Learning Heuristics over Large Graphs via Deep Reinforcement Learning

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Abstract

In this paper, we propose a deep reinforcement learning framework called GCOMB to learn algorithms that can solve combinatorial problems over large graphs. GCOMB mimics the greedy algorithm in the original problem and incrementally constructs a solution. The proposed framework utilizes Graph Convolutional Network (GCN) to generate node embeddings that predicts the potential nodes in the solution set from the entire node set. These embeddings enable an efficient training process to learn the greedy policy via Q-learning. Through extensive evaluation on several real and synthetic datasets containing up to a million nodes, we establish that GCOMB is up to 41% better than the state of the art, up to 7 times faster than the greedy algorithm, robust and scalable to large dynamic networks.

1 Introduction

Optimization problems on graphs appear routinely in various applications such as viral marketing in social networks [Kempe et al., 2003], computational sustainability [Dilkina et al., 2011], and health-care [Wilder et al., 2018]. These optimization problems are often combinatorial in nature, which results in NP-hardness. Therefore, designing an exact algorithm is infeasible and polynomial-time algorithms, with or without approximation guarantees, are often desired and used in practice [Goyal et al., 2011; Jung et al., 2012; Medya et al., 2018]. Furthermore, these graphs are often dynamic in nature and the approximation algorithms need to be run repeatedly at regular intervals. Since real-world graphs may contain millions of nodes and edges, this entire process becomes tedious and time-consuming.

To provide a concrete example, consider the problem of viral marketing on social networks. Given a graph $G$ and a budget $b$, the goal is to select $b$ nodes (users) from the graph such that their endorsement of a certain product (ex: through a tweet) is expected to initiate a cascade that reaches the largest number of nodes in the graph. It has been shown that this problem is NP-hard by reducing it to the max-coverage problem [Kempe et al., 2003]. Advertising through social networks is a common practice today and needs to solved repeatedly due to the networks being dynamic in nature. Furthermore, even the greedy approximation algorithm has been shown to not scale on large networks [Arora et al., 2017].

At this juncture, we highlight two key observations. First, although the graph is changing, the underlying model generating the graph is likely to remain the same. Second, the nodes that get selected in the answer set of the approximation algorithm may have certain properties common in them. Motivated by these observations, we ask the following question: Given an optimization problem $P$ on graph $G$ from a distribution $D$ of graph instances, can we learn an approximation algorithm and solve the problem on an unseen graph generated from distribution $D$? In this paper, we show that this is indeed possible.

The above observation was first highlighted by Khalil et al. [Khalil et al., 2017], where they proposed an algorithm to learn combinatorial algorithms on graphs. Unfortunately, this study is limited to networks containing less than 5000 nodes and hence performance on real networks containing millions of nodes and edges remains to be seen. In this work, we bridge this gap. Specifically, we develop a deep reinforcement learning based architecture, called GCOMB, to learn combinatorial algorithms on graphs at scale. We also show that GCOMB outperforms [Khalil et al., 2017].

Our contributions are summarized as follows:

- **Novel Framework.** We propose a deep reinforcement learning based framework called GCOMB to learn algorithms for combinatorial problems on graphs. GCOMB first generates node embeddings through Graph Convolutional Networks (GCN). These embeddings encode the effect of a node on the budget-constrained solution set. Next, these embeddings are fed to a neural network to learn a $Q$-function and predict the solution set.

- **Application.** We benchmark GCOMB on datasets containing up to 1 million nodes. The results show that GCOMB is 7 times faster than greedy, up to 41% better than the state-of-the-art neural method for learning algorithms [Khalil et al., 2017], and scalable. More significantly, GCOMB can be operationalized on real networks to solve practical problems.

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2 Problem Formulation and Preliminaries

Our goal is to learn algorithms for solving combinatorial optimization problems on graphs. Formally, we define our learning task as follows.

**Problem 1.** Given a combinatorial optimization problem \( P \) over graphs drawn from distribution \( D \), learn a heuristic to solve problem \( P \) on an unseen graph \( G \) generated from \( D \).

The input to our problem is therefore a set of training graphs \( \{G_1,\ldots,G_n\} \) from distribution \( D \) and the set of solution sets \( \{S_1,\cdots,S_n\} \) from an approximation algorithm for problem \( P \) on each of these graphs. Given an unseen graph \( G \) from \( D \), we need to predict its solution set \( S \) corresponding to problem \( P \).

### 2.1 Instances of the proposed problem

To motivate our work, we discuss some graph combinatorial problems that have practical applications and fit well within our framework.

**Definition 1** (Maximum Coverage Problem (MCP)). Given a collection of subsets \( S = \{S_1,S_2,\cdots,S_m\} \) from a universal set of items \( U = \{u_1,u_2,\cdots,u_n\} \), the problem is to choose at most \( b \) sets to cover as many items as possible.

The MCP problem is the optimization version of the classical Set Cover decision problem. The MCP problem can be equivalently expressed on bipartite graph \( G = (V,E) \) (with \( m+n \) nodes) as follows: There are two sets \( V = A \cup B \) of nodes; \( A = \{i|S_i \in S\} \) and \( B = \{j|u_j \in U\} \). There is an undirected edge \((i,j)\) whenever \( u_j \in S_i \). Given a budget \( b \), the goal is to find a set \( S^* \) of \( b \) nodes in \( A \) such that \( |X| \) is maximized, where \( X = \{j|(i,j) \in E, i \in S^*, j \in B\} \).

The MCP problem is used as a building block of many problems on graphs. Influence maximization on social networks [Kempe et al., 2003] is one such prominent example.

**Definition 2** (Minimum Vertex Cover (MVC)). Given an undirected graph \( G = (V,E) \), find the smallest subset of vertices \( S \subseteq V \) such that each edge in the graph is incident to at least one vertex in \( S \).

MVC is a decision problem. An optimization version of MVC can be defined in the same manner as MCP [Apollonio and Simeone, 2014]. Specifically, given a graph \( G = (V,E) \) and a budget \( b \), find a set \( S^* \) of \( b \) nodes such that \( |X| \) is maximized, where \( X = \{(i,j)|(i,j) \in E, i \in S^*, j \in V\} \). The MVC problem has applications in several domains with drug discovery being one of the highlights [Guha et al., 2002].

### 2.2 The greedy approach

The greedy approach is one of the most popular and well-performing strategies to solve combinatorial problems on graphs. Alg. 1 presents the pseudocode. The input to the algorithm is a graph \( G = (V,E) \), an optimization function \( f(S) \) on a set of nodes \( S \), and budget \( b \). Starting from an empty solution set \( S \), the solution is built iteratively by adding the “best” node to \( S \) in each iteration (lines 3-5). The best node \( v^* \in V \backslash S \) is the one that provides the highest marginal gain on the optimization function (line 4). The process ends after \( b \) iterations where \( b \) is the budget.

### 3 GCOMB

GCOMB consists of two phases: the training phase and the testing phase. The input to the training phase is a set of graphs and the optimization function \( f(.) \) corresponding to the combinatorial problem being solved. The output of the training phase is a sequence of two different neural networks with their corresponding learned parameters. In the testing phase, the inputs are identical as in the greedy algorithm, which are the graph \( G = (V,E) \), the optimization function \( f(.) \) and the budget \( b \). The output of the testing phase is the solution set, which is constructed using the learned neural networks from the training phase.

Fig. 1 presents the pipeline of the training phase. The training phase can be divided into two parts: a network embedding phase through Graph Convolutional Network (GCN) and a Q-learning phase. Given a training graph and its solution set, the GCN learns network embeddings that separates the potential solution nodes from the rest. Next, the embeddings of only the potential solution nodes are fed to a Q-learning framework, which allows us to predict those nodes that collectively form a good solution set. The next sections elaborate further on these two key components of the training phase.

### 3.1 Embedding via GCN

Our goal is to learn embeddings of the nodes such that they can predict the nodes that are likely to be part of the answer set. Towards that, one can set up a classification-based pipeline, where, given a training graph \( G = (V,E) \) and its greedy solution set \( S \) corresponding to the optimization function \( f(S) \), a node \( v \) is called positive if \( v \in S \); otherwise it is negative. One can next train a neural network to learn node embeddings with an appropriate loss function such as cross-entropy loss. This approach, however, has two key weaknesses. First, it assumes all nodes that are not a part of \( S \) to be equally bad. In reality this may not be the case. To elaborate, consider the case where \( f(\{v_1\}) = f(\{v_2\}) \), but the marginal gain of node \( v_2 \) given \( S = \{v_1\} \), i.e., \( f(\{v_1,v_2\}) - f(\{v_1\}) \), is 0 and vice versa. In this scenario, only one of \( v_1 \) and \( v_2 \) would be selected in the answer set although both are of equal quality on their own.

To capture the above aspect of a combinatorial optimization problem, we sample from the solution space and learn embeddings that reflect the probability of a node being part of the solution. To sample from the solution space, we perform a probabilistic version of the greedy search in Alg. 1. Specifically, in each iteration, instead of selecting the node with the highest marginal gain, we choose a node with probability proportional to its marginal gain. The probabilistic
Graph Convolutional Network (GCN)

**Require:** \( G = (V, E), \{\text{score}(v)\}, \) input features \( x_v \), \( \forall v \in V \), depth \( K \), weight matrices \( \mathbb{W}^k, \forall k \in [1, K] \) and weight vector \( w \), dimension size \( d \).

**Ensure:** \( d \)-dimensional vector representations \( \mu_v, \forall v \in V \)

1: \( h^0_v \leftarrow x_v, \forall v \in V \)
2: for \( k \in [1, K] \) do
3: for \( v \in V \) do
4: \( N(v) \leftarrow \{u \mid (v, u) \in E\} \)
5: \( h^k_v \leftarrow \text{MAXPOOL} \left( \{h^{k-1}_u, \forall u \in N(v)\} \right) \)
6: \( h^k_v \leftarrow \text{ReLU} \left( \mathbb{W}^k \cdot \text{CONCAT} \left( h^k_v, h^{k-1}_v \right) \right) \)
7: \( h_v \leftarrow \frac{1}{|N(v)|} \sum_{u \in \text{ReLU} \left( \mathbb{W}^k \cdot \text{CONCAT} \left( h^k_v, h^{k-1}_u \right) \right) \} \)
8: \( \mu_v \leftarrow \frac{1}{|N(v)|} \sum_{u \in \text{ReLU} \left( \mathbb{W}^k \cdot \text{CONCAT} \left( h^k_v, h^{k-1}_u \right) \right) \} \)
9: \( \text{score}(v) = w^T \cdot \mu_v, \forall v \in V \)

Learning Q-function

**Require:** \( \mu_v, \forall v \in V \), hyper-parameters \( M, N \) related to fitted \( Q \)-learning, number of episodes \( I \) and sample size \( T \).

**Ensure:** Learn parameter set \( \Theta \)

1: Initialize experience replay memory \( M \) to capacity \( N \)
2: for episode \( e \leftarrow 1 \) to \( L \) do
3: for step \( t \leftarrow 1 \) to \( T \) do
4: \( v_t \leftarrow \begin{cases} \text{random node } v \notin S_t, \text{with probability } \epsilon & \\
\text{argmax}_{v \in S_t} Q(S_t, v, \Theta) \text{ otherwise} & \end{cases} \)
5: \( S_{t+1} \leftarrow S_t \cup \{v_t\} \)
6: if \( t \geq n \) then
7: \( S_{t+n} \leftarrow S_{t+n}, \sum_{i=t}^{t+n} r(S_i, v_i), t \) to \( M \)
8: Sample random batch \( B \) from \( M \)
9: Update the parameters \( \Theta \) by SGD for \( B \)
10: return \( \Theta \)

**Defining \( x_v \):** The initial feature vector \( x_v \) at depth 0 should have the raw features that are relevant with respect to the combinatorial problem being solved. For example, in MCP and MVC, the degree of a node is an indicator of its own coverage. As we discuss later in Sec. 4, we use only node degree as the node feature. In principle, any feature can be used including node labels.

While in Alg. 2, the parameters are learned by minimizing the loss function across all nodes, in practice, we use mini-batches of a small sample of nodes.

3.2 Learning Q-function

While GCN captures the individual importance of a node towards a particular combinatorial problem, through \( Q \)-learning [Sutton and Barto, 2018], we capture nodes that collectively form a good solution set. More specifically, given some set of nodes \( S \) and a node \( v \notin S \), we aim to predict \( Q(S, v) \) (intuitively long-term reward for adding \( v \) to \( S \)) through the surrogate function \( Q'(S, v; \Theta) \). For any \( Q \)-learning task, we need to define the following five aspects: state space, actions, rewards, policy and termination.

- **State space:** A state is the aggregation of two sets of nodes: nodes selected in the current solution set \( S \) and...
those not selected, i.e., \( V \setminus S \). Thus, the state corresponding to solution set \( S \) is captured using two vectors: \( \mathbf{\mu}_S = \text{MAXPOOL}(\{ \mathbf{\mu}_v, v \in S \}) \) and \( \mathbf{\mu}_{V \setminus S} = \text{MAXPOOL}(\{ \mathbf{\mu}_v, v \notin S \}) \).

- **Action**: An action corresponds to adding a node \( v \notin S \) (represented as \( \mathbf{\mu}_v \)) to the solution set.
- **Rewards**: The reward function at state \( S \) is the marginal gain of adding node \( v \) to \( S \), i.e. \( r(S, v) = f(S \cup \{ v \}) - f(S) \).
- **Policy**: The policy \( \pi(v|S) \) (given state \( S \) and action) is deterministic and, as in the greedy policy, selects the node with the highest predicted marginal, i.e.,

\[
\pi(v|S) = \arg \max_{v \notin S} Q(S, v; \Theta)
\]

- **Termination**: We terminate when \( |S| = b \); \( b \) is the budget.

**Learning \( \Theta \):** Alg. 3 presents the pseudocode of learning the parameter set \( \Theta \). We partition \( \Theta \) into four weight vectors \( \Theta_1, \Theta_2, \Theta_3, \Theta_4 \) such that, \( Q'(S, v; \Theta) = \Theta_1 \cdot \mathbf{\mu}_S, v \), where

\[
\mathbf{\mu}_{S,v} = \text{ReLU} \left\{ \text{CONCAT} \left( \Theta_1 \cdot \mathbf{\mu}_S, \Theta_2 \cdot \mathbf{\mu}_{V \setminus S}, \Theta_3 \cdot \mathbf{\mu}_v \right) \right\}
\]

If the dimension of the initial node embeddings is \( d \), the dimensions of the weight vectors are as follows: \( \Theta_1 \in \mathbb{R}^{d \times 1}, \Theta_2, \Theta_3 \in \mathbb{R}^{d \times d} \). In Eq. 3, ReLU is applied element-wise to its input vector.

The standard Q-learning updates parameters in a single episode via a SGD step to minimize the squared loss.

\[
J(\Theta) = (y - Q'(S_t, v_t; \Theta))^2
\]

where \( y = \gamma \cdot \max_{v} (Q'(S_{t+1}, v; \Theta)) + r(S_t, v_t) \)

\[
S_t \text{ denotes current solution set, } \gamma \text{ is the discount factor, and } v_t \text{ is the considered node. To better learn the parameters, we perform } n \text{-step } Q\text{-learning instead of } 1\text{-step } Q\text{-learning. } n\text{-step } Q\text{-learning incorporates delayed rewards, where the final reward of interest is received later in the future during an episode (lines 6-9). This avoids the myopic setting of } 1\text{-step update. The key idea here is to wait for } n \text{ steps so that the approximator’s parameters are updated and therefore, more accurately estimate future rewards. To incorporate } n \text{-step rewards, Eq. 5 is modified as follows.}

\[
y = \gamma \cdot \max_{v} (Q'(S_{t+n}, v; \Theta)) + \sum_{t=0}^{n-1} r(S_t, v_t)
\]

**Efficiency:** For efficient learning of the parameters, we perform two optimizations. First, we exploit fitted Q-iteration [Riedmiller, 2005], which results in faster convergence using a neural network as a function approximator [Mnih et al., 2013]. Specifically, instead of updating the Q-function sample-by-sample, the fitted Q-iteration approach uses experience replay with a batch of samples from a previously populated dataset \( M \) defined in line 1 of Alg. 3. Second, we reduce the state space, by learning marginal gains only for the top-10% nodes with the predicted values learned during the GCN step.

### 3.3 Summary

The entire pipeline of GCOMB works as follows.

| Name                | \(|V|\)  | \(|E|\)  |
|---------------------|---------|---------|
| loc-Gowalla (LG)    | 196.5K  | 950.3K  |
| loc-Brightkite (LB) | 58.2K   | 274K    |
| sx-mathoverflow (SM)| 24.8K   | 506.5K  |

Table 1: Dataset description and statistics of real networks.

- **Training Phase**: Given a training graph \( G \), and optimization function \( f(S) \), learn parameter set \( \theta_{GCN} \) and \( \theta_Q \) corresponding to the GCN component and Q-learning component. This is a one-time, offline computation. The sub-tasks in the training phase are:
  - Learn node embeddings \( \mathbf{\mu}_v, \forall v \in V \) along with \( \theta_{GCN} \).
  - Feed \( \mathbf{\mu}_v, \forall v \in V \) to Q-learning framework and learn \( \theta_Q \).
- **Testing Phase**: Given an unseen graph \( G \),
  - Embed all nodes using \( \theta_{GCN} \).
  - Iteratively compute the solution set based on the learned \( Q \) function. Specifically, in each iteration we add the node \( v^* = \arg \max_{v \in V} Q'(S_t, v; \Theta_Q) \), where \( S_t \) is the solution set in the \( t \)th iteration. As in greedy (Alg. 1), we iterate for \( b \) iterations, where \( b \) is the budget.

### 4 Experimental Results

In this section, we benchmark GCOMB and establish:

- **Quality**: GCOMB is up to 41% better in quality than the state of the art technique [Khalil et al., 2017].
- **Scalability**: GCOMB scales to million-sized networks where [Khalil et al., 2017] crashes. Furthermore, GCOMB achieves almost the same quality as the greedy algorithm, while being 7 times faster.
- **Application**: GCOMB is applicable to dynamic networks and achieves quality at par with the greedy algorithm, which is the best possible polynomial-time approximation scheme for MCP unless \( P = NP \).

#### 4.1 Experimental Setup

All experiments are performed on a machine running Intel Xeon E5-2698v4 processor with 20 cores, having 8 Nvidia 1080 Ti GPU cards and 512 GB RAM with Ubuntu 16.04 operating system. All our codes are written in Python with the support of TensorFlow.

**Datasets:** We use both synthetic and real datasets for our experiments. For synthetic dataset, we generate graphs from two different models:

- **Barabási–Albert (BA):** In BA, the default edge density is set to 4, i.e., \(|E| = 4|V|\). We use the notation BA-\( X \) to denote the size of the generated network, where \( X \) is the number of nodes.
- **Bipartite Graph (BP):** [Khalil et al., 2017] proposes a model to generate bipartite graphs as follows: Given the number of nodes, they are partitioned into two sets with \( \% \) nodes in one side and the rest in other. The edge between any pair of nodes from different partitions is generated with probability 0.1.

In addition, we also use the real datasets\(^1\) listed in Table 1. Among them, sx-mathoverflow (SM) is a dynamic (temporal) network where each edge is annotated with a timestamp.

\(^1\)http://snap.stanford.edu/data/index.html
Baselines: We denote our method as GCOMB, the greedy algorithm as GR, the state-of-the-art method from Khalil et al., 2017 as SoA. For SoA, we use the code shared by the authors. Note that computing the optimal solution is not feasible since the problems being learned, such as MCP and MVC, are NP-hard. GR guarantees a \(1 - 1/e\) approximation for both MCP and MVC (optimization version). Given a budget \(b\), we compute a random selection of \(b\) nodes. This baseline is called Random.

Other Settings: GCN is trained for 200 epochs with a learning rate of 0.0005, a dropout rate of 0.1 and a convolution depth \((K)\) of 2. For training the n-step Q-Learning neural network, \(n\) is set to 2 and a learning rate of 0.0001 is used. In each epoch of training, 8 training examples are sampled uniformly from the Replay Memory \(M\) as described in Alg. 3. This Q Learning network is trained for 5-10 graph instances with \(b = 30\).

### 4.2 Comparison with State-of-the-art

First, we benchmark GCOMB against the state-of-the-art learning method by Khalil et al., 2017 (SoA) on the bipartite graph model proposed by Khalil et al., 2017. We measure the quality of the solution sets obtained by these two methods on both MCP and MVC. For a fair comparison, we keep the training time (1 hour), training dataset and testing dataset same for both methods. Furthermore, to measure robustness, all results are reported by averaging the quality over 5 training instances.

As Khalil et al. show results on small graphs, we first test both GCOMB and SoA on relatively small graphs. Both the methods are trained on a graph with 1000 nodes and tested for the MCP problem (Section 2) with budget 15. As presented in Table 2, GCOMB outperforms SoA across all graph sizes.

Next, we show the results for BA datasets with larger sizes on the MVC problem with budget as \(b = 30\). Both methods are trained on BA graphs with \(1k\) nodes. Table 3 shows that our method produces better results consistently with the quality being up to 41% better than SoA. Furthermore, SoA fails to scale on large graphs (100k nodes and beyond).

GCOMB is not only better in quality, but also more robust. This property is captured in Table 4, which shows the variance in quality across the different training instances. The variance is SoA is up to 3 times higher than GCOMB. Overall, GCOMB is up to 41% better in quality, more scalable, and robust when compared to SoA.

Next, we move to evaluating GCOMB on large graphs. We omit SoA from the next set of experiments since it crashes on these datasets due to scalability issues.

### 4.3 Comparison with Greedy

In this section, we benchmark GCOMB against GR.

**Quality:** Table 5 shows the results on the MCP problem over multiple synthetic and real datasets. GCOMB is trained on BA-1000. The “Ratio” column in Table 5 denotes the ratio between the quality produced by GCOMB against GR. While GCOMB consistently produces quality above 80% on synthetic graphs, it improves further to 91% on real datasets. For MVC problem, the results are around 50% (Table 6).

**Efficiency (MVC):** The real benefit of using GCOMB for combinatorial optimization problems comes from the property that it is significantly faster than greedy. Specifically, once the parameters have been learned in the training phase and the node embeddings have been constructed on the unseen graph, for any given budget \(b\), we only need to pass the top-10% nodes through the \(Q\)-learning neural network. This is an extremely lightweight task when compared to the greedy solution, and therefore, significantly faster.

To bring out this aspect, we present the online running times of GCOMB and greedy in Fig. 2b as the budget is increased. As clearly visible, GCOMB is more than 7 times faster with a lower growth rate than GR. The quality, although slightly lower than GR, grows at par with GR (Fig. 2a).

**Impact of dimension (MCP):** We run GCOMB for MCP by varying the node embedding dimension in GCN. This experiment is performed on BP datasets of different sizes. The model is trained on a BP graph with 1000 nodes. Table 7...
Table 6: MVC: Comparison of our method with baselines on large graphs. Ratio denotes the ratio between the quality produced by GCOMB and GR.

| Graph  | GR   | Random | GCOMB | Ratio |
|--------|------|--------|-------|-------|
| BA-100k| 14490| 270    | 7975  | .55   |
| BA-500k| 30723| 268    | 14911 | .49   |
| LB     | 14787| 238    | 7468  | .50   |
| LG     | 76793| 416    | 29531 | .38   |

Table 7: MCP: Performance of GCOMB with varying embedding dimensions.

| Graph | d = 64 | d = 128 | d = 256 |
|-------|--------|---------|---------|
| BP-4k | 2678   | 2668    | 2589    |
| BP-5k | 3344   | 3296    | 3250    |
| BP-10k| 6603   | 6565    | 6443    |

Figure 2: MVC: (a) Quality and (b) running Time of GCOMB and GR on BA graphs with 1 million nodes against budget.

Figure 3: Quality of the solution sets produced by GCOMB and GR on temporal networks.

and MVC problems respectively and then test on all of the remaining graphs.

Figure 3 presents the performance of GCOMB. As visible, the quality of GCOMB’s solutions sets are almost identical to GR across all test graphs.

5 Previous Work

Many combinatorial graph problems lead to NP-hardness [Karp, 1972]. There are classical NP-hard problems on graphs such as Minimum Vertex Cover, Minimum Set Cover, Travelling Salesman Problem (TSP); as well as other important combinatorial problems with many applications. Examples include finding top influential nodes [Kempe et al., 2003], maximizing centrality of nodes [Yoshida, 2014], and optimizing networks [Medya et al., 2018; Dilkina et al., 2011].

There has been recent interest in solving graph combinatorial problems with neural networks and reinforcement learning [Bello et al., 2016; Khalil et al., 2017]. Learning-based approaches are useful in producing good empirical results for NP-hard problems. The methods proposed in [Bello et al., 2016] are generic and do not explore structural properties of graphs, and use sample-inefficient policy gradient methods. Khalil et al. [Khalil et al., 2017] has investigated the same problem with a network embedding approach combined with a reinforcement learning technique. The same problem has been studied by Li et al. [Li et al., 2018] via a supervised approach using GCN. Among other interesting work, for branch-and-bound algorithms, He et al. studied the problem of learning a node selection policy [He et al., 2014]. Another examples include pointer networks [Vinyals et al., 2015] proposed by Vinyals et al. and reinforcement learning approaches by Silver et al. [Silver et al., 2016] to learn strategies for the game Go.

6 Conclusion

In this paper, we have proposed a deep reinforcement learning based framework called GCOMB to learn algorithms for combinatorial problems on graphs. GCOMB first generates node embeddings through Graph Convolutional Networks (GCN). These embeddings encode the effect of a node on the budget-constrained solution set. Next, these embeddings are fed to a neural network to learn a Q-function and predict the solution set. Through extensive experiments on both real and synthetic datasets containing up to a million nodes, we show that GCOMB is up to 41% better in quality...
over the state-of-the-art neural method, more robust and more scalable. In addition, GCOMB is up to 7 times faster than the greedy approach, while being of comparable quality. Overall, with these qualities, GCOMB can be operationalized on real dynamic networks to solve practical problems at scale.

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