Community Search: Learn from Small Data

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1 INTRODUCTION

Community is a cohesive subgraph that is densely intra-connected and loosely inter-connected in a graph. Given any query nodes, community search (CS) aims to find communities covering the query nodes, i.e., local query-dependent communities, which has a wide range of real applications, e.g., friend recommendation, advertisement in e-commerce and protein complex identification. To deal with this problem, an effective solution is to inject prior knowledge which is always shared by different tasks and also serves as the design intuition. For diversified communities in real-world graphs, there is no universal community constraint which is the overall best. One constraint may be either too loose or too tight. Even for one graph, the topology is diverse in different regions so that a fixed community constraint may not be consistently applicable for different local queries. To this end, it is quite difficult to choose a proper $k$ value as well as one community metric to pursue high accuracy. To tackle the structural inflexibility of traditional CS algorithms, ML/DL-based solutions are arising as an attractive research direction. These approaches build ML/DL models from given ground-truth communities and expect the model to generalize to unknown community-member relationships. For one thing, these data-driven approaches get rid of the inflexible constraint instead adapt to implicit structural patterns from data. For the other thing, the model can learn via error feedback from its predictions over the queries with community membership ground-truth in an end-to-end fashion.

It has been shown that compared with algorithmic approaches, the learning-based approaches are more successful in finding high-quality solutions. Nevertheless, the success heavily relies on sufficient training ground-truth. Specifically, [14] collects user feedback to update a model incrementally and interactively. The model is trained for a specific query node, whose effectiveness is fully determined by the quality of the given ground-truth of that query node. The effectiveness will be degraded if the user cannot provide enough high-quality ground-truth for that query node. [24] proposes a graph neural network based model that is trained by a collection of query nodes with their community labeling, and makes predictions for unseen query nodes. For one graph, a large volume of query nodes with community membership ground-truth are necessary for training, which ensure the model well generalize to other local queries.

In reality, collecting and labeling ground-truth are expensive and labor-intensive, especially for various local queries and diversified graphs. When deploying the data-driven approaches, users are always stuck in the dilemma that there is no sufficient training data. To deal with this problem, an effective solution is to inject prior knowledge extracted from multiple tasks into the ML model, instead of training one model from scratch over the insufficient training data of one task. Here, one task is a graph with only a few query nodes and ground-truth for training. Fortunately, the implicit prior knowledge of the CS task is rather intuitive, i.e., for any local query of any graph, its communities are the nearby densely connected nodes, which also share similar attributes with the query. Although the real-world graph and the local queries are diverse, this intuition is always shared by different tasks and also serves as the design

ABSTRACT

Community Search (CS) is one of the fundamental graph analysis tasks, which is a building block of various real applications. Given any query nodes, CS aims to find cohesive subgraphs that query nodes belong to. Recently, a large number of CS algorithms are designed. These algorithms adopt pre-defined subgraph patterns to model the communities, which cannot find communities that do not have such pre-defined patterns in real-world graphs. Thereby, machine learning based approaches are proposed to capture flexible community structures by learning from community ground-truth in a data-driven fashion. However, existing approaches rely on sufficient training data to provide enough generalization for machine learning models.

In this paper, we study ML-based approaches for community search, under the circumstance that the training data is scarce. To learn from small data, we extract prior knowledge which is shared across different graphs as CS tasks in advance. Subsequent small training data from a new CS task are combined with the learned prior knowledge to help the model well adapt to that specific task. A novel meta-learning based framework, called CGNP, is designed and implemented to fulfill this learning procedure. A meta CGNP model is a task-common node embedding function for clustering by nature, learned by metric-based learning. To the best of our knowledge, CGNP is the first meta model solution for CS. We compare CGNP with traditional CS algorithms, e.g., CTC, ATC, ACQ, and ML baselines on real graph datasets with ground-truth. Our experiments show that CGNP outperforms the native graph algorithms and ML baselines 147% and 113% on F1-score by average.
The principle of existing CS algorithms, in different forms, e.g., different \( k \)-related subgraph patterns. Hence, in this paper, we concentrate on learning a meta-model to capture this prior by meta-learning, in the multi-task scenarios. The prior knowledge synthesizes similar or complementary inductive bias across different tasks to compensate the insufficient knowledge from small training data, thus can be swiftly adapted to a new task.

There are existing meta-learning algorithms, e.g., simple feature transfer and model-agnostic meta-learning. However, trivial adaptations to CS tasks fail to achieve high performance since they do not try to exploit the intrinsic characteristic of the CS task. For CS, what a model needs to justify for each node in a graph is whether or not it has a community membership with any given query node. To facilitate such binary justification, we propose a novel model, Conditional Graph Neural Process (CGNP) to generate node embeddings conditioned on the small training data, and the distance between a node embedding to that of the query node explicitly indicates their community membership. Furthermore, as a graph specification of Conditional Neuronal Process (CNP) [15], CGNP inherits the main ideas of CNP that implicitly learns a kernel function between a training query node and a query node to be predicted. In a nutshell, our learned CGNP is a common embedding function that transforms the nodes of every graph into a distance-aware hidden space, as well as a common kernel function between query nodes across different graphs, which captures the CS prior knowledge. Combining with graph neural network, the metric-based learning approach, CGNP is particularly suitable for classification tasks over graphs with small training data.

Roadmap: The rest of the paper is organized as follows. Section 2 reviews the relative work. In section 3, we give the problem statement followed by two naive solutions introduced in section 4. We introduce the main idea of our approach, CGNP in section 5, and elaborate on its architecture design in section 6. Section 7 presents the training and test algorithms of CGNP. We present our comprehensive experimental studies in section 8 and conclude the paper in section 9.

2 RELATED WORK

Community Search. The problem of community search (CS) is to find densely connected subgraphs containing given query nodes. A comprehensive survey of CS problems and approaches can be found in [12, 22]. In a nutshell, CS problem can be divided into two categories. One is non-attributed community search which only concerns the structural cohesiveness over simple graphs and the other is attributed community search (ACS) which concerns both the structural cohesiveness and content overlapping or similarities over attributed graphs. Regarding capturing the structural cohesiveness, various community metrics have been proposed, including, \( k \)-core [9, 27, 36], \( k \)-truss [3, 20], \( k \)-clique [8, 45] and \( k \)-edge connected component [6, 18]. These metrics are inflexible to adapt to complex real-world graphs and applications. For one thing, the constraint may be either too loose like \( k \)-core or too tight like \( k \)-clique. For the other thing, choosing a proper \( k \) value as well as one metric is not an easy task for diversified graphs.

In addition to only exploiting the structural information, attributed community search leverages both the structural constraint and attributes such as keywords [11, 21], location [41], temporal [28], etc. As two representative approaches for ACS, ATC [21] finds \( k \)-truss community with the maximum pre-defined attribute score. And ACQ [11] finds \( k \)-core communities whose nodes share the maximum attributes with the query attributes. Both ATC and ACQ adopt a two-stage process. First, they find the candidate communities based on the structural constraints. Then, the candidates are verified based on the computed attribute score or the appearance of attribute set. However, the quality of the found communities of the two approaches are unpromising since the independent two stages fail to capture the correlations between structures and attributes in a joint fashion.

As the development of ML/DL, recently, GNN has been adopted to community search task [14]. By recasting the community membership determination to a classification task, a model can learn via its prediction error feedback gain the training samples and can adapt to a specific graph in an end-to-end way. Recently, Gao et al. proposed ICS-GNN [14] for interactive community search, which allows users to provide ground-truth for online incremental learning. The model learned is a query-specific model that fails to generalize to new query nodes. In other words, the model has to be retrained from scratch for each encountered query.

Meta-Learning. Meta-learning is a learning paradigm that learns the prior knowledge from multiple tasks, which can be swiftly transferred to a new task with only a few observed data. In general, the meta-learning approaches fall into three categories, i.e., black-box adaption [16, 31, 34, 42], optimization-based [13, 32, 33], and metric-based [35, 37, 40] approaches. Black-box adaption relies on specific neural network architecture, e.g., recurrent neural network to encode each task sequentially. These approaches have powerful expressive capability to model the task priors but are data inefficient and challenging for optimization. The optimization-based approaches learn the hierarchy by explicit gradient-based
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| Symbols | Definitions |
|---------|-------------|
| \(G(V, E)\) | An undirected graph with nodes \(V(G)\) and edges \(E(G)\) |
| \(N(v)\) | The neighbors of node \(v\) |
| \(\mathcal{A}\) | The node attributes |
| \(C_q(G)\) | The communities containing node \(q\) in graph \(G\) |
| \(T = (\mathcal{L}, Q, L)\) | A learning task with graph \(G\), queries \(Q\) and ground-truth \(L\) |
| \(f_{\psi}(\cdot)/f_{\theta}(\cdot)\) | The aggregate/combine function of a GNN layer |
| \(h_{\psi}^{(k)}\) | Representation of node \(v\) in the \(k\)-layer of GNN |
| \(\mathcal{L}(\cdot; \theta)\) | The loss of query \(q\) with model parameters \(\theta\) |
| \(l_q^{q}\) | The ground-truth/binary prediction of query node \(q\) |
| \(S/Q\) | The support/query set |
| \(\phi_{\psi}/\phi_{\theta}\) | The encoder/decoder of CGNP with parameter \(\theta\) |
| \(l_q^{q}/l_q\) | The query/label identifier of node \(v\) |
| \(H_q\) | The representation view specific to query node \(q\) |
| \(H\) | The representation combined by multiple \(H_q\) views |

backpropagation. These algorithms are usually model-agnostic and effective regarding learning the meta-model. However, their computations are time and memory-consuming due to the hierarchical optimization paradigm. The metric-based approaches borrow the idea from clustering algorithms and KNN that learn embeddings or additional attributes \(A(G)\) associated with the \(v\) is denoted as \(A(G) = \{u(u, v) \in E(G)\}\). The nodes may have \(d\) additional attributes \(\mathcal{A} = \{A_1, \cdots, A_d\}\). For each node \(v\), a one-hot \(d\)-dimensional vector \(A(v) \in \{0, 1\}^d\) encodes whether \(v\) is associated with the \(d\) attributes in \(\mathcal{A}\). A community of \(G\) is a cohesive subgraph \(G' = (V', E')\) induced by a node set \(V'(G') \subseteq V(G)\). The nodes \(V'(G')\) are intensively connected within the community whereas are sparsely connected with other nodes in the graph, i.e., \(|E'(G')| \gg |(u, v)u \in V'(G'), v \in V(G) \setminus V'(G')|\).

### Table 1: Frequently Used Notations

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### 3 PROBLEM STATEMENT

We consider an undirected simple graph \(G = (V, E)\), where \(V(G)\) is the node set and \(E(G)\) is the edge set. Let \(n = |V(G)|\) and \(m = |E(G)|\) denote the number of nodes and edges, respectively. The neighborhood of node \(v\) is denoted as \(N(v) = \{u(u, v) \in E(G)\}\). The nodes may have \(d\) additional attributes \(\mathcal{A} = \{A_1, \cdots, A_d\}\). For each node \(v\), a one-hot \(d\)-dimensional vector \(A(v) \in \{0, 1\}^d\) encodes whether \(v\) is associated with the \(d\) attributes in \(\mathcal{A}\). A community of \(G\) is a cohesive subgraph \(G' = (V', E')\) induced by a node set \(V'(G') \subseteq V(G)\). The nodes \(V'(G')\) are intensively connected within the community whereas are sparsely connected with other nodes in the graph, i.e., \(|E'(G')| \gg |(u, v)u \in V'(G'), v \in V(G) \setminus V'(G')|\).

### Community Search: For a graph \(G = (V, E)\), given a query node \(q \in V(G)\), the community search problem is to find the query-dependent community \(C_q(G) \subset V(G)\), where \(q \in C_q(G)\). Distinguished from prior algorithmic approaches [11, 21, 23], the community \(C_q(G)\) in this paper is not restricted in a single \(k\)-related subgraph, instead, it is learned from given community membership ground-truth.

#### Problem Statement: Our problem is to construct a meta model \(M\) to support community search queries for multiple tasks. The model \(M\) is trained on a set of training tasks \(\mathcal{D} = \{\mathcal{T}_i\}_{i=1}^N\). Each training task is a triplet \(\mathcal{T} = (G, Q, L)\), where \(G\) is a graph, \(Q = \{q_1, \cdots, q_j|q_j \in V(G)\}\) is a set of \(j\) query nodes in \(G\), and \(L = \{l_1, \cdots, l_j\}\) is the ground-truth of the \(j\) query nodes, respectively. Specifically, \(l_q\) is a set of nodes in \(G\) w.r.t. the query node \(q\), containing a set of positive samples, \(l_q^+ \subset C_q(G)\) and a set of negative samples, \(l_q^- \subset (V(G) \setminus C_q(G))\). For a new test task \(\mathcal{T}^* = (G^*, Q^*, L^*)\), the meta-model \(M\) will exploit the query node set \(Q^*\) associated with the ground-truth \(L^*\) to adapt to task \(\mathcal{T}^*\) and make community search prediction for nodes in \(V(G^*)\) \(\setminus Q^*\). Note that for test task, the number of query nodes in \(Q^*\), named shots, is rather limited, i.e., \(|Q^*| \ll |V(G^*)|\). Table 1 lists the frequently used notations throughout this paper.

There are many possible scenarios with different ways that the training task set \(\mathcal{D}\) is constituted, and new tasks are also encountered in different ways. In this paper, we explore the following three task structures, whose diagrammatic sketches are shown in Fig. 1.

- **Single Graph with Shared Communities** (Fig. 1(a)). The graphs in any training task, \(G\), and test task, \(G^*\), are local subgraphs of a single large graph \(G_0\). The query nodes from the training task and test task are from the same communities in \(G_0\).
- **Single Graph with Disjoint Communities** (Fig. 1(b)). The graphs in any training task, \(G\), and test task \(G^*\), are local subgraphs of a single large graph \(G_0\). The query nodes from the training task and test task are from different communities in \(G_0\), i.e., \(C_q(G) \cap C_q(G^*) = \emptyset, \forall q \in Q, q^* \in Q^*\).
- **Multiple Graphs with Disjoint Communities** (Fig. 1(c)). The graphs in any training task, \(G\), and testing task, \(G^*\), are from different graphs. Naturally, the query nodes from the training task and test task are from different communities. \(G\) and \(G^*\) can be different graphs in the same domain, or in different domains. But all the graphs in the training tasks are from the same domain.

### 4 NAIVE APPROACHES

To construct a meta-model, one naive approach is to pre-train a graph neural network (GNN) model over \(D\) and finetune the model for a new task \(\mathcal{T}^*\). Below, we first introduce tackling community search as multi-label classification by GNN, which serves as the basis of the naive approaches and our meta-learning approach.

Given a graph \(G\), a \(K\)-layer GNN follows a neighborhood aggregation paradigm to generate a new representation for each node by aggregating the representations of its neighbors in \(K\) iterations. Let \(h_{\psi}^{(k)}(v)\) denote the representation of a node \(v\) generated in the \(k\)-th iteration, which is a \(d^{(k)}\) dimensional vector. In the GNN \(k\)-th
iteration (layer), for each node $v \in V(G)$, an aggregate function $f_{\mathcal{A}}^{(k)}$ aggregates the representations of the neighbors of $v$ that are generated in the $(k - 1)$-th iteration as Eq. (1). Then, a combine function $f_{\mathcal{C}}^{(k)}$ updates the representation of $v$ by the aggregated representation $a_v^{(k)}$ and previous representation $h_v^{(k-1)}$ as Eq. (2).

$$a_v^{(k)} = f_{\mathcal{A}}^{(k)} ([x_u^{(k-1)} | u \in N(v)])$$

$$h_v^{(k)} = f_{\mathcal{C}}^{(k)} (h_v^{(k-1)}, a_v^{(k)})$$

The functions $f_{\mathcal{A}}^{(k)}$ and $f_{\mathcal{C}}^{(k)}$ are neural networks, e.g., linear transformation with non-linearities and optional Dropout for preventing overfitting. They transform $d^{(k-1)}$, dimensional node representation $h_v^{(k-1)}$ into $d^{(k)}$, dimensional representation $h_v^{(k)}$. The neural network parameters from $f_{\mathcal{A}}^{(k)}$ and $f_{\mathcal{C}}^{(k)}$ are shared by all the nodes.

For a given task $T = (G, Q, L)$, a GNN can be built by training over $Q$ and $L$, then is deployed to make prediction for any node $q^* \in V(G) \setminus Q$ as a query. Concretely, a binary query identifier $I_q(v) \in \{0, 1\}$ is concatenated with the attribute feature vector $\mathcal{A}(v)$ to form the initial node representation $h_v^{(0)}$, where $I_q(v) = 1$ if $v$ is the query node $q^*$ otherwise $I_q(v) = 0$. Through transformation of K layers, the 1-dimensional node representation $h_v^{(K)}$ is activated by a sigmoid function, i.e., $\hat{y}(v) = \text{sigmoid}(h_v^{(K)})$, which is the likelihood that $v$ is in the same community with query node $q^*$. The given query node set $Q$ and the ground-truth $L$ provide the training data for the GNN model. For a known query $q \in Q$ and its ground-truth $l_q^* = (l_q^+, l_q^-)$, where $l_q^+$ and $l_q^-$ are the positive and negative samples regarding query node $q$, respectively. The binary cross entropy (BCE) loss in Eq. (3) evaluates the divergence between the predictive probability of the nodes from the positive and negative samples under the GNN with parameter $\theta$.

$$L(q; \theta) = -\left[ \sum_{v: q^+ \in I_q} \log \hat{y}(v^+) + \sum_{v: q^- \in I_q} \log (1 - \hat{y}(v^-)) \right]$$

Based on the simple GNN approach, then we review two straightforward approaches to learn a meta-model for tasks with small training data, one is direct feature transfer and the other is GNN-based model-agnostic meta-learning.

**Feature Transfer.** The parameters of shallow layers in neural network trained by one or multiple tasks can be transferred to new tasks, instead of learning from scratch. The intuition is that the pre-trained low-level feature transformation can be shared with a new task. Usually, the parameters of the final layer of the neural network are updated by the training data of the new task by several gradient steps, whereas other parameters in the former layers are frozen in this procedure. Thereby, we can train a GNN by the union of all the $Q$ and $L$ of the training task $T$ in the training set $\mathcal{D}$. When a new task $T^*$ arrives, the parameters of $f_{\mathcal{A}}^{(k)}$ and $f_{\mathcal{C}}^{(k)}$ will be updated by minimizing the BCE loss in Eq. (3) over $Q^*$ and $L^*$. However, the effectiveness of simple feature transfer is limited. For one thing, this approach is originally proposed for convolutional neural network (CNN) to process image data, which has an explicit feature hierarchy to be transferred. However, whether the same transfer mechanism well suits GNN over graph data still needs exploration. For the other thing, it is hard to control the gradient steps in the fine-tuning procedure for various test tasks. Too many steps will incur overfitting whereas too few will incur underfitting.

**Model-Agnostic Meta-Learning (MAML).** A meta GNN model can be built by a general meta-learning algorithm, MAML [13], over a set of training tasks $\mathcal{D}$. MAML is a two-level end-to-end optimization algorithm, where the lower level is to optimize task-specific parameters $\theta_i$ for one task $T_i$ and the upper level is to optimize the task-common parameters $\theta$ over the training task set $\mathcal{D}$. The learned task-common parameters $\theta^*$ will be used as the neural network initialization and updated by a few gradient steps to generalize a new task $T^*$, given the few-shot task-specific data $Q^*$ and $L^*$. To be concrete, training data $Q_i = \{q_j\}_{j=1}^J$ and $L_i = \{l_q\}_{j=1}^J$ of one training task $T_i$ are divided into two sets, $S_i = \{(q_j, l_j)\}_{j=1}^J$ and $Q_i = \{(q_j, l_q)\}_{j=1}^J$, $S_i$ is called support set and $Q_i$ is called query set. The task-specific parameters $\theta_i$ is updated by the support set of $T_i$ as Eq. (4) in an inner loop, and the task-common parameters $\theta^*$ is updated by the query set over $\mathcal{D}$ in an outer loop as Eq. (5), by gradient descent with learning rates $\alpha$ and $\beta$, respectively. Fig. 2(a) delineates this two-level optimization framework.

$$\theta_i \leftarrow \theta - \alpha \nabla_\theta \sum_{(q_i, l_q) \in S_i} L(q; \theta)$$

$$\theta^* \leftarrow \theta - \beta \nabla_\theta \sum_{T_i \sim \mathcal{D}} \sum_{(q_i, l_q) \in Q_i} L(q; \theta_i)$$
Although MAML is an effective and fairly general framework, it suffers from a variety of problems, including training instability, restrictive model generalization performance and extensive computational overhead [4].

5 CNP & CGNP FOR CS

Considering to overcome the disadvantages of the naive approaches, we devise a novel meta-learning framework for CS, named Conditional Graph Neural Process (CGNP), in the family of Conditional Neural Process (CNP) [15]. In this section, we present the core idea of CNP and CGNP for CS as an overview. Firstly, we briefly introduce CNP.

CNP is a neural network approximation of stochastic process, e.g., Gaussian Process (GP). It directly models the predictive distribution conditioned on an arbitrary number of context observations by neural networks, in contrast to GP that specifies the prior of the model explicitly and infer the predictive distribution by Bayes rule and Bayesian model average. Specifically, given observed data set \( X = \{x_i\}_{i=1}^N \) with corresponding ground-truth \( Y = \{y_i\}_{i=1}^N \), CNP models the predictive distribution of new data \( x^* \) with the target \( y^* \), \( p(y^*|x^*,X,Y) \), by the neural network architecture in Eq. (6).

\[
p(y^*|x^*,X,Y) = \rho_\theta(x^*, \bigoplus_{i=1}^N \phi_{\theta}(x_i, y_i))
\]  

Here, \( \phi_{\theta} : X \times Y \rightarrow \mathbb{R}^d \) and \( \rho_{\theta} : X \times \mathbb{R}^d \rightarrow \mathbb{R}^c \) are neural networks. The big \( \oplus \) is a commutative operation that takes elements in \( \mathbb{R}^d \) and aggregates them into a single element of fixed length \( \mathbb{R}^d \). \( \phi_{\theta} \) is the encoder that transforms pairs of \( (x_i, y_i) \) into \( d \)-dimensional hidden representations. The big \( \oplus \) aggregates \( N \) representations into a context representation in a permutation-invariant fashion which memorizes the whole dataset \( X \) and \( Y \). To deal with a query for new observation \( x^* \), a decoder \( \rho_{\theta} \) takes the context and \( x^* \) as inputs and makes a final prediction for \( x^* \).

Similar to stochastic process, CNP can be used to build meta-models via learning the prior of data generation, where each data instance is a collection of \( (x_i, y_i) \), i.e., a task. The difference lies in that stochastic process, e.g., GP, explicitly specifies the prior distribution, and optimizes the hyper-parameters of the prior by maximum likelihood. The CNP instead explicitly parameterizes the predictive distribution as neural networks thereby learning the prior implicitly.

The model we propose, CGNP, is a graph specification of CNP for query-dependent node classification. For a CS task \( \mathcal{T} = (G, Q, L) \), CGNP directly models the predictive distribution \( p(l_q^*|q^*, \mathcal{T}) \) for a new query node \( q^* \in V(G) \setminus Q \), where \( l_q^* = \{l_{q^*}(v)\}_{v \in V(G)} \in \{0, 1\}^N \) is the binary target prediction for all the nodes in \( G \). CGNP preserves the property of CNP for meta-learning, which learns a kernel function \( \mathcal{K}_\theta(\cdot, \cdot) \) for input pairs as what GP does [15]. In this kernel-based perspective, CGNP can be regarded as reinterpreting the predictive distribution as Eq. (7)-(8), which is a sum of the observed ground-truth \( l \), weighted by the similarity between an observed query node \( q \) and the target query node \( q^* \). The similarity is specified by a kernel function \( \mathcal{K}_\theta(\cdot, \cdot, \cdot) \). As shown in Fig. 2(b), what CNP learns is a common kernel function \( \mathcal{K}_\theta(\cdot, \cdot, \cdot) \) between \( q \) and \( q^* \), shared by all the tasks. This implicit kernel learning prompts CNP and CGNP to be metric-based-meta-learning.

\[
p(l_q^*|q^*, \mathcal{T}) = p_\theta(q^*, \bigoplus_{(q,l_q) \in (Q,L)} \phi_{\theta}(q, l_q))
\]  

\[
= \sum_{(q,l_q) \in (Q,L)} \mathcal{K}_\theta(q^*, q) \odot l_q
\]  

For metric-based meta-learning framework, e.g., Matching Network [40], whose core idea is from KNN, a distance kernel is explicitly defined to derive the predictive distribution as Eq. (8). For CNP and CGNP, the kernel function \( \mathcal{K}_\theta(\cdot, \cdot) \), as well as the multiplication operation \( \odot \) is implicitly learned from the data by the defined \( p_\theta \), \( \phi_{\theta} \) and big \( \oplus \). However, KNN and CNP memorize the input data in different ways. KNN persists the input data by simple concatenation whereas CNP persists it by a more abstract operation, i.e., big \( \oplus \). Similar to KNN, the metric learning intuition of CNP makes it promising for small samples and classification tasks as CS.
We elaborate on how to design a CGNP model for the query-dependent node classification over graphs. Fig. 3 delineates the architecture of CGNP, which is composed of a GNN based encoder, a commutative pooling operation, big ⊕, and a decoder associated with inner product operation.

GNN Encoder. For each query node \( q \in Q \) and its corresponding ground-truth \( l \in L \), the encoder \( \phi_{q,l}(q,l,G) \) is a K-layer GNN that maps the pair \((q,l)\) together with the graph \( G \) to a node embedding matrix \( H_q = \{h_{v}^{(K)}\}_{v \in V(G)} \in \mathbb{R}^{n \times d_{v}} \). Here, \( h_{v}^{(K)} \) is a \( d \times K \)-dimensional output of the \( K \)-th layer of GNN for node \( v \). The subscript \( q \) of \( H_q \) indicates the node embedding \( H_q \) is generated particularly for query node \( q \), as all the query nodes \( Q \) share the same GNN encoder to generate their \( H \) matrix. Specifically, as the inputs of GNN, the adjacency matrix of graph \( G \) is used for message passing of GNN, and \((q,l)\) determines the initial node \( h_{v}^{(0)} \) as Eq. (10), where \( \| \) is the vector/bit concatenation operation, \( A(v) \) is the attribute features of node \( v \). In Eq. (10), \( I_{q}(v) \in \{0,1\} \) is a binary ground-truth identifier which distinguishes nodes within and without a same community, under the close world assumption.

\[
\begin{align*}
    h_{v}^{(0)} &= [I_{q}(v)\|A(v)], I_{q}(v) = \\
    &\begin{cases}
        1 & v \in I_{q}^{+} \cup \{q\} \\
        0 & \text{otherwise}
    \end{cases}
\end{align*}
\]

For graphs without node attributes, we can concatenate auxiliary features, for instance, the normalized core number and local clustering coefficient of a node. The intuition of the GNN encoder is to generate a view, \( H_q \), for the whole graph given an observation \((q,l)\) by message passing. The collection of views will be aggregated by the commutative operation big \( \oplus \). This idea is enlightened by a CNP specialization for 3D scene understanding and rendering, Generative Query Network (GQN) [10], where few-shot observed 3D views are summed up for predicting the view of a new query perspective. It is worth mentioning that, to the best of our knowledge, we are the first to introduce the insight of GQN to graph query processing.

Commutative Operation. To combine the view matrices \( H_q \) for all query node \( q \in Q \) into one context representation, CGNP is equipped with three choices of commutative operations, sum, average and self-attention. All of the three operations are permutation-invariant.

\[
H = \sum_{q \in Q} H_q
\]
**Self-Attention** is inspired by Attentive Neural Process (ANP) [25] and GP. Instead of giving the same weight to aggregate multiple data points, ANP and GP aggregate observed data by self-adaptive weights by self-attention [38] and GP’s kernel function, respectively. Thereby, CGNP leverages the self-attention to combine the node representations derived from all the query nodes, weighted by a set of learnable weights \( \{w_q\}_{q \in Q} \in \mathbb{R}^{|Q|} \) as Eq. (12). The weights \( \{w_q\}_{q \in Q} \) are shared by all the nodes in \( G \).

\[
H = \sum_{q \in Q} w_q H_q \tag{12}
\]

Here, to compute the attention weight \( \{w_q\}_{q \in Q} \) by the multiple views \( \{H_q\}_{q \in Q} \), let \( H = \{H_q[v]\}_{q \in Q} \in \mathbb{R}^{|Q| \times d_h} \) be the matrix stacked by the \( |Q| \) node embeddings in \( \{H_q\}_{q \in Q} \) for an arbitrary node \( q \). In Eq. (13), \( H_1, H_2 \in \mathbb{R}^{|Q| \times d_h} \) are transformed by linear weight matrices \( W_1, W_2 \in \mathbb{R}^{d_h \times d_r} \), respectively. \( \{w_q\}_{q \in Q} \) is computed by the inner product of \( H_1 \) and the transpose of \( H_2 \) followed by a softmax function that normalizes the weights to a probability distribution, as Eq. (14) shows.

\[
\begin{align*}
H_1 &= H W_1, \quad H_2 = H W_2, \\
\{w_q\}_{q \in Q} &= \text{softmax} \left( \frac{<H_1, H_2^T>}{\sqrt{d}} \right) \tag{14}
\end{align*}
\]

**Decoder.** Given the combined context representation \( H \), a decoder network \( \rho(\cdot|q^*, H) \) estimates the membership prediction for a new query node \( q^* \), \( p(\cdot|q^*, H) \in \mathbb{R}^{|Q| \times 1} \) conditioned on the memorized context \( H \). For CGNP, we design three decoders with different complexities, a simple inner product decoder, multi-layer perception (MLP) decoder and GNN decoder. The latter two decoders MLP and GNN decoder are also based on inner product.

**Inner Product Decoder** is free of parameters and only operates on the context \( H \). Since \( H \) is a node embedding combined by multiple views, we can directly compute the node similarities between the embedding of a query node \( q \) and all the other nodes. We use the inner product operation, \( <\cdot, \cdot> \), to compute the similarity score as Eq. (15), followed by a sigmoid function to predict the probability that one node is in the same community with query node \( q^* \). The inner product operation indicates the smaller the angle of two node embeddings in the vector space, the more likely the two nodes are from the same community.

\[
p(\cdot|q^*, \mathcal{T}) = \text{sigmoid}(H[q^*], H) \tag{15}
\]

**MLP Decoder** first transforms the context matrix \( H \) by a two-layer MLP as Eq. (16), then feeds the transformed \( H \) to an inner product decoder of Eq. (15).

\[
H \leftarrow \text{ReLU}(H W_1) W_2 \tag{16}
\]

**GNN Decoder** first transforms the context matrix \( H \) by a K-layer GNN as Eq. (17), then feeds the transformed \( H \) to an inner product decoder of Eq. (15). In Eq. (17), we use \( W = \{f_A^{(0)}, f_C^{(0)}, \ldots, f_A^{(K)}, f_C^{(K)}\} \) to denote the weights in the K-layer GNN. Note the GNN here is independent to the GNN in the encoder.

\[
H \leftarrow \text{GNN}(H, G, W) \tag{17}
\]

In contrast to the inner product decoder, the MLP and GNN encoder impose additional parametric transformations on the combined context embedding \( H \) to improve the modeling capability of the decoder. The difference between MLP and GNN lies that GNN further allows message passing among the nodes whereas the MLP transforms each node independently.

### 7 META-LEARNING BY CGNP

In this section, we present the learning algorithms to train a meta CGNP model \( \mathcal{M} \) and adapt the model to new tasks. Given the set of training tasks \( \mathcal{D} = \{\mathcal{T}_i\}_{i=1}^N \), recall that CGNP is to model a generative process of tasks \( f \sim \mathcal{D} \). Suppose the tasks are independent and the query nodes are independent in each task. The marginal likelihood of CGNP over \( \mathcal{D} \) is

\[
p(\{L_1, \ldots, L_N\}|\{Q_1, \ldots, Q_N\}, \Theta) = \prod_{\mathcal{T}_i \in \mathcal{D}} p(L_i|Q_i) \tag{18}
\]

Similar to MAML, for one training task \( \mathcal{T}_i \), we split the training data \( Q_i = \{q_j\}_{j=1}^{|Q_i|} \) and \( L_i = \{l_q\}_{q \in Q_i} \) into the support set \( S_i = \{(q_j, l_{q_j})\}_{j=1}^{|Q_i|} \) and query set \( Q_i = \{q_j\}_{j=|Q_i|+1}^{|Q_i|+|Q_N|} \). The learning objective is to minimize the negative log-likelihood of the query set \( Q_i \), conditioned on the support set \( S_i \) across all the tasks in \( \mathcal{D} \) as Eq. (19). The negative log-likelihood loss in Eq. (19) is in accordance with the BCE loss (Eq. (3)) of the query nodes in the query set \( Q_i \) as shown in Eq. (20).

\[
L(q; \Theta) = -\sum_{\mathcal{T}_i \in \mathcal{D}} \sum_{q \in Q_i} \log p(l_q|q, S_i) = -\sum_{\mathcal{T}_i \in \mathcal{D}} \sum_{q \in Q_i} \log \hat{y}(\sigma^a) + \sum_{\omega \in \Omega} \log (1 - \hat{y}(\sigma^a)) \tag{19}
\]

**Meta Training.** In the training stage, given the training task set \( \mathcal{D} \), learning rate \( \alpha \), and the number of epochs \( T \), a meta CGNP model is trained by optimizing the negative log-likelihood by stochastic gradient descent. Algorithm 1 presents the training process. In each epoch (line 1-12), all the training tasks are randomly shuffled in line 2. For each task \( \mathcal{T}_i \), we get the allocated support set \( S_i \) and query set \( Q_i \) from the given query node and ground-truth (line 4). First, each query node \( q \) associated with the ground-truth \( l \) in the support set \( S_i \), together with the graph structure \( G_i \), is fed into the GNN encoder, \( \phi_q \), to generate a query-specific view \( H_q \) (line 5-6). Second, in line 7, all the views are aggregated into the context matrix \( H \) by the permutation-invariant operation big \( \mathcal{G} \). Third, for each query node in the query set \( Q_i \), we compute its predictive distribution and loss in line 9-10. Fourth, the model is updated by one gradient step of the aggregated task-specific loss (line 11-12).

**Meta Testing.** For a test task \( \mathcal{T} \) with graph \( G^* \), few-shot query nodes \( Q^* \) and the associated ground-truth \( L^* \), Algorithm 2 presents the steps to predict the community members for a query node \( q^* \). The whole \( Q^* \) and \( L^* \) serve as the support set \( S^* \) (line 1), followed by computing the context representation \( H \) (line 2-4). Finally, the query node \( q^* \) and context \( H \) are fed into the decoder network \( \rho_0 \) to obtain the prediction.

**Computation Complexity.** We analyze the time complexity of CGNP in brief. To be concise, we assume fixed dimension vector.
Algorithm 1: CGNP Meta Train

Input: training task set \( \mathcal{D} = \{ T_i \}_{i=1}^N \), learning rate \( \alpha \), number of epochs \( T \)

Output: parameters \( \theta \) of meta model \( M \)

1. for epoch \( \leftarrow 1 \) to \( T \) do
   2. Shuffle the task set \( \mathcal{D} = \{ T_i \}_{i=1}^N \);
   3. for \( T_i = (G_i, Q_i, L_i) \in \mathcal{D} \) do
      4. \( S_i, Q_i \sim (Q_i, L_i) \);
      5. for \( (q, l_q) \in S_i \) do
         6. \( H_q \leftarrow \phi(q, l_q; G_i) \);
         7. \( H \leftarrow \bigoplus_{(q, l_q) \in S_i} H_q \);
      8. for \( (q, l_q) \in Q_i \) do
         9. \( p(l_q|q, S_i) \leftarrow \rho_q(q, H) \);
      10. Compute the Loss \( L(q) \) by \( p(l_q|q, S_i) \) and \( l_q \);
      11. \( L \leftarrow \sum_{(q, l_q) \in Q_i} L(q) \);
      12. \( \theta \leftarrow \theta - \alpha \nabla_{\theta} L \);
   13. return \( \theta \);

Algorithm 2: CGNP Meta Test

Input: test task \( T^* = (G^*, Q^*, L^*) \), parameter \( \theta \) of meta model \( M \), a query node \( q^* \in V(G^*) \setminus Q^* \)

Output: predictive distribution of \( q^* \)

1. \( S^* \leftarrow (Q^*, L^*) \);
2. for \( (q, l_q) \in S^* \) do
   3. \( H_q \leftarrow \phi(q, l_q, G^*) \);
   4. \( H \leftarrow \bigoplus_{q \in S^*} H_q \);
   5. \( p(l_q|q^*, S^*) \leftarrow \rho_q(q^*, H) \);
   6. return \( p(l_q^*|q^*, S^*) \);

add, multiplication, inner product take constant time when the dimension is far smaller than the graph node number \( n \). For the GNN encoder of CGNP, the time complexity is \( O(Km|S|) \) for a single task, where \( K \) is the number of GNN layers, \( m \) is the number of edges and \( |S| \) denotes the number of shots. The complexity of the big \( \oplus \) operation is \( O(n|S|) \) for the sum and average pooling and \( O(n|S|^2) \) for the self-attention, respectively. For the decoders, the inner product operation takes \( O(n|Q|) \) time, and an MLP decoder and \( K' \) layer GNN decoder takes extra \( O(n|Q|) \) and \( O(K'm|Q|) \) cost, respectively. In total, the complexity of the meta test algorithm, Algorithm 2, is \( O(c(n + m)) \), where \( c \) is a constant determined by \( K, K', |S|, |Q| \). And the training complexity of Algorithm 1 is \( O(TNc(n + m)) \), where \( T \) and \( N \) are the numbers of iterations and training tasks.

8 EXPERIMENTAL STUDIES

In this section, we introduce the experimental setup (section 8.1) and report our substantial results in the following facets: ① compare the effectiveness of CGNP with the baseline approaches under different task configurations (section 8.2), ② evaluate the train and test efficiency of CGNP compared with the baselines, and conduct scalability test for learning-based approaches (section 8.3). ③ investigate the effect of the volume of the ground-truth on the performance of CGNP for different tasks (section 8.4). ④ conduct the ablation studies on the CGNP model regarding the GNN layer and the commutative operation (section 8.5).

8.1 Experimental Setup

Datasets: We use six real-world graph datasets, including five datasets of single graph, Cora, Citeseer, Arxiv, Reddit, DBLP, and one dataset of multiple graphs, Facebook. Table 2 lists the profile of the six datasets. Cora, Citeseer and Arxiv are citation networks whose nodes represent research papers and edges represent citation relationships. We use node class labels to simulate the communities derived from the paper citation, which reveal the research topics that papers belong to. DBLP [44] is a co-authorship network where nodes represent authors and two authors are connected if they collaborate on at least one paper. The publication venue defines a ground-truth community. This dataset has ground-truth communities, i.e., the publication venues of the papers. Reddit is collected from an online discussion forum, where nodes refer to posts, and an edge between two posts exists if a user comments on both of the posts. The ground-truth is the communities that posts belong to. Facebook is a dataset containing 10 ego-centric social networks, which have friendship community ground-truth. Cora, Citeseer, and Facebook have discrete node attributes. The attributes of Cora and Citeseer are the keywords in the paper and the attributes of Facebook are the user properties. For the three datasets, we use one-hot representations of the attributes as the node features, concatenating with the core number and local cluster coefficient of the node. Arxiv, DBLP and Reddit do not have node attributes. Thereby, we use core number and local cluster coefficient alone as the node features.

Tasks & Queries: To test our CGNP in different local regions of one graph, different graphs, and different application scenarios, we use the datasets in Table 2 to construct 4 different types of task as described in section 3: ① Single Graph with Shared Communities Task (SGSC) ② Single Graph with Disjoint Communities Task (SGDC) ③ Multiple Graphs from One Domain Task (MGOD) ④ Multiple Graphs from Different Domains Task (MGDD). For SGSC and SGDC and MGDD, one task is generated by sampling a subgraph of 200 nodes by BFS in Cora, Citeseer, Arxiv, DBLP. While in Reddit, a
subgraph of 100 nodes is generated. The query nodes are randomly drawn from the sampled subgraph, \( G \), where we assign 1 or 5 query nodes to the support set \( S \), i.e., 1-shot or 5-shot tasks, and assign 30 query nodes to the query set \( Q \) disjointly. It is worth noting the difference between SGSC and SGDC lies in that the query nodes in \( S \) and \( Q \) may be from the same ground-truth communities for SGSC whereas the query nodes must be from disjoint communities for SGDC. For each query \( q \), we randomly drawn 5 positive samples from the community of \( q \), \( C_q(G) \), to construct \( I_q^+ \) and 10 negative samples from \( V(G) \setminus C_q(G) \) to construct \( I_q^- \). Following this way, for task types of SGSC and SGDC, we generate 32 training tasks for Citeseer and 100 training tasks for Reddit, Arxiv, and DBLP and generate 10 test tasks for the four datasets, respectively. For \( \text{MGDD} \), we directly use one Facebook ego-network as the graph of one task and sample the same numbers of queries and labels with the above setting. The 10 tasks are split into 7 for training and 3 for testing. For \( \text{MGOD} \), 32 tasks of Cora are generated for training and 10 tasks of Citeseer are used for testing, denoted as Cora_Citeseer.

**Baselines:** To evaluate the performance of CGNP framework for community search, we compare CGNP with six baseline approaches, including the two naive proposals in section 4, three native community search algorithms and a supervise-learned GNN model.

- **Feature Transfer (FeaTrans).** A base GNN model is pre-trained on all the training tasks. For a test task \( T^* = (S^*, Q^*) \), the final layer of the GNN is finetuned on the support set \( S^* \) by a gradient step, while all the other parameters are kept intact.
- **Model-Agnostic Meta-Learning (MAML) [13].** We use a GNN as the base model. The task-specific parameters of the GNN are trained by gradient update in an inner loop as Eq. 4 and the task-common parameters are trained by gradient update in an outer loop as Eq. (5) over all training tasks.
- **Attributed Truss Community Search (ATC) [21] is an attributed community search algorithms given the input of query nodes and attributes. Firstly, it finds the maximal \((k, d)\)-truss containing the query nodes. Then, the algorithm iteratively removes unpromising nodes from the truss, which has a small attribute score. The time and space complexity of ATC is \( O(m|\mathcal{A}_q| + m + n \log n) \) and \( O(m + \sum_{v \in V(G)} |\mathcal{A}(v)|) \), respectively, where \( n \) and \( m \) are the numbers of nodes and edges of the graph, and \(|\mathcal{A}_q|\) is the number of query given attributes.
- **Attributed Community Query (ACQ) [11] aims to find subgraph whose nodes are tightly connected and share common attributes with the given query node. The algorithm is impractical for query nodes with a large number of attributes due to combinatorial explosion during enumerating the shared attribute sets.
- **Closest Truss Community (CTC) [23] is a k-truss based community search framework for non-attributed graphs. Given a set of query nodes, \( Q \), a greedy algorithm finds a k-truss with the largest \( k \) that contains \( Q \) and has the minimum diameter among the truss. CTC takes \( O((|Q|t + \rho)m) \) time and \( O(m) \) space, where \( \rho \) is the arboricity of the graph, \( t \) is the number of iterations and \( m \) is the number of edges for the maximal connected k-truss.
- **Supervised GNN (Supervised).** In contrast to meta-learning, we train one GNN model for each test task from scratch by the few-shot data in \( S^* \). The GNN specifically fits the test task and directly makes predictions for new queries of the task.

We do not compare with ICS-GNN [14] since in our setting, for any query node to be tested, no ground-truth is known in advance. In other words, the model should be fully generalized to unseen query nodes. ICS-GNN does not consider this generalization.

**Implementation and Settings:** We give the settings of the ML approaches, i.e., CGNP, MAML, FeaTrans and Supervised. For the GNN encoder in CGNP and the base GNN model in MAML, FeaTrans and Supervised, the number of the GNN layers is 3, where each GNN layer has 128 hidden units and a Dropout probability of 0.2 by default. We investigate popular GNN layers, including the vanilla Graph Convolutional Network (GCN) [26], Graph Attention Network (GAT) [39] and GraphSAGE [17], and finally choose GAT by default due to its high performance. For the MLP decoder of CGNP, we use a two-layer MLP with 512 hidden units. For the GNN decoder of CGNP, we use a two-layer GNN which has the same configuration as the encoder.

The learning framework of CGNP and the 3 ML baselines are built on PyTorch [1] with PyTorch Geometric [2]. We use Adam optimizer with a learning rate of \( 10^{-4} \) to train all the models by 200 epochs. For MAML, the inner loop performs 10 gradient steps for training and 20 steps for testing, with a larger learning rate of \( 10^{-3} \). It is worth mentioning that the performance of CGNP is robust in the range of empirical training hyper-parameters. By default, the training and prediction are conducted on a Tesla V100 with 16GB memory, ATC, ACQ and CTC are tested on the same Linux server with 32 Intel(R) Silver 4215 CPUs and 128GB RAM.

**Evaluation Metrics:** To evaluate the quality of the found result, we use accuracy, precision, recall and F1-score between the prediction and the ground-truth. Suppose \( l \in \{0, 1\}^{|\mathcal{A}^*|} \) and \( l' \in \{0, 1\}^{|\mathcal{A}^*|} \) are the binary representations of the prediction result and the ground-truth of a query \( q \). Precision, recall and F1-score are defined as below:

\[
\text{Prec}(\hat{l}, l) = \frac{\sum_{v \in V(G)} \hat{l}(v) \& l(v)}{\sum_{v \in V(G)} \hat{l}(v)}, \quad \text{Rec}(\hat{l}, l) = \frac{\sum_{v \in V(G)} \hat{l}(v) \& l(v)}{\sum_{v \in V(G)} l(v)}
\]

\[
\text{F1}(\hat{l}, l) = \frac{2 \cdot \text{Prec}(\hat{l}, l) \cdot \text{Rec}(\hat{l}, l)}{\text{Prec}(\hat{l}, l) + \text{Rec}(\hat{l}, l)}
\]

F1-score is the harmonic average of precision and recall, which better reflects the overall performance.

**8.2 Effectiveness**

We investigate the overall performance of CGNP on the four types of task, i.e., SGSC, SGDC, MGDD and MGOD, for 1-shot and 5-shot learning. The number of shots is the number of query nodes provided in the support set. The three variants of CGNP, CGNP with the simple inner product decoder (CGNP_IP), CGNP with MLP decoder (CGNP_MLP), and CGNP with GNN decoder (CGNP_GNN) are compared with six baseline approaches. In general, the 3 variants of CGNP consistently outperform other approaches in all the datasets.
Table 3: Performance on S6GC and S6GC Tasks

| Dataset   | Task config. | Single Graph with Shared Communities | Single Graph with Disjoint Communities |
|-----------|--------------|--------------------------------------|----------------------------------------|
|           |              | 1-shot                               | 1-shot                                 | 5-shot                                 | 5-shot                                 |
|           |              | Acc | Pre | Rec | F1  | Acc | Pre | Rec | F1  | Acc | Pre | Rec | F1  |
|           | Methods      |     |     |     |     |     |     |     |     |     |     |     |     |
|           |              | 0.3561 | 0.4953 | 0.2339 | 0.3179 | 0.4162 | 0.3878 | 0.1916 | 0.2565 | 0.5486 | 0.5089 | 0.3327 | 0.4204 | 0.3508 | 0.5322 | 0.3591 | 0.4289 |
|           | MAML         | FeaTrans     | Supervised | ATC   | CTC  | CNGP_IP | CNGP_MLP | CNGP_GNN | CNGP_IP | CNGP_MLP | CNGP_GNN |
|           |              | 0.5497 | 0.5089 | 0.3327 | 0.4204 | 0.3508 | 0.5322 | 0.3591 | 0.4289 |
|           |              | 0.6997 | 0.0459 | 0.5039 | 0.1334 | 0.0808 | 0.9751 | 0.6012 | 0.5420 | 0.0923 | 0.9116 |
|           |              | 0.0781 | 1.0000 | 0.4154 | 0.3182 | 0.5547 | 0.8291 | 0.9633 | 0.0781 | 0.5497 | 0.8291 | 0.9633 |

Table 4: Performance on MGDO and MGDD Tasks

| Dataset   | Task config. | 1-shot                               | 5-shot                                 |
|-----------|--------------|--------------------------------------|----------------------------------------|
|           |              | Acc | Pre | Rec | F1  | Acc | Pre | Rec | F1  |
|           | Methods      |     |     |     |     |     |     |     |     |
|           |              | 0.7476 | 0.2194 | 0.2982 | 0.8274 | 0.7476 | 0.2194 | 0.2982 | 0.8274 |
|           | CNGP_IP      | CNGP_MLP | CNGP_GNN | CNGP_IP | CNGP_MLP | CNGP_GNN | CNGP_IP | CNGP_MLP | CNGP_GNN |
|           |              | 0.7476 | 0.2194 | 0.2982 | 0.8274 | 0.7476 | 0.2194 | 0.2982 | 0.8274 |
|           |              | 0.6158 | 0.1658 | 0.7432 | 0.1968 | 0.6158 | 0.1658 | 0.7432 | 0.1968 |

significantly, where the F1 of CNGP is larger than that of other approaches 0.29 on average.

Table 3 presents the performance of tasks of multiple graphs with shared communities and disjoint communities. Here, we highlight the best result and underline the second best result. CNGP improves 0.32 of F1-score on average. The superiority of our CNGP is reflected in improving the recall significantly, while keeping a relative high accuracy and precision. We observe that from 1-shot to 5-shot, the performance of all the learning-based approaches tends to become better generally. Specifically, the performance of Supervised is influenced by the number of training queries to the largest extent, which even surpasses CNGP on the 5-shot Citesee. CNGP is the most robust learner due to its metric-based learning, and this phenomenon is similar to KNN and GP, which fully validates the effectiveness of CNGP for small graphs.

Table 4 shows the performance for tasks of multiple graphs. The tasks of multiple graphs are harder than that of the single graph, and the tasks across domains are even harder. We can observe that for the testing Citesee tasks, the F1 of Cora_Citesee in Table 4 is lower than that of Citesee in Table 3 in all the learning-based approaches. Fortunately, the F1 of CNGP variants dominate the top two best results, which achieves an increment of 0.26 on F1 by average. This demonstrates that CNGP can effectively learn prior knowledge from only a few data of one graph and adapt to other graphs even from different domains, and the learned prior is indeed helpful. In fact, transferring the prior of a shared node embedding function for clustering, as what CNGP does, is much easier than transferring model parameters, as what MAML and FeaTrans do.

CNGP with different decoders may bring different performance to the result. The difference between them is subtle i.e. less than 5%. However, in most cases, they are better than all other baselines. Meta-learning methods, MAML and FeaTrans are significantly less effective than CNGP in all cases. We can come to a conclusion that CNGP is the most effective meta method for community search. While for Supervised, as we can observe, the performance can be
compared or even outperform CGNP when training data is enough i.e. 5-shots setting. We will discuss the efficiency of this method to illustrate some drawbacks in the following parts. Traditional algorithm ATC, ACQ and CTC also fail to outperform CGNP due to low recall. We can finally make a conclusion that our CGNP can get excellent results compared with meta methods, supervised learning methods and traditional algorithms.

8.3 Efficiency
We compare the efficiency of CGNP and the baseline approaches regarding the test and training time. Fig. 4(a) presents the total test time of the compared approaches. Regarding the prediction efficiency, our CGNP is the best ML-based approach and the second-best among all the approaches, which is over one order of magnitude faster than CTC, ACQ, MAML and Supervised, and slightly faster than FeaTrans. For one test task, MAML and FeaTrans apply the backward propagation algorithm to update the parameters online, and Supervised trains the parameters from scratch. The algorithm ACQ needs to enumerate all the sets of attributes that are shared by the query node and candidates, so that it fails to return the results for Cora, Citeseer and Citeseer in 12 hours. For CTC, the intermediate candidate communities of Reddit and Facebook are large, it takes much longer time to compute the diameter and maintain the $k$-truss structure.

Fig. 4(b) shows the meta training time of the learning-based approaches on the training task set, where all the models are trained by the same epoch of 200. Note that ATC, ACQ, CTC and Supervised do not involve this meta training stage. Our CGNP is two orders of magnitude faster than MAML and its training efficiency is close to the simplest transfer strategy. FeaTrans. MAML is quite time-consuming due to its two-level optimization paradigm. For the three CGNP variants, due to different model complexities, training CGNP_GNN is slightly slower than that of CGNP_MLP, which is further slightly slower than that of CGNP_IP. We observe that these differences are negligible in the testing stage in Fig. 4(a).

Scalability Test. We explore the scalability of the learning-based approaches. Fig. 5 shows the GPU training time and test time of CGNP, MAML, FeaTrans and Supervised, as the number of node of graph in each task increases from 1,000 to 10,000. It is worth mentioning that our CGNP can scale to graphs of 10,000 nodes in the limited 16GB GPU, whereas FeaTrans runs out of memory and MAML even fails for 1,000 nodes. Although CGNP spends longer time than FeaTrans for testing, their gap shrinks as the size of graphs becomes larger. That is because the larger the graph, the longer time FeaTrans spends in the finetuning step, which CGNP do not incur.

8.4 Effect of the ground-truth number
We further evaluate how the number of ground-truth samples influence the performance of the learning-based approaches. For each query node $q$ in the support set, its number of positive/negative samples, i.e., $\frac{|E^+|}{|E^-|}$, is varying from 2%/10% to 20%/100% of the total number of the nodes. Fig. 6 shows the F1-score of the 3 CGNP variants and 3 ML baselines on the 6 different tasks in the one-shot scenario.

In Fig. 6, CGNP variants surpass the ML baselines by 40% on average, particularly under the circumstances of the small number of ground-truth, which indicates the superiority of CGNP on learning from small samples. For small training samples, Supervised suffers from severe over-fitting and FeaTrans and MAML also face a high risk of over-fitting in their adaption step. As the number of ground-truth increases, the performance of Supervised and MAML increase in general. And Supervised will overtake CGNP as shown in Fig. 6(e)-(f), when the number of ground-truth is at a high level. Given sufficient training data, a task-specific Supervised model can better adapt to the task, compared with a meta-model. Furthermore, we find that the performance of CGNP is robust to the number of ground-truth. That is in accordance with the nature of metric-based learning, where only a few training samples can achieve high performance for KNN and kernel learning.

8.5 Ablation Study
In this section, we conduct ablation studies to investigate the effect of different options for the GNN layer and the commutative operation on the performance of CGNP. CGNP_MLP, the CGNP with an MLP decoder, is tested as the base CGNP model and all the model variants are trained by the same hyper-parameters. These model variants are tested on the 5-shot Citeseer task, Arxiv SGSC task, DBLP SGDC task, Facebook MGDD task and Cora_Citeseer MGDD task, respectively.
Figure 6: F1 under different ratio of ground-truth

GNN Layer. We adopt three popular GNN layers, GCN [26], GAT [39] and GraphSAGE [17] as the GNN layer of the encoder, where the commutative operation is fixed to the average pooling. Table 5 lists the performance of the CGNP_MLP variants on the 4 tasks. In general, the GAT encoder consistently outperforms GCN and GraphSAGE encoders. That is because GAT aggregates the node representation weighted by learnable weights via self-attention, where the importance of each neighbor regarding its local structure, possible features and positive/negative labels are considered. The higher F1 of GAT demonstrates the attention mechanism can also contribute to improving the performance of CGNP in the encoder part.

Commutative Operation. We adopt the sum, average pooling and self-attention, introduced in section 6 as the commutative operation big @ of CGNP_MLP, by fixing GAT as the encoder GNN. Table 6 shows the corresponding performance of the 3 model variants. Attention performs best for the same graph tasks Arxiv, DBLP and Citeseer, while average pooling performs best of the different graphs task Facebook. And the differences between the three variants are relatively slight. We speculate that different tasks, graphs or ground-truth distributions may benefit from different commutative operations, and the effect of the type of commutative operation is not as remarkable as that of the GNN encoder.

9 CONCLUSION

In this paper, we study leveraging ML/DL approaches for community search, under the circumstance that the training data is scarce. We propose a metric-based meta-learning framework, Conditional Graph Neural Process (CGNP) to learn a meta-model to capture the prior knowledge of community search. The meta model is adapted to a new task swiftly to make predictions of the community membership, where a task is a graph with only a few given ground-truth. To the best of our knowledge, CGNP is the first meta-learning model for community search that utilizes the generalization ability of neural networks to the greatest extent. Compared with algorithmic approaches, CGNP supports flexible community structures learned from the data. Compared with general meta-learning algorithms, CGNP further exploits the characteristic of community search. Our extensive experiments demonstrate that CGNP outperforms the two lines of approaches significantly regarding accuracy.

REFERENCES

[1] PyTorch. https://github.com/pytorch/pytorch.
[2] PyTorch Geometric. https://github.com/rusty1s/pytorch_geometric.
[3] Ehsan Akbas and Peixiang Zhao. 2017. Truss-equivalence Based Indexing Approach. Proc. VLDB Endow. 10, 11 (2017), 1298–1309.
[4] Antreas Antoniou, Harrison Edwards, and Amos J. Storkey. 2019. How to train your MAML In Proc. ICLR.

Table 5: Performance with Different GNN layers

| Dataset  | Layer     | Acc   | Pre   | Rec   | F1    |
|----------|-----------|-------|-------|-------|-------|
| Citeseer | GCN       | 0.5220| 0.5347| 0.5631| 0.5486|
|          | GAT       | 0.5260| 0.5341| 0.6347| 0.5800|
|          | GraphSAGE | 0.5105| 0.5248| 0.5402| 0.5323|
| Arxiv    | GCN       | 0.5081| 0.4645| 0.7140| 0.5628|
|          | GAT       | 0.4968| 0.4625| 0.8297| 0.5939|
|          | GraphSAGE | 0.5116| 0.4636| 0.6461| 0.5399|
| DBLP     | GCN       | 0.5274| 0.4326| 0.7267| 0.5424|
|          | GAT       | 0.5618| 0.4584| 0.7542| 0.5702|
|          | GraphSAGE | 0.5609| 0.4491| 0.6145| 0.5189|
| Facebook | GCN       | 0.2838| 0.2395| 0.9334| 0.3812|
|          | GAT       | 0.4309| 0.2880| 0.9564| 0.4427|
|          | GraphSAGE | 0.5575| 0.3036| 0.6747| 0.4188|
| Cora_Citeseer | GCN    | 0.5191| 0.5122| 0.6901| 0.5880|
|          | GAT       | 0.5351| 0.5209| 0.8115| 0.6345|
|          | GraphSAGE | 0.5112| 0.5060| 0.7046| 0.5890|

Table 6: Performance with Different Commutative Op.

| Dataset     | Com. Op. | Acc     | Pre     | Rec     | F1      |
|-------------|----------|---------|---------|---------|---------|
| Citeseer    | Attention| 0.5442  | 0.5485  | 0.6579  | 0.5982  |
|              | Sum      | 0.5435  | 0.5480  | 0.6557  | 0.5971  |
|              | Average  | 0.5260  | 0.5341  | 0.6347  | 0.5800  |
| Arxiv       | Attention| 0.4480  | 0.4450  | 0.9898  | 0.6140  |
|              | Sum      | 0.4476  | 0.4448  | 0.9891  | 0.6126  |
|              | Average  | 0.4968  | 0.4625  | 0.8297  | 0.5939  |
| DBLP        | Attention| 0.5211  | 0.4393  | 0.8779  | 0.5856  |
|              | Sum      | 0.5172  | 0.4369  | 0.8750  | 0.5828  |
|              | Average  | 0.5618  | 0.4584  | 0.7542  | 0.5702  |
| Facebook    | Attention| 0.3403  | 0.2611  | 0.9791  | 0.4123  |
|              | Sum      | 0.3376  | 0.2603  | 0.9792  | 0.4113  |
|              | Average  | 0.4309  | 0.2880  | 0.9564  | 0.4427  |
| Cora_Citeseer | Attention| 0.5130  | 0.5061  | 0.8583  | 0.6367  |
|              | Sum      | 0.5144  | 0.5070  | 0.8460  | 0.6340  |
|              | Average  | 0.5351  | 0.5209  | 0.8115  | 0.6345  |
