Reinforcement Learning for Combinatorial Optimization: A Survey

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Abstract
Combinatorial optimization (CO) is the workhorse of numerous important applications in operations research, engineering and other fields and, thus, has been attracting enormous attention from the research community for over a century. Many efficient solutions to common problems involve using hand-crafted heuristics to sequentially construct a solution. Therefore, it is intriguing to see how a combinatorial optimization problem can be formulated as a sequential decision making process and whether efficient heuristics can be implicitly learned by a reinforcement learning agent to find a solution. This survey explores the synergy between CO and reinforcement learning (RL) framework, which can become a promising direction for solving combinatorial problems.

1 Introduction
Optimization problems are concerned with finding the best configuration or "value" among different possibilities and they naturally fall into one of the two buckets: configurations with continuous and with discrete variables. For example, finding a solution to a convex programming problem is a continuous optimization problem, while finding the shortest path among all paths in a graph is a discrete optimization problem. Sometimes the line between the two can not be drawn that easily. For example, the linear programming task in the continuous space can be regarded as a discrete combinatorial problem because its solution lies in a finite set of vertices of the convex polytope as it has been demonstrated by Dantzig’s algorithm. Conventionally, optimization problems in the discrete space are called combinatorial optimization (CO) problems and, typically, have different types of solutions comparing to the ones in the continuous space. One can formulate CO problem as follows:

**Definition 1.** Let $S$ be a set of elements and $f : S \rightarrow \mathbb{R}$ is a cost function. **Combinatorial optimization problem** aims to find optimal value of the function $f$ and any corresponding optimal element that achieves that optimal value on the domain $S$.

Typically the set $S$ is finite, in which case there is a global optimum, and a trivial solution exists for any CO problem by comparing values of all elements $s \in S$. Note that the definition 1 also includes the case of decision problems, when the solution is binary (or, more generally, multi-class), by associating a higher cost for the wrong answer than for the right one.

One common example of a combinatorial problem is a Travelling Salesman Problem (TSP). The goal is to provide the shortest route that visits each vertex and returns to the initial endpoint, or, in other words, to find a Hamiltonian circuit $H$ with minimal length in a fully-connected weighted graph. In this case, a set of elements is defined by all Hamiltonian circuits, i.e. $S = \{ \text{all Hamiltonian paths} \}$, and the cost associated with each Hamiltonian circuit is the sum of the edges on the circuit, i.e. $f(H) = \sum_{e \in E} w(e)$. Another example of CO problem is Mixed-Integer Linear Program (MILP), for which the objective is to minimize $c^\top x$ for a given vector $c \in \mathbb{R}^d$ such that the vector $x \in \mathbb{Z}^d$ satisfies the constraints $Ax \leq b$ for the parameters $A$ and $b$.

We note that CO is a popular type of combinatorial problem but not the only one. Other kinds of combinatorial problems include generation problems, the main goal of which is to find all elements in the set $S$ that possess some property and enumeration problems that focus on computing the total number of elements of a particular type. For example, finding all possible graph automorphisms, i.e. isomorphism of a graph on itself, is a generation problem, while finding the cardinality of the automorphism group is an enumeration problem. Solving these problems often requires some group-theoretic algorithms, which differ in the nature of the proposed solutions, so we focus only on combinatorial optimization problems in this work.

The primary scope of this survey is the reinforcement learning methods designed for the CO problems. In RL, an agent acts on an environment through Markov Decision Process (MDP), collecting rewards and updating its future actions. The environment consists of some states forming the state set $S$, which could be either discrete or continuous. For example, a state $s \in S$ can be described as the position of the agent in some labyrinth (discrete) or the torque that should be applied to the motor (continuous). The actions that agents can perform create the action space $A$, and the main goal of the agent is to increase the reward $R$ it gets for executing these actions. The probabilities of rewards for each of the possi-
allowable actions are provided by some policy, which is a function depending on the state, usually denoted as \( \pi(s) \). Hence, it is natural to state that to solve an MDP means to find the optimal policy \( \pi^* \), which maximizes the expected rewards, when following this particular policy:

\[
\pi^* = \arg\max_\pi \mathbb{E}[R|\pi],
\]

where the reward can be expressed as \( R = \sum_{t=0}^{N-1} \gamma^t r_{t+1} \) in the case when the agent interacts with the environment in an episodic manner, i.e. the environment’s state is restarted after some number of steps \( N \); or as \( R = \sum_{t=0}^{\infty} \gamma^t r_{t+1} \) in the case of non-episodic MDP, where the agent has the potential to go on forever. In general, \( \gamma \) encourages the agent to pay more attention to the short-term rewards, however, in the last case the discount factor \( \gamma \), which satisfies \( \gamma < 1 \), prevents the accumulated reward from approaching infinity.

RL methods have been integrated with CO via two different paradigms: principal and joint learning. In principal learning, an agent directly takes the decision that constitutes a part or the complete solution of the problem and does not have the feedback from the off-the-shelf solver. For example, in the TSP problem, the agent can be parameterized by a neural network that incrementally builds a path from a set of vertices and then receives the reward in the form of the length of the constructed path, which is used to update the policy of the agent. Another approach is to learn the RL agent in the joint training with already existing solvers, so that it can improve some of the metrics for a particular problem. For example, in MILP problems a commonly used approach is the Branch & Bound method, which at every step selects a branching rule on the node of the tree. This can have a significant impact on the overall size of the tree and, hence, the running time of the algorithm. A branching rule is a heuristic that typically requires either some domain expertise or a hyperparameter tuning procedure. However, given a dataset of already solved instances of the problem, a parameterized RL agent can learn to imitate the policy of node selection that in turn reduces the running time.

Our work is motivated by the recent success in the application of the techniques and methods of the RL field to solve CO problems. Although there are many practical combinatorial optimization problems that can be, in principle, solved by reinforcement learning algorithms, and relevant literature exists in the operations research community, we will focus on machine learning perspective to the problem. This survey covers the most recent papers on the topic that show how reinforcement learning algorithms can be applied to formulate and solve some of the canonical optimization problems, such as Travelling Salesman Problem (TSP), Vehicle Routing Problem (VRP), Graph Coloring Problem, Maximum Independent Set Problem, Bin Packing Problem, Knapsack Problem, and several others.

Despite the promising results demonstrated recently, the appeal of the proposed solutions is largely unknown to the audience of mathematicians and ML practitioners. Our goal is to provide the researchers with an overview of the major results achieved in this area during the course of the last five years. While there are other surveys [Bengio et al., 2018, Lombardi and Milano, 2018] that mention this particular topic, in this work we aim to deep-dive into RL methods that have demonstrated superior quality for popular CO problems. We, therefore, hope that this timely review can facilitate further research in this field.

| Approach | Problems | Example works |
|----------|----------|---------------|
| Value    | MIS      | [Cappart et al., 2019] |
|          | MC       | [Cappart et al., 2019] |
|          | MCS      | [Bai et al., 2020] |
|          | MVC      | [Song et al., 2019] |
| Policy   | TSP      | [Kool et al., 2018, Ma et al., 2019] |
|          | KP       | [Bello et al., 2016] |
|          | VRP      | [Nazari et al., 2018] |
|          | 3DBP     | [Hu et al., 2017, Duan et al., 2018] |
| MCTS     | 3DBP     | [Laterre et al., 2018] |
|          | GC       | [Huang et al., 2019] |
|          | MIS      | [Abe et al., 2019] |

Table 1: Categorization of the main approaches (Value-based, Policy-based, MCTS) used for solving CO problems with RL. Problems include Maximum Independent Set (MIS), Maximum Coverage (MC), Maximum Common Subgraph (MCS), Minimum Vertex Cover (MVC), Traveling Salesman Problem (TSP), Knapsack Problem (KP), Vehicle Routing Problem (VRP), 3D Bin Packing Problem (3DBP), Graph Coloring (GC). For brevity we omit some of the problems and works, which we describe in detail in the remainder of the paper.

The survey is split into three parts - each covers a particular type of RL methods applied to solve CO problems. Among different approaches, we distinguish value-based, policy-based, and Monte Carlo Tree Search methods, which are shown in Table 1. For each method, we first provide a theoretical explanation that describes the main definitions and ideas, followed by the applications of each method to the specific CO problems. We conclude the survey by providing some future directions in Section 5.

## 2 Value-based methods

The focus of value-based reinforcement learning methods is finding an optimal policy by obtaining an optimal value function \( V^*(s) \) or action-value function \( Q^*(s, a) \).

### 2.1 Theoretical explanation

In the context of an MDP, the value function of a state following some particular policy is the expected set of discounted rewards of the sequence of states induced by that policy:

\[
V^*(s) = \mathbb{E} \left[ \sum_{t=0}^{\infty} \gamma^t R(s_t) | \pi, s_0 = s \right].
\]

Value function allows us to evaluate how promising, in terms of future rewards, is being in some state and following some specific policy in the long run.
At the same time, we can think of the reward and the value function as the functions depending not only on the state but also on the action. This way, we can introduce the state-action value function $Q(s, a)$. It can also be seen that $V(s)$ can be interpreted in terms of the state-action value function as:

$$V^\pi(s) = \max_a Q(s, a).$$

Consequently, the $Q$-function can also be rewritten in a more general form:

$$Q^\pi(s, a) = \mathbb{E}_\pi \left[ \sum_{t=0}^{\infty} \gamma^t R(s_t, a_t) | s_0 = s, a_0 = a \right].$$

It is clear, that the optimality of the state-action function, as well as the state-value function, is closely connected to the optimality of the policy. The state-action value function of an MDP is called optimal if it is the maximum of state-action value functions across all policies:

$$Q^*(s, a) = \max_\pi Q^\pi(s, a), \forall s \in S, \forall a \in A.$$  

One of the fundamental equations used for solving MDPs is called the Bellman equation [Bellman, 1952] and has the following form:

$$Q^\pi(s, a) = R(s, a) + \gamma \sum_{s'} T(s, a, s') \max_{a'} Q^\pi(s', a'),$$

where $T(s, a, s')$ is the transition function, representing the probability of transitioning from $s$ to $s'$ while performing $a$.

To iteratively find the solution to the Bellman equation, when the transition function is not known, we can use the TD(0) update rule [Sutton, 1988]. It has been shown that performed on the finite data and repeated infinite number of times, the TD(0) rule will allow to approximate the maximum likelihood estimate of the optimal state-value function. Based on this fact there can be derived an algorithm known as Q-learning [Watkins and Dayan, 1992].

Q-learning is a very powerful algorithm for solving MDP tasks. However, we can imagine that for real-world problems many tasks are much harder to solve, especially when the state and action spaces are continuous or too big to cover. Consequently, sometimes it can be more convenient to approximate the $Q$-function directly.

With the rise of Deep Learning, neural networks have proven to achieve state-of-the-art results on various datasets by learning useful function approximations through the high-dimensional inputs. This led researchers to explore the potential of neural network approximations of the $Q$-functions resulting in the emergence of one of the fundamental articles [Mnih et al., 2015] on Deep Q-network (DQN). DQN, being a convolutional neural network defined by the parameters $\theta$, can learn the policies directly using end-to-end reinforcement learning. The network outputs the approximate $Q$-values for each action depending on the current input state.

To train the Q-network, the authors, firstly, have addressed the instability and divergence problems that are common for many RL tasks. One of the solutions they have implemented is the experience replay technique. The main idea behind it is to collect and store $(s, a, r, s')$ trajectories in some replay memory set $D$. The second technique for stabilizing the training is used when constructing the loss function, which has the following form:

$$L(\theta_i) = \mathbb{E}_{(s, a, r, s') \sim D} \left[ (r + \gamma \max_{a'} Q_{\theta^-}(s', a') - Q_{\theta^i}(s, a))^2 \right].$$

(1)

Here we would like to minimize the mean-squared error between the current approximation of the $Q$-function and some maximized target value $r + \gamma \max_{a'} Q_{\theta^-}(s', a')$. It is worth noting that $\theta$ and $\theta^-$ are two different sets of neural network’s weights: the second set of parameters $\theta^-$ is achieved by cloning the current neural network every $C$ steps. This makes training more stable by creating a delay between the target update $Q_{\theta^-}(s', a')$ and the update to the current learnable approximation $Q_\theta(s', a')$.

As it has been said before, this work on DQN has given rise to the whole field of Deep Reinforcement Learning methods, being a state-of-the-art approach on the Atari benchmark. Consequently, there followed numerous articles on the improvement of the initially proposed DQN algorithm, which have achieved even better stability, generalization and benchmark results. These works, however, are not covered in this survey.

### 2.2 Value-based methods for Combinatorial Optimization

DQN is one of the most popular methods for solving many reinforcement learning problems. This claim is also true for a wide variety of combinatorial optimization tasks. In particular, some fundamental problems covered in this section, which have been solved specifically by DQN are the Maximum Cut [Barrett et al., 2019], Minimum Vertex Cover [Khalil et al., 2017, Song et al., 2019], Traveling Salesman [Khalil et al., 2017]. Set Covering Problem [Khalil et al., 2017], Maximum Independent Set [Cappart et al., 2019] and Maximum Common Subgraph [Bai et al., 2020].

The common strategy of finding an optimal solution to the CO task used in the majority of the mentioned works is the principal learning. However, there is another approach to solving combinatorial optimization problems, which has been introduced by [Cappart et al., 2019], where an RL algorithm is used to find the optimal ordering of the variables in a Decision Diagram (DD), in order to tighten the relaxation bounds for the Maximum Independent Set Problem and the Maximum Cut Problem. Authors also showed that using reinforcement learning for a restricted DD formulation allows finding the good heuristic solutions to the mentioned problems.

In terms of the RL approach used in the cited works above, we can make one big generalization — they all use Q-learning to find the optimal solutions to the stated problems. However, every article carries out some specific modifications either to the Q-learning algorithm itself, or to the graph network representation, or in the case of [Barrett et al., 2019, Bai et al., 2020] to both.

As for the more classical formulations of the Q-learning algorithm, we can refer to the articles by
method. The authors create the linear programming approach solved by the branch & bound construct sequential policies for the CO tasks. The arti-

tuitively similar to the Imitation Learning, in which the two

While the mentioned articles use the same algorithmic approaches, they still aim to solve different problems. Hence, the main difference between the articles is the state, action and reward representation. In the case of [Khalil et al., 2017], the state is a p-dimensional graph embedding vector, for the current sequence of nodes at the time step \( t \), while the action is picking another node, which has not been used at the current state. The reward is defined as the difference in the cost functions after transitioning from the state \( s \) to the state \( s' \) when taking some action \( a: r(s,a) = c(h(s'), G) − c(h(s), G) \), where \( h \) is the graph embedding function, \( G \) is the whole graph, \( c \) is the cost function.

In the work by [Cappart et al., 2019] the state \( s \) is a tuple \((s_L, s_B)\), where \( s_L \) is the ordered sequence of variables and \( s_B \) is the DD constructed on \( s_L \). The action, in this case, is picking a not yet chosen variable, and the reward is calculated based on the change of the upper and lower bounds after adding a variable to the decision graph. The lower and upper bounds are associated with the longest path of the partially constructed DD and, consequently, the reward for both cases can be represented as the difference in the longest path’s length. For the upper bound case, this reward is penalized, so that not to increase it, and the gain in the lower bound is on the contrary positively rewarded.

Lastly, the article by [Bai et al., 2020] is focused on solving the Maximum Common Subgraph problem, hence the authors construct a novel graph embedding network called Joint Subgraph-Node (JSNE), in order to use just one network to embed two graphs in a meaningful way. The updates to the weights of the network are performed according to the same approach as in [Mnih et al., 2015].

However, these three works meet the same problems as [Mnih et al., 2015], namely, constructing the optimal solution recursively does not allow the algorithm to reconsider the previous decisions leading to the suboptimal solutions. To deal with these problems, authors of [Barrett et al., 2019], [Song et al., 2019] have added some alterations to the common neural Q-learning method.

Namely, [Song et al., 2019] uses the co-training approach, which has gained popularity in the classification domain, to construct sequential policies for the CO tasks. The article describes the two policy-learning strategies for the minimum vertex cover problem: the first strategy copies the one described in [Khalil et al., 2017], i.e. S2V with neural Q-learning from [Mnih et al., 2015], the second is the integer linear programming approach solved by the branch & bound method. The authors create the CoPTEr algorithm that is intuitively similar to the Imitation Learning, in which the two strategies induce two policies, estimate them to figure out which one is better, exchange the information between them and, finally, make the update.

ECO-DQN [Barrett et al., 2019] directly targets the task of the better state-space exploration and the scalability of the learned Q-function. To achieve that, they propose a special training framework different from the one in [Khalil et al., 2017], i.e. it does not learn a part of the solution one step at a time. Instead, at the beginning of each episode, some solution is randomly instantiated, and the agent is allowed to “flip” its vertices. The reward, specifically constructed to motivate exploration, does not penalize the agent for performing actions, which will not increase the current reward. On the contrary, the algorithm provides a small reward of \( \frac{1}{\text{number of vertices}} \), when an agent finds some locally optimal solution, which has not been yet explored. The graph embedding network used by the authors is the Message Passing Neural Network [Gilmer et al., 2017], the weights of which, in the same manner as in the previous articles, parameterize the Q-function.

## 3 Policy-based methods

The main goal of policy-based methods of reinforcement learning algorithms is to find optimal behavioral strategy by directly optimizing a policy represented by some parametric function \( \pi_\theta(a|s) \).

### 3.1 Theoretical explanation

The optimization objective is formulated as follows:

\[
J(\theta) = \mathbb{E}_{\pi_\theta} \left[ \sum_{t=0}^{\infty} \gamma^t R(s_t)|s_0 = s \right].
\]

where \( R \) is a reward and \( \gamma \) is a discount factor, \( 0 \leq \gamma \leq 1 \).

The policy gradient theorem proves that the gradients of the aforementioned objective with respect to the policy parameters \( \theta \) can be obtained by:

\[
\nabla_\theta J(\theta) = \mathbb{E}_{\pi_\theta} \left[ Q^\pi_{\pi_\theta}(s,a) \nabla_\theta \ln \pi_\theta(a|s) \right].
\]

In order to calculate the gradients of the objective function, REINFORCE algorithm has been proposed [Williams, 1992].

The main idea of this method is to get the estimation of the state-action value function \( Q^\pi(s,a) \) using Monte Carlo rollouts. The calculated estimates of these gradients can then be used to improve \( \pi_\theta(a|s) \) by applying the gradient descent optimization algorithms.

A commonly used extension of REINFORCE algorithm subtracts a baseline value \( b(s) \) from Monte Carlo estimates of \( Q^\pi(s,a) \), in order to reduce variance of gradient estimates of the objective without changing its bias:

\[
\nabla_\theta J(\theta) = \mathbb{E}_{\pi_\theta} \left[ (Q^\pi_{\pi_\theta}(s,a) − b(s)) \nabla_\theta \ln \pi_\theta(a|s) \right].
\]

For example, one common variation of REINFORCE uses the estimation of the parametric state value function \( V_\pi(s) \), which is optimized by the return obtained with Monte Carlo rollouts.

The family of Actor-Critic (A2C, A3C) algorithms further extend REINFORCE with baseline by using bootstrapping — updating the state-value estimates from the values of
subsequent states. Although this approach introduces bias to the gradient estimates, it often reduces variance even further. Moreover, the actor-critic methods can be applied to online and continual learning, as they no longer rely on Monte Carlo rollouts.

Further development of this group of reinforcement learning algorithms has resulted in the appearance of several more advanced methods such as PPO [Schulman et al., 2017] or DDPG [Lillicrap et al., 2015], a detailed explanation of which lays out of the scope of this work.

In addition to the policy-based methods discussed in this section, we also would like to pay some attention to a conceptually different way of approaching an RL problem, which is Hierarchical Reinforcement Learning. Most of the families of RL methods described in this survey have one specific flaw — to find a good policy, the algorithm requires a huge amount of training iterations, which is proportional to the complexity of the task. The main idea behind Hierarchical RL that takes further inspiration from behavioral biology, is to group some sequences of primitive actions into one single macro-action. In Deep Reinforcement Learning, to facilitate this kind of action abstraction, most of the algorithms create a “manager-learner” framework. This framework usually consists of one top-level policy, which is trained to choose from the set of several sub-policies, which, in turn, are trained to achieve some specific subgoals. The representation of the primary goals and primitive subgoals can also vary, from [Sukhbaatar et al., 2018, Rafati and Noelle, 2019] to the handcrafted ones [Bacon et al., 2017], such as the particular intermediate states of the environment, for example. All in all, for some specific tasks Hierarchical RL helps to significantly reduce the action space as well as the number of training iterations and increase generalization.

3.2 Policy-based methods for Combinatorial Optimization

One of the first attempts to apply policy gradient algorithms to combinatorial optimization problems has been made by [Bello et al., 2016] to solve TSP and Knapsack problems using REINFORCE algorithm with learned baseline. Here, pointer network architecture proposed by [Vinyals et al., 2015] is used to encode the input sequence. The solution is constructed sequentially from a distribution over the input using the pointer mechanism of the decoder, and trained in parallel asynchronously similar to [Mnih et al., 2016]. Moreover, several inference strategies are proposed to construct a solution — along with greedy decoding and sampling. Active Search approach is suggested. Active Search allows learning the solution for the single test problem instance, either starting from a trained or untrained model.

The approach suggested by [Bello et al., 2016] can not be applied directly to solve Vehicle Routing Problem due to its dynamic nature, i.e. the demand in the node becoming zero once the node has been visited. [Nazari et al., 2018] extend the previous methods used for solving TSP to circumvent this problem and find the solutions to VRP and its stochastic variant. Specifically, they simplify the encoder by replacing the LSTM unit with the 1-d convolutional embedding layers, so that the model is invariant to the input sequence order, consequently, being able to handle the dynamic state change. The policy learning is then performed by using REINFORCE algorithm for TSP and VRP while using A3C ([Mnih et al., 2016]) for stochastic VRP.

[Deudon et al., 2018] solve TSP by modifying the approach of [Bello et al., 2016] with the enhanced encoder-decoder architecture. Specifically, instead of including LSTM units, this architecture is based solely on the attention mechanisms so that the input is encoded as a set and not as a sequence. Additionally, the authors have looked into combining a solution provided by the reinforcement learning agent with the 2-opt heuristic [Croes, 1958], in order to further improve the inference results.

Parallel to [Deudon et al., 2018], an approach to solve TSP, two variants of VRP (Capacitated VRP and Split Delivery VRP), Orienteering Problem (OP), Prize Collecting TSP (PCTSP) and Stochastic PCTSP (SPCTSP) has been proposed by [Kool et al., 2018]. In this work, the authors have implemented similar encoder-decoder architecture and used a simple rollout baseline instead of the learned critic one.

Another important CO problem — 3D Bin Packing — has been tackled by [Hu et al., 2017] in a manner similar to [Bello et al., 2016]. They have utilized reinforcement learning to produce the policy, which represents an optimal packing order of items. The algorithm is trained on the features of the provided sequence of incoming items, while the resulting policy is evaluated by calculating the values of the surface area of packed items. As the baseline, authors propose to use the surface area of a packing plan, which is generated by a heuristic algorithm. For inference, greedy decoding as well as sampling with beam search are used. Further work of [Duan et al., 2018] extends this approach to learning orientations along with sequence order of items by combining reinforcement and supervised learning.

A work by [Chen and Tian, 2018] proposes a different take on solving VRP, expression simplification and online job scheduling problems by iteratively improving the existing solution. The algorithm rewrites the different parts of the solution until convergence instead of constructing the solution in the sequential order. The state space is represented as a set of all solutions to the problem, while the action set consists of regions and their corresponding rewriting rules. The authors use an LSTM encoder, specific to each of the covered problems and train region-picking and rule-picking policies jointly by applying Q-Actor-Critic algorithm.

In order to learn to build a complete solution instead of constructing it sequentially, one specific approach has been proposed by [Emami and Ranka, 2018]. The authors have designed the policy gradient method, Sinkhorn Policy Gradient (SPG), specifically for the class of combinatorial optimization problems involving permutations. The action space, in this case, is a set of permutation matrices. Using a special Sinkhorn layer to produce continuous and differentiable relaxations of permutation matrices, authors were able to train actor-critic algorithms similar to Deep Deterministic Policy Gradient (DDPG) [Lillicrap et al., 2015] and produce competitive solutions to Maximum Weight Matching Problem, Euclidian TSP and Integer Sorting Problem.
Another approach to solving the variant of TSP with time windows has been suggested by [Ma et al., 2019], which solves the constrained Travelling Salesman Problem. The main idea of this work is to use a layered hierarchical RL framework inspired by [Haarnoja et al., 2018], in which there are several layers, each representing policies of different complexity: from the lowest - making the solution satisfy the problem’s constraints, to the highest, which is responsible for finding the solution to the original TSP optimization problem. This behavior of different layers of policies is made possible by the manually designed layer-specific reward functions and tied together by sharing the latent vectors \( h_i^{(k)} \). In principle, latent vector is outputted by the policy of some layer \( k \) and used as the additional condition for sampling an action from the policy of the next layer \( k + 1 \). To find the optimal policies of each layer, the authors use REINFORCE with their own central self-critic baseline, which is similar to the self-critic baseline [Rennie et al., 2017] and the rollout baseline in [Kool et al., 2018].

4 Neural Monte Carlo Tree Search with Self-play

Recently, algorithms combining deep neural networks with the tree search and self-play mechanisms showed great success in two-player games. In particular, AlphaZero and Expert Iteration have achieved super-human performance in games like chess, shogi, go and hex, learning exclusively through self-play. Moreover, the most recent algorithm, MuZero [Schrittwieser et al., 2019], was able to achieve super-human performance by extending previous approaches using the learned dynamics model in challenging visually complex domains, such as Atari games, go and shogi without the knowledge of game rules.

4.1 Theoretical explanation

We refer to this class of algorithms as Neural Monte Carlo Tree Search with Self-Play. The algorithm alternates between simulation and play phases. Simulation follows general procedure of Monte Carlo Tree Search (MCTS) [Browne et al., 2012] consisting of selection, expansion, rollout and backup steps. However, instead of evaluating leaf nodes in a tree by making a roll-out step, a neural network with parameters \( \theta \) is used to provide policy \( p_{\theta}(s) \) and state value estimates \( v_{\theta}(s) \) for the new state in the game. Then the usual backup step is used to get the improved policy \( \pi(s) \) to be used in the play phase. Alternation of phases is performed until the end of the game: the improved policies obtained by MCTS as well as the game’s results are used to train the neural network, which aims to improve the estimates of the state-value and policy functions, which, in turn, are used for MCTS in the subsequent episodes. Using a neural network to “guide” MCTS reduces the complexity of the algorithm, and integrating self-play provides a natural learning curriculum.

4.2 Neural MCTS with Self-play for Combinatorial Optimization

A combination of learnable policy and value function along with MCTS and self-play has been adopted in [Laterre et al., 2018]. In order to solve 2D and 3D Bin Packing Problems formulated as single-player games, Neural MCTS constructs the optimal solution with the addition of ranked rewards mechanism that reshapes the rewards according to relative performance in the recent games. This mechanism aims to provide a natural curriculum for a single agent similar to the natural adversary in two-player games.

In a similar fashion, [Xu and Lieberherr, 2019] have introduced a different approach to solving combinatorial optimization problems by converting them into Zermelo Games. Neural MCTS with Self-play is used to learn the winning strategy that can be interpreted as the solution of a specific instance of the original combinatorial problem.

[Huang et al., 2019] have used a similar approach to solve Graph Coloring Problem for large graphs by adding efficient policy and value function neural network architecture called FastColorNet. In addition, they have used some techniques to reduce MCTS to a limited number of moves to handle learning on graphs with millions of vertices.

Similarly, [Abe et al., 2019] has proposed to use Graph Neural Network, namely Graph Isomorphism Network (GIN), to account for variable size of the state representation in a search tree and to modify AlphaGoZero algorithm by normalizing the value function. These techniques were used to solve Maximum Independent Set Problem and other NP-hard problems on graphs.

5 Conclusion and future directions

Previous sections discussed several approaches to solving canonical combinatorial optimization problems by utilizing reinforcement learning algorithms. This field is rapidly developing, and we are expecting new algorithms and approaches to emerge to tackle several shortcomings and limitations of current works.

One of such issues is handling large problem instances from the perspective of computation time since we feel it is an important factor to compare with the traditional algorithms in the field. Another problem to address is developing the specific algorithms and training strategies to improve generalization, i.e. training on smaller problem instances and generalizing to larger ones. In the same line of research, generalizing to the other problem instances with different distributions should be investigated. Working towards devising more general algorithms that can work with various combinatorial problem classes to some specific problems’ formulations is also a promising research direction to pursue. Finally, the current approaches often use some basic variations of the reinforcement learning algorithms, so utilizing state-of-the-art approaches from the field could prove beneficial in the future because of the increased sample efficiency and stability, as well as the incorporation of more efficient representation learning techniques.

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