Learning Lower Bounds for Graph Exploration With Reinforcement Learning

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Abstract

We explore the usage of reinforcement learning for theoretical computer science. Reinforcement learning has shown to find solutions in challenging domains such as Chess or Go. Theoretical problems, such as finding the worst possible input for an algorithm come with even more vast, combinatorial search spaces. In this paper, we look at the example of online graph exploration. Here we want to find graphs that yield a high competitive ratio for a greedy explorer. The search space consists of having every edge being either present or absent. Given there are quadratically many possible edges in a graph and each subset of edges is a possible solution, this yields unfeasibly large search spaces even for few nodes. We show experimentally how clever constraints can keep such search spaces manageable. As a result, we can learn graphs that resemble those known from literature and even improve them to yield higher competitive ratios.

1 Introduction

We have seen reinforcement learning achieve some remarkable results in recent years. Some of the remarkable results, in our opinion, show the ability to navigate search spaces for games such as Chess or Go [Silver et al., 2017], achieving superhuman performance. While these games have perfect information, the models evaluate positions deeply, which requires navigating a combinatorially exploding search space. At the same time, we have seen that machine learning finds solutions to classical difficult combinatorial problems such as the traveling salesman problem [Khalil et al., 2017] or the satisfiability problem [Selsam et al., 2019]. These papers show that machine learning is promising in finding solutions, even when we know the problems are difficult ($\mathcal{NP}$-hard) and come with large combinatorial spaces. In this paper, we turn this setting around. We look at a problem, that is not yet fully understood (graph exploration). For graph exploration, we want to more closely understand the limits of a particular solution (greedy exploration). To understand this better, let us first give a brief introduction to (online) graph exploration.

Online Graph Exploration. Online graph exploration is closely related to the traveling salesman problem (TSP). Both problems have an explorer that wants to visit all nodes in the graph while minimizing the edge traversals. In TSP, we are given the complete graph as input. On the other hand, graph exploration is an online algorithm. That means the input graph is gradually revealed as we walk around. At every point, the explorer only received information about the explored nodes and which nodes are adjacent to them (see Figure 1 for an example). The relevant metric for comparing the two problems is the *competitive ratio*. This ratio measures the ratio of the best possible online

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(a) Information in travelling salesman

(b) Information in graph exploration

Figure 1: Comparison of information for travelling salesman (left) and graph exploration (right). Dark nodes are explored, bright nodes part of the input. Non-colored nodes and dashed edges are not part of the input.

graph exploration algorithm versus the best possible offline graph exploration algorithm (i.e., a TSP solution). That is, how much more difficult the problem becomes by not having full information about the input from the very beginning.

From the perspective of competitive ratio, graph exploration is not yet well understood. On the one hand, we know that the competitive ratio is at least $\frac{10}{3}$ [Birx et al., 2020] which is a very recent improvement over the old lower bound of 2.5 [Dobrev et al., 2012]. This bound means that no matter the exploration algorithm, there exists a graph where the offline computed TSP tour will be shorter by a factor of at least $\frac{10}{3}$. The theoretical gap here is that we do not know how "correct" this factor is or even if this factor is independent of the number of nodes. For a particular approach to solve graph exploration, we know more: the greedy explorer is an intuitive, reasonable heuristic that always goes to the nearest unexplored node. For greedy we know, that its competitive ratio is indeed dependent on the graph size; the greedy explorer has a competitive ratio of $\Theta(\log n)$ [Hurkens and Woeginger, 2004].

Reinforcement Learning for Online Graph Exploration. In this paper, we take a closer look at this asymptotic bound, and we want to better understand this bound in terms of constant factors hidden inside the asymptotic notation. In this paper, we focus our analysis on unweighted undirected graphs. Hurkens and Woeginger [2004] show a construction yielding a competitive ratio of $\frac{1}{4}(3 + \log n)$. We explore if we can improve this lower bound using reinforcement learning. Doing this, we want to advance the research to find the still unknown worst competitive ratio for the greedy explorer in non-asymptotic terms. Note that for a graph with n nodes, there are $\frac{n\cdot(n+1)}{2}$ many possible edges, each of which can be independently present or not. Thus, the search space is in the order of $2^{\Theta(n^2)}$ and explodes even for small values of n, while the solutions constitute a small part of this space only. Thus, we present heuristics to keep this search space manageable. Indeed, experiments show that we can discover structures such as those in Hurkens and Woeginger [2004] and modify them to reach larger competitive ratios. We found that without these heuristics, models fail to learn good solutions and converge before sufficient exploration of the space.

2 Related Work

Reinforcement Learning for Combinatorial Problems. Previous work has used machine learning, and in particular reinforcement learning, to provide good solutions for several combinatorial and NP-hard problems [Khalil et al., 2017, Vinyals et al., 2015, Bello et al., 2017, Selsam et al., 2019, Amizadeh et al., 2019]. In these works, the authors give a well-understood problem class and use machine learning to solve instances of these problems. The other way around, Sato et al. [2019] want to learn a generative model that constructs difficult problem instances of a difficult problem class. Our work is more in the second spirit, we learn instances that are expensive for a given algorithm (the greedy explorer) to solve.

Algorithm Inference with Machine Learning. In the related field of algorithm inference, learning-based methods infer algorithmic structures from input-output examples and execution traces. The learning is enhanced with new architectures [Kaiser and Sutskever, 2016, Freivalds and Liepins, 2017, Neelakantan et al., 2016, Velickovic et al., 2020], differentiable storage components [Graves et al., 2014, 2016, Grefenstette et al., 2015, Zaremba and Sutskever, 2016], composition of smaller sub-programms [Reed and de Freitas, 2016, Zaremba et al., 2016], recursion Cai et al. [2017], or

logic reasoning [Evans and Grefenstette, 2018, Dong et al., 2019]. The case of this paper instead is to learn more about the limitations of a known, given algorithm.

3 The Reinforcement Learning Model

We learn a construction agent (constructer) to create a graph with a maximal competitive ratio against an exploring agent (explorer). Principally, the constructer plays the explorer in rounds in a problem-setter versus problem-solver framework. The constructer is given the current position (a node) of the explorer and decides how to connect this node to the rest of the graph. Then, the explorer decides which node to visit next. In our scenario of the greedy explorer, it computes the distances to all nodes that are adjacent to at least one explored node and moves to the closest one. In the case of ties — that might happen since we look at unweighted graphs — the explorer tiebreaks to the node with a lower node ID. After moving to this node, the constructer takes another turn to connect this node, ... until all nodes have been explored.

State Space. We design the state space to provide "full" observability, where full refers to all the available information of the graph reinforcement learning framework. For this, the constructer receives three inputs:

- The ID of the currently explored node given as a one-hot vector
- A binary vector denoting which nodes have already been explored
- The adjacency matrix of the graph up to this point. In the scope of this paper, we look at undirected graphs so it suffices to only give the upper triangle of the adjacency matrix

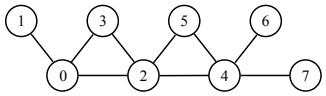
Action Space. The action space are n binary decision variables. Per action each of these variables decides whether to add an edge or not. Concretely, if the explorer currently is on node c, the i-th variable decides if we add the edge $\{c, i\}$ to the graph. We ignore self edges ($c = i$) and edges that we already decided on before (if i is already explored). This is because we tackle undirected, that is symmetric, graphs.

Managing the state space dimensionality. Even with uniform weights and undirected edges, there are $\frac{n\cdot(n-1)}{2}$ possible edges. Each subset of those edges is a valid solution, giving the constructer a total of $2^{\frac{n\cdot(n-1)}{2}}$ possible graphs to search. Exploring this state-space becomes very quickly infeasible, even for moderately small numbers of nodes. Thus, we employ heuristic constraints on the state space. Let us consider the initial situation, where the constructer connects node 0 to other nodes. Principally, the exact nodes to connect to are less important than the number of nodes. All different combinations of a certain number of edges lead to isomorphic graphs that largely behave the same (apart maybe from some cases of tiebreaking). However, the constructer is oblivious to this isomorphism and has to learn the properties of every graph individually. For adding k edges, there are $\binom{n\cdot(n-1)/2}{k}$ many possibilities. We propose to choose one canonical representative for this set of graphs that we use consistently instead. This collapses all permutations to just one, giving an *exponential* speedup in the search space — *per round*.

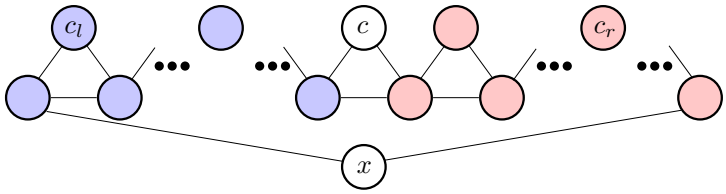
Concretely, let V be the set of nodes in the graph. We can partition V into 3 sets: the set E of all nodes that have been explored, the set B of all nodes adjacent to nodes in E, and the set of remaining nodes U. Nodes in U are those that the explorer does not know about, yet. This is the property we exploit. We add a new output to the action space that decides how many edges in U the newly explored node is connected to. Then we pick this number of nodes in U canonically — in this paper we take the lowest numbered nodes from U. We ignore all decision variables for nodes in U.

4 Experimental Investigation

We investigate the efficacy of this state-space model, action space model, and search space heuristic by experimental tests. In particular, we want to investigate if our constructer can find graphs that match or surpass the competitive ratio of known theoretical constructions. We experiment with different graphs sizes $n = 2^i$ for different i. We follow the known constructions, such as Hurkens and Woeginger [2004] that use graphs with where the number of nodes is a power of two. We learn



(a) Example triangle structure found by the constructer.



(b) Recursive triangle structure. Two smaller structures (left in blue, right in red) are merged through node c. Node x connects the left and right ends.

the neural networks and outputs with proximal policy optimization [Schulman et al., 2017]. One episode is a full exploration cycle when the explorer visited every node for which we give a reward of the achieved competitive ratio minus 1 (ratio 1 means the online algorithm was just as good as the offline algorithm). In total, we train constructers for 500.000 decisions, which gives a differing amount of episodes depending on the graph size.

We found that graph construction using the vanilla architecture without the heuristic search space constraints does not allow us to find graphs with a high competitive ratio, apart from very small graphs with $n = 8$ nodes. Without much influence from hyperparameters, the models converge before they start finding good solutions. We had some success with increasing the exploration-exploitation tradeoff parameter but this comes with *much* higher (exponentially more) computational cost. Thanks to the heuristic, we can cut down this search space to find good solutions also for larger graphs. In general, the graphs we find this way follow a triangle structure similar to Figure 2a. This structure resembles the construction from Hurkens and Woeginger [2004].

Triangle Improvements In the second line of experiments, we tried if we can improve on the construction of Hurkens and Woeginger [2004]. They employ a recursive structure. The base graph is a triangle with three nodes. Upper levels are constructed by combining two lower-level structures and merging them to a long chain of triangles, adding a new center node. They also add a node x to connect the leftmost and rightmost nodes. Refer to Figure 2b for a visualization.

In this set of experiments we run the constructer but mask the edges from Hurkens and Woeginger [2004] to 1, such that at least these edges are always present. This structure imposes a strong bias on the constructions for the constructer, so we do not employ our heuristic as well. We find that our constructer learns to improve on the provided structure systematically.

The idea lies in misleading the greedy explorer to finish the exploration. Consider the situation when the explorer already explored both recursive structures, thus is at node c_r. Now there are three steps left to do: explore c and x in any order and return to the starting node l. In the construction of Hurkens and Woeginger [2004], the explorer will first explore c, then x, then return to l. The reinforcement learning agent learns that exploring x first and then c is better because now it costs $\frac{n}{4}$ to move back to l in the end, instead of 1 if c was explored first. In the original construction, the nodes x and c are equidistant, so the agent learns to create a "shortcut" in the right half. This shortcut connects two nodes that are two hops away directly. Now x is closer to c_r, and greedy explores there first. On the other hand, this shortcut might also compromise earlier exploration; however, we found that shortcuts that provide just this intended effect exist. With this approach we are able to improve the known competitive ratio from $\frac{1}{4}(3 + \log n)$ to $\frac{1}{4}(4 + \log n) - \frac{3}{n}$.

5 Conclusions and Outlook

We see many interesting avenues to continue this line of research. On the one hand, much remains unexplored in terms of online graph exploration. Future work could look at training constructers against other exploration algorithms than greedy. For example, blocking [Kalyanasundaram and Pruhs, 1994, Megow et al., 2012] is a proposed algorithm that is supposed to perform better than the greedy explorer. One more alternative would be to realize the explorer through another reinforcement learning agent and learn both constructers and explorers with self-play. Last, we saw that the constructer had difficulties catching recursive structures, this might be a promising area to explore further modeling approaches that come with recursive inductive biases.

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