Curriculum learning for multilevel budgeted combinatorial problems

Adel Nabli Margarida Carvalho
CIRRELT and Département d’Informatique et de Recherche Opérationnelle
Université de Montréal
adel.nabli@umontreal.ca
carvalho@iro.umontreal.ca

Abstract

Learning heuristics for combinatorial optimization problems through graph neural networks have recently shown promising results on some classic NP-hard problems. These are single-level optimization problems with only one player. Multilevel combinatorial optimization problems are their generalization, encompassing situations with multiple players taking decisions sequentially. By framing them in a multi-agent reinforcement learning setting, we devise a value-based method to learn to solve multilevel budgeted combinatorial problems involving two players in a zero-sum game over a graph. Our framework is based on a simple curriculum: if an agent knows how to estimate the value of instances with budgets up to $B$, then solving instances with budget $B + 1$ can be done in polynomial time regardless of the direction of the optimization by checking the value of every possible afterstate. Thus, in a bottom-up approach, we generate datasets of heuristically solved instances with increasingly larger budgets to train our agent. We report results close to optimality on graphs up to 100 nodes and a $185 \times$ speedup on average compared to the quickest exact solver known for the Multilevel Critical Node problem, a max-min-max trilevel problem that has been shown to be at least $\Sigma^P_2$-hard.

1 Introduction

The design of heuristics to tackle real-world instances of NP-hard combinatorial optimization problems over graphs has attracted the attention of many Computer Scientists over the years [31]. With advances in Deep Learning [32] and Graph Neural Networks [69], the idea of leveraging the recurrent structures appearing in the combinatorial objects belonging to a distribution of instances of a given problem to learn efficient heuristics with a Reinforcement Learning (RL) framework has received an increased interest [7, 52]. Although these approaches show promising results on many fundamental NP-hard problems over graphs, such as Maximum Cut [5] or the Traveling Salesman Problem [41], the range of combinatorial challenges on which they are directly applicable is still limited.

Indeed, most of the combinatorial problems over graphs solved heuristically with Deep Learning [3, 5, 6, 14, 17, 41, 45, 51] are classic NP-hard problems for which the canonical optimization formulation is a single-level Mixed Integer Linear Program: there is one decision-maker seeking to minimize a linear cost subject to linear constraints and integer requirements. However, in many real-world situations, decision-makers interact with each other. A particular case of such setting are sequential games with a hierarchy between players: an upper level authority (a leader) optimizes its goal subject to the response of a sequence of followers seeking to optimize their own objectives given

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1 We will use interchangeably the words decision-maker, agent and player. Note that decision-maker, player and agent are usually used in Operations Research, Game Theory and Reinforcement Learning, respectively. Similarly for the words decision, strategy and policy.
the actions previously made by others higher in the hierarchy. These problems are naturally modeled
as Multilevel Programming problems (MPs) and can be seen as a succession of nested optimization
tasks, i.e. mathematical programs with optimization problems in the constraints [10][13][71].

Thus, finding an optimal strategy for the leader in the multilevel setting may be harder than for single-
level problems as evaluating the cost of a given strategy might not be possible in polynomial time: it
requires solving the followers optimization problems. In fact, even Multilevel Linear Programming
with a sequence of \( L + 1 \) players (levels) is \( \Sigma P^3 \)-hard [9][19][38]. In practice, exact methods capable
to tackle medium-sized instances in reasonable time have been developed for max-min-max Trilevels,
min-max Bilevels and more general Bilevel Programs (e.g. [15][24][25][30][65]).

Despite the computational challenges intrinsic to MPs, these formulations are of practical interest as
they properly model hierarchical decision problems. Originally appearing in economics in the
bilevel form, designated as Stackelberg competitions [68], they have since been extended to more
than two agents and seen their use explode in Operations Research [42][62]. Thus, research efforts
have been directed at finding good quality heuristics to solve those problems, e.g. [18][26][28][66].

Therefore, one can ask whether we can make an agent learn how to solve a wide range of instances of
a given multilevel problem, extending the success of recent Deep Learning approaches on solving
single-level combinatorial problems to higher levels.

In this paper, we propose a simple curriculum to learn to solve a common type of multilevel
combinatorial optimization problem: budgeted ones that are zero-sum games played in a graph.
Although the framework we devise is set to be general, we center our attention on the Multilevel
Critical Node problem (MCN) [2] and its variants. The reasons for such a choice are manifold. First,
the MCN is an example of a Defender-Attacker-Defender game [11] which received much attention
lately as it aims to find the best preventive strategies to defend critical network infrastructures against
malicious attacks. As it falls under the global framework of network interdiction games, it is also
related to many other interdiction problems with applications ranging from floods control [56] to the
decomposition of matrices into blocks [29]. Moreover, an exact method to solve the problem has
been presented in [2] along with a publicly available dataset of solved instances [2] which we can use
to assess the quality of our heuristic. Lastly, complexity results are available for several variants and
sub-problems of MCN, indicating its challenging nature [54].

Contributions. Our contribution rests on several steps. First, we frame generic Multilevel Budgeted
Combinatorial problems (MBC) as Alternating Markov Games [47][48]. This allows us to devise a
first algorithm, MultiL-DQN, to learn \( Q \)-values. By leveraging both the combinatorial setting (the
environment is deterministic) and the budgeted case (the length of an episode is known in advance),
we motivate a curriculum, MultiL-Cur. Introducing a Graph Neural Networks based agent, we
empirically demonstrate the efficiency of our curriculum on 3 versions of the MCN, reporting results
close to optimality on graphs of size up to 100.

Paper structure. Section 2 formalizes the MBC problem. In Section 3 we provide an overview of
the relevant literature. The MBC is formulated within the Multi-Agent RL setting in Section 4 along
with the presentation of our algorithmic approaches: MultiL-DQN and MultiL-Cur. Section 5 states
the particular game MCN in which our methodology is validated in Section 6.

2 Problem statement

The general setting for the MPs we are considering is the following: given a graph \( G = (V,A) \), two
concurrent players, the leader and the follower, compete over the same combinatorial quantity \( S \),
with the leader aiming to maximize it and the follower to minimize it. They are given a total number
of moves \( L \in \mathbb{N} \) and a sequence of budgets \( (b_1,...,b_L) \in \mathbb{N}^L \). Although our study and algorithms
also apply to general integer cost functions \( c \), for the sake of clarity, we will only consider situations
where the cost of a move is its cardinality. We focus on perfect-information games, i.e. both players
have full knowledge of the budgets allocated and previous moves. The leader always begins and
the last move is attributed by the parity of \( L \). At each turn \( l \in [1,L] \), the player concerned makes
a set of \( b_l \) decisions about the graph. This set is denoted by \( A_l \) and constrained by the previous
moves \( (A_1,...,A_{l-1}) \). We consider games where players can only improve their objective by taking a
decision: there is no incentive to pass. Without loss of generality, we can assume that \( L \) is odd. Then,

\[https://github.com/mxmmargarida/Critical-Node-Problem\]
the Multilevel Budgeted Combinatorial problem (MBC) can be formalized as:

\[
\text{(MBC)} \quad \max_{|A_1| \leq b_1} \min_{|A_2| \leq b_2} \ldots \max_{|A_L| \leq b_L} S(G, A_1, A_2, \ldots, A_L).
\] (1)

MBC is a zero-sum game as both leader and follower have the same objective function but their direction of optimization is opposite. A particular combinatorial optimization problem is defined by specifying the quantity \( S \), fixing \( L \), and by characterizing the nature of both the graph (e.g. directed, weighted) and of the actions allowed at each turn (e.g. labeling edges, removing nodes). The problem being fixed, a distribution \( \mathcal{D} \) of instances \( i \sim \mathcal{D} \) is determined by setting a sampling law for random graphs and for the other parameters, having specified bounds beforehand: \( n = |V| \in [n_{\min}, n_{\max}] \), \( |A| \in [d_{\min} \times n(n-1), d_{\max} \times n(n-1)] \), \( (b_1, \ldots, b_L) \in [b_{\min}^1, b_{\max}^1] \times \ldots \times [b_{\min}^L, b_{\max}^L] \). Our ultimate goal is thus to learn good quality heuristics that manage to solve each \( i \sim \mathcal{D} \).

In order to achieve that, we aim to leverage the recurrent structures appearing in the combinatorial objects in the distribution \( \mathcal{D} \) by learning graph embeddings that could guide the decision process. As data is usually very scarce (datasets of exactly solved instances being hard to produce), the go-to framework to learn useful representations in these situations is Reinforcement Learning [64].

3 Related Work

The combination of graph embedding with reinforcement learning to learn to solve distributions of instances of combinatorial problems was introduced by Dai et al. [17]. Thanks to their S2V-DQN meta-algorithm, they managed to show promising results on three classic budget-free NP-hard problems. Thenceforth, there is a growing number of methods proposed to either improve upon S2V-DQN results [5, 14, 41, 45, 51] or tackle other types of NP-hard problems on graphs [3]. As all these approaches focus on single player games, they are not directly applicable to MBC.

To tackle the multiplayer case, Multi-Agent Reinforcement Learning (MARL) [46, 60] appears as the natural toolbox. The combination of Deep Learning with RL recently led to one of the most significant breakthrough in perfect-information, sequential two-player games: AlphaGo [61]. Although neural network based agents managed to exceed human abilities on other combinatorial games (e.g. backgammon [67]), these approaches focus on one fixed board game. Thus, they effectively learn to solve only one (particularly hard) instance of a combinatorial problem, whereas we aim to solve a whole distribution of them. Hence, the MBC problem we propose to study is at crossroads between previous works on MARL and deep learning for combinatorial optimization.

An MBC with \( L \) levels is potentially \( \Sigma^P_L \)-hard, and hence, it can be challenging to solve. One of the strategies used to learn to solve complex problems is to break them down in a sequence of learning tasks that are increasingly harder, a concept known as Curriculum Learning [8]. For supervised learning, Bengio et al. [8] showed that gradually increasing the entropy of the training distribution helped. However in RL, breaking down a task in sub-problems that can be ordered by difficulty is non trivial [3]. In robotics, [27, 37] proposed to start from the goal (e.g., open a door) and give a starting state that is gradually further from that goal. These methods assume at least one known goal state that is used as a seed for expansion. For video games, [57] adapted the concept with a starting state increasingly further from the end of a demonstration. However, here, the goal is not to “reach a particular end state”: there is no goal state at all. Rather, what we want is to “take an optimal decision at each level”, and, particularly, take optimal decisions at the beginning of the game, i.e., at the highest level of the multilevel optimization problem, given that all subsequent actions will be optimal. To do that, we show that we can start training our agent on the penultimate states of the sequential decision processes, where the optimization problems are easy to solve as there is only one unit of budget left, and, gradually, consider instances with larger budgets, which effectively corresponds to problems arriving earlier in the sequence of decisions, until we return to the original problem. Thus, contrary to [27, 37, 57], we do not “reverse time” to artificially build a sequence of tasks starting further from a goal state and, subsequently, harder to solve it in the hope of learning how to reach this goal from all possible starting states. Rather, we stack new optimization problems on top of previous ones, which gradually increases the computational complexity of the task, in order to learn to act optimally in optimization problems with an increasing number of levels.

Finally, taking another direction, some shifted their attention from specific problems to rather focus on general purpose solvers. For example, methodologies have been proposed to speed up the branch-and-bound implementations for (single-level) linear combinatorial problems by learning to branch [4]
We now have all the elements to frame the MBC in the Alternating Markov Game framework. The write the generalized Bellman equations for Alternating Markov Games [47]:

An Alternating Markov Game involves two players: a maximizer and a minimizer. It is defined by the tuple \( (S_1, S_2, A_1, A_2, P, R) \) with \( S_i \) and \( A_i \) the set of states and actions, respectively, for player \( i \). The transition function mapping state-actions pairs to probabilities of next states and \( R \) a reward function. For \( s \in S = S_1 \cup S_2 \), we define \( V^*(s) \) as the expected reward of the concerned agent for the optimal minimax policy against an optimal opponent starting from state \( s \). In a similar fashion, \( Q^*(s, a) \) is the expected reward for the player taking action \( a \) in state \( s \) and both agents behaving optimally thereafter. Finally, with the introduction of the discount factor \( \gamma \), we can write the generalized Bellman equations for Alternating Markov Games [47]:

\[
V^*(s) = \begin{cases} 
\max_{a_1 \in A_1} Q^*(s, a_1) & \text{if } s \in S_1 \\
\min_{a_2 \in A_2} Q^*(s, a_2) & \text{otherwise}
\end{cases}
\]

(2)

\[
Q^*(s, a) = R(s, a) + \gamma \sum_{s'} P(s, a, s') V^*(s').
\]

(3)

## 4 Multi-Agent Reinforcement Learning framework

Whereas single agent RL is usually described with Markov Decision Processes, the framework needs to be extended to account for multiple agents. This has been done in the seminal work of Shapley [58] by introducing Markov Games. In our case, we want to model two-player games in which moves are not played simultaneously but alternately. The natural setting for such situation was introduced by Littman in [40, 47, 48] under the name of Alternating Markov Games.

### 4.1 Alternating Markov Games

An Alternating Markov Game involves two players: a maximizer and a minimizer. It is defined by the tuple \( (S, A, P, R) \) with \( S \) and \( A \) the set of states and actions, respectively, for player \( i \). The transition function mapping state-actions pairs to probabilities of next states and \( R \) a reward function. For \( s \in S = S_1 \cup S_2 \), we define \( V^*(s) \) as the expected reward of the concerned agent for following the optimal minimax policy against an optimal opponent starting from state \( s \). In a similar fashion, \( Q^*(s, a) \) is the expected reward for the player taking action \( a \) in state \( s \) and both agents behaving optimally thereafter. Finally, with the introduction of the discount factor \( \gamma \), we can write the generalized Bellman equations for Alternating Markov Games [47]:

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V^*(s) = \begin{cases} 
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\min_{a_2 \in A_2} Q^*(s, a_2) & \text{otherwise}
\end{cases}
\]

(2)

\[
Q^*(s, a) = R(s, a) + \gamma \sum_{s'} P(s, a, s') V^*(s').
\]

(3)

## 4.2 MARL formulation of the Multilevel Budgeted Combinatorial problem

We now have all the elements to frame the MBC in the Alternating Markov Game framework. The \textit{leader} is the maximizer and the \textit{follower} the minimizer. The states \( s_t \) consist of a graph \( G_t \) and a tuple of budgets \( B_t = (b_t^1, ..., b_t^L) = (0, ..., 0, k, b_{t+1}, ..., b_L) \) with \( k \leq b_1 \), beginning with \( s_0 \sim \mathcal{D} \). Thus, the value function is defined with:

\[
V^*(s_0) = \max_{|A_1| \leq b_1^1} \min_{|A_2| \leq b_2^1} \max_{|A_L| \leq b_L^1} S(G_0, A_1, A_2, ..., A_L).
\]

(4)

The game is naturally sequential with an episode length of \( L \): each time step \( t \) corresponds to a level \( t \in [1, L] \). The challenge of such formulation is the size of the action space that can become large quickly. Indeed, in a graph \( G \) with \( n \) nodes, and \textit{leader’s} budget \( b_1 \), if the action that he/she can perform is "removing a set of nodes from the graph" (a common move in network interdiction games), then the size of the action space for the first move of the game is \( \binom{n}{b_1} \). To remedy this, we redefine what is a step in the sequential decision process. We define \( A_1, ..., A_L \), the sets of \textit{individual} decisions available at each level \( t \). Then, we make the simplifying observation that a player making a set of \( b_t \) decisions \( A_t \) in one move is the same as he/she making \( b_t \) decisions \( (a_t^1, ..., a_t^{b_t}) \in A_t \times \cdots \times A_t \) in one strike. More formally, we have the simple lemma (proof in [Appendix A.1]):

**Lemma 4.1.** The Multilevel Budgeted Combinatorial optimization problem ([47]) is equivalent to:

\[
\max_{a_1^1 \in A_1} \cdots \max_{a_1^{b_1} \in A_1} \min_{a_2^1 \in A_2 \setminus \{a_1^1, ..., a_1^{b_1-1}\}} \cdots \max_{a_L^L \in A_L \setminus \{a_1^1, ..., a_L^{b_L-1}\}} S(G, \{a_1^1, ..., a_1^{b_1}\}, ..., \{a_L^1, ..., a_L^{b_L}\}).
\]

In this setting, the length of an episode is no longer \( L \) but \( B = b_1 + \cdots + b_L \): the \textit{leader} makes \( b_1 \) sequential actions, then the \textit{follower} the \( b_2 \) following ones, etc. To simplify the notations, we
re-define the $\mathcal{A}_t$ as the sets of actions available for the agent playing at time $t$. As each action takes place on the graph, $\mathcal{A}_t$ is readable from $s_t$. Moreover, we now have $|\mathcal{A}_t| = \mathcal{O}(|V| + |A|)$.

The environments considered in MBC are deterministic and their dynamics are completely known. Indeed, given a graph $G_t$, a tuple of budgets $B_t = (b^1_t, ..., b^L_t)$ and a chosen action $a_t \in \mathcal{A}_t$ (e.g. removing the node $a_t$), the subsequent graph $G_{t+1}$, tuple of budgets $B_{t+1}$ and next player are completely and uniquely determined. Thus, we can introduce the next state function $N$ that maps state-action couples $(s_t, a_t)$ to the resulting afterstate $s_{t+1}$, and $p$ as the function that maps the current state $s_t$ to the player $p \in \{1, 2\}$ whose turn it is to play. As early rewards weight the same as late ones, we set $\gamma = 1$. Finally, we can re-write equations (2) and (3) as:

$$
V^*(s_t) = \begin{cases} 
\max_{a_t \in \mathcal{A}_t} \left( R(s_t, a_t) + V^*(N(s_t, a_t)) \right) & \text{if } p(s_t) = 1 \\
\min_{a_t \in \mathcal{A}_t} \left( R(s_t, a_t) + V^*(N(s_t, a_t)) \right) & \text{otherwise}
\end{cases}
$$

$$
Q^*(s_t, a_t) = R(s_t, a_t) + V^*(N(s_t, a_t)).
$$

The definition of $R$ depends on the combinatorial quantity $S$ and the nature of the actions allowed.

### 4.3 Q-learning for the greedy policy

Having framed the MBC in the Markov Game framework, the next step is to look at established algorithms to learn $Q^*$ in this setup. Littman originally presented minimax Q-learning [46][47] to do so, but in matrix games, where all possible outcomes are enumerated. An extension using a neural network $\hat{Q}$ to estimate $Q$ has been discussed in [22]. However, their algorithm, Minimax-DQN, is suited for the simultaneous setting and not the alternating one. The main difference being that the former requires the extra work of solving a Nash game between the two players at each step, which is unnecessary in the later as a greedy policy exists [46]. To bring Minimax-DQN to the alternating case, we present MultiL-DQN, an algorithm inspired by S2V-DQN [17] but extended to the multilevel setting: we alternate between a min and a max in both the greedy rollout and the target definition. See Appendix B.1 for the pseudo-code.

### 4.4 A curriculum taking advantage of the budgeted combinatorial setting

With [MultiL-DQN] the learning agent directly tries to solve instances drawn from $\mathbb{D}$, which can be very hard theoretically speaking. However, Lemma 4.1 shows that, at the finest level of granularity, MBC is actually made of $B$ nested sub-problems. As we know $B_{\text{max}} = b^1_{\text{max}} + ... + b^L_{\text{max}}$, the maximum number of levels considered in $\mathbb{D}$, instead of directly trying to learn the values of the instances from this distribution, we can ask whether beginning by focusing on the simpler sub-problems and gradually build our way up to the hard ones would result in better final results.

This reasoning is motivated by the work done by Bengio et al. [8] on Curriculum Learning. Indeed, it has been shown empirically that breaking down the target training distribution into a sequence of increasingly harder ones actually results in better generalization abilities for the learning agent. But, contrary to the continuous setting devised in their work, where the parameter governing the hardness (entropy) of the distributions considered is continuously varying between 0 and 1, here we have a natural discrete sequence of increasingly harder distributions to sample instances from.

Indeed, our ultimate goal is to learn an approximate function $\hat{Q}$ to $Q^*$ (or equivalently $\hat{V}$ to $V^*$ [46]) so that we can apply the subsequent greedy policy to take a decision. Thus, $\hat{Q}$ has to estimate the state-action values of every instance appearing in a sequence of $B$ decisions. Although the leader makes the first move on instances from $\mathbb{D}$, as our game is played on the graph itself, the distribution of instances on which the second decision is made is no longer $\mathbb{D}$ but instances from $\mathbb{D}$ on which a first optimal action for the leader has been made. If we introduce the function

$$
N^k_{i, \pi^*}: \mathcal{S} \rightarrow \mathcal{S}
$$

$$
s_t = (G_t, B_t) \rightarrow \begin{cases} 
N(s_t, a^*_t \sim \pi^*(A_t)) & \text{if } B_t = (0, ..., 0, k, b_{t+1}, ..., b_L) \\
\text{otherwise}
\end{cases}
$$

then, from top to bottom, we want $\hat{Q}$ to estimate the values of taking an action starting from the states $\mathbb{D}^1 = \mathbb{D}$ where the first action is made, then $\mathbb{D}^2 = N^b_{\text{max}}\mathbb{D}$, then $\mathbb{D}^3 = N^b_{\text{max}} \circ N^b_{\text{max}} \circ N^b_{\text{max}} \circ \cdots \circ N^b_{\text{max}} \circ N^b_{\text{max}} \circ \mathbb{D}$. Thus, we can re-write equations (2) and (3) as:

$$
\mathbb{D}^b_{B_{\text{max}}} = N^1_{L, \pi^*} \circ \cdots \circ N^b_{L, \pi^*} \circ \cdots \circ N^b_{1, \pi^*} \circ \mathbb{D}.
$$
As the maximum total budget is \(B_{\text{max}}\), \(\hat{Q}\) has to effectively learn to estimate values from \(B_{\text{max}}\) different distributions of instances, one for each possible budget in \([1, b_{\text{max}}]\) for each \(l \in [1, L]\). But the instances in these distributions are not all equally hard to solve. Actually, the tendency is that the deeper in the sequence of decisions a distribution is, the easier to solve are the instances sampled from it. For example, the last distribution \(D_{\text{train}}^{l, \pi}\) contains all the instances with a total remaining budget of at most 1 that it is possible to obtain for the last move of the game when every previous action was optimal. The values of these instances can be computed exactly in polynomial time by checking the reward obtained with every possible action. Thus, if we had access to the \(\{D_{\text{train}}^{l, \pi}\}\), then a natural curriculum would be to begin by sampling a dataset of instances \(s_{B_{\text{max}}}^* \sim D_{\text{train}}^{l, \pi}\), find their exact value in polynomial time, and train a neural network \(\hat{V}\) on the couples \((s_{B_{\text{max}}}^*, \hat{V}(s_{B_{\text{max}}}^*))\).

Once this is done, we could pass to the \(s_{B_{\text{max}}-1}^* \sim D_{\text{train}}^{l, \pi}\) or \(N_{l, \pi_{l-1}}\). As these instances have a total budget of at most 2, we can heuristically solve them by generating every possible sequence of moves, i.e., we use \(N_{l, \pi_{l-1}}\) instead of \(N_{l, \pi_{l}}\). Doing so still allows us to learn the values of the instances we actually care about (proof in Appendix B.2).

**Lemma 4.2.** \(\forall j \in [2, B_{\text{max}}]\), \(\text{supp}(D_{\text{train}}^{l, \pi}) \subseteq \text{supp}(D_{\text{train}}^{l, \pi})\).

Thus, by learning the value of instances sampled from \(D_{\text{train}}^{l, \pi}\), we also learn values of instances from \(D^{l, \pi}\). To avoid the pitfall of catastrophic forgetting happening when a neural network switches of training distribution, each time it finishes to learn from a \(D_{\text{train}}^{l, \pi}\) and before the transition \(j \rightarrow j - 1\), we freeze a copy of \(\hat{V}\) and save it in memory as an “expert of level \(j\)”. Hence, at level \(l \in [1, L]\) with budget \(k_l \in [1, b_{\text{max}}]\), we have access to a list of trained experts \(\mathbb{L}_j\) that can take decisions for each next step in the sequences, corresponding to instances with either a lower level \(l' < l\) or a lower budget \(k_{l'} < k_l\). To train \(\hat{V}\), we first sample a dataset \(\{s_{l, \pi_{l-1}}^{(i)}\}_{i=1}^N\) of instances from \(\mathbb{D}\). Then, for each instance, we take a sequence of random decisions to arrive at level \(l\) and budget at most \(k_l\) by applying the operator \(N_{l, \pi_{l-1}}\). Finally, to retrieve the approximate targets of the subsequent instances that we will use to train the current \(\hat{V}\), we generate every possible afterstate and use the previously trained \(\mathbb{L}_j\). The complete procedure is formalized in Algorithm 1.

```
Algorithm 1: MultiL-Cur
1. Initialize the value-network \(\hat{V}\) with weights \(\hat{\theta}\).
2. Initialize the list of experts \(\mathbb{L}_j\) to be empty.
3. for \(j = B_{\text{max}}, \ldots, 2\) do
4. Create \(D_{\text{train}}^{l, \pi}_{\text{val}}\) by sampling \((s_j^{*} \sim D_{\text{train}}^{l, \pi}_{\text{val}}, \text{GreedyRollout}(s_j^{*}, \mathbb{L}_j))\);
5. Initialize \(V_j\), the expert of level \(j\) with \(\hat{\theta}_j = \hat{\theta}\);
6. Initialize the loss on the validation set \(L_j^{\text{val}}\) to \(\infty\).
7. for epoch \(e = 1, \ldots, E\) do
8. for batches \((s_i, \hat{y}_i)^{m}_{i=1} \in D_{\text{train}}^{l, \pi}_{\text{train}}\) do
9. Update \(\hat{\theta}\) over \(\frac{1}{m} \sum_{i=1}^{m} (\hat{y}_i - \hat{V}(s_i))^2\) with Adam.
10. if number of new updates \(= T_{\text{val}}\) then
11. \(\text{if } L_{\text{val}}^{\text{new}} = \frac{1}{N_{\text{val}}} \sum_{k=1}^{N_{\text{val}}} (\hat{y}_k - \hat{V}(s_k))^2 < L_{\text{val}}^{\text{old}}\) then
12. \(\hat{\theta}_j \leftarrow \hat{\theta}; L_j^{\text{val}} \leftarrow L_{\text{val}}^{\text{new}}\).
13. Add \(V_j\) to \(\mathbb{L}_j\).
14. return \(\text{the trained list of experts } \mathbb{L}_j\).
```

\(\text{The pseudo-code for the GreedyRollout function is available in Appendix B.2}\).

5 The Multilevel Critical Node Problem

The MCN [2] is a trilevel budgeted combinatorial problem on a weighted graph \(G = (V, A)\). The leader is called the defender and the follower is the attacker. The defender begins by removing (vaccinate) a set \(D\) of \(\Omega\) nodes, then the attacker labels a set \(I\) of \(\Phi\) nodes as attacked (infected), and finally the defender removes (protects) a set \(P\) of \(\Lambda\) new nodes that were not attacked. Once all the

\(^3\text{Assuming the quantity } S \text{ is computable in polynomial time.}\)
moves are done, attacked nodes are the source of a cascade of infections that propagate through arcs from node to node. All nodes that are not infected are saved. As \( D \) and \( P \) were removed from the graph, they are automatically saved and the leader receives \( w(D) \) and \( w(P) \), the weights of the nodes in \( D \) and \( P \), as reward when performing those actions. The quantity \( S \) that the defender seeks to maximize is thus the sum of the weights of the saved nodes in the end of the game, while the attacker aims to minimize it. An example of a game is presented in Figure 1. The problem can be written as:

\[
\max_{D \subseteq V} \min_{I \subseteq V \setminus D} \max_{P \subseteq V \setminus (D \cup I)} S(G, D, I, P).
\]

(9)

With unit weights, the MCN has been shown to be at least NP-hard on undirected graphs and at least \( \Sigma_2^p \)-hard on directed ones. In the more general version, with positive weights and costs associated to each node, the problem is \( \Sigma_3^p \)-complete [54].

6 Computational Results

Instances. We studied 3 versions of the MCN: undirected with unit weights (MCN), undirected with positive weights (MCN\(_w\)), and directed with unit weights (MCN\(_{dir}\)). The first distribution of instances considered is \( \mathbb{D}^{(1)} \), constituted of Erdos-Renyi graphs [20] with size \( |V|^{(1)} \in [10, 23] \) and arc density \( d^{(1)} \in [0.1, 0.2] \). For the weighted case, we considered integer weights \( w \in [1, 5] \). The second distribution of instances \( \mathbb{D}^{(2)} \) focused on larger graphs with \( |V|^{(2)} \in [20, 60] \), \( d^{(2)} \in [0.05, 0.15] \). To compare our results with exact ones, we used the budgets reported in the experiments of the original MCN paper [2]: \( \Omega \in [0, 3] \), \( \Phi \in [1, 3] \) and \( \Lambda \in [0, 3] \).

Graph embedding. The architectures presented in Figure 2 was implemented with Pytorch Geo-Metric [23] and Pytorch 1.4 [55]. At the beginning, a node \( v \in V \) has only 2 features \((w_v, 1_{v \in V})\): its weight and an indicator of whether it is attacked or not. The first step of our node embedding method is to concatenate the node’s two features with its Local Degree Profile [12] consisting in 5 simple statistics on its degree. Following the success of Attention on routing problems reported in [41], we then apply their Attention Layer. As infected nodes are the ones in the same connected component as
attacked ones in the graph, we sought to propagate the information of each node to all the others it is connected to. That way, the attacker could know which nodes are already infected before spending the rest of his/her budget, and the defender could realize which nodes are to protect in his/her last move. So, after the Attention Layers, we used an APPNP layer \[40\] that, given the matrix of nodes embedding \(X^{(0)}\), the adjacency matrix with inserted self-loops \(\hat{A}\), \(\hat{D}\) its corresponding diagonal degree matrix, and a coefficient \(\alpha \in [0, 1]\), recursively applies \(K\) times:

\[
X^{(k)} = (1 - \alpha)\hat{D}^{-1/2}\hat{A}\hat{D}^{-1/2}X^{(k-1)} + \alpha X^{(0)},
\]

To achieve our goal, the value of \(K\) must be at least equal to the size of the largest connected component possible to have in the distribution of instances \(\mathcal{D}^{(i)}\). We thus used \(K = \max(|V|^{(i)})\). Finally, the graph embedding method we used is the one presented in \[44\]. Given two neural networks \(h_{\text{gate}}\) and \(h_v\) which compute, respectively, a score \(\in \mathbb{R}\) and a projection to \(\mathbb{R}^r\), the graph level representation vector it outputs is:

\[
r = \sum_{i=1}^{n} \text{softmax}(h_{\text{gate}}(x_i)) \odot h_v(x_i).
\]

To train our agent and at inference, we used one gpu of a cluster of NVidia V100SXM2 with 16G of memory\(^4\). Further details of the implementation are discussed in Appendix D.

**Algorithms.** We compared our algorithms on \(\mathcal{D}^{(1)}\) and trained our best performing one on \(\mathcal{D}^{(2)}\). But as it is, comparing MultiL-DQN with MultiL-Cur may be unfair. Indeed, MultiL-DQN uses a \(Q\)-network whereas MultiL-Cur uses a value network. The reason why we used \(V\) instead of \(Q\) in our second algorithm are twofold. First, as our curriculum leans on the abilities of experts trained on smaller budgets to create the next training dataset, computing values of afterstates is necessary to heuristically solve instances with larger budgets. Second, as MCN is a game with one player removing nodes from the graph, symmetries can be leveraged in the afterstates. Indeed, given the graph \(G'\) resulting of a node deletion, many couples \((G, v)\) of graph and node to delete could have resulted in \(G'\). Thus, \(Q\) has to learn that all these possibilities are similar, while \(V\) only needs to learn the value of the shared afterstate, which is more efficient \[44\]. To fairly compare the algorithms, we thus introduce MultiL-MC, a version of MultiL-DQN based on a value network and using Monte-Carlo samples as in MultiL-Cur. Its pseudo-code is available in Appendix B.3.

**Table 1:** Evolution during training of the loss on 8 test sets of 1000 exactly solved instances \(\in \mathcal{D}^{(1)}\). Averaged on 3 runs. We measured the loss on distributions arriving at different stages of the curriculum. The approximation ratio and optimality gap were measured after training and averaged over all the tests sets.

|          | opt gap (%) | approx ratio |          | opt gap (%) | approx ratio |          | opt gap (%) | approx ratio |
|----------|-------------|--------------|----------|-------------|--------------|----------|-------------|--------------|
| MultiL-Cur | 0.51        | 1.006        | MultiL-MC | 3.34        | 1.036        | MultiL-DQN | 14.53       | 1.158        |

**Baselines.** Results from Table 1 indicate that MultiL-Cur is the best performing algorithm on \(\mathcal{D}^{(1)}\). Thus, we trained our learning agent with it on \(\mathcal{D}^{(2)}\) and tested its performance on the datasets generated in \[2\]. We compare the results with 2 other heuristics: the random policy (for each instance, we average the value given by 10 random episodes), and the DA-AD heuristic \[2\]. The latter consists in separately solving the two bilevel problems inside MCN: \(D\) is chosen by setting \(\lambda\) to 0 and exactly

\[\text{https://github.com/AdelNabli/MCN}\]
solving the Defender-Attacker problem, while I and P are determined by solving the subsequent Attacker-Defender problem. The metrics we use are the optimality gap $\eta$ and the approximation ratio $\zeta$. Given $n_i$, the number of instances of a said type for which the optimal value $v^*$ is available, $\eta = \frac{1}{n_i} \sum_{k=1}^{n_i} \frac{|v_k^* - v^*_k|}{v^*_k}$ and $\zeta = \frac{1}{n_i} \sum_{k=1}^{n_i} \max \left( \frac{v^*_k}{v_k}, \frac{v_k}{v^*_k} \right)$. In Table 2, we report the inference times $t$ in seconds for our trained agents. The ones for the exact method and DA-AD are from [2].

### Table 2: Comparison between several heuristics and exact methods. Results on MCN are computed on the dataset of the original paper [2]. For MCN$_{dir}$ and MCN$_w$, we generated our own datasets by making small adaptations to the exact solver of [2] originally suited for MCN, see Appendix C for details.

| $|V|$ | exact | random | DA-AD | MCN$_{dir}$ | MCN$_w$ |
|---|---|---|---|---|---|
| $t(s)$ | $\eta(\%)$ | $\zeta$ | $t(s)$ | $\eta(\%)$ | $\zeta$ | $t(s)$ | $\eta(\%)$ | $\zeta$ | $t(s)$ | $\eta(\%)$ | $\zeta$ |
| 20 | 29 | 68 | 3.32 | 0.3 | 1.00 | 0.4 | 0.5 | 1.00 | 5.7 | 1.07 | 6.9 | 1.07 |
| 40 | 241 | 52 | 2.64 | 13 | 7.6 | 1.09 | 0.9 | 5.0 | 1.06 | 11.9 | 1.13 | 6.5 | 1.07 |
| 60 | 405 | 68 | 3.24 | 38 | 7.3 | 1.09 | 1.5 | 4.4 | 1.05 | 4.4 | 1.05 | 3.7 | 1.04 |
| 80 | 636 | 55 | 2.28 | 60 | 3.8 | 1.04 | 2.8 | 2.7 | 1.03 | 1.6 | 1.02 | 2.8 | 1.03 |
| 100 | 848 | 45 | 1.86 | 207 | 2.7 | 1.03 | 8.7 | 49.6 | 1.50 | 1.8 | 1.02 | 4.1 | 1.05 |

**Discussion.** Although the results in Table 1 are the outcome of a total of $\sim 900000$ episodes and $\sim 350000$ optimization steps for all 3 algorithms, our experiments show that we can divide by 2 the data and 4 the number of steps without sacrificing much the results on $D^{(1)}$ for the curriculum, which cannot be said of Multi-L-DQN that is data hungry, see Appendix E for details. The major drawback of Multi-L-Cur is that it needs to compute all possible afterstates at each step of the rollout. This does not scale well with the graph’s size: having 100 nodes for the first step means that there are 100 graphs of size 99 to check. Thus, the curriculum we present is a promising step towards automatic design of heuristics, while opening new research directions on restricting the exploration of rollouts.

Table 2 reveals that the results given by the Multi-L-Cur algorithm are close to the optimum for a fraction of the time necessary to both DA-AD and the quickest exact solver known (MCN$_{MIX}$, presented in [2]). For the MCN instances, the jump in the metrics for graphs of size 100 is due to one outlier among the 85 exactly solved instances of this size. When removed, the values of $\eta$ and $\zeta$ drop to 17.8 and 1.18. The performances measured are consistent across different problems as we also report low values of $\eta$ and $\zeta$ for MCN$_{dir}$ and MCN$_w$. The curriculum we devised is thus a robust and efficient way to train agents in a Multilevel Budgeted setting.

**Conclusion**

In this paper, we proposed a new method for learning to solve Multilevel Budgeted Combinatorial problems by framing them in the Alternative Markov Game framework. To train our agent, we broke down the classical multilevel formulation into a sequence of unitary steps, allowing us to devise a curriculum leveraging the simple observation that the further down in the decision process a problem is, the lower its computational complexity is. Using a bottom up approach, we demonstrated that this learning strategy outperforms more classical RL algorithms on a trilevel problem, the MCN. This study also restates the difficulty of scaling up methods for multilevel optimization due to their theoretical and empirical complexity. This motivates the development of heuristics that can both serve as stand-alone methods or warm-start exact solvers. However, the one we devised is based on an afterstate value function, raising scalability issues. But, our work being the first looking to such problems, it sets the ground for less expensive curricula, which we leave as a future direction.

Finally, we highlight the need for further study on the metrics necessary to properly report the optimality gaps in the multilevel setting. The main drawback of heuristics for multilevel optimization is on their evaluation: given a leader’s strategy, its associated value can only be evaluated if the remaining levels are solved to optimality. This means that in opposition to single-level optimization, one must be very careful on the interpretation of the estimated reward associated with an heuristic method: we can be overestimating or underestimating it. In other words, it means that in the remaining levels, players might be failing to behave in an optimal way. Consequently, further research is necessary to provide guarantees on the quality of the obtained solution, namely, on dual bounds.
Broader Impact

We propose a general framework for training agents to tackle a class of Multilevel Budgeted Combinatorial problems. Such models are widely used in Economics and Operations Research. In this study, we particularly focused on the Multilevel Critical Node problem (MCN). Regarding the usefulness of such problem for practical scenarios, the MCN could fit on several applications, e.g. to limit the fake news spread in social networks or in cyber security for the protection of a botnet against malware injections \[2\]. Thus, this could represent a step towards the design of more robust networks, but could also be used to identify their critical weaknesses for malicious agents. We do not anticipate that our work will advantage or disadvantage any particular group.

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Appendices

A Proofs

Lemma A.1. The Multilevel Budgeted Combinatorial optimization problem \( \mathcal{P} \) is equivalent to:

\[
\max_{a_1^t \in A_1} \ldots \max_{a_{b_1}^t \in A_{b_1}} \min_{a_{b_2}^t \in A_{b_2}} \max_{a_{b_3}^t \in A_{b_3}} \cdots \max_{a_{b_L}^t \in A_{b_L}} S(G, \{a_1^t, \ldots, a_{b_1}^t\}, \ldots, \{a_{b_2}^t, \ldots, a_{b_L}^t\}).
\]

Proof. We immediately have the following relation:

\[
\max_{|A_1| \leq b_1} \ldots \max_{|A_L| \leq b_L} S(G, A_1, A_2, \ldots, A_L) = \max_{a_i \in A_i} \max_{A' \subseteq A_i} S(G, \{a_i\} \cup A', A_2, \ldots, A_L).
\]

As the same reasoning holds with \( \in \), we can apply it recursively, which closes the proof.

Lemma A.2. \( \forall j \in [2, B_{max}], \text{supp}(D_j) \subseteq \text{supp}(D_j^*) \)

Proof. For all \( s_0 \sim \mathcal{D} \), for all \( t \in [0, B-1] \), we define \( A_t^* = (a_0, \ldots, a_{t-1}) \subseteq A_t(a_0, \ldots, a_{t-1}) \) as the set of optimal actions at time \( t \) in state \( s_t \) for the player \( p(s_t) \), where we made evident the dependence of \( s_t \) on previous actions. As by assumption we consider games where players can only improve their objective by taking a decision, we have that \( \forall t \), \( A_t \neq \emptyset \implies A_t^* \neq \emptyset \). For a given \( s_t \) and subsequent \( A_t \), recall that \( a_t^* \) is defined as a random variable with values in \( A_t \) and following the uniform law. Given \( s_0 \sim \mathcal{D} \), we take \( (a_0^*, \ldots, a_{B-1}^*) \in A_0^* \times \cdots \times A_{B-1}^* \), one of the possible sequence of optimal decisions. Then, using the chain rule, it is easy to show by recurrence that \( \forall t \in [0, B-1] \), \( F(a_0^*, \ldots, a_{t}^*) > 0 \). In words, every optimal sequence of decisions is generated with a strictly positive probability.

B Algorithms

B.1 MultiL-DQN

As the player currently playing is completely determined from \( s_t \), we can use the same neural network \( \hat{Q} \) to estimate all the state-action values, regardless of the player. We call \( B_t \) the sum of all the budgets in \( B_t \) such that an episode stops when \( B_t = 0 \).

Algorithm 2: MultiL-DQN

1. Initialize the replay memory \( \mathcal{M} \) to capacity \( C \);
2. Initialize the \( Q \)-network \( \hat{Q} \) with weights \( \hat{\theta} \);
3. Initialize the target-network \( \tilde{Q} \) with weights \( \tilde{\theta} = \hat{\theta} \);
4. for episode \( e = 1, \ldots, E \) do
5. \( s_0 = (G_0, B_0) \sim \mathcal{D} \);
6. \( t \leftarrow 0 \);
7. while \( B_t \geq 1 \) do
8. \( a_t = \begin{cases} \text{random action } a_t \in A_t & \text{w.p. } \epsilon \\ \arg \max_{a_t \in A_t} Q(s_t, a_t) & \text{otherwise if } p(s_t) = 1 \\ \arg \min_{a_t \in A_t} Q(s_t, a_t) & \text{otherwise if } p(s_t) = 2 \end{cases} \)
9. \( s_{t+1} \leftarrow N(s_t, a_t) \);
10. \( t \leftarrow t + 1 \);
11. if \( t \geq 1 \) then
12. Add \((s_{t-1}, a_{t-1}, R(s_{t-1}, a_{t-1}), s_t)\) to \( \mathcal{M} \);
13. Sample a random batch \( \{(s_i, a_i, r_i, s_i')\}_{i=1}^m \sim \mathcal{M} \);
14. for \( i = 1, \ldots, m \) do
15. \( y_i = r_i + \mathbb{I}_{p(s_i')=0} \max_{a_i' \in A_i'} \hat{Q}(s_i', a_i') + \mathbb{I}_{p(s_i')=2} \min_{a_i' \in A_i'} \hat{Q}(s_i', a_i') \)
16. Update \( \tilde{\theta} \) over \( \frac{1}{m} \sum_{i=1}^m (y_i - \hat{Q}(s_i, a_i))^2 \) with Adam [39];
17. Update \( \hat{\theta} \leftarrow \theta \) every \( T_{\text{target}} \) steps
18. return the trained \( Q \)-network \( \hat{Q} \)
B.2 Greedy Rollout

Algorithm 3: Greedy Rollout

Input: A state $s_t$ with total budget $B_t$ and a list of experts value networks $\mathbb{L}_p$
1. Initialize the value $\hat{v} \leftarrow 0$
2. while $B_t \geq 1$ do
3. Retrieve the expert of the next level $\hat{V}_{t+1}$ from the list $\mathbb{L}_p$
4. Generate every possible afterstate $S_t' \leftarrow \{ N(s_t, a_t) \}_{a_t \in A_t}$
5. $s_{t+1} = \begin{cases} 
\arg \max_{a_t \in A_t} \hat{V}_{t+1}(s') & \text{if } p(s_t) = 1 \\
\arg \min_{a_t \in A_t} \hat{V}_{t+1}(s') & \text{if } p(s_t) = 2 
\end{cases}$
6. $\hat{v} \leftarrow \hat{v} + R(s_t, s_{t+1})$
7. $t \leftarrow t + 1$
8. return the value $\hat{v}$

B.3 MultiL-MC

As we use Monte-Carlo samples as targets, the values of the targets sampled from the replay memory $\mathcal{M}$ is not dependent on the current expert as in DQN [53] but on a previous version of $\hat{V}$, which can become outdated quickly. Thus, to easily control the number of times an old estimate is used, we decided to perform an epoch on the memory every time $m$ new samples were pushed, and used a capacity $C = k \times m$ so that the total number of times a Monte-Carlo sample is seen is directly $k$.

Algorithm 4: MultiL-MC

1. Initialize the replay memory $\mathcal{M}$ to capacity $C$
2. Initialize the value-network $\hat{V}$ with weights $\theta$
3. for episode $e = 1, ..., E$ do
4. Sample $s_0 = (G_0, B_0) \sim \mathcal{D}$
5. Initialize the memory of the episode $\mathcal{M}_e$ to be empty
6. Initialize the length of the episode $T \leftarrow 0$
7. while $B_t \geq 1$ do // perform a Monte Carlo sample
8. random action $a_t \in A_t$ w.p. $\epsilon$
9. $a_t = \begin{cases} 
\arg \max_{a_t \in A_t} \hat{V}(N(s_t, a_t)) & \text{otherwise if } p(s_t) = 1 \\
\arg \min_{a_t \in A_t} \hat{V}(N(s_t, a_t)) & \text{otherwise if } p(s_t) = 2 
\end{cases}$
10. $s_{t+1} = N(s_t, a_t)$
11. Add $(s_t, R(s_t, a_t))$ to $\mathcal{M}_e$
12. $T \leftarrow T + 1$
13. Initialize the target $y_T \leftarrow 0$
14. for $t = 1, ..., T$ do // associate each state to its value
15. Recover $(s_{T-1}, R(s_{T-1}, a_{T-1}))$ from $\mathcal{M}_e$
16. $y_{T-1} \leftarrow y_{T-1} + R(s_{T-1}, a_{T-1})$
17. Add $(s_{T-1}, y_{T-1})$ to $\mathcal{M}$
18. if there are more than $m$ new couples in $\mathcal{M}$ then
19. Create a random permutation $\sigma \in S_N$
20. for batches $\{ (s_i, y_i) \}_{i=1}^m \sim \sigma(\mathcal{M})$ do // perform an epoch on the memory
21. Update $\hat{\theta}$ over the loss $\frac{1}{m} \sum_{i=1}^m (y_i - \hat{V}(s_i))^2$ with Adam [39]
21. return the trained value-network $\hat{V}$

C Broadening the scope of the exact algorithm

In order to constitute a test set to compare the results given by our heuristics to exact ones, we used the exact method described in [2] to solve a small amount of instances. The algorithm they described was thought for the MCN problem, but is directly applicable without change on MCN$_{mc}$. However, in order to monitor the learning at each stage of the curriculum for MCN as in Table 1 there is a need to solve instances where node infections were already performed in the sequence of previous moves but there is still some budget left to spend for the attacker, which is not possible as it is in [2]. Moreover, small changes need to be made in order to solve instances of MCN$_{w}$. 
C.1 Adding nodes that are already infected

We denote by $J$ the set of nodes that are already infected at the attack stage and $\beta_v = 1_{v \in J}$ the indicator of whether node $v$ is in $J$ or not. Then, the total set of infected nodes after the attacker spend his/her remaining budget $\Lambda$ and infect new nodes $I$ is $J \cup I$. In order to find $I$, we use the AP algorithm of [2], with the following modification to the rlxAP optimization problem:

$$\min \quad \Lambda p + \sum_{v \in V} \gamma_v$$
$$\sum_{v \in V} y_v \leq \Lambda$$
$$y_v \leq 1 - \beta_v \quad \forall v \in V$$
$$h_v + \sum_{(u,v) \in A} q(u,v) - \sum_{(u,v) \in A} q(v,u) \geq 1 \quad \forall v \in V$$
$$p - \sum_{(u,v) \in A} q(u,v) \geq 0 \quad \forall v \in V$$
$$\gamma_v + |V|y_v - h_v \geq -|V|\beta_v \quad \forall v \in V$$
$$p, h_v, \gamma_v, q(u,v) \geq 0 \quad \forall v \in V, (u,v) \in A$$
$$y_v \in \{0,1\} \quad \forall v \in V$$

We indicated changes in blue. The notations for the variables being the ones from [2].

C.2 Adding weights

Taking the weights $w_v$ of the nodes $v \in V$ into account in the optimization problems is even more straightforward. As the criterion to optimize is no longer the number of saved nodes but the sum of their weights, each time a cardinal of a set appears in the algorithms AP and MCN in [2], we replace it by the sum of the weights of its elements. As for the optimization problems that are solved during the routines, we replace, in the Defender problem and in the 1lvlMIP:

$$\sum_{v \in V} \alpha_v \rightarrow \sum_{v \in V} w_v \alpha_v$$

and in the rlxAP problem:

$$h_v + \sum_{(u,v) \in A} q(u,v) - \sum_{(u,v) \in A} q(v,u) \geq 1 \rightarrow h_v + \sum_{(u,v) \in A} q(u,v) - \sum_{(u,v) \in A} q(v,u) \geq w_v$$

D Experiments details

D.1 Architecture details

Nodes embedding . The first step of the method described in Figure 2 is the node embedding part. Each node $v \in V$ begins with two features $x_v = (w_v, 1_{v \in I})$: its weight and an indicator of whether it is attacked or not. First, we normalize the weights by dividing them with the sum of the weights in the graph such that each $w_v \in [0,1]$. We extend the two features with the Local Degree Profile of each node [12], which consists in 5 features on the degree:

$$x_v = x_v ||(\text{deg}(v), \min(\text{DN}(v)), \max(\text{DN}(v)), \text{mean}(\text{DN}(v)), \text{std}(\text{DN}(v)))$$

with $\text{deg}$ the degree of a node, and $\text{DN}$ the degrees of $\mathcal{N}(v)$ - the neighbors of $v$ in the graph. Then, we project our features $x_v \in \mathbb{R}^7$ into $\mathbb{R}^{d_e}$ with a linear layer. After that, we replicated the Multihead Attention Layer described in Kool et al. [41] using a Graph Attention Network (GAT) [16]. Thus, we apply one GAT layer such that:

$$x_v' = \mu_{v,v} \Theta x_v + \sum_{u \in \mathcal{N}(v)} \mu_{v,u} \Theta x_u$$

(13)
with \( \mu \) defined by:

\[
\mu_{v,u} = \frac{\exp(\text{LeakyReLU}(a^\top(\Theta x_v || \Theta x_u)))}{\sum_{k \in N(v) \cup \{v\}} \exp(\text{LeakyReLU}(a^\top(\Theta x_v || \Theta x_k)))},
\]

where \( a \in \mathbb{R}^{2 \times d_e} \) and \( \Theta \in \mathbb{R}^{d_e \times d_e} \) are the trainable parameters. Here, \( d_e \) is the original embedding dimension of \( x_v \), \( d_h \) is the dimension of \( x'_v \). We apply these equations with \( n_h \) different \( \Theta \) and \( a \), \( n_h \) being the number of heads used in the attention layer. Then, we project back in \( \mathbb{R}^{d_e} \) the \( x'_v \) with a linear layer, and sum the \( n_h \) resulting vectors. After that, we apply a skip connection and a Batch-Normalization layer such that:

\[
x'_v = \text{BN}(x_v + x'_v).
\]

Finally, we introduce a feedforward network FF which is a 2-layer fully connected network with ReLU activation functions. The input and output dimensions are \( d_e \) and the hidden dimension is \( d_h \). The final output is then:

\[
x_v = \text{BN}(x'_v + \text{FF}(x'_v)).
\]

We repeated the process described between equation (13) and equation (16) a total of \( n_a \) times. Then, to propagate the information of each node to the others in the same connected component, we use an APPNP layer. Given the matrix of nodes embedding \( X^{(0)} \), the adjacency matrix with inserted self-loops \( \hat{A}, \hat{D} \) its corresponding diagonal degree matrix, and a coefficient \( \alpha \in [0, 1] \), it recursively applies \( K \) times:

\[
X^{(k)} = (1 - \alpha)\hat{D}^{-1/2} \hat{A} \hat{D}^{-1/2} X^{(k-1)} + \alpha X^{(0)}.
\]

We used \( K = 23 \) when we trained on instances from \( \mathbb{D}^{(1)} \) and \( K = 60 \) when we trained on \( \mathbb{D}^{(2)} \).

**Graph embedding.** Given the resulting nodes embedding \( x_v \in \mathbb{R}^{d_e} \), in a skip-connection fashion, we concatenate the \( x_v \) back with the original two features \( (w'_v, 1_{v \in I}) \) (\( w'_v \) being the normalized weights). Then, the graph level representation vector is, for a graph of size \( n \):

\[
r = \sum_{i=1}^{n} \text{softmax}(h_{\text{gate}}(x_i)) \odot h_v(x_i).
\]

Here, \( h_{\text{gate}} \) and \( h_v \) are feedforward neural networks with 2 layers and using ReLU activation functions. For both, the input dimension is \( d_e + 2 \) and the hidden dimension is \( d_h \). For \( h_v \), the output dimension is \( d_e \) whereas for \( h_{\text{gate}} \), it is 1. We used \( n_p \) different versions of the parameters and concatenated the \( n_p \) different outputs such that the final graph embedding has a dimension of \( n_p \times d_e \).

**Final steps.** We now have the nodes embedding \( x_v \in \mathbb{R}^{d_e} \) and a graph representation \( r \) of dimension \( d_e \times n_p \). But the context for each node is not entirely contained in \( r \): the budgets, the size of the graph \( n \) and the total sum of weights in the graph are still missing. Thus, we form a context vector \( c_o \) as follows:

\[
c_o = r || (n, \Omega, \Phi, \Lambda, \Omega/n, \Phi/n, \Lambda/n, \sum_{u \in V} w_v).
\]

When this is done, we perform, for each node, the concatenation \( x_v || c_o \). This is the entry of a feedforward neural network, FF\( V \) or FF\( Q \), that computes, for \( \hat{V} \), the probability of each node being saved given the context, and the state-action values for \( \hat{Q} \). The two feedforward networks are 3-layers deep, with the first hidden dimension being \( d_h \) and the second \( d_e \). We used LeakyReLU activation functions, Batch Norm and dropout with parameter \( p \). Indeed, our experiment shows that using dropout at this stage helps prevent overfitting, and Batch Norm speedups the training. The last activation function for FF\( Q \) is ReLU whereas for FF\( V \) we use a sigmoid. Finally, for FF\( V \), we output:

\[
\hat{V}(s) = \sum_{v \in V} P(v \text{ is saved} \mid \text{context})w_v.
\]

For FF\( Q \), we just mask the actions not available, i.e. the nodes that are already labeled as attacked.
Hyperparameters. All the negative slopes in the LeakyReLU we used were set by default at 0.2. The value of all the other hyperparameters we introduced here were fixed using Optuna with a TPE sampler and a Median pruner. The objective we defined was the value of the loss of \( \hat{V} \) on a test set of exactly solved instances \( \in \mathbb{D}^{(1)} \) with budgets \( \Omega = 0 \), \( \Phi = 1 \), \( \Lambda \in [0, 3] \). After running Optuna for 100 trials, we fixed the following values for the hyperparameters: \( d_v = 200 \), \( d_h = 400 \), \( d_x = 100 \), \( \alpha = 0.2 \), \( \beta = 0.2 \), \( n_a = 7 \), \( n_h = 3 \), \( n_p = 3 \). It represents a total of 2,8 million parameters to train for both \( \hat{V} \) and \( \hat{Q} \).

D.2 Parameters of the training algorithms

Comparison between the 3 algorithms. For all 3 algorithms, we used roughly the same values of parameters in order to make the comparison fair. All three algorithms were compared on instances from \( \mathbb{D}^{(1)} \). The batch size was fixed to \( m = 256 \). Although we share our training times for the sake of transparency and to compare the methods, we want to highlight that our code is hardly optimized and that cutting the times presented here may be easy with a few improvements.

For MultiL-Cur, we used a training set of size 100 000 and a validation set of 1000 instances at each stage of the curriculum. As there are 8 distributions to learn from (as we use afterstates, there is no need to learn the values of instances having \( \Omega = 3 \), \( \Phi = 3 \), \( \Lambda = 3 \) as budgets), this amounts for a total of 808 000 episodes. At each stage \( j \), we trained our expert \( \hat{V}_j \) for 120 epochs, meaning that we used a total of 375 000 training steps to finish the curriculum, which necessitated a total of 36 hours. Most of the training time was directed towards generating the training sets, i.e. performing the greedy rollouts. Moreover, a few hours in this training time is also possible if we do not monitor the evolution of the training on the test sets (computing the loss on the test sets regularly takes time).

For MultiL-MC, we fixed \( C \), the capacity of the replay memory to be equal to \( 27 \times 256 \) so that each Monte-Carlo sample is exactly seen 27 times. We used a total of 700 000 episodes here, resulting in an average of 377 000 training steps, which took 56 hours. Indeed, the length of the episodes here is longer on average than the ones used in the curriculum as we directly begin from instances sampled from \( \mathbb{D}^{(1)} \) and not the ones where moves were already performed randomly. So the rollout process lasts longer, which is what takes time in our algorithm.

Finally, for MultiL-DQN, we used a capacity \( C = 10 \ 240 \). In order to perform the same number of training steps for the same number of episodes than the other two algorithms, we generated our data in batches of size of 16: at each time step, there are 16 new instances pushed in memory. We used a total of 16 \( \times 60 \ 000 = 960 \ 000 \) episodes. The number of training steps performed was 370 000 on average. The time necessary for that was 29 hours. Although this is lower than the other two methods (due to a much quicker rollout), the optimality gap and approximation ratio were so high (\( \eta = 32.55\% \), \( \zeta = 1.54 \)) with this amount of data that we actually decided to re-launch an experiment using more episodes. The graphs in Table 1 show the behaviour during training of the 3 algorithms with the setting described until now, however the results of optimality gap and approximation ratio for the MultiL-DQN algorithm are those from a different training setting where we used much more episodes. We made a second experiment were we generated batches of size 128 instead of 16, amounting the number of episodes used to 7 080 000 for the same number of training steps. This second experiment took 72 hours, proving that MultiL-DQN actually necessitates way more data than the two other algorithms, for worse results.

For both MultiL-MC and MultiL-DQN, we used a probability \( \epsilon \) with an exponential decay: \( \epsilon_{\text{start}} = 0.9 \), \( \epsilon_{\text{end}} = 0.05 \) and a temperature \( T_{\text{decay}} = 1000 \).

Curriculum on larger graphs. For the results in Table 2, we trained our experts on \( \mathbb{D}^{(2)} \). As these instances are of larger size and theoretically harder to solve, we decided to train for longer our experts \( \hat{V}_j \). We used a training set of size 120 000, a validation set of size 2000 and a number of epoch per stage of 200 for the MCN problem. For MCNdir and MCNw, we used a training set of size 60 000, a validation set of size 1000 and 400 epochs at each stage. The MCN training took roughly a week to run, for MCNw and MCNdir, it took 5 days: the rollout on larger graphs takes a long time.

D.3 Details on the test sets

The test sets we used for the results in Table 1 consisted in 1000 exactly solved instances for each of the 8 different training distributions used during the curriculum. For the results in Table 2, we gathered the instances from [2] for the MCN. As they put a threshold of 2 hours for their solver
MCN^{MIX}, the number of instances solved for each of the sizes is different. Moreover, an extensive study of the graphs of size 40 has been done in their paper. For MCN_{dir} and MCN_{w}, we used the solvers described in Appendix C. The size of the training sets considered in Table 2 are then:

| size of \( |V| \) | \( \text{size of } D_{\text{test}} \) | MCN | MCN_{dir} | MCN_{w} |
|---|---|---|---|---|
| 20 | 120 | 36 | 36 |
| 40 | 876 | 35 | 34 |
| 60 | 110 | 23 | 29 |
| 80 | 101 | 12 | 30 |
| 100 | 85 | 11 | 27 |

### E Extended Results

#### E.1 Training the Q network with more data

As discussed earlier, we trained an agent on \( D^{(1)} \) with MultiL-DQN using two configurations. First, we used 960 000 episode for 370 000 optimization steps. Faced with the poor results, we re-trained our agent using more data: 7 680 000 episodes for the same number of steps. We compare the results of the two methods in Table 4. We clearly see that training with more data radically impacts the results. More than that, there is a necessity of training with many episodes to obtain reasonable results. We also notice a worse behaviour at the attack stage compared to the other two where it is the defender’s turn to play. Thus, we may benefit from adapting the MultiL-DQN algorithms to use two Q networks, one for each player.

#### E.2 Training the Value network with less data

In order to assess the capacity of our curriculum to use less data and less training steps, we trained our value network on \( D^{(1)} \) using a second configuration. We re-trained our experts using 50 000 instances in the training sets, with 60 epochs at each stage, instead of 100 000 and 120 originally.
Table 5: Comparison between two configurations of curriculum for $\hat{Y}$. In Config. 1, we trained with a total of 800 000 episodes and 375 000 optimization steps while in Config. 2 we used 400 000 episodes and 93 750 steps. We display the evolution of the losses during training on 8 test sets of size 1000 arriving at different stages of the curriculum. We measure the resulting optimality gap $\eta$ and approximation ratio $\zeta$ on 3 different test sets, one for each of the 3 levels of the problem.

| Level       | $\eta$ (%) | $\zeta$   | $\eta$ (%) | $\zeta$   |
|-------------|------------|-----------|------------|-----------|
| Vaccination | 0.955      | 1.011     | 1.126      | 1.013     |
| Attack      | 0.409      | 1.004     | 0.913      | 1.009     |
| Protection  | 0.005      | 1.000     | 0.005      | 1.000     |

The results in Table 5 clearly show that training with half the data and a quarter of the steps in the curriculum hardly affects the end results, demonstrating the efficiency of the method. Training with Config. 2 took 15 hours compared to the 36 necessary with Config. 1.

E.3 Comparing the difficulty to learn to solve the 3 problems

In this part, we propose to compare the difficulty our curriculum has on learning to solve the 3 different problems MCN, MCN$_{dir}$, and MCN$_w$ on instances from $\mathcal{D}^{(1)}$. For that, we ran our curriculum in exactly the same way 3 times, except for the distribution of graphs from which we sampled our instances: undirected with unit weights for the MCN, directed with unit weights for MCN$_{dir}$, and undirected with integer weights for MCN$_w$. In Figure 3, we compare the values of the 3 validation losses during the training, along with the values of the approximation ratio $\zeta$ and optimality gap $\eta$ on 3 test sets of 9000 exactly solved instances from $\mathcal{D}^{(1)}$ in Table 6.

| Problem   | $\eta$ (%) | $\zeta$   |
|-----------|------------|-----------|
| MCN$_w$   | 7.08       | 1.069     |
| MCN$_{dir}$ | 2.84   | 1.032     |
| MCN       | 0.51       | 1.006     |

Table 6: Values of the approximation ratio and optimality gap on a test sets of exactly solved instances from $\mathcal{D}^{(1)}$ for each of the 3 problems.

Figure 3: Evolution of the loss on the successive validation sets during the curriculum for the 3 problem considered.

Both the table and the figure seem to tell the same story: the easiest problem to learn to solve with our curriculum is the MCN, followed by MCN$_{dir}$, the hardest one being MCN$_w$. 

20
E.4 Assessing the ability to generalize to larger graphs

Previous work on learning to solve single level combinatorial problems with graph neural networks such as [17, 41] reported that their trained agent managed to satisfyingly solve instances with larger graphs at test time than the ones used in their training distributions. In order to assess if this holds for agents trained with our curriculum on the multilevel combinatorial problem, we trained, for each of the 3 problems, our agents on both $D^{(1)}$ and $D^{(2)}$, then measured how well they behaved on increasingly larger graphs at test time. We report our results in Table 7.

Table 7: Evolution of the optimality gap $\eta$ and the approximation ratio $\zeta$ with the size of the graphs at test time for each of the 3 problems considered.

![Graphs showing the evolution of optimality gap and approximation ratio](image)

We clearly see in Table 7 that the experts trained on $D^{(2)}$, i.e. on larger graphs, perform better than the ones trained on $D^{(1)}$. From the curves, it seems that our experts can generalize to graphs up to 2 times larger than the ones they were trained on. The fact that for the curves about $D^{(1)}$ there is first an increase of the values of the metrics and a sudden decrease around $|V| = 80$ may be explained by the fact that $\eta$ and $\zeta$ do not directly measure the goodness of our heuristics. Indeed, if we were to measure how good the decisions taken at a certain level are, we should solve to optimality the subsequent lower levels, which is not what we do here: we use our heuristics everywhere. Thus, when our heuristics perform too badly at each level, i.e. defending poorly but also attacking poorly, there is a chance that the value measured in the end of the game is actually not too far from the one
that would have followed optimal decisions. To produce the graphs in Table 7, we generated 3 test sets, one for each problem, using the solver described in Appendix C with IBM ILOG CPLEX 12.9.0. The number of instances in those datasets for each value of $|V|$ are listed in Table 8.

Table 8: Sizes of the test sets used for the results in Table 7.

| $|V|$ | 20  | 25  | 30  | 35  | 40  | 45  | 50  | 55  | 60  | 65  | 70  | 75  | 80  | 85  | 90  | 95  | 100 |
|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MCNw | 36  | 36  | 36  | 35  | 34  | 33  | 29  | 29  | 28  | 31  | 29  | 30  | 28  | 29  | 29  | 27  |
| MCNdir | 36  | 36  | 36  | 34  | 35  | 32  | 29  | 27  | 23  | 17  | 13  | -   | 12  | -   | 10  | -   | 11  |
| MCN  | 36  | 36  | 36  | 32  | 30  | 27  | 29  | 26  | 24  | 22  | 17  | 15  | 14  | -   | 9   | -   | 10  |

E.5 Identifying multiple optimal solutions

In many situations, there exists multiple solutions to an instance of a combinatorial problem. For some methods, this can represent a challenge as it clouds the decision-making process [45]. However, being able to produce multiple optimal solutions to a combinatorial problem is of interest. Here, the formulation we used naturally allows to identify many of the optimal solutions, assuming our value networks correctly approximate the values of each afterstate. Indeed, if our agents correctly label each node with its value (i.e. the value of the afterstate if the action is performed on the node, plus reward), then identifying all the possible ways of acting optimally is directly readable from them, as shown in the example presented in Figure 4.

Figure 4: Exact values and approximate values on an instance of MCN constituted of a graph $G$ and budgets $\Omega = 1$, $\Phi = 1$, $\Lambda = 2$. The exact value of each node is obtained by removing (vaccinating) the said node from $G$ and solving exactly the subsequent afterstate with $\Omega$ set to 0. The approximate values are obtained by feeding the afterstates to the expert trained on budgets $\Phi = 1$, $\Lambda \in [0, 3]$ during the curriculum for instances from $D^{(1)}$.

In Figure 4 there are 2 optimal vaccinations: the two blue nodes with value 12. Although the approximate values are not perfectly aligned with the exact ones, the two optimal decisions are clearly identifiable from them, demonstrating the ability of our method to detect multiple optimal solutions.