
META-LEARNING WITH GRAPH NEURAL NETWORKS: METHODS AND APPLICATIONS

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ABSTRACT

Graph Neural Networks (GNNs), a generalization of deep neural networks on graph data have been widely used in various domains, ranging from drug discovery to recommender systems. However, GNNs on such applications are limited when there are few available samples. Meta-learning has been an important framework to address the lack of samples in machine learning, and in recent years, the researchers have started to apply meta-learning to GNNs. In this work, we provide a comprehensive survey of different meta-learning approaches involving GNNs on various graph problems showing the power of using these two approaches together. We categorize the literature based on proposed architectures, shared representations, and applications. Finally, we discuss several exciting future research directions and open problems.

1 Introduction

The methods of artificial intelligence (AI) and machine learning have found tremendous success in various applications, ranging from natural language processing [Dev+19] to cancer screening [Wu+19]. The success of AI systems can be attributed to various architectural innovations, and the ability of deep neural networks (DNN) to extract meaningful representations from Euclidean data (e.g. image, video etc.). However, in many applications, the data is graph-structured. For example, in drug discovery, the goal is to predict whether a given molecule is a potential candidate for a new drug, where the input molecules are represented by graphs. In a recommender system, the interaction between the users and the items are represented by a graph, and such non-Euclidean data is crucial in designing a better system.

The proliferation of graph structured data in various applications has led to a Graph Neural Network (GNN), a generalization of DNN for graph-structured inputs. The main goal of GNNs is to learn effective representations of the graphs. Such representations map the vertices, edges, and/or graphs to a low-dimensional space (e.g. \mathbb{R}^d), so that the structural relationships in the graph are reflected by the geometric relationships in the representations [HYL17b]. In recent years, GNNs have been applied in diverse domains, often with surprising positive results like discovery of a new antibiotic [Sto+20], accurate traffic forecasting [Cui+19] etc.

Despite of recent success of GNNs in various domains, GNN frameworks have their own shortcomings. One of the major challenges in applying GNNs, particularly for large graph-structured datasets, is the limited number of samples. Furthermore, real-world systems like recommender systems often need to handle a diverse type of problems, and must adapt to a new problem with very few observations. In recent years, meta-learning has turned out to be an important framework to address these shortcomings of deep learning systems. The main idea behind meta-learning is to design learning algorithms that can leverage prior learning experience to adapt to a new problem quickly, and learn a useful algorithm with few samples. Such approaches have been quite successful in diverse applications like natural language processing [Liu+19], robotics [Nag+20], and healthcare [Zha+19].

Recently, several meta learning methods to train GNNs have been proposed for various applications. The main challenge in applying meta-learning to graph-structured data is to determine the type of representation that is shared across tasks, and devise an effective training strategy. In this survey, we review the growing literature on meta learning with GNNs. There are several thorough individual surveys on GNN [Zho+18; Wu+20] and meta-learning [Hos+20], but we believe this survey is the first effort to categorize and comprehensively review the existing papers on meta learning with GNNs.

Our Contribution Besides providing background on meta-learning and GNN architectures individually, our contributions can be summarized as follows.

- **Comprehensive review:** We provide a comprehensive review of meta learning techniques with GNNs on several graph problems. We categorize the literature based on methods, representations and applications and show various scenarios where limitations of GNNs are addressed via meta learning.
- **Future directions:** We discuss how meta learning and GNNs can address some of the challenges in several areas: (i) combinatorial graph problems, (ii) graph mining problems, and (iii) other emerging applications such as traffic flow prediction and network alignment.

The rest of this paper is organized as follows. Section 2 provides background on key graph neural network frameworks. Section 3 also outlines the background on meta-learning and key theoretical advances. Besides an overview in Section 4, a comprehensive categorization of the papers that use the framework of meta-learning equipped with GNNs on important graph related problems is described in Sections 5 and 6. Section 7 suggests some exciting future directions.

2 Background on GNN

Generalizing deep learning on graphs has given birth to an exciting area of Graph Neural networks (GNNs). Here we briefly describe the key GNN architectures. A primary contribution in applying neural architectures on graphs has been made by [KW17] with the introduction of Graph Convolutional Networks (GCNs). GCNs are analogous version of convolutional neural networks (CNNs) on graphs. Inspired by the idea of representing a pixel with information from its nearby pixels (filter in CNNs), graph convolutions also apply the key idea of aggregating feature information from a node’s local neighborhood. More formally, GCNs are neural network architectures that produces a d -dimensional embeddings for each node by taking as input adjacency matrix A and features and node features X ; $\text{GCN}(A, X) : \mathbb{R}^{n \times n} \times \mathbb{R}^{n \times p} \rightarrow \mathbb{R}^{n \times d}$. The idea is to aggregate feature information from a node’s neighborhood (can be generalized to multiple hops) and its own features to produce the final embedding. A 2-layer (neighbourhood is 2-hops) *GCN* can be defined as follows:

$$\text{GCN}(A, X) = \sigma(\hat{A}\sigma(\hat{A}XW^{(1)})W^{(2)})$$

where $\hat{A} = \tilde{D}^{-\frac{1}{2}}\tilde{A}\tilde{D}^{-\frac{1}{2}}$ is the normalized adjacency matrix with \tilde{D} as weighted degree matrix and $\tilde{A} = I_n + A$ with I_n being an $n \times n$ identity matrix and σ is an activation function. Moreover, $W^{(i)}$ is a weight matrix for the i -th layer to be learned during training, with $W^{(1)} \in \mathbb{R}^{p \times d'}$, $W^{(2)} \in \mathbb{R}^{d' \times d}$, and d (d') being the number of neural network nodes in the output (hidden) layer.

Hamilton et al. [HYL17a] proposed an inductive GNN framework with an aggregation function that is able to share weight parameters (\mathbb{W}^k) across nodes, can be generalized to unseen nodes and scale to large datasets. To learn representation h_v^k of a node v , it iterates over all nodes which are in their K -hop neighborhood. While iterating over node v , it *aggregates* (with AGGREGATE_k) the current representations of v ’s neighbors ($\mathbf{h}_N^k(v)$) and *concatenate* with the current representation of v (h_v^{k-1}), which is then fed through a fully connected layer with an activation function. Intuitively, with more iterations, nodes incrementally receive information from neighbors of higher depth (i.e., distance). More specifically for k -th iteration,

$$\begin{aligned} \mathbf{h}_N^k(v) &= \text{AGGREGATE}_k(\{h_u^{k-1}, \forall u \in N(v)\}) \\ \mathbf{h}_v^k &= \sigma(\mathbb{W}^k \cdot \text{CONCAT}(\mathbf{h}_N^k(v), h_v^{k-1})) \end{aligned}$$

There are several variations of GNNs that are based on different mechanisms: Graph Attention Networks (GATs) [Vel+18; Zha+18] learn edge weights using attention mechanisms; Graph Autoencoders [CLX16; KW16] encode nodes/graphs into a latent vector space and further reconstruct the graph related data depending on the application from this encoding in an unsupervised fashion; Recurrent GNNs [Sca+08; Li+16] apply the same set of parameters recurrently over nodes to extract high-level node representations. For a comprehensive survey on GNNs, please refer to [Wu+20].

Applications. GNNs outperform traditional approaches for semi-supervised learning tasks (e.g. node classification) on graphs. The high level applications of GNNs can be categorized in three major tasks: node classification, link prediction, and graph classification. For node classification and link prediction traditionally four benchmark datasets are used: Cora, Citeseer, Pubmed, and PPI. Shchur et al. [Shc+18] and Errica et al. [Err+19] provide a detailed comparison of performances of the main GNN architectures on node and graph classification respectively. GNNs are also used in link prediction task that has applications in many domains such as friend or movie recommendation, knowledge graph completion, and metabolic network reconstruction [ZC18].

3 Background on Meta-Learning

Meta-learning has turned out to be an important strategy the problem of limited data in various machine learning applications. The main idea behind meta-learning is to design learning algorithms that can leverage prior learning experience to adapt to a new problem quickly, and learn a useful algorithm with few samples [Sch87].

Framework. In standard supervised learning, we are given a training dataset $\mathcal{D} = \{\mathbf{x}_i, y_i\}_{i=1}^n$, a loss function ℓ , and we aim to find a predictive model of the form $\hat{y} = f_\theta(\mathbf{x})$.

$$\theta^* = \operatorname{argmin}_\theta \mathcal{L}(\mathcal{D}, \theta) = \operatorname{argmin}_\theta \sum_{i=1}^n \ell(f_\theta(\mathbf{x}_i), y_i)$$

In meta-learning, we are given samples from a number of different tasks and the goal is to learn an algorithm that generalizes across tasks. In particular, the tasks are drawn from a distribution $p(\mathcal{T})$, and the meta-objective is to find a common parameter that works across the distribution of tasks.

$$\omega^* = \operatorname{argmin}_\omega \sum_{\substack{\mathcal{T}_i \sim p(\mathcal{T}) \\ \mathcal{D}_i \sim \mathcal{T}_i}} \mathcal{L}_i(\mathcal{D}_i, \omega) \quad (1)$$

In the meta-test phase, we are given a target task (say task 0) and we use the meta-knowledge ω^* to obtain the best parameter for the target with few samples.

$$\theta_0^* = \operatorname{argmin}_\theta \mathcal{L}_0(\mathcal{D}_0, \theta | \omega^*)$$

Training. Many popular meta-learning algorithms are based on gradient descent on the meta-parameter ω [FAL17; RL17]. In order to understand how to perform gradient descent with respect to ω , it is insightful to frame Eq. 1 as a bi-level optimization problem.

$$\begin{aligned} \omega^* &= \operatorname{argmin}_\omega \sum_{\substack{\mathcal{T}_i \sim p(\mathcal{T}) \\ \mathcal{D}_i \sim \mathcal{T}_i}} \mathcal{L}(\mathcal{D}_i, \theta_i^*(\omega), \omega) \\ \text{s.t. } \theta_i^*(\omega) &= \operatorname{argmin}_\theta \mathcal{L}_i(\theta, \omega, \mathcal{D}_i) \quad \forall i \end{aligned}$$

If we have a model for the inner-optimization method, then a gradient of the objective with respect to ω can be computed by using the chain rule e.g. $\nabla_\omega \mathcal{L}(\mathcal{D}_i, \theta_i^*(\omega), \omega) = \nabla_{\theta_i^*(\omega)} \mathcal{L}(\mathcal{D}_i, \theta_i^*(\omega), \omega) \frac{d\theta_i^*(\omega)}{d\omega}$. However, often the inner objective function is non-convex, and hard to solve. So model agnostic meta learning (MAML), introduced by [FAL17] suggests first taking a gradient step for each task i ($\theta'_i = \theta - \alpha \nabla_\theta \mathcal{L}_i(\theta, \omega, \mathcal{D}_i)$) and then replacing $\theta_i^*(\omega)$ in the outer objective i.e. $\omega = \omega - \beta \nabla_\omega \sum_i \mathcal{L}(\mathcal{D}_i, \theta'_i, \omega)$.

Theory. Despite immense success, we are yet to fully understand the theoretical foundations of meta-learning algorithms. Baxter [Bax00] first proved generalization bound for multitask learning problem, by considering a model where tasks with shared representation are sampled from a generative model. Pontil et al. [PM13], and Maurer et al. [MPRP16] developed general uniform-convergence based framework to analyze multitask representation learning. However, they assume oracle access to a global empirical risk minimizer. The most promising theoretical direction stems from representation learning. The main idea is that the tasks share a common shared representation and a task-specific representation [TJJ20b; TJJ20a]. If the shared representation is learned from the training tasks, then the task-specific representation for the new task can be learned with only a few samples.

4 Overview

We review the literature on meta learning with graph neural networks in two sections. First, section 5 covers applications of meta-learning framework for solving some classical graph problems. Here, the problem doesn't explicitly

come with a multi-task settings, rather the meta-learning framework is applied to a fixed graph. Then, in section 6 we cover the literature on graph meta learning when there are multiple tasks and the graph might change with the tasks. Although various GNNs have been proposed for graph meta-learning, they can be categorized broadly based on the type of shared representation, which can be either at a local level (node/edge based) or at the global level (graph based). Table 1 provides an overview of various papers categorized by the type of shared representation and application considered.

Representation	Graph applications		
	Node classification	Link Prediction	Graph Classification
Node/Edge Level	[Zho+19]	[Che+19]	
	[Din+20]	[BLH20]	
	[Liu+21]		
	[Wan+20]		
	[BV20]	[BV20]	[BV20]
Graph Level		[Bos+19]	[CNK20]
			[Ma+20]

Table 1: Organization of the papers on Meta-learning and GNN based on applications and underlying graph-related representations.

5 Meta-Learning Applied to Graph Problems

In this section, we review applications of meta-learning for solving some classical problems on graphs. Here we consider the setting when the underlying graph is fixed and the node/edge features do not change with different tasks. In fact, we are not in a multitask framework where there are a number of tasks and few samples are available from each task. Rather, the framework of meta-learning is applied to various graph problems by creating multiple tasks either considering the nodes or the edges.

Node Embedding. The goal of node embedding is to learn representations for the nodes in the graph so that any downstream application can directly work with these representations, without considering the original graph. This problem is often challenging in practice because the degree distributions of most graphs follow a power law distribution and there are many nodes with very few connections. Liu et al. [Liu+20] address this issue by applying meta-learning to the problem of node embedding of graphs. They set up a regression problem with a common prior to learn the node embeddings. Since the base representations of high-degree nodes are accurate, they are used as meta training set to learn the common prior. The low degree nodes have only a few neighbors (samples), the regression problem for learning their representations is formulated as a meta-testing problem, and the common prior is adapted with a small number of samples for learning the embeddings of such nodes.

Node Classification. The node classification task aims to infer the missing labels of nodes of a given partially labeled graph. This problem often appears in diverse contexts such as document categorization and protein classification [Tan+08; Bor+05], and have received significant attention in recent years. However, often many classes are novel i.e., they have very few labeled nodes. This makes meta-learning or few-shot learning particularly suitable for this problem. Zhou et al. [Zho+19] apply a meta-learning framework for the node classification problem on graphs by learning a transferable representation using data from classes that have many labeled examples. Then, during the meta-test phase, this shared representation is used to make predictions for novel classes with few labeled samples. Ding et al. [Din+20] improve upon the previous method by considering a prototype representation of each class and meta-learning the prototype representation as an average of weighted representations of each class. Subsequently, Liu et al. [Liu+21] point out that it is important to also learn the dependencies among the nodes in a task, and propose to use nodes with high centrality scores (or hub nodes) to update the representations learned by a GNN. This is done by selecting a small set of hub nodes and for each node v , considering all the paths to the node v from the set of hub nodes.

Link Prediction. Meta-learning is useful for learning new relationship via edges/links in multi-relational graphs. In multi-relational graphs, an edge is represented by a triple of two end points and a relation. Such graphs appear in many important domains such as drug-drug interaction prediction. The goal of link prediction in multi-relation graphs is to predict new triples given one end point of a relation r with observing a few triples about r . This problem is challenging

Papers	Meta-learning parameters	
	Inner Loop (Task-Specific)	Outer Loop (Shared)
[HZ20]	Node embeddings	Classification
[Wan+20]	Node embeddings	Feature matrix
[CNK20]	Graph feature, Super-class	graph label/ actual class
[Ma+20]	Graph feature, Graph embedding	graph embedding/ Classification
[BV20]	Node Embedding	Output Layer
[Bos+19]	VGAE Initialization	Graph Signature (GCN + MLP)
[Liu+20]	High-degree node embedding	node specific embedding

Table 2: Organization of the papers in Section 6 based on the corresponding meta-learning approaches.

as only few associative triples are usually available. Chen et al. [Che+19] use meta-learning to solve link prediction in two steps: (1) A Relation-Meta Learner generates relation meta from heads’ and tails’ embeddings in the support set, and (2) An Embedding Learner that calculates the truth values of triples in support set via end points’ embeddings and relation meta.

Multi-relational graphs are even more difficult to manage with their dynamic nature (addition of new nodes) over time and the learning is even more difficult when these newly evolved nodes have only few links among them. Baek et al. [BLH20] introduce a few-shot out-of-graph link prediction technique, where they predict the links between the seen and unseen nodes as well as between the unseen nodes. The main idea is to randomly split the entities in a given graph into the meta-training set for simulated unseen entities, and the meta-test set for real unseen entities.

6 Meta-Learning on GNN

We now discuss the growing and exciting literature on graph meta learning where there are multiple tasks and the graph changes across the tasks. Changes in graphs occur if either the node/edge feature changes, or the underlying network structure changes with the tasks. In the context of meta-learning, several architectures have been proposed in recent years. However, a common thread underlying all of them is a shared representation of the graph, either at a local node/edge level, or at a global graph level. Based on the type of shared representation, we categorize the existing works into two groups. Most of the existing literature adopt the MAML algorithm [FAL17] to train the GNNs. The outer loop of MAML updates the shared parameter, whereas the inner loop updates the task-specific parameter for the current task. Table 2 lists the shared and the task-specific parameters for all the papers in this section.

6.1 Node/Edge Level Shared Representation

First, we consider the setting where the shared representation is local i.e. node/edge based. Huang et al. [HZ20] consider the node classification problem where the input graphs as well as the labels can be different across tasks. They learn a representation for each node u in two steps. First, extract a subgraph S_u corresponding to the set of nodes $\{v : d(u, v) \leq h\}$ where $d(u, v)$ is the distance of the shortest path between nodes u and v . Then feed the subgraph S_u through a GCN to learn a representation for node u . The theoretical motivation behind considering the graph S_u is that the influence of a node v on u decreases exponentially as the shortest-path distance between them increases. Once the nodes are encoded, one can learn any function f_θ that maps the encodings to class labels. Huang et al. [HZ20] use MAML to learn this function with very few samples on a new task, enjoying the benefits of node-level shared representations in node classification.

Wang et al. [Wan+20] also consider the few shot node classification problem for a setting where the network structure is fixed, but the features of the nodes change with tasks. In particular, given a base graph with node feature matrix $X \in \mathbb{R}^{n \times d}$, the proposed model learns a new feature matrix $X_t = X \odot \alpha_t(\phi) + \beta_t(\phi)$ for the t -th task, and then use a GNN $f_\theta(X_t)$ to learn the node representations for the t -th task. During training, the outer loop updates the ϕ parameters, whereas the inner loop of MAML only updates the θ -parameter. This enables quick adaptation to the new task.

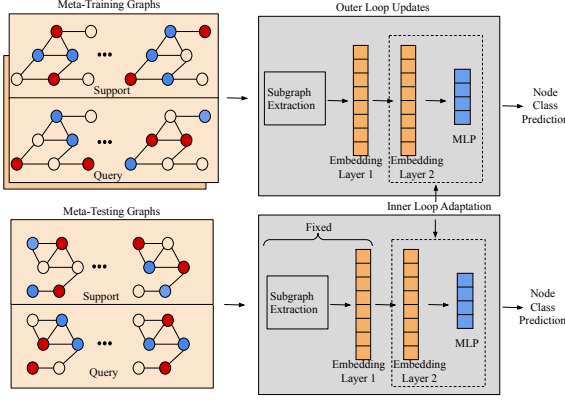


Figure 1: A prototype of the meta learning framework with GNN for solving node classification problem. This is based on the architectures proposed by [HZ20] and [Wan+20]. Following [HZ20], we propose to use the neighborhoods of each node for node embedding. Embedding layer 1 is trained in the outer loop of MAML, whereas the other layers are adapted for particular tasks.

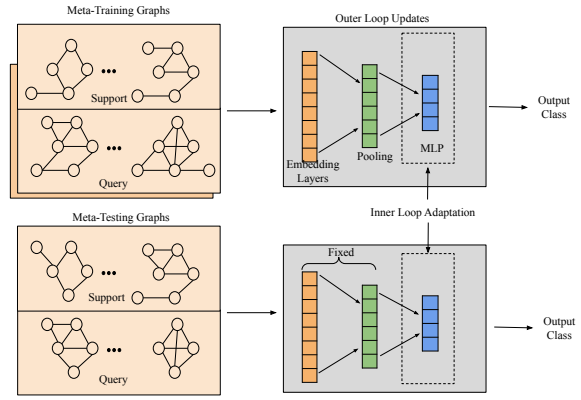


Figure 2: A prototype of the meta learning framework with GNN for solving graph classification problem. This is based on the architectures proposed by [Ma+20], and [BV20]. The embedding and pooling layers learn global representation of the input graph, and are trained in the outer loop of MAML. The final multi-layer perceptron (MLP) is used for classification and is adapted to the particular task at meta-test.

6.2 Graph Level Shared Representation

In this subsection, we discuss the setting when the shared representation is global i.e. graph-level. A canonical application of this representation is the *graph classification* problem, where the goal is to classify a given graph to one of many possible classes. Graph classification often requires a large number of samples for high quality prediction. Thus, learning with few labeled graph data is challenging for practical applications and can be addressed by meta-learning. The existing papers on using meta-learning for graph classification usually learn an underlying shared representation and then adapts the representation for a new task.

Chauhan et al. [CNK20] proposed few-shot graph classification based on graph spectral measures. In particular, they train a feature-extractor $F_\theta(\cdot)$ to extract features from the graphs in meta-training. For classification, they use two units C^{sup} to predict the super-class probability of a graph, and C^{att} , an attention network to predict the actual class label. During the meta-test phase, the weights of the networks $F_\theta(\cdot)$ and C^{sup} are fixed, and the network C^{att} is retrained on the new test classes. As the feature extractor F_θ is the common shared structure, and is not retrained on the test tasks, this approach requires few samples from new classes.

Although Chauhan et al. [CNK20] propose a novel meta-learning architecture for graph classification, there are several limitations. First, the architecture assumes significant overlap between the super-class structure of the test and the training set. Second, the fixed feature extractor cannot be updated for the new tasks. Ma et al. [Ma+20] design a better meta-learning technique by allowing the feature extractor to adapt efficiently for new tasks. They apply two networks – embedding layers (θ_e), followed by classification layers (θ_c) to classify a given graph. However, for a new task, both θ_e and θ_c are updated. In particular, the authors use MAML [FAL17] to update the parameters and use a reinforcement learning based controller to determine how the inner loop is run i.e., what is the optimal adaptation step for a new task. The parameters of the controller is updated using the graph’s embedding quality and the meta-learner’s training state.

Finally, Buffelli et al. [BV20] attempt to develop a framework that can adapt to three different tasks – graph classification, node classification, and link prediction. Like [CNK20; Ma+20] they use two different layers; one generates node embeddings and convert the graph to a representation, and another was a multi-head output layer for the three types of tasks. The node embedding layer is trained during the initialization phase of MAML and the multi-head output layer is updated in the inner loop of MAML based on the type of task.

Bose et al. [Bos+19] consider the few shot link prediction problem, where the goal is to predict labels of links/edges that contain only a small fraction of their true labels. They assume that the graphs are generated from a common distribution $p(\cdot)$ and learn a meta link prediction model that can be quickly adapted to a new graph $G \sim p(\cdot)$. In particular, the authors use Variational Graph Autoencoder (VGAE) [KW16] to model the base link prediction model. There are two sets of parameters – global initialization parameters for the VGAE, and local graph signature $s_G = \psi(G)$

which is obtained by passing the graph G through GCN and then using a k -layer MLP. The training is done using MAML and only the graph signature is updated for the test graph.

7 Future Directions

The application of meta-learning to GNNs for graph specific applications is a growing but exciting area of research. In this section, we suggest several future directions for research.

7.1 Emerging Applications

We have discussed applications of meta-learning equipped with GNNs on node/graph classification and link prediction. In fact, this framework is quite general, and one can consider other relevant problems.

Traffic Prediction: Recently, the traffic prediction problem [Pan+20] has been addressed via meta-learning. In traffic prediction, the main challenges are modeling complex spatio-temporal correlations of traffic and capturing the diversity of such correlations varying locations. An important question is the following: *how do we apply meta-learning to learn these correlations and use these meta knowledge to have high quality predictions in diverse locations?*

Network Alignment (NA): Another potential problem where meta-learning could be helpful is network alignment. NA aims to map or link entities from different networks and relevant in many application domains such as cross-domain recommendation and advertising. Zhou et al. [Zho+20] address this alignment problem via meta-learning. The idea is to use the meta-metric learning from known anchor nodes to obtain latent priors for linking unknown anchor nodes. The existing approaches of NA is also difficult to scale. An interesting direction of research would consider meta-learning to overcome this scalability challenge.

Molecular Property Prediction: GNNs have been also used in predicting molecular properties. However, one of the main challenges is that molecules are heterogeneous structure where each atom has connection with different neighboring atoms via different types of bonds. Secondly, often a limited amount of data on labeled molecular property are available; and thus, to predict new molecular properties, meta-learning techniques [Guo+21] can be relevant and effective.

7.2 Graph Combinatorial Optimization Problems

Combinatorial optimization problems appearing in graphs have applications in many domains such as viral marketing in social networks [KKT03], health-care [Wil+18], and infrastructure development [Med+18], and several GNN based architectures have been proposed for solving them [Dai+17; LCK18; Gas+19; Man+20]. These optimization problems are often NP-hard, and polynomial-time algorithms, with or without approximation guarantees, are often desirable and used in practice. However, some techniques [LCK18; Man+20] based on GNNs need to generate candidate solution nodes/edges before generating the actual solution set. Note that, labels in the form of importance of each node in a solution set of these problems are often difficult to get. Meta-learning can be used when there are scarcity of labels. Furthermore, these combinatorial problems often share similar structures. For instance, the influence maximization problem [KKT03] have similarity with the Max Cover problem. However, even performing a greedy iterative algorithm to generate solutions/labels for influence maximization problem is computationally expensive. The idea of using meta-learning in solving a harder combinatorial problem (unseen task) with a fewer node labels will be to learn on the easier problems (seen tasks) where labels can be generated at a lower cost. Solving combinatorial optimization problems on graphs via neural approaches has recently gained a lot of attention and we refer the readers to [Cap+21] for further reading.

7.3 Graph Mining Problems

There has been recent attempt to solve classical graph mining problems with GNN frameworks. For instance, a popular problem is to find graph edit distance (similarity) between two graphs [Bai+19]. When the notion of similarity changes and there are not enough data to learn via a standard supervised learning method, can meta-learning be helpful? Another popular graph mining problem is detecting the Maximum Common Subgraph (MCS) between two input graphs with applications in biomedical analysis and malware detection. In drug design, common substructures in compounds can reduce the number of human-conducted experiments. However, MCS computation is NP-hard, and state-of-the-art exact MCS solvers are not scalable to large graphs. Designing learning based models [Bai+20] for the MCS problem while utilizing as few labeled MCS instances as possible remains to be a challenging task and meta-learning could be helpful in mitigating this challenge.

7.4 Dynamic Graphs

In many applications, graphs arise with their dynamic nature, i.e., nodes and edges along with their attributes can change (addition or deletion) over time. Most of the discussed papers that use frameworks built on meta-learning and GNNs focus on static graphs. An interesting direction would be to extend this framework for dynamic graphs [BLH20].

7.5 Theory

We pose two important theoretical questions in the context of meta learning with GNNs. The most natural question is understanding the benefits of transfer learning in GNNs. Garg et al. [GJJ20] and Scarselli et al. [STH18] have recently established generalization bounds for GNNs. On the other hand, in the context of meta-learning, Tripuraneni et al. [TJJ20b] considers functions of the form $f_j \cdot h$, where $f_j \in \mathcal{F}$ is the task-specific function and h is the shared function. Then the number of samples required in the meta-test phase grows as $C(\mathcal{F})$, which can be significantly lower than learning $f_j \cdot h$ from scratch. It would be interesting to see if one can prove similar speedup results for GNNs by generalizing the results of [GJJ20] and [STH18]. Another interesting question is determining the right level of shared representation and figuring out the expressiveness of such structures. The seminal work of Xu et al. [Xu+18] proves that GNN variants like GCN and GraphSAGE are no more discriminative than the Weisfeiler-Leman (WL) test. Since GNNs for meta-learning further limit the type of architecture used, an interesting question is whether it comes with any additional cost on expressiveness.

8 Conclusion

In this survey, we have performed a comprehensive review of the works that are combination of graph neural networks (GNNs) and meta-learning. Besides outlining backgrounds on GNNs and meta-learning, we have organized the past research in an organized manner in multiple categories. We have also provided a thorough review, summary of methods, and applications in these categories. Furthermore, we have described several future research directions where meta learning with GNN can be useful. The application of meta-learning to GNNs is a growing and exciting field and we believe many graph problems will benefit immensely from the combination of the two approaches.

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