | Letter-High |
|---------|-------|----------------|-----------|-------------|
| GSM     | 5-shot| 71.40 ± 4.34   | 69.91 ± 5.90 |
|         | 10-shot| 75.60 ± 3.67  | 73.28 ± 3.46 |
| Ours    | 5-shot| 86.47 ± 0.74   | 76.29 ± 0.89 |
|         | 10-shot| 87.26 ± 0.69  | 77.87 ± 0.75 |

Table 3: Accuracies evaluated from GSM and AS-MAML we proposed. For AS-MAML, we tested 200 N-way-K-shot tasks on both datasets. For GSM, we use the best results in their paper.

5.6 Ablation Study

In this section, we show the effect of controller module by ablation study. First of all, without the adaptive step (AS), we evaluated the performance of our framework by just putting GraphSAGE, SAGPool into meta-learner. From Table 2, we found that under 2-way-10-shot setting on Graph-R52, AS-MAML (wo/AS) brings about 3.06% improvement compared with finetuning baseline. Furthermore, the step controller brings about 2.28% improvement under 2-way-10-shot setting on Graph-R52 and 3.51% improvement under 5-way-5-shot setting on COIL-DEL.

We did deeper analysis for ANI and give more details of the step controller module under 5-way-10-shot setting on COIL-DEL dataset. The scatter diagram (Figure 2(a)) shows that ANIs have positive correlation with classification accuracies, which means larger ANI indicates better graph embedding for the MLP classifier module. The advantage of ANI over classification accuracy is that a larger ANI implies more discriminative graph embedding modules, while a better classification accuracy may mean that the MLP classifier module is over fitted on poor graph embedding modules. Figure 2(b) shows the variations of the adaptation step produced by the controller. In the beginning, the controller receives larger loss and smaller ANI, so it gives more adaptation steps to meta-learner for encouraging exploration. When the meta-learner has been trained well, the controller receives smaller loss and larger ANI, so it outputs smaller step size to alleviate overfitting.

Figure 2: Illustrations of the learning process under the 5-way-10-shot setting on COIL-DEL dataset. (a) The normalized ANIs and training accuracies in the first 50 epochs. Both of them are extracted from support graphs of the training set. (b) The variations of adaptation step on the training stage. the value at epoch 0 is the initial adaptation step, and then we calculate an average for every 5 epochs.

6 Conclusion and Future Works

Modelling real-world data by graphs is becoming more and more important for solving complex problems. In this paper, we address the problem of graph data dependency and propose few-shot graph classification with Model Agnostic Meta-Learning. By training GNNs with the meta-learning paradigm, we proposed AS-MAML and found that the framework works well with a few training graphs. For controlling the meta-learner’s adaptation step, we use ANI to demonstrate embedding quality. Beyond that, ANI is calculated by unsupervised way like estimating Mutual Information on graphs [Veličković et al., 2019]. Exploring and utilizing them for graph representation learning is an interesting future work. Moreover, we expect better graph embedding methods to improve the performance of our framework, and we also expect our work can be expanded to other graph classification tasks like skeleton based action recognition and subgraph analysis of social networks.
References

[Antoniou et al., 2019] Antreas Antoniou, Harrison Edwards, and Amos Storkey. How to train your MAML. In ICLR, 2019.

[Baxter, 2000] Jonathan Baxter. A model of inductive bias learning. Journal of Artificial Intelligence Research, 2000.

[Borgwardt and Kriegel, 2005] Karsten M Borgwardt and Hans-Peter Kriegel. Shortest-path kernels on graphs. In ICDM. IEEE, 2005.

[Chauhan et al., 2020] Jatin Chauhan, Deepak Nathani, and Manohar Kaul. Few-shot learning on graphs via superclasses based on graph spectral measures. In KDD’19, page 2895–2904, 2019.

[Diehl, 2019] Frederik Diehl. Edge contraction pooling for graph neural networks. arXiv preprint arXiv:1905.10990, 2019.

[Du et al., 2019] Zhengxiao Du, Xiaowei Wang, Hongxia Yang, Jingren Zhou, and Jie Tang. Sequential scenario-specific meta learner for online recommendation. In ICLR, 2020.

[Finn et al., 2017] Chelsea Finn, Pieter Abbeel, and Sergey Levine. Model-agnostic meta-learning for fast adaptation of deep networks. In ICML, 2017.

[Gao and Ji, 2019] Hongyang Gao and Shuiwang Ji. Graph u-nets. In Kamalika Chaudhuri and Ruslan Salakhutdinov, editors, ICML, volume 97 of PMLR, pages 2083–2092, Long Beach, California, USA, 09–15 Jun 2019.

[Hamilton et al., 2017] Will Hamilton, Zhitao Ying, and Jure Leskovec. Inductive representation learning on large graphs. In NeurIPS. 2017.

[J., 1992] Williams Ronald J. Simple statistical gradient-following algorithms for connectionist reinforcement learning. Machine Learning, 8:229–256, 1992.

[Kim et al., 2019] Jongmin Kim, Taesup Kim, Sungwoong Kim, and Chang D. Yoo. Edge-labeling graph neural network for few-shot learning. In CVPR, June 2019.

[Kipf and Welling, 2017] Thomas N Kipf and Max Welling. Semi-supervised classification with graph convolutional networks. ICLR, 2017.

[Knyazev et al., 2019] Boris Knyazev, Graham W Taylor, and Mohamed Amer. Understanding attention and generalization in graph neural networks. In NeurIPS, 2019.

[Lee et al., 2017] Jaekoo Lee, Hyunjae Kim, Jongsun Lee, and Sungroh Yoon. Transfer learning for deep learning on graph-structured data. In AAAI, 2017.

[Lee et al., 2019] Junhyun Lee, Inyeop Lee, and Jaewoo Kang. Self-attention graph pooling. In ICML, pages 3734–3743, 2019.

[Li et al., 2018] Zhenguo Li, Fengwei Zhou, Fei Chen, and Hang Li. Meta-sgd: Learning to learn quickly for few shot learning. In ICML, 2018.

[Liu et al., 2019] Lu Liu, Tianyi Zhou, Guodong Long, Jing Jiang, and Chengqi Zhang. Learning to propagate for graph meta-learning. In NeurIPS, 2019.

[Ravi and Larochelle, 2017] Sachin Ravi and Hugo Larochelle. Optimization as a model for few-shot learning. In ICLR, 2017.

[Riesen and Bunke, 2008] Kaspar Riesen and Horst Bunke. “iam graph database repository for graph based pattern recognition and machine learning”. In Niels da Vitoria Lobo, Takis Kasparis, Fabio Rolli, James T. Kwok, Michael Georgiopoulos, Georgios C. Anagnostopoulos, and Marco Loog, editors, Structural, Syntactic, and Statistical Pattern Recognition, 2008.

[Rusu et al., 2019] Andrei A. Rusu, Dushyant Rao, Jakub Sygnowski, Oriol Vinyals, Razvan Pascanu, Simon Osindero, and Raia Hadsell. Meta-learning with latent embedding optimization. In ICLR, 2019.

[Santoro et al., 2016] Adam Santoro, Sergey Bartunov, Matthew Botvinick, Daan Wierstra, and Timothy P. Lillicrap. Meta-learning with memory-augmented neural networks. In ICML, 2016.

[Satorras and Estrach, 2018] Victor Garcia Satorras and Joan Bruna Estrach. Few-shot learning with graph neural networks. In ICLR, 2018.

[Shervashidze et al., 2009] Nino Shervashidze, SVN Vishwanathan, Tobias Petri, Kurt Mehlhorn, and Karsten Borgwardt. Efficient graphlet kernels for large graph comparison. In AISTATS, pages 488–495, 2009.

[Shervashidze et al., 2011] Nino Shervashidze, Pascal Schweitzer, Erik Jan van Leeuwen, Kurt Mehlhorn, and Karsten M Borgwardt. Weisfeiler-lehman graph kernels. JMLR, 12(Sep):2539–2561, 2011.

[Snell et al., 2017] Jake Snell, Kevin Swersky, and Richard S. Zemel. Prototypical networks for few-shot learning. In NIPS, 2017.

[Veličković et al., 2018] Petar Veličković, Guillem Cucurull, Arantxa Casanova, Adriana Romero, Pietro Liò, and Yoshua Bengio. Graph attention networks. In ICLR, 2018.

[Veličković et al., 2019] Petar Veličković, William Fedus, William L. Hamilton, Pietro Liò, Yoshua Bengio, and R Devon Hjelm. Deep graph infomax. In ICLR, 2019.

[Vinyals et al., 2016] Oriol Vinyals, Charles Blundell, Tim Lillicrap, Koray Kavukcuoglu, and Daan Wierstra. Matching networks for one shot learning. In NIPS, 2016.

[Xu et al., 2019] Keyulu Xu, Weihua Hu, Jure Leskovec, and Stefanie Jegelka. How powerful are graph neural networks? In ICLR, 2019.

[Yao et al., 2020] Huaxiu Yao, Xin Wu, Zhiqiang Tao, Yaliang Li, Bolin Ding, Ruirui Li, and Zhenhui Li. Hierarchical graph pooling with structure learning. arXiv preprint arXiv:1911.05954, 2019.