Uncertainty-sensitive Learning and Planning with Ensembles

Piotr Miłoś* 1 2  Łukasz Kuciński* 1 Konrad Czechowski* 3 Piotr Kozakowski 3 Maciej Klimek 3

Abstract
We propose a reinforcement learning framework for discrete environments in which an agent makes both strategic and tactical decisions. The former manifests itself through the use of value function, while the latter is powered by a tree search planner. These tools complement each other. The planning module performs a local what-if analysis, which allows avoiding tactical pitfalls and boosts backups of the value function. The value function, being global in nature, compensates for the inherent locality of the planner. In order to further solidify this synergy, we introduce an exploration mechanism with two components: uncertainty modelling and risk measurement. To model the uncertainty, we use value function ensembles, and to reflect risk, we use several functionals that summarize the uncertainty implied by the ensemble. We show that our method performs well on hard exploration environments: Deep-sea, toy Montezuma’s Revenge, and Sokoban. In all the cases, we obtain speed-up in learning and boost in performance.

1. Introduction
The model-free and model-based approaches to reinforcement learning (RL) have complementary sets of strengths and weaknesses. While the former offers good asymptotic performance, it suffers from inferior sample complexity. In contrast, the latter usually needs significantly less training samples, but often fails to achieve state-of-the-art results on complex tasks (which is primarily attributed to the model’s imperfections). The interplay of model-based and model-free approaches in RL has received a lot of research attention. This led, for example, to strong AI systems like Silver et al. (2017; 2018) or more recently to Lowrey et al. (2018), which is closely related to our work.

When dealing with challenging RL domains, it is helpful to address strategic and tactical decision-making. These two perspectives complement each other: the strategic perspective is global, static, and often approximate, while the tactical perspective is local, dynamic, and exact. A neural network value function can be considered as an implementation of the former, while a planner as an example of the latter. Indeed, neural network value functions provide noisy estimates (approximate) of values (static) to every state (global). Conversely, planning provides high-quality control which, starting from a given state (local), generates actions (dynamic) that are temporally coherent and result in better executed trajectories (exact).

In this paper we propose a framework combining the aforementioned components into a single system. We test our approach on the sparse reward variants of the following environments: Sokoban, a classic logical puzzle known for its combinatorial complexity (in fact, answering the question of whether a Sokoban level is solvable is NP-hard, see e.g. Dor & Zwick (1999)) and a recent benchmark for RL, ChainEnv, a seemingly impossible task referred to as a ‘hay in a needle-stack’ problem (see Osband et al. (2018)), and Toy Montezuma’s Revenge, environment notoriously known for its exploration difficulty (see Guo et al. (2019)).

Put differently, we consider a situation of an agent with limited memory and computational resources, being dropped into a complex and diverse environment. We assume that solving for an optimal trajectory is out of reach, and a limited depth planner has to be used. Plugging the value function into the planner provides guided heuristics in the local search, shortens the search horizon, and thus makes the search computationally efficient. For complex problems, this setup has to be supplemented by an exploration scheme. We develop a scheme based on modelling uncertainty of the value function approximation using ensembles. The uncertainty is quantified by a risk measure, which is then utilized by a planner to drive exploration.

The main contribution of this work is showing how recent progress in AI can be brought together to improve planning, value function learning, and exploration, in a way that forms robust algorithms for solving challenging reinforcement learning environments. In particular:
1. For uncertainty modeling, we assume the point of view of Osband et al. (2018), which uses ensembles to approximate posterior distribution.

2. In the spirit of Lowrey et al. (2018), we incorporate risk measures to guide exploration.

3. For the planner, we base on AlphaZero Monte-Carlo Tree Search, see Silver et al. (2017).

4. In the value function training protocol, we introduce several improvements, including a version of prioritized replay buffer and hindsight (Andrychowicz et al. (2017)). We found it beneficial to calculate targets for value function learning using the planner search history.

The rest of the paper is organized as follows. In the next subsection we provide an overview of related work. In Section 2 we present and discuss our method in detail. Experiments are gathered in Section 3. Section 4 concludes the paper. Some details concerning the algorithm’s pseudo-code, neural network architecture and training, and ablations can be found in the Appendix. We provide source code to our work https://github.com/learningandplanningICLR/learningandplanning and a dedicated website https://sites.google.com/view/learn-and-plan-with-ensembles with more details and movies.

1.1. Related work

The ideas of mixing model-based and model-free learning were perhaps first stated explicitly in Sutton (1990). Many approaches followed. More recently, in the groundbreaking series of papers Silver et al. (2017; 2018) culminating in AlphaZero, the authors have developed an elaborate system that plans and performs model-free training to master the game of Go (and others). Similar ideas were also studied in Anthony et al. (2017). A recent paper Schrittwieser et al. (2019) presents impressive results of joint model learning and planning in the latent space.

Perhaps, the work which is closest to ours is Lowrey et al. (2018). It is argued in the paper that an agent with limited computational resources in a complex environment needs both to plan and learn from the incoming stream of experience. Importantly, the value function in Lowrey et al. (2018) is modeled by an ensemble of value functions. The risk measure used to combine them is given by the ‘log-sum-exp formula’, Lowrey et al. (2018, equation 6). The authors show experimentally that this approach leads to improvements in various continuous control tasks, including Humanoid. Similar line of research was followed in recent Lu et al. (2019). In our work, we deal with a discrete action setting, which enforces a different planning module (here MCTS-based). Moreover, we treat a more diverse class of risk measures (see Section 2).

Constructing neural network models that would incorporate uncertainty in a principled Bayesian way has proven to be challenging and remains an open problem. A promising new results using ensembles include Osband et al. (2018; 2017); Lakshminarayanan et al. (2017). Including uncertainty in RL dates at least to Strens (2000) who proposes learning a model of an MDP in a Bayesian framework. Practical initiations have been proposed e.g. Janz et al. (2019). In our work, we use an ensemble approach of Osband et al. (2018; 2017), which can also be viewed in this setting; see discussion in Janz et al. (2019, Section 2). Another interesting idea has been presented in O’Donoghue et al. (2017), to relate uncertainty at any time-step to the expected uncertainties at subsequent time-steps. Moerland et al. (2017) proposes to disentangle epistemic and aleatoric uncertainties, using Bayesian drop-out to treat the former and Gaussian distributions for modelling the latter. Ensembles of models were successfully used to improve model-based RL training, see Kurutach et al. (2018); Chua et al. (2018), and the references therein. We note that RL practitioners willingly use unprincipled ensemble methods. For example, in a recent competition Kidzinski et al. (2019) aimed to train an agent able to use a prosthetic leg, four top-ten solutions used some ensemble-based techniques.

Another work similar to ours is Guo et al. (2014), in which the authors use MCTS in the role of an ‘expert’ from which a neural policy is learnt using the DAgger algorithm, Ross & Bagnell (2014). The basic difference is that Guo et al. (2014) uses a classical MCTS without value function nor ensembles.

Many works aim to build planning and learning into neural network architectures, see e.g. Oh et al. (2017); Farquhar et al. (2017). Kaiser et al. (2019), a recent work on model-based Atari, has shown the possibility of sample efficient reinforcement learning with an explicit visual model. Gu et al. (2016) uses model-based methods at the initial phase of training and model-free methods during ‘fine-tuning’. Furthermore, there is a body of work that attempts to learn the planning module, see Pascaru et al. (2017); Racanière et al. (2017); Guez et al. (2019).

Finally, our paper is related to research focusing on study of exploration. Fundamental results in this area concern the multi-arm bandits problem, see Lattimore & Szepesvári (2018) and the references therein. Methods developed in this area have been successfully applied in planning algorithms, see Kocsis et al. (2006) and Silver et al. (2017; 2018). Furthermore, a measure with a loading on variance (defined in Section 2) is related to UCB-V algorithm developed in Audibert et al. (2007). Another set of methods has been...
developed in an attempt to solve notoriously hard Montezuma’s Revenge, see for example Ecaoffet et al. (2019); Guo et al. (2019).

In our work we also use hindsight, see Andrychowicz et al. (2017). Its primarily motivation is to enrich the learning signal and train a universal value function. However, from a certain point of view it can be seen as an exploration algorithm.

### 2. Method

In this section, we describe our method: the planning and exploration components, as well as the training protocol. Algorithm 1 shows how the components are brought together in the training loop. The pseudo-code for planner.run.episode is listed in Algorithm 2 and, for the sake of clarity, the remainder of pseudo-code was moved to Appendix A.1. For the model-based planner component, we develop an MCTS-inspired algorithm.\(^1\)

The main novelty is using a risk-sensitive policy (for tree traversal and action choice) intended to guide exploration. We also investigate techniques exploiting the graph structure, including cycle avoidance\(^2\) and develop a novel method of calculating targets for value function training.

Loop avoidance is an extension of the transposition table techniques, see Childs et al. (2008); Gelly et al. (2012); Swiechowski et al. (2018) and is closely related to the virtual loss method of Segal (2010); McAleer et al. (2019). It is achieved in two ways: by backpropagation of some fixed negative value through the in-tree path ending with a leaf having no unvisited neighbors (see the pseudo-code in Appendix A.1 related to dead_ends), and during tree traversal, when the agent is encouraged to avoid actions leading to previously visited states on the path (see pseudo-code related to penalty_ε in Appendix A.1). To strengthen this effect, the agent is also encouraged to avoid actions leading to previously visited states on the episode level (see parameter penalty_ε in Algorithm 2).

These enhancements combined make it possible to learn even in sparse rewards scenarios, which is experimentally demonstrated in Section 3 (all used environments have sparse rewards). We note that Algorithm 1 is not MCTS specific and other planners could be used as well.

The logic of our MCTS is laid out in Algorithm 2. We assume that any node of the search tree, say n, stores a visit count n.count, accumulated value n.value, accumulated reward n.reward(a), and its children are denoted by n.child(a) for each action \(a \in A\). We define

\[
\hat{Q}_\theta(n) = n.reward(a) + \gamma n.child(a).value,
\]

where \(\gamma > 0\) is a discount rate.

Our proposed risk-sensitive exploration method is implemented in Algorithm 3, see line 7. It is used by the planner both in the action selection step (Algorithm 2, line 9) and during the tree traversal stage (Algorithm 4, line 5). Its key defining elements are uncertainty modeling and risk measurement. A risk-sensitive tree traversal policy is defined as follows:

\[
a^*(n) := \arg \max_a \mathbb{E}_{\theta \sim \Theta} \phi_a(\hat{Q}_\theta(n))
\]

\[
\hat{Q}_\theta(n) := (\hat{Q}_\theta(n,a') : a' \in A),
\]

where \(A\) is the action space, \(\phi_a : \mathbb{R}^{|A|} \rightarrow \mathbb{R}\) is a risk measure, and \(\hat{Q}_\theta\) is an estimator of the \(Q\)-function. The posterior distribution \(\Theta\) models uncertainty in the value estimation.

We approximate the expected value from equation 1, \(\mathbb{E}_{\theta \sim \Theta} \phi_a(\hat{Q}_\theta(n))\), using Monte-Carlo and ensembles, by \(\frac{1}{K} \sum_{i=1}^{K} \phi_a(\hat{Q}_{\theta_i}(n))\), where \(K\) is the size of ensemble. This approximation is motivated by Osband et al. (2018, Lemma 3), see Appendix A.3. In our case we use an ensemble of value functions. In some cases, we "sub-sample" from \(\Theta\), which is inspired by (Osband et al., 2016) and the classical Thomson sampling (see Appendix A.3 for details).

\begin{algorithm}
\caption{planner.run.episode()}
\begin{algorithmic}[1]
\Require
max_episode_len
num_mcts_passes
model
penalty_ε  \triangleright Episode penalty
V_θ  \triangleright Value function
\EndRequire
\Input
episode  \leftarrow \emptyset
\For{step = 1 to max_episode_len}
\State root  \leftarrow s
\State root.value  \leftarrow root.value - penalty_ε
\EndFor
\For{1 to num_mcts_passes}
\State path.leaf  \leftarrow traversal(root)
\State value  \leftarrow expand_leaf(leaf; V_θ; model)
\State backpropagate(value, path)
\EndFor
\State a  \leftarrow choose_action(root, {root})
\State s, r, done  \leftarrow env.step(a)
\If{done} \textbf{break} \EndIf
\State episode.append((root, a, r))
\EndFor
\Return episode, done
\end{algorithmic}
\end{algorithm}
The intuitions behind the aforementioned choices of $\phi_a$’s are as follows. One can think of $\phi_a(x) = e^{\kappa x_a}$, used in Lowrey et al. (2018), as a measure capturing all moments of value ensemble. For small values of $\kappa \approx 0$, it behaves like the measure with a loading on variance (via the Tylor expansion). The mean approximates the value of a given action, while the variance quantifies the epistemic uncertainty. Taking weighted sum of these terms has the aim of balancing exploitation and exploration. It is also related to UCB-V algorithm, see Audibert et al. (2007). Voting, on the other hand, is a well established approach when combining ensembles, see e.g. Breiman (1996) or Rokach (2010). A relative majority vote, in particular, is simple and it can lead to good performance, see e.g. in Osband et al. (2016, Section 6.4). In the context of planning and RL, it has several interesting properties. In particular, the distribution of votes across ensembles encodes the uncertainty related to the optimal action in a given state. High uncertainty may result in stochastic movement (caused by uniform tie breaking), and consequently lead to higher exploration. On the other hand, low uncertainty may result in an exploitative behavior of an agent and, as a result, less exploration. Additionally, voting may improve decision making of an agent in the states, where some action can be dangerous (e.g. lead to irreversible states).

We conclude this section by describing the part of Algorithm 1 related to the update of value functions. The episodes are collected and stored in a prioritized replay buffer. The replay buffer performs some bookkeeping by storing, for each transition, information whether it comes from a solved

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**Algorithm 1** Learning and planning with ensembles

**Require:** Environment `env`, Model `model`

1: Initialize parameters of value function ensemble $\theta = (\theta_1, \ldots, \theta_K)$, $V_\theta = (V_{\theta_1}, \ldots, V_{\theta_K})$

2: Initialize replay_buffer

3: **repeat**

4: $s \leftarrow$ env.reset()

5: episode, solved $\leftarrow$ planner.run_episode$(s; \text{model}, V_\theta)$ $\triangleright$ see Algorithm 2

6: values $\leftarrow$ evaluate_episode$(episode)$ $\triangleright$ see Algorithm 8

7: Optionally calculate a mask $\triangleright$ see Appendix A.3

8: replay_buffer.add$(episode, \text{values, solved, mask})$ $\triangleright$ see Algorithm 9

9: $B \leftarrow$ replay_buffer.batch() $\triangleright$ $B = \{(s_k, v_k, m_k)\}$, see Algorithm 10

10: Update $V_\theta$ by one step of gradient descent

$$\nabla_{\theta_i} \left( \frac{1}{|B|} \sum_{(s, v, m) \in B} m_i (V_{\theta_i}(s) - v)^2 + \zeta ||\theta_i||^2 \right), \text{ for } i \in \{1, \ldots, K\}$$

11: **until** convergence

**Algorithm 3** choose_action()

**Require:** avoid_loops $\triangleright$ Bool

**Input:** n, seen

1: if avoid_loops then

2: $A \leftarrow \{a \in A(n) : \text{n.child}(a) \notin \text{seen}\}$

3: if $A = \emptyset$ then $\triangleright$ Terminal or dead-end

4: return None

5: else

6: $A \leftarrow A(n)$

7: Choose action according to equation 1 from set of available actions $A$

$$a^* \leftarrow \arg \max_{a \in A} E_{\theta \sim \Theta} \left[ \phi_a(\hat{Q}_\theta(n)) \right]$$

8: return $a^*$

Utilizing a risk measure is inspired by Lowrey et al. (2018), who used $\phi_a(x) = e^{\kappa x_a}$ for $x \in \mathbb{R}^{|A|}$ and $\kappa > 0$. In this paper we consider the following choices of $\phi_a$:

- A measure with a loading on variance, $\phi_a(x) = x_a + \kappa x_a^2$, $\kappa > 0$. This includes second moments and can be easily generalized to include variance, standard deviation and exploration bonuses.

- A relative majority vote (also known as plurality vote) measure,

$$\phi_a(x) = 1 \left( \arg \max_{a'} x_{a'} = a \right). \quad (2)$$

Contrary to the other cases, $\phi_a$ defined in equation 2, depends not only on marginal values of its input, but

the whole input (i.e. the estimator vector $\hat{Q}_\theta$). It leads to a rule resembling optimal Bayes classifier form, i.e. the one which chooses $a$ minimizing $\mathbb{P}(a^*_b(s) \neq a)$. 
We utilize various neural network architectures, see Appendix A.2. We measure uncertainty using standard deviation except for the case of Sokoban with randomly-generated boards, where voting was used, see equation 2. Configuration of the experiments is summarized in Table 3 in Appendix A.3.

### 3. Experiments

In this section, we provide experimental evidence to show that using ensembles and risk measures is useful. We chose three environments: Deep-sea, toy Montezuma’s Revenge, and Sokoban. In all cases we work with sparse reward versions of the environments i.e. the agent’s is rewarded only upon successful completion of the task.

We use an MCTS planner with the number of passes equal to 10 (see line 4 of Algorithm 2), which is rather modest for MCTS-like planning methods. Interestingly, we observed that such a relatively weak planner is sufficient to obtain a well-preforming algorithm.

In the Sokoban multi-board experiments, we use a learned model; otherwise we assume access to the perfect model. A good model for the Sokoban environment could be acquired from random trajectories, which is improbable for other domains. Extending our algorithm to these cases is an exciting research direction, which will require development of planning methods robust to model errors, possibly again using ensembles (see e.g. Kurutach et al. (2018)) and training the model and the policy in an interlaced fashion (e.g. similar to Kaiser et al. (2019)).

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3For example, the recent work Schrittwieser et al. (2019) uses 800 passes to plan in board games.

### 3.1. Deep-sea

Deep-sea environment was introduced in Osband et al. (2018, Section 4) and later included in Osband et al. (2019) as a benchmark for exploration. The agent is located in the upper-left corner (position (0, 0)) on a \( N \times N \) grid, \( N \in \mathbb{N} \).

In each timestep, its \( y \)-coordinate is increased, while \( x \) is controlled. The agent issues actions in \{−1, 1\}. These are translated to step left or step right (increasing \( x \) by −1 or +1, respectively, as long as \( x \geq 0 \); otherwise \( x \) remains unchanged) according to a prescribed action mask (not to be confused with transition masks in Algorithm 1). For each step right the agent is punished with \( 0.01/N \). After \( N \) steps, the game ends, and the agent receives reward +1 if and only if it reaches position \((N, N)\). The action mask mentioned above is randomized at each field at the beginning of training (and kept fixed).

Such a game is purposely constructed so that naive random exploration schemes fail already for small \( N \)'s. Indeed, a random agent has chance \((1/2)^N\) of reaching the goal even if we disregard misleading rewards for step right. The exploration progress for our method is shown in Figure 1. In Figure 2, one can see a comparison of non-ensemble models, ensemble models with Thomson sampling (see Appendix A.3) but without uncertainty bonus (\( \kappa = 0 \)), and our final ensemble model with uncertainty bonus \( \kappa = 50 \). We conclude that using both sub-sampling and ensembles is essential to achieving good exploration (for details see also Appendix A.3).

### 3.2. Toy Montezuma’s Revenge

Toy Montezuma’s Revenge is a navigation maze-like environment. It was introduced in Roderick et al. (2018) to evaluate ideas of using higher-level abstractions in long-horizon problems.

While its visual layer is greatly reduced version of the actual Montezuma’s Revenge Atari game, it retains much of the original’s exploration problems. This makes it a useful test environment for exploration algorithms, see e.g. Guo et al. (2019). In our experiments we work with with the biggest map with 24 rooms, see Figure 5. In order to concentrate on the evaluation of exploration we chose to work with sparse rewards. The agent gets reward 1 only if it reaches the treasure room, otherwise the episode is terminated after 300 steps.

It is expected that any simple exploration technique would fail in this case (we provide some baselines in Table 1). Guo et al. (2019) benchmarks PPO, PPO with self imitation learning (PPO+SIL), PPO with count based exploration

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4We use a slightly modified code from https://github.com/chrisgrimm/deep_abstract_q_network
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Figure 1. The heatmaps of standard deviations of ensemble values in the Deep-sea environment. High values are marked in blue and low in white. At the beginning of training (left picture) the standard deviation is high for all states. Gradually it is decreased in the states that have been explored. Finally (the right) the reward state is found. Note that the upper-right part of the board is unreachable.

Figure 2. Comparison of number of steps needed to solve the deep-sea environment with given grid size $N$. Orange dots marks trials which were unable to solve problem in 1400000 steps. Large problem instances ($N > 20$) are solved only when exploration bonus is used (right-most plot, $\kappa = 50$).

DTSIL builds on the intermediate partial solutions, which are ranked according to their reward, thus we suspect it would fail in the sparse reward case.

The results are summarized in Table 1. We have three setups: no-ensemble, ensemble, no std, ensemble, std. In the first case, we train using Algorithm 1 with a single neural-network. In the second case, for each episode we sub-sample 10 members of an ensemble of size 20 to be used and MCTS is guided by their mean. In the final, third case, we follow the same protocol but we add to the mean the standard deviation. In our experiments we observe that no-ensemble in 30 out of 43 cases does not leave behind the first room. The setup without explicit exploration bonus, ensemble, no std, perform only slightly better. Finally, we observe that ensemble, std behaves very well.

Further experimental details and the network architecture are presented in Appendix A.2 and A.3.

| Setup          | Solved / no. seeds | Av. visited rooms |
|----------------|-------------------|------------------|
| no-ensemble    | 0 / 43            | 4.7              |
| ensemble, no std | 2 / 40           | 5.8              |
| ensemble, std  | 30 / 37           | 17.5             |

Table 1. Result for toy Montezuma’s Revenge. We report the number of runs which found solution in $1.2 \times 10^6$ steps and the number of seeds of network initialization. We also show the average number of visited rooms, which is a proxy of the learning progress.

3.3. Sokoban

Sokoban is an environment known for its combinatorial complexity. The agent’s goal is to push all boxes (marked as yellow, crossed squares) to the designed spots (marked as squares with a red dot in the middle), see Figure 3. Apart from the navigational challenge, the difficulty of this game is greatly increased by the fact that some actions are irreversible. A canonical example of such an action is pushing a box into a corner, though there are multiple less obvious cases. Formally, this difficulty manifests itself in the fact that deciding whether a level of Sokoban is solvable or not, is NP-hard, see e.g. Dor & Zwick (1999). Due to these
challenges the game has been considered as a test bed for reinforcement learning and planning methods.

Operationally, to generate Sokoban levels we use an automated procedure proposed by Racanière et al. (2017). Some RL approaches to solving Sokoban (e.g. Racanière et al. (2017); Guez et al. (2019)) assume additional reward signal in the game, e.g. for pushing a box into a designed spot. In this work we use sparse setting, that is the agent is rewarded only when all the boxes are put in place.

It is interesting to note, that Sokoban offers two exploration problems: single-level-centric, where a level-specific exploration is needed, and multi-level-centric, where a ‘meta-exploration’ strategy is required, which works in a level-agnostic manner or can quickly adapt. As a result, we conducted three lines of experiments using ensembles: a) learning to solve randomly generated boards (dubbed as multiple-boards Sokoban), b) learning to solve a single board (dubbed as single-boards Sokoban), c) transfer and learnable ensembles.

In our experiment we use Sokoban with board of size (10, 10) and 4 boxes. We use the limit of 200 steps in the experiment a) and 100 in the remaining ones.

**Multiple-board Sokoban: learning to solve randomly generated boards** In this experiment we measure the ability of our approach to solve randomly generated Sokoban boards. We show also that the approach is flexible enough to accommodate for the use of a learned model of dynamics. More precisely, the planning described in Algorithm 2 is performed using this model.

The model is trained using a set of trajectories obtained by a random (uniform) agent. The major difficulty in obtaining the model is learning (sparse) rewards. The ratio of non-zero reward transitions is less than 3e-6. To tackle this problem we generated a dataset consisting of boards with 1, 2, 3, 4 boxes and substantially upsample rewarded transitions. Details are provided in Appendix A.3.

**Single-board Sokoban: learning to solve a single board** In this experiment we measure the extent in which our methods can plan and learn on single boards. We note that this setting differs substantially from the one in the previous paragraph. In the multiple-boards Sokoban there is a possibility of generalization from easier to harder scenarios (e.g. MCTS with randomly initialized value network solves \( \approx 0.7 \) % of boards). Such a transfer is not possible in the single-board case studied here. On the other hand, the algorithm gathers multiple episodes from the same board, which enables the agent to explore the board’s state space.

For the single-board Sokoban we used experimental settings similar to the one in Section 3.2, see also details in Appendix A.3. We observe that the setup with ensembles solves 73% compared to 50% the standard training without ensembles (experiments with and without ensembles were performed on a common set of 250 randomly generated boards). The latter might seem surprisingly good, taking into account the sparse reward. This follows by the loop avoidance described...
Table 2. Results of transfer experiments. We test transfers from one value function (Trans. 1) and transfer from ensembles of 2 and 3 value functions (Trans. 2 and Trans. 3). In the later two cases the aggregation of values is learned. The results are averaged over 20 seeds.

| Architecture | Random | Trans. 1 | Trans. 2 | Trans. 3 |
|--------------|--------|----------|----------|----------|
| 5-layers     | 0.7%   | 4.9%     | 7.1%     | 8.5%     |
| 4-layers     | 0.7%   | 4.3%     | 5.6%     | 7.3%     |

in Section 2. If during planning the agent finds itself in a situation from which it cannot find a novel state (i.e. encounters dead_end in Algorithm 6) a negative value, set to −2 in our experiments, is backpropagated in Algorithm 5 to already seen vertices. We speculate that this introduces a form of implicit exploration.

In the single-board Sokoban case we performed also experiments on (8, 8) boards with 4 boxes obtaining success rate of 94% compared to 64% on the standard non-ensemble settings.

Sokoban: transfer and learnable ensembles Generating any new board can be seen as a cost dimension along with sample complexity. This quite naturally happens in meta-learning problems. We tested how value functions learned on small number of boards perform on new, previously unseen, ones. We used the following protocol: we trained value function on fixed number of 10 games. To ease the training, we used relabelling akin to Andrychowicz et al. (2017). We evaluated these functions on other boards. It turns out that they are typically quite weak, which is not very surprising, as solving 10 boards does not give much chance to infer ‘the general’ solutions. Next, we used ensembles of the value functions. More precisely, we calculated the values of \( n = 2, 3 \) models and aggregated them using a small neural network with one fully connected hidden layer. This network is learnable and trained using the standard setup. We observe that the quality increases with the number of value functions in the ensemble as summarized in Table 2. We observed high variability of the results over seeds, which is to be expected as Sokoban levels significantly vary in difficulty. We also observe that maximal results for transfer increase with the number of value function, being approximately 10%, 11% and 12%. This further supports the claim that ensembling may lead to improved performance. In 5-layer experiment we use a network with 5 hidden convolutional neural network layers, see details in Appendix A.2, we compare this with an analogous 4 layers network. In the latter case, we obtain a weaker result. We speculate this might be due to the fact that larger networks generalize better, see e.g. Cobbe et al. (2019).

4. Conclusions and further work

In this paper, we introduced a reinforcement learning method that blends planning, learning, and risk-sensitive approach to exploration. We verified experimentally that such a setup is useful in solving hard exploration problems, i.e. problems characterized by sparse rewards and long episodes (e.g. spanning even hundreds of steps).

We believe that this opens promising future research directions. There are multiple ensemble design choices, and we tested only a selected few. Additionally, there are more ways to combine the results of ensembles and it would be interesting to see if one, relatively general, method can be found. Such a result would be a step towards deep Bayesian learning.

In our work, we used a learned model in the case Sokoban, in which a relatively good model could be obtained from random trajectories. It would to interesting to cover a general case, when learning model and agent’s behaviour needs to occur simultaneously. Perhaps the most challenging problem is making planner robust to model errors. Equally important research direction would be related to solving stochastic environments. This might be considerably more difficult as such a task requires disentangling epistemic (studied in this work) and aleatoric (coming from the environment) uncertainties.

We focused our attention on MCTS, but there is a priori no reason why some other planning method should not yield better results. In some initial experiments we obtained promising, but yet inconclusive, results using the Levin tree search (see Orseau et al. (2018)). Another tempting direction is training both value function and a policy, akin to methods of Silver et al. (2017).

It would also be interesting to isolate the proposed exploration method from the planner and see how it fares when coupled with model-free algorithms. This fits along the lines of some recent research directions, see e.g. Agarwal et al. (2019).

Going further, we speculate that it may be possible to use the methods developed for Sokoban in meta-learning and continual learning grounds problems, perhaps akin to recent Lu et al. (2019). Measures of uncertainty can possibly enable a learning system to adapt to a changing environment. In an archetypical case, this might be obtained by choosing from ensemble a model (a skill) which is useful at the moment and understanding situations that such a model is not yet present.
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A.1. Algorithm

In this section we detail the building blocks of Algorithm 1. Our algorithm takes into account the graph structure of the underlying environment. Following inspiration of the transposition table techniques, see Childs et al. (2008); Gelly et al. (2012); Swiechowski et al. (2018), we calculate and store values corresponding to the nodes of the graph (i.e. the states of the environment). These nodes are clearly different than the nodes of the tree search. To ease the notation, we write node.value, node.value instead of node.state.value, node.state.value, respectively (with the exception of Algorithm 6, where these are explicit). Importantly, in our approach these values are vectors of dimension equal to the size of ensemble.

As mentioned in Section 2, the key elements of MCTS (see Algorithm 2) are: tree traversal, leaf expansion and backpropagation (shown in Algorithm 4, Algorithm 6 and Algorithm 5, respectively).

Algorithm 6 shows how the model and value function enter the picture. The model is used for generating next states (line 10) and the value function evaluates new, previously unvisited, states. The visited states are kept in a global transposition table. Algorithm 7 shows the update of a tree node.

Algorithm 4 and Algorithm 5 both use variable penalty\_p. This is a penalty corresponding to entering the same states during tree traversal stage (hence is operates on the planner level) and the change is applied during traversal, and undone during backpropagation.

---

### Algorithm 4 traversal()

**Require:** penalty\_p  
**Input:** root  
1: n ← root  
2: path ← ∅  
3: while n is not a leaf do  
4: n.value ← n.value − penalty\_p  
5: a ← choose_action(n.path)  
6: if a is None then break  
7: path.append((n,a))  
8: n ← n.child(a)  
9: if n not yet visited then  
10: return path, n

### Algorithm 5 backpropagate()

**Require:** penalty\_p, γ  
**Input:** v, path  
1: for (n, a) in reversed(path) do  
2: n.value ← n.value + penalty\_p  
3: v ← n.reward + γv  
4: update(n, v)

### Algorithm 6 expand_leaf()

**Require:** dead_end_value, V\_θ, model  
**Input:** leaf  
1: if leaf is terminal then  
2: update(leaf, 0)  
3: return 0.  
4: else if leaf is a dead end then  
5: update(leaf, dead_end_value)  
6: return dead_end_value  
7: else  
8: for a ∈ A(leaf) do  
9: new_tree_node ← create_tree_node()  
10: next_state ← model(leaf.state,a)  
11: new_tree_node.state ← next_state  
12: if next_state not yet visited then  
13: next_state.value ← V\_θ(next_state)  
14: leaf.child(a) ← new_tree_node  
15: return leaf.value

### Algorithm 7 update()

**Input:** n, value  
1: n.value ← n.value + value  
2: n.count ← n.count + 1

---

The following blocks of code are related to the training setup. Algorithm 8 is responsible for computing an appropriate value for each element of the episode. There are two available modes: bootstrap, which utilizes the values accumulated during the MCTS phase, and factual, which represents the sum of discounted rewards in the episode. In the bootstrap mode we undo the penalty applied during the episode generation stage (line 5 in the Algorithm 2). We recall also that s\_i.value is a vector of dimension equal to the ensemble size; we take its mean in line 4. Up to our knowledge, the bootstrap mode is novel and performed favourably in experiments, see Appendix A.5.3.

The inner details of replay buffer, in particular Hindsight and prioritisation, are given in Algorithm 9 and Algorithm 10. Hindsight refers to any method that processes episode, and potentially overrides states values (see lines 1-2 in Algorithm 9). Algorithm 10 shows the way a batch is generated. First, for each transition it is determined whether it should be sampled
from a solved or unsolved episode (according to a fixed ratio). Second, a game is sampled from a population determined in
the previous step, with probability proportional to the game length. Finally, given a game a transition is chosen uniformly.

Algorithm 8 evaluate_episode()

Require: mode \(\triangleright\) String
penalty \(\triangleright\) Episode penalty

Input: episode \(\triangleright\) \(\{(s_t, a_t, r_t)\}\)
solved \(\triangleright\) Bool
\(\gamma\) \(\triangleright\) Discount rate

1: \(T \leftarrow \text{len(episode)}\)
2: values \(\leftarrow [0, \ldots, 0] \in \mathbb{R}^T\)
3: if mode = "bootstrap" then
4: \(\text{values} \leftarrow \text{mean}(s_t, \text{value}), t \in 0, \ldots, T - 1\]
5: \(\text{values} \leftarrow \text{values} + \text{penalty}_e\)
6: else if mode = "factual" then
7: \(r \leftarrow [0, \ldots, 0, 1_{\text{solved}}]\)
8: for \(t = T - 1 \text{ to } 1\) do
9: \(\text{values}_{t-1} \leftarrow \gamma \text{values}_t + r_t\)
10: return values

Algorithm 9 replay_buffer.add()

Require: \(\mathcal{D}\) \(\triangleright\) Replay Buffer
\(H\) \(\triangleright\) Hindsight mapping

Input: episode \(\triangleright\) \(\{(s_t, a_t, r_t, w_t)\}\)
value \(\triangleright\) \{\(v_t\}\)
solved \(\triangleright\) Bool
mask \(\triangleright\) Binary vector

1: for \(t = 0 \text{ to } T - 1\) do
2: \(v_t \leftarrow H(\text{episode})_t\)
3: \(\mathcal{D} \leftarrow \mathcal{D} \cup \{(s_t, v_t), \text{solved}, \text{mask}\}\)

Algorithm 10 replay_buffer.batch()

Require: \(\mathcal{D}\) \(\triangleright\) Replay Buffer
size \(\triangleright\) Batch size
ratio \(\triangleright\) Solved/unsolved

1: Initialize \(B \leftarrow \emptyset\)
2: for \(b = 1 \text{ to } \text{size}\) do
3: if \(b \times \text{ratio}\%1 = 0\) then
4: \(\text{select} \leftarrow \text{False}\)
5: else
6: \(\text{select} \leftarrow \text{True}\)
7: \(D' \leftarrow \{d \in \mathcal{D}: d.\text{solved} = \text{select}\}\)
8: Sample \(d \in D'\) with
\(\text{prob}(d) \propto \text{len}(d.\text{episode})\)
9: Sample \((s, v, m)\) uniformly from \(d\)
10: \(B \leftarrow B \cup \{(s, v, m)\}\)
11: return \(B\)

A.2. Architectures and input formats

Deep-sea For the Deep-sea environment we encode a state as a one hot vector of size \(N^2\), and learn a simple linear
transformation for the value estimation.

Toy Montezuma Revenge Observations are represented as tuples containing the location of the current room, the agent's
position within the room and the status of all keys and doors on the board. To estimate value, we use fully-connected neural
networks with two hidden layers of 50 neurons each.

Single-board Sokoban Observations have shape \((10, 10, 7)\), where the first two coordinates are spatial and the third one
is a one-hot encoding of the type of a state (e.g. box, target, agent, wall). To estimate the value, we flatten the observation
and apply fully-connected neural networks with two hidden layers of 50 neurons each.

Multiple-boards Sokoban We use the same observation type as in the single-board problem. Each value function network
is composed of five \(3 \times 3\) convolutional layers with with stride 1, followed by two fully connected layers with 128 units and
1 unit, respectively.

Now we describe details of the model architecture. The input consists of a one-hot representation of a board (as above)
and an action in \(\{1, \ldots, 4\}\). The one-hot representation of the action is concatenated with the board resulting in a tensor of
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shape (10, 10, 11). It is processed through two convolutional layers with the kernel sizes (5, 5) and 64 channels. We then apply a neural network with two heads. The first one applies a point-wise dense layer to produce the next Sokoban frame (again one-hot encoded). The second uses the global average pooling and a linear layer to predict if input state and action generates a reward (which in our sparse setup is equivalent to solving the board).

Sokoban: transfer and learnable ensembles In the 5-layer experiment we use the same architecture as in the multiple-boards Sokoban. In the 5-layer we remove one of inner hidden convolutional layers.

Figure 5. The biggest toy Montezuma’s Revenge map, consisting of 24 room. The goal is to reach the room marked with G. The agent needs to avoid traps (marked in red) and pass through doors (marked in blue). Doors are open using keys (marked in yellow).

A.3. Training details

Masks An important decision for training is how to assign transitions to the particular elements of value functions ensemble. This is implemented using masks, see Algorithm 1. Suppose a batch \( B \) is to be used in an update step (see lines 9-10 of Algorithm 1) and let \( \tau = (s, v, m) \in B \) be a transition. A mask \( m \in \{0, 1\} \) has the following interpretation: \( m_i = 1 \) if and only if the transition \( \tau \) is used to train \( V_{\theta_i}, i = 1, \ldots, K \).

We experimented with the following versions of masking:

- dynamic masks: masks are generated anew whenever transition is sampled from replay buffer,
- static masks: each transition is assigned a fixed mask generated when added to the replay buffer.

In the cases of dynamic masks, each batch was split equally among the elements of ensemble (for this we kept the batch size to be the multiplicity of the number of ensembles). The static masks were inspired by the Bootstrapped DQN, see Osband et al. (2016, Appendix B), where it is a core idea. We experimented with applying a different mask to each transition according to the Bernoulli distribution, or to assign the same masks for all transitions in the same trajectory.

We found it useful to use static masks in the Deep-sea, Toy Montezuma’s Revenge and Single-board Sokoban experiments, and dynamic masks in Multiple-board Sokoban experiments.

Ensembles sampling Recall that equation 1 involves calculating the expected value, \( E_{\theta \sim \Theta} \), with respect to the posterior distribution \( \Theta \). In some experiments we instead sub-sample from \( \Theta \). Such an approach follows Osband et al. (2016), which itself is inspired by the classical Thomson sampling (see discussion Osband et al. (2016, Section 4) and the original Thompson (1933)). To be concrete, for a given a risk measure \( \phi_a \), equation 1 reduces to

\[
a^*(n) := \arg\max_a \sum_{i \in \mathcal{E}} \left[ \phi_a(Q_{\theta_i}(n)) \right],
\]

where \( \mathcal{E} = \{1, \ldots, K\} \). Sub-sampling, with a fixed parameter \( \ell \), is equivalent to computing equation 3, with \( \mathcal{E} \) taken as a random subset of \( \{1, \ldots, K\} \) of cardinality \( \ell \).

Model training In this section, we describe the details of training of the environment model used for planning in the multi-board Sokoban experiments, see Section 3.3. As noted in the main text, we found out that randomly generated
trajectories very rarely solve boards with 4 boxes (in fact less than $3e^{-6}$ of transitions contains solved boards). To ensure enough transitions resulting in a solved board, we sampled 100000 episodes of length 40 using boards containing $\{1, 2, 3, 4\}$ boxes. In total, only 0.05% of transitions were labeled as solved. To enable neural network training, we upsample positive transitions 100 times. The model of the environment was not fine-tuned while training the RL agent; however, it was quite good. During this phase, we logged errors in model predictions encountered on the top-level trajectory (enrolled with the real environment). In 99.5% of cases, the Sokoban frames predicted by the learned model matched the ground truth. Events of false reward predictions were even less frequent $\leq 1e^{-6}$. However, we did not measure how many errors were made in the rollouts inside the search tree.

**Randomized priors** It was shown in Osband et al. (2018, Lemma 3) that for Bayesian linear regression setting with Gaussian prior and noise model, generating samples from posterior distribution is equivalent to solving an appropriate optimization problem. To be exact, suppose $D = \{(x_i, y_i)\}$ is the dataset, $f_\theta(x) = x^T\theta$ is the regression function, $\epsilon_i$ is a Gaussian noise, $\theta$ comes from a Gaussian prior, and $\tilde{y}_i = y_i + \epsilon_i$. Then the solution of the following problem

$$\arg\min_{\theta} (||\tilde{y}_i - (f_\theta + f_\theta)(x_i)||^2_2 + \zeta||\theta||^2_2),$$

for some $\zeta > 0$, enables one to sample from the posterior $\theta|D$. Consequently, Osband et al. (2018) propose to use equation 4 as a training objective and include randomized prior in the value function approximator. This objective is matched with the one used in Algorithm 1. We observed that the presence of randomized priors did not improve performance, hence we did not include them in final experiments.

### A.4. Hyperparameters

We summarize the parameters of the training used in Deep-sea, Toy Montezuma’s Revenge, Single-board Sokoban and Multiple-boards Sokoban experiments presented in Section 3.

| Parameter                              | Deep-sea | Toy MR | Single-b. Sok. | Multiple-b. Sok. |
|-----------------------------------------|----------|--------|----------------|------------------|
| Number of MCTS passes                   | 10       | 10     | 10             | 10               |
| Ensemble size $K$                       | 20       | 20     | 20             | 3                |
| Ensemble sub-sampling $\ell$            | 10       | 10     | 10             | no               |
| Risk measure $\kappa$                   | mean+std, mean+std, mean+std, voting |
| VF target $\kappa$                      | 50       | 3      | 9              | n/a              |
| Discounting $\gamma$                    | 0.99     | 0.99   | 0.99           | 0.99             |
| Randomized prior $\zeta$                | no       | no     | no             | no               |
| Optimizer $\zeta$                       | RMSProp  | RMSProp | RMSProp       | RMSProp          |
| Learning rate                           | $2.5e^{-4}$ | $2.5e^{-4}$ | $2.5e^{-4}$ | $2.5e^{-4}$ |
| Batch size                              | 32       | 32     | 32             | 32               |
| Mask                                    | static   | static | static         | dynamic          |

1. `num_mcts_passes` in the MCTS algorithm, see Algorithm 2
2. the number of value functions in ensemble in Algorithm 1
3. the parameter of ensemble sub-sampling, see the second paragraph of Section A.3
4. `mean+std` stands for mean $+ \kappa \cdot$ std, where mean is the mean of the ensemble predictions and std is its standard deviation. `voting` stands for using as given by equation 2
5. see footnote 4
6. see description in Section 2 and Algorithm 8
7. as used in Algorithm 8
8. see Section 2 and Appendix A.3
9. the optimizer used in line 10 of Algorithm 1
10. the optimizer’s learning rate
11. cardinality of batch $B$ in line 9 of Algorithm 1
12. line 10 of Algorithm 1

*Table 3. Default values of hyperparameters used in our experiments.*
A.5. Ablations

In this section we analyze various experiment design choices.

A.5.1. Masks

We conjecture that masks prevent premature convergence of the members of the ensemble to the same values. We found that using masks (see Algorithm 1 and Appendix A.3) was crucial in the Deep-sea environment. In Figure 6 we observe failures of the setup without masks occurring on larger boards. Their careful analysis revealed that the agent often get stuck on a single, sub-optimal, trajectory. Masks also played important role also in the Toy Montezuma’s Revenge environment, see Table 4.

![Figure 6. Deep-sea training with or without splitting training data between ensemble members.](image)

| Setup       | solved / no. runs | av. visited rooms |
|-------------|-------------------|-------------------|
| without mask| 22 / 50           | 13.0              |
| with mask   | 30 / 37           | 17.5              |

*Table 4. Toy Montezuma’s Revenge - ratio of successful runs when learning ensembles with or without mask. Different runs were performed with different random seeds.*

A.5.2. Ensemble size

Using ensembles is crucial to our method as it enables us to define a risk-sensitive tree traversal policy, as indicated in equation 1 and Algorithm 3. The optimal number of ensembles seems to depend on the environment and probably other hyper-parameters. In Figure 7 we compare the training behavior for different ensemble sizes for the Deep-sea (recall also Figure 2). Ensemble sizes as high as 20 are needed in this case. For multi-board Sokoban experiments, see Section 3.3, we found out that the ensemble of size 3 was enough to improve over no-ensemble baseline. Increasing the size of the ensemble offers only marginal further gains, see Figure 8.

A.5.3. Value target

Using bootstrap, see Section 2 and Algorithm 8, is a technical novelty of our work. We found that it works better than the standard factual method in all our experiments. In Figure 9 and Figure 10 we offer a comparison for the Deep-sea and Sokoban, respectively.
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Figure 7. Deep Sea training with different ensemble sizes.

Figure 8. Multiple-boards Sokoban with different sizes of ensemble. Values 3, 5 and 7 result in similar performance.
Figure 9. Deep-sea training with different training targets.

Figure 10. Multiple-boards Sokoban. Comparison of factual and bootstrap training targets.
A.5.4. Search size

The parameter `num_mcts_passes` (see Algorithm 2) is perhaps the most important parameter of the planner. Increasing `num_mcts_passes` increases the computational costs and improves the quality of the planner. In this paper we purposefully focused on studies of exploration in the low computational-complexity regime setting `num_mcts_passes = 10`. This number is very modest compared to other works, for example in a recent paper Schrittwieser et al. (2019) declares 800 passes was used to plan in board games. In Figure 11 we present a comparison of performance for various numbers of MCTS passes.

Another important parameter is `max_episode_len`. In the environments in which the episode does not have a fixed length, longer planning may yield positive results. In the multi-board Sokoban setting, increasing the values of `max_episode_len` slows down initial learning (weak agent will collect episodes of maximal length), but they ensure better learning at later phases of the training. We found 200 to be a sweet-spot, which is \( \approx 4 \) times higher than the average solution length. See Figure 12 for details.

Figure 11. Multiple-boards Sokoban. Ensemble agent with different number of MCTS passes.
Figure 12. Multiple-boards Sokoban. Ensemble agent with different environment step limit per episode.