Graph Convolutional Policy for Solving Tree Decomposition via Reinforcement Learning Heuristics

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Abstract

We propose a Reinforcement Learning based approach to approximately solve the Tree Decomposition (TD) problem. TD is a combinatorial problem, which is central to the analysis of graph minor structure and computational complexity, as well as in the algorithms of probabilistic inference, register allocation, and other practical tasks. Recently, it has been shown that combinatorial problems can be successively solved by learned heuristics. However, the majority of existing works do not address the question of the generalization of learning-based solutions. Our model is based on the graph convolution neural network (GCN) for learning graph representations. We show that the agent built on GCN and trained on a single graph using an Actor-Critic method can efficiently generalize to real-world TD problem instances. We establish that our method successfully generalizes from small graphs, where TD can be found by exact algorithms, to large instances of practical interest, while still having very low time-to-solution. On the other hand, the agent-based approach surpasses all greedy heuristics by the quality of the solution.

1 Introduction

At the core of many practical tasks, such as probabilistic inference, decision making, planning, etc., lies a combinatorial (NP-hard) optimization problem. The solution of huge NP problems is often possible only with the help of approximate algorithms or heuristics. These heuristics are often designed manually, which is a complicated and time-consuming process. The resulting algorithm is also typically domain-specific and can not be reused. Recently, an application of reinforcement learning (RL) to design heuristics gained significant attention [Bello et al., 2016] [Kool et al., 2018] [Khalil et al., 2017]. RL is a natural framework for the automatic design of approximation algorithms for problems with an inherent cost function and large search space, which is the essence of combinatorial optimization.

The specific NP problem we consider here is the Tree Decomposition, first introduced by Robertson & Seymour [1986]. The Tree Decomposition (TD) is central to the analysis of the complexity and the topological structure of graphs. Also, if the TD of a graph is known, then several NP-hard problems can be solved in linear time using it. Examples are Independent Set, Clique, Satisfiability, Graph Coloring, Travelling Salesman Problem (TSP), and many others. Associated with the solution of a TD problem is an integer number treewidth. The treewidth quantifies the complexity of many NP-problems; the computational cost of solving these problems is exponential in the treewidth, but only polynomial in the problem’s graph size. Tree Decomposition emerges as a core step in various contexts, such as probabilistic inference [Kask et al., 2011] or shortest path search [Chatterjee et al., 2016]. The TD problem is usually solved on non-Euclidean graphs, as opposed to the traveling salesman problem (TSP), which is the most common target of recent trainable heuristics studies [Kool et al., 2018; Bello et al., 2016].

Multiple exact [Gogate & Dechter, 2012; Tamaki, 2019] Bodlaender et al. [2006] and approximate [Berry et al., 2003] algorithms exist to solve the TD problem. We are the first (to the best of our knowledge) to propose a Machine Learning based solution. To learn heuristics, we utilize Markov Decision Process (MDP) formalism, considering TD as a Reinforcement Learning task with graph-structured data. We demonstrate that our agent can be successfully trained using a single graph, and the resulting policy can generalize on massive problem instances. Our setting contrasts previous work on learned heuristics for combinatorial optimization where usually large datasets are used. The quality of the solution of our agent-based procedure is superior compared to all simple greedy heuristics, and
the time-to-solution is much lower compared to advanced algorithms. The experiments also indicate that our agent improves over previous RL-based methods.

The goal of this work is not to outperform the existing state of the art TD algorithms, but rather to highlight the new challenges for representation learning and to provide a direction in the study of RL approaches to fundamental NP-hard problems. The progress towards producing a heuristic from a small number of graphs is essential to improve the quality of learning-based methods.

Main contributions of the paper are:

- A method proposed to learn a heuristic for Tree Decomposition Problem, which is more accurate than simple polynomial solvers and has similar low time-to-solution at the same time.
- It is shown that the agent trained on a small single graph generalizes to large real-world instances of TD problem and preserves the high quality of the solution.
- We demonstrate that our stochastic policy generalizes better across different graph structures compared to the previous reinforcement learning-based approach.

2 Background

In this section, we introduce the problem and the techniques we use. We start with a formulation of Tree decomposition as a linear ordering problem. Then the embedding method using Graph Convolution Networks (Kipf & Welling 2016) is explained. Finally, we formulate the problem in the Reinforcement Learning framework.

2.1 Tree decomposition problem

A full definition of a Tree Decomposition can be found in the original works by Robertson & Seymour (1986) or in more recent reviews (Bodlaender 1994). Informally, the Tree Decomposition measures how close a given graph resembles a tree.

Formally, a tree decomposition is a mapping of the initial graph \( G = (U, E) \) into a tree graph \( F = (B, T) \).

Here \( U \) is the set of nodes and \( E \) is the set of edges of the initial graph; \( B \) is the set of bags (nodes) and \( T \) are the edges of the tree graph. Each bag \( b \in B \) is a subset of nodes of the graph \( G \), e.g. \( b \subseteq U \). A tree decomposition has to fulfill three criteria to be valid:

1. Every node of \( G \) is in some bag, i.e., \( \cup_{b \in B} b = U \).

2. For every edge \((u, v) \in E\) there must be a bag such that both endpoints are in that bag, i.e., \( \exists b : u \in b, v \in b \).

3. For every node \( u \) of \( G \), the subgraph of the tree \( F \), induced by all bags that contain \( u \) is a connected tree.

The tree decomposition problem is a follows. For a given graph \( G \) one needs to find a tree \( F \) satisfying the conditions above, such that the size of the maximal bag \( b \in B \) minus one, called treewidth, is minimized across all possible tree graphs. It can be shown that this problem is NP-hard (Berg & Järväalo 2014). Instead of building the tree \( F \) directly, in this work we will search for TD by using its relation to the ordering of vertices (Blair & Peyton 1991). The procedure to build a tree \( F \) given a permutation of vertices is provided in the Appendix A.

A permutation \( \pi \) of vertices of a graph \( G \) is called an elimination order. The elimination order of the graph yields the following procedure:

1. For \( t \in [1 \ldots |U|] \), take the \( t \)-th node \( u = \pi^{-1}(t) \).

2. Remove \( u \) and connect all neighbors of \( u \) into a clique (fully connected subgraph).

If \( G \) has treewidth at most \( k \), then there is an elimination order \( \pi \) of \( G \), such that each vertex has at most \( k \) neighbors in the elimination procedure with respect to \( \pi \) (Amit 2001). We define the maximal number of neighbors associated with a permutation \( \pi \) as \( c_\pi \). The treewidth is a minimum of \( c_\pi \) across all possible permutations, e.g. \( tw(G) = \min_\pi c_\pi \). If the treewidth of a graph is small, then it is tree-like. In particular, a tree has treewidth 1.

We define our problem as follows: given an undirected graph \( G \) find an elimination order, i.e., a permutation of the vertices, such that the number of neighbors in the elimination procedure along \( \pi \) is minimized across all permutations.

As an example, consider two elimination procedures of the same graph in Figure 1. In the first case (upper part), the size of the maximal clique is 3 (and hence the treewidth corresponding to this order is 2). In the second case, the treewidth is 1, and the order is optimal (since the graph is a tree). Note that the optimal order may not be unique: the order of nodes number 1 and 2 can be swapped, for example, but the same treewidth is achieved.
2.2 Graph Convolution Networks

Our problem has a non-Euclidean structure, and we need a method that can utilize this for the arbitrary graphs. One of the most popular options is graph convolutional networks.

Recent graph architectures follow the aggregation scheme that consists of three types of functions: message passing, aggregation, and update function. In GCN (Kipf & Welling, 2016; Defferrard et al., 2016), message passing is a simple multiplication by weights; aggregation is a sum, and update is an activation function. Let $A$ be the adjacency matrix of a graph of $n$ vertices, let $\tilde{A} = A + I_n$ be an adjacency matrix with self-connections, and let $H^{(0)}$ be a feature matrix defined on the nodes of $G$. The propagation rule of a GCN layer is:

$$f(H^{(l)}, A) = \sigma \left( D^{-\frac{1}{2}} \tilde{A} D^{-\frac{1}{2}} H^{(l)} W^{(l)} \right)$$

(1)

Here $D$ is the diagonal matrix with elements defined as $D_{ii} = \sum_j \tilde{A}_{ij}$, $H^{(l)}$ is a feature matrix at $l$-th layer, $W^{(l)}$ are weights of the $l$-th layer and $\sigma$ is an activation function.

After $l$ layers, the features of GCN contain knowledge about $l$-hop neighborhoods in $G$. If a network of sufficient depth is used, the GCN embedding provides rich structural information about the graph to the higher layers of the network.

2.3 Reinforcement Learning for Graph Elimination

In order to put the TD problem into the RL framework, we should define a Markov decision process (MDP) over our task. At each time step $t$, the agent selects a node of the graph $G_t$ based on the observed information, represented by state features. The node is then eliminated from $G_t$ and a graph $G_{t+1}$ is produced. We define the environment $(S, A, P, r, \gamma)$ as follows:

- $S$ is a set of states. Each state $s_t \in S$ is defined as the embedding matrix $H_t^{(l)}$ of the graph $G_t$. To extract features on every step we use GCN.
- $A$ is a set of actions and consists of nodes $u \in U_t \subset U$, which have not been eliminated at the current step.
- $P$ is a transition function $P = p(s, u, s')$, where $p(s, u, s')$ is a probability distribution, $s, s' \in S, u \in A$.
- $r$ is a naturally defined cost for the sequential combinatorial problem; in our case, $r$ is the size of a maximal clique in the graph, which is obtained during the elimination process. This reward provides an estimation of the treewidth for the current elimination order.
- $\gamma \in [0, 1]$ is a discount factor responsible for trading off the preferences between the current reward and a future reward.

Now, as the TD problem is reduced to MDP, our goal is to maximize the return. Solving an MDP means finding an optimal policy $\Pi$, a mapping which outputs a distribution of actions. In the next section, we apply an Actor-Critic (Konda, 2002) algorithm for this problem.

3 Method

3.1 Graph Convolution Policy

We represent graphs $G_t$ with $n$ nodes as pairs $(A_t, H_t)$, where $A_t$ is the adjacency matrix and $H_t \in \mathbb{R}^{n \times d}$ is the node feature matrix, assuming that the graph has $d$ features. In our case we define $H_t$ as a vector of the inverse node’s degree.

In order to work with dense reward signal in the setting of the TD problem we define a reward function as follows:

$$r(s_t, u) = \begin{cases} -c_t(u), & \text{if } t \text{ is terminal}, \\ -\log c_t(u), & \text{otherwise} \end{cases}$$

(2)

where $c_t(u) = \max\{\text{degree}(u), c_{t-1}(u)\}$, and $u$ is the node of the graph $G_t$ which defines a state $s_t$. Such
A reward will yield $tw(G)$ in the end of the elimination process (which we are trying to minimize), and at the same time it does not restrict agent trajectories during the search for optimal ordering.

Our node selection policy $\Pi_\theta(u|s_t)$ is parameterized by a three layers of GCN [Kipf & Welling, 2016] [Defferrard et al., 2016] with ELU activations [Clevert et al., 2016] and two heads based on two-layer perceptron for value and policy functions. Here $\theta$ denotes all weights of the network. An attractive property of GCN in our setting is permutation invariance of state representation, which allows us to learn the pattern of heuristic irrespective of the order of the initial adjacency matrix. Figure 3 summarizes our method in the diagram.

### 3.2 Policy Optimization

The MDP for the agent is explicitly defined above, and we can use the Actor-Critic method [Konda, 2002] (a modification of the REINFORCE algorithm by Williams [1992]) to search for the optimal policy. The intuition to use the Actor-Critic is the following: we need a sufficient sample efficient algorithm, which converges faster than DQN [Hasselt et al., 2010] and can converge to the optimal policy that lies far from a random one. Let us briefly describe the Actor-Critic method below.

To find an optimal policy $\Pi_\theta$, one needs to maximize the expectation of the reward, defined as:

$$L_{\Pi_\theta}(s) = \mathbb{E}_{u \sim \Pi_\theta(s|s)} [r(s, u)]$$  \hfill (3)

To reduce the variance we use a trainable value function $V_{\Pi_\theta}(s)$ as a baseline, which is usual for Actor-Critic methods [Konda, 2002]. The purpose of a baseline is to estimate the complexity of the current state $s$. The value function is parameterized as a two-layer perceptron network, the same as the policy network. The value network takes as input a global average of node embeddings and is trained with a standard $L_2$ loss function. We take the loss of the value network as:

$$L_{\text{value}}(s, u) = \sum_t \left( \hat{A}(s_t, u_t) - V_{\Pi_\theta}(s_t) \right)^2$$  \hfill (4)

Here $\hat{A}(s_t, u_t)$ is the advantage estimation function. We defined the advantage according to the Generalized Advantage Estimator (GAE) method by [Schulman et al., 2015]. For a given trajectory $\pi$ for each step $t$, the GAE method implements an exponential average of advantage estimations along with all future steps in the trajectory. The GAE achieves the trade-off between the bias and variance by adjusting the weight $\lambda$ in the exponential average. The estimate of advantage is expressed as:

$$\hat{A}^{\text{GAE}}(s_t, u_t) = \sum_{l=0}^{[U]-t} (\gamma \lambda)^l \delta_{t+l},$$  \hfill (5)

$$\delta_t = r_t + \gamma V(s_{t+1}) - V(s_t)$$

We also included an entropy term in the loss function to increase the exploration of our agent. The entropy loss is defined as:

$$L_{\text{entropy}}(s, u) = -\sum_t \Pi_\theta(u_t|s_t) \log \Pi_\theta(u_t|s_t)$$  \hfill (6)

The total loss function for simultaneous training of graph representation, policy, and value function is a weighted sum of the terms described above:

$$L_{\text{total}}(s, u) = L_{\Pi_\theta} + \beta_{\text{value}} L_{\text{value}} - \beta_{\text{entropy}} L_{\text{entropy}}$$  \hfill (7)

### 4 Experiments

In this section, we demonstrate that provided a good representation of the state graph the agent can successfully learn a heuristic. We present our comparative results against common human-designed heuristics and show that our neural heuristic trained on a single graph can generalize.

#### 4.1 Data

For the experiments, three types of data were used. The first type is random ErdsRnyi (ER) graphs [Erdos & Rnyi, 1960] with edge probability $5/n$, where $n$ is the number of nodes. It was found experimentally that this choice of probability leads to graphs where the TD problem is not trivial (the ER graphs contain many loops and are not too dense). For validation we use a fixed dataset $D$ of 100 ErdsRnyi graphs with 10 to 1000 nodes.

The second dataset is taken from the PACE2017 competition [Dell et al., 2017] on designing TD algorithms. The last type is graphs that emerge in the simulation of random quantum circuits [Boixo et al., 2017], a common framework in the study of quantum computing supremacy.

The main reason for using ER graphs is to simplify the reproducibility of the experiments. Our main results are obtained on the PACE2017 dataset, which was created specifically to test TD algorithms and contains severe problem instances. The third one selected as a real-world TD applications.

[https://github.com/PACE-challenge/Treewidth-PACE-2017-instances](https://github.com/PACE-challenge/Treewidth-PACE-2017-instances)
[https://github.com/qbit-/boixo_circuits.git](https://github.com/qbit-/boixo_circuits.git)
Figure 3: Performance of agents trained on six different graphs. The agents are compared using a fixed ErdesRnyi dataset.

4.2 Training Details

All models were implemented with PyTorch Geometric (Fey & Lenssen, 2019) and trained with Adam optimizer (Kingma & Ba, 2015) with parameters $\beta_1 = 0.9$ and $\beta_2 = 0.999$. For GCN layers and the policy head we fix the learning rate ($lr$) to 0.01 for faster convergence, while the value head is optimized with $lr = 0.001$. We also set the parameters of the RL algorithm as follows: discount factor $\gamma = 0.999$, GAE weight $\lambda = 0.95$, the weight of the value loss $\beta_{\text{value}} = 1.0$ and the multiplier of the entropy regularization term $\beta_{\text{entropy}} = 0.001$. The GCN subnetwork contains 3 layers, and we fix the hidden feature size to 64 as in (Khalil et al., 2017). Policy and value heads are parameterized by a 2-layer perceptron with a hidden dimension equal to 64. We train our model on the NVIDIA 1080ti with one thread for sampling.

| Learnable Heuristic | 10 | 50 | 100 | Std. Dev. |
|---------------------|----|----|-----|-----------|
| GCN-agent           | 1.08 | 1.09 | 1.09 | 0.024 |
| S2V-DQN             | 1.67 | 1.10 | 1.11 | 0.028 |
| Random agent        | 1.78 |    | 0.18 |           |

Table 1: Performance of RL-based algorithms on the ER validation dataset. The agents are trained for 50 and 100 epochs (shown in braces) on 5 single different graphs with 50 nodes. The AR is calculated for all graphs in the hold-out dataset, and averaged over the trained agents.

The reinforcement learning approach we compared to is the S2V-DQN by Khalil et al. (2017). This algorithm was previously used to solve sequential optimization problems on graphs, such as Minimum Vertex Cover, and we adapted it to use the cost function from Eq. 2. It has to be noted that the original algorithm was trained on a large set of graphs, but here we try to obtain a heuristic using a single graph. We trained the S2V-DQN model

3our implementation with the author’s parameters

To produce a solution from the our RL-based solver we sample 10 trajectories and take the one with the lowest treewidth.

We compared the performance of different solvers with respect to the solver of Tamaki (2019). As a performance metric an Approximation Ratio (AR), $\text{AR} = \frac{\text{tw}_{\text{method}}(G)}{\text{tw}_{\text{Tamaki}}(G)}$ is used. The AR metric is standard in the literature on approximation algorithms. The treewidth was calculated from the elimination order $\pi$ produced by the solvers.

4.4 Convergence of RL approaches

To test the speed of learning of our Actor-Critic based agent, we trained it on 5 single graphs with 50 nodes from the ER dataset and stopped the training after different number of epochs. We found that typically, the efficient way is to train policy 100 epochs (no significant improvement occurs in further training), and
save the model with best score on the validation set. Turns out it is sufficient to train our agent for \( \sim 10 \) epochs (around 20 minutes).

In contrast, the S2V-DQN requires around 100 epochs to find a good policy, which is expected due to the low sample efficiency of standard DQN \([\text{Hasselt et al., 2016}]\). Still, the quality of the DQN-based agent is lower. The comparative results are listed in Table 1.

### 4.5 Choice of the Training Graph

In this series of experiments, we would like to check how does the choice of the training example affects the performance of the resulting agent. For this purpose, we chose 5 graphs of different kinds with around 50 nodes and trained our agent on each of them separately. We used two ER graphs with 50 nodes and \( p = 0.02 \), one graph from the quantum circuit dataset ("circuit4x4_46") and three different graphs from the PACE dataset ("he050", "he077", "he083"). The performance of the agents was compared on the validation dataset of ErdosRenyi graphs. The results are shown in Figure 3.

Surprisingly, we found that the score of the agent does not significantly depend on the source of the training graph, despite the graphs we used had very different structures. This fact may be attributed to the inefficiency of the agent or to the uniform structure of the TD problem already for average-sized graphs (with 50 nodes). We admit that this intriguing fact may need additional investigation. To simplify the reproducibility of our experiments, we chose ErdosRenyi graphs for further tests.

Another choice is the size of the training graph. It is known that if the action space is huge, the RL methods have problems with convergence due to the significant variance of the gradients. It is then desirable to keep the training graph size small (for example, less than 100 nodes); however, training on larger instances may produce agents with better performance. To check the influence of the training graph size on the accuracy of the learned heuristic, we trained separate agents on ER graphs with 10 to 210 nodes. The dependence of the AR is shown in Figure 4.

As can be seen from Figure 4, the accuracy of the GCN-agent depends on the number of nodes only slightly. Also, it can be noted that better accuracy was obtained for the graphs with 70 and 130 nodes, which is approximately the GCN feature size or twice feature size. For further experiments, we selected a graph with 70 nodes.

### 4.6 Comparison with Other Solvers

In this section, we will compare the performance of our agent to other methods on graphs of different sizes and structures. The agent was trained on the ER graph with 70 nodes. The results of all experiments are summarized in Figure 5.

| Method            | Approx. Ratio | Ratio Max. | Avg. Time, sec |
|-------------------|---------------|------------|----------------|
| Tamaki (2019)    | 1.0           | 1.0        | 17.01          |
| QuickBB           | 1.07 ± 0.08   | 1.41       | 1617.27        |
| Min-Fill          | 1.16 ± 0.14   | 1.78       | 153.52         |
| Min-Degree        | 1.21 ± 0.21   | 2.13       | 0.04           |
| GCN-Agent (ours) | 1.12 ± 0.13   | 1.44       | 10.93          |
| S2V-DQN           | 1.39 ± 0.35   | 1.79       | 0.9            |
| Random agent      | 1.84          | -          | -              |

Table 2: A summary of the agent’s performance on the PACE2017 dataset. The values are averaged over all graphs with sizes from 10 to 1000 nodes.

In all cases, the agent achieves a better score than greedy heuristics. It is interesting to see that one can learn a relatively useful heuristic using only a single graph.

The quality of the agent’s solution deteriorates as the size of the test graph grows, but usually slower than the quality of the solution of greedy heuristics.

Our Actor-Critic based agent performs well on all three datasets, despite being trained on a single ER graph, and achieves a significant level of generalization. In contrast, a DQN agent trained on the ER graph generally performs poorly on graphs with different structure. In contrast, the S2V-DQN outperforms our agent on large ER graphs. These observations may be explained by the fact that DQN-based methods se-
Figure 5: Approximation Ratio (less is better) of different methods averaged over all graphs in the respective dataset. The red line shows the AR compared to Tamaki solver with 30 minutes time bound.

The policy greedily, which can be incorrect if the distribution of the test data is different from the training data. In contrast, once a high-quality deterministic policy is found, the DQN-based method is more efficient than the Actor-Critic, which can learn a policy with a high proportion of stochastic behavior.

The results on the PACE2017 dataset, which we consider the most representative, are summarized in Table 2. We note that in addition to high accuracy comparing to greedy heuristics (both on average and in the worst cases) the RL-based heuristic has very competitive time-to-solution, which is important for solving NP problems. Furthermore, this time can be significantly decreased, as sampling can be trivially performed in parallel.

At last we would like to discuss the ways to improve our approach, as the agent still can rarely reach the accuracy of specialized algorithms. Recall that we formulated TD as a search for the optimal order of nodes. At each step the reward is closely related to the degree of the vertex, and hence the policy/value networks are guided to use local structure of the graph. In contrast, current state of the art algorithms for TD are based on finding vertex separators, which are global structures relating distant parts of the graph. We would speculate that the TD problem is hard in the ordering formulation. The reward we use, despite natural, provides a poor feedback to the RL algorithm during the search of the solution. Reformulation of the RL task may be a way to produce better heuristics.

Nevertheless, it is fascinating that a high-quality heuristic can be produced using a single graph, and that this heuristic agent can produce a near-optimal solution of a combinatorial problem in a fixed time.

4.7 Agent Decision Making

In this section, we will analyze the agent’s decision making process in order to get insights about the structure of the TD problem.

As mentioned earlier in all experiments, we use sampling to get candidate solutions and select the one with the best score. We use a small sample of 10 trajectories, which is a stronger result comparing to other works on neural-based heuristics, where samples of size 1000 are common [Kool et al., 2018]. The efficiency with small samples suggests that the agent learns a distribution that may be close to the "true" distribution of the solution.

Another evidence in support of the high quality of the learned distribution is the behavior of the agent on complete graphs. A fully connected graph with \(n\) nodes has treewidth \(n - 1\), and any elimination order on it is equivalent. The policy learned by our agent produces a uniform distribution on complete graphs (appeared during the elimination process), as shown.
in Figure 6. Also, we provide additional numerical experiments in Appendix B which clarify the distribution over remaining cliques in the agent decisions.

5 Related Works

In recent years several pioneering works concentrated on applying neural networks to learn heuristics for NP-hard problems due to the desire to get an approximate near-optimal algorithm without using domain-specific knowledge. Pointer Network (Vinyals et al., 2015) is the first neural-based sequence-to-sequence model applied in this context. The authors used attention over the input architecture to solve permutation-based combinatorial optimization problems, such as Euclidean TSP. Another work by Bello et al. (2016) improved the heuristics for TSP using the Actor-Critic (Konda, 2002) algorithm. A more recent article by Nazari et al. (2018) focuses on the Vehicle Routing Problem, which is also defined on the 2D Euclidean space, similar to TSP. Another approach for 2D TSP variants was proposed in Kool et al. (2018). The authors created a very efficient way to solve small TSP instances using modern techniques from machine translation, but their method is not very effective numerically as more than 1000 agent trajectories were sampled to find the solution.

The main drawback of previous approaches to 2D TSP is an explicit utilization of the Euclidean structure of the problem, which prevents the application of these techniques to other combinatorial problems on graphs. Recently Dai et al. (2016) proposed a graph embedding model that can be naturally applied to arbitrary graphs. In a subsequent paper Khalil et al. (2017) the authors used these embeddings to create an RL-based solution for Minimum Vertex Cover, Euclidean TSP and Maximum Cut problems and demonstrated that near-optimal solutions can be generated by the agent. Unfortunately, their graph embeddings should be trained on a large number of graphs, which can be computationally expensive. The method the authors used to train the agent is based on the DQN (Hasselt et al., 2016) and may produce a simple greedy result, which can be a drawback in some applications.

One of the best results in finding neural-based heuristics was presented by Li et al. (2018). Their approach is based on the combination of neural graph representation and a classical heuristic. The authors use GCN with a guided tree-search in a supervised setting. The only drawback of their method is the need for supervised learning for the embedding of the input graph i.e., the method requires a large number of solved NP problem instances for training. Summarizing previous works, it seems that efficient agent-based heuristics have to use a trainable graph embedding as a representation module necessarily.

6 Conclusion and Future Work

This paper presents the Tree Decomposition problem as a new task for representation learning. We propose a model, which can directly learn how to solve this combinatorial optimization problem using only a single graph for training. The training procedure also can be performed using a large set of graphs, but this work aims to show the generalization ability of a simple agent trained on a single graph. We show that a learnable heuristic can beat greedy, manually designed ones. Our method can generalize to large problem instances without significantly increasing the time-to-solution. We extensively verify the performance of the learnable heuristic using three datasets containing graphs with very different structures.

Our preliminary results suggest that this approach is a good starting point for learning heuristics on the graph-structured data. Beating specialized algorithms is a big challenge to our problem. We are planning to generalize our result to different NP problems which can be formulated in a sequential decision framework. Another perspective direction of research is a combination of RL based heuristics with local-search methods.
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A Reconstruction of the Tree Decomposition from an Ordering of Vertices

Here we provide a procedure to produce a tree decomposition of a graph \( G = (U, E) \) given an ordering of vertices \( \pi : U \rightarrow 1, \ldots, |U| \). An extensive presentation of the procedure with proofs can be found in [Blair & Peyton, 1991] and in [Bodlaender, 1994]. Here we merely list our variant of the algorithm for the reader’s reference.

We denote the neighborhood of node \( u \) by \( \mathcal{N}(u) \). We present here an algorithm that builds a tree decomposition in the breadth-first search fashion starting from the leaves of the tree. Given an ordering of vertices \( \pi \) of a graph \( G = (U, E) \), one can build its tree decomposition \( F = (B, T) \) with the following procedure: The algorithm runs an elimination procedure and builds a TD simultaneously. The neighborhoods of each node in the elimination order \( \pi \) are bags in the TD. Here we skip bags, which are subsets of their child bags.

The idea behind the algorithm is that parent bags in the tree emerge later in the elimination sequence than their children. If there is an intersection between two bags, then an edge has to exist in the tree. The algorithm keeps a queue of current leaf bags and checks the next bag against this list. If the parent of a leaf bag is found, the child is removed from the queue, and an edge is introduced in the tree graph \( F \).

B Entropy in agent decision

To get a better insight into the structure of the learned policy, we study the behavior of the entropy. At each step of the elimination trajectory, \( \pi \) the entropy of policy \( \Pi(u|s) \) is defined as:

\[
H(s) = - \sum_u \Pi(u|s) \log \Pi(u|s)
\]

As the size of the action space is not the same for different states in our problem, we define a normalized entropy:

\[
\hat{H}(s) = \frac{H(s)}{\log |U_s|}
\]  

Here \( |U_s| \) is the size of the action space for state \( s \).

We plot normalized entropies for several trajectories on different graphs in Figure 7.

A clear pattern is seen in the learned policies. The agent eliminates vertices in such a way that the largest clique appears at the end of the ordering. If the treewidth of the order found by the agent is \( k \), then the size of the largest clique in the elimination sequence is also \( k \). After this last clique is formed, the order of elimination is irrelevant (it does not increase the treewidth). This fact is reflected by the plateaus on the right side of the normalized entropy graphs (the normalized entropy of the uniform distribution is 1). Also, we can see in most cases the normalized entropy is far from zero. Consequently, there are multiple choices that lead to the orderings of the same treewidth according to the policy. We assume that the learned policy is close to the distribution of the solution, which is a plausible assumption considering low values of AR and a correct behavior of the agent on fully connected graphs.
Figure 7: Normalized entropy $\hat{H}(s)$ evaluated on every step of elimination procedure for four Erdős-Rényi’s graphs and four randomly sampled PACE2017 graphs (names of the graphs are provided in quotes). Every caption contains information about the AR for the first ordering sampled from the policy. $|U|$ is the number of nodes in the corresponding graph. The vertical red line shows the treewidth (the line intersects $x$ axis at $|U| - tw$).