Tackling Decision Processes with Non-Cumulative Objectives using Reinforcement Learning

Abstract

Markov decision processes (MDPs) are used to model a wide variety of applications ranging from game playing over robotics to finance. Their optimal policy typically maximizes the expected sum of rewards given at each step of the decision process. However, many real-world problems do not fit straightforwardly into this framework: Non-cumulative Markov decision processes (NCMDPs), where instead of the expected sum of rewards, the expected value of an arbitrary function of the rewards is maximized. Example functions include the maximum of the rewards or their mean divided by their standard deviation. In this work, we introduce a general mapping of NCMDPs to standard MDPs. This allows all techniques developed to find optimal policies for MDPs, such as reinforcement learning or dynamic programming, to be directly applied to the larger class of NCMDPs. We demonstrate the effectiveness of our approach in diverse reinforcement learning tasks, including classical control, financial portfolio optimization, and discrete optimization. Our approach improves both final performance and training efficiency compared to relying on standard MDPs.

1 Introduction

Markov decision processes (MDPs) are used to model a wide range of applications where an agent iteratively interacts with an environment during a trajectory. Important examples include robotic control (Andrychowicz et al., 2020a), game playing (Mnih et al., 2015), or discovering algorithms (Mankowitz et al., 2023). At each time step t of the MDP, the agent chooses an action based on the state of the environment and receives a reward r_t. The agent's goal is to follow an ideal policy that maximizes

$$\mathbb{E}_\pi \left[\sum_{t=0}^{T-1} r_t \right], \tag{1}$$

where T is the length of the trajectory and the expectation value is taken over both the agent's probabilistic policy π and the probabilistic environment. There exist a multitude of established strategies for finding (approximately) ideal policies of MDPs, such as dynamic programming and reinforcement learning (Sutton & Barto, 2018).

A limitation of the framework of MDPs is the restriction to ideal policies that maximize Equation (1), while a large class of problems cannot straightforwardly be formulated this way. For example, in weakest-link problems, the goal is to maximize the minimum rather than the sum of rewards, e.g. in network routing one wants to maximize the minimum bandwidths along a path (Cui & Yu, 2023). In finance, the Sharpe ratio, i.e. the mean divided by the standard deviation of portfolio gains, is an important figure of merit of an investment strategy, since maximizing it will yield more risk-averse strategies than maximizing the sum of portfolio gains (Sharpe, 1966). We therefore require a method to tackle non-cumulative Markov decision processes (NCMDPs), where instead of the expected sum of rewards, the expectation value of an arbitrary function of the rewards is maximized. The main contribution of this paper is twofold:

1. We expand the scope of reinforcement learning by introducing a theoretical framework that maps NCMDPs to standard MDPs. This mapping enables direct application of advanced MDP solvers,

Figure 1: Mapping of a decision process with non-cumulative objective (blue) to a corresponding Markov decision process with adapted states and rewards (orange) that can be solved by standard methods (black). For details and notation, see Section 2.

    including reinforcement learning and dynamic programming, to NCMDPs without modification. Our approach accommodates general non-cumulative objectives and is straightforward to implement.

2. We conduct numerical experiments demonstrating the effectiveness of deep reinforcement learning on NCMDPs across complex applications with large state and action spaces, including portfolio optimization, classical control, and discrete optimization. Our results indicate improvements in training efficiency and final performance compared to prior reinforcement learning approaches.

2 Theoretical Analysis

2.1 Preliminaries

In an MDP, an agent iteratively interacts with an environment during a trajectory. At each time step t, the agent receives the current state s_t of the environment and selects an action a_t by sampling from its policy $\pi(a_t|s_t)$, which is a probability distribution over all possible actions given a state. The next state of the environment s_{t+1} and the agent's immediate reward r_t are then sampled from the transition probability distribution $p(r_t, s_{t+1}|s_t, a_t)$, which depends on the MDP. This process repeats until it reaches a terminal state. The ideal policy of the agent maximizes the expected sum of immediate rewards, i.e. Equation (1). Note that we take this ideal policy to be part of the definition of an MDP to distinguish MDPs from NCMDPs with different ideal policies. For simplicity, we discuss only non-discounted, episodic MDPs. However, generalization to discounted settings is straightforward.

2.2 Non-cumulative Markov Decision Processes

In the following, we denote states and rewards related to NCMDPs by $\tilde{s}_t$ and $\tilde{r}_t$, respectively, to distinguish them from MDPs. We define NCMDPs equivalently to MDPs except for their ideal policies maximizing the expectation value of an arbitrary scalar function f of the immediate rewards $\tilde{r}_t$ instead of their sum, i.e.

$$\mathbb{E}_\pi \left[f(\tilde{r}_0, \tilde{r}_1, \ldots, \tilde{r}_{T-1}) \right]. \tag{2}$$

To accommodate trajectories of arbitrary finite length, we require f to be a family of functions consisting of a function $f_t : \mathbb{R}^t \to \mathbb{R}$ for each $t \in \mathbb{N}$. For brevity, we denote $f_t(\tilde{r}_0, \tilde{r}_1, \ldots, \tilde{r}_{t-1}) = f(\tilde{r}_0, \tilde{r}_1, \ldots, \tilde{r}_{t-1})$. NCMDPs still have a Markovian transition probability distribution but their return, i.e. Equation (2), can depend on the rewards in a non-cumulative and therefore non-Markovian way. Thus, NCMDPs are a generalization of MDPs. Due to this distinction, MDP solvers cannot straightforwardly be used for NCMDPs. To solve this problem, we describe a general mapping from an NCMDP $\tilde{M}$ to a corresponding MDP M with adapted states and adapted rewards but the same actions. The mapping is chosen such that the optimal

Table 1: Examples of non-cumulative objective functions f.

$f(\tilde{r}_0,\ldots,\tilde{r}_t)$	Additional state information h_t	Adapted reward r_t
$\max(\tilde{r}_0,\ldots,\tilde{r}_t)$	$h_0 = -\infty,\ h_{t+1} = \max(h_t, \tilde{r}_t)$	$r_0 = \tilde{r}_0$
$r_t = \max(0, \tilde{r}_t - h_t), t > 0$
$\min(\tilde{r}_0,\ldots,\tilde{r}_t)$	$h_0 = \infty,\ h_{t+1} = \min(h_t, \tilde{r}_t)$	$r_0 = \tilde{r}_0$
$r_t = \min(0, \tilde{r}_t - h_t), t > 0$
Sharpe ratio
$\frac{\mathrm{MEAN}(\tilde{r}_0,\ldots,\tilde{r}_t)}{\mathrm{STD}(\tilde{r}_0,\ldots,\tilde{r}_t)}$	$h_0 = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix},\ h_{t+1} = \begin{bmatrix} \frac{h_t^{(2)}}{h_t^{(2)}+1} h_t^{(0)} + \frac{1}{h_t^{(2)}+1}\tilde{r}_t \\ \frac{h_t^{(2)}}{h_t^{(2)}+1} h_t^{(1)} + \frac{1}{h_t^{(2)}+1}\tilde{r}_t^2 \\ h_t^{(2)} + 1 \end{bmatrix}$	$r_t = \frac{h_{t+1}^{(0)}}{\sqrt{h_{t+1}^{(1)} - h_{t+1}^{(0)2}}}$
$- \frac{h_t^{(0)}}{\sqrt{h_t^{(1)} - h_t^{(0)2}}}$
$\max_{k \in [-1,t]} \sum_{i=0}^{k} \tilde{r}_i$	$h_0 = 0,\ h_{t+1} = \max(0, h_t - \tilde{r}_t)$	$r_t = \max(0, \tilde{r}_t - h_t)$
$\tilde{r}_0 \tilde{r}_1 \ldots \tilde{r}_t$	$h_0 = 1,\ h_{t+1} = \tilde{r}_t h_t$	$r_0 = \tilde{r}_0,$
$r_t = h_{t+1} - h_t, t > 0$
Harmonic mean
$\frac{1}{\frac{1}{\tilde{r}_0} + \cdots + \frac{1}{\tilde{r}_t}}$	$h_0 = 0, h_{t+1} = h_t + \frac{1}{\tilde{r}_t}$	$r_0 = \tilde{r}_0,$
$r_t = \frac{1}{h_{t+1}} - \frac{1}{h_t}, t > 0$
$\delta^t \sum_{k=0}^{t} \tilde{r}_k,$
$\delta \in (0,1)$	$h_0 = \begin{bmatrix} 0 \\ 0 \end{bmatrix},\ h_{t+1} = \begin{bmatrix} h_t^{(0)} + \tilde{r}_t \\ h_t^{(1)} + 1 \end{bmatrix}$	$r_t = \delta^{h_{t+1}^{(1)}} h_{t+1}^{(0)}$
$- \delta^{h_t^{(1)}} h_t^{(0)}$
$\frac{1}{t+1} \sum_{k=0}^{t} \tilde{r}_k$	$h_0 = \begin{bmatrix} 0 \\ 0 \end{bmatrix},\ h_{t+1} = \begin{bmatrix} h_t^{(0)} + \tilde{r}_t \\ h_t^{(1)} + 1 \end{bmatrix}$	$r_t = \frac{1}{h_{t+1}^{(1)}} h_{t+1}^{(0)}$
$- \frac{1}{h_t^{(1)}} h_t^{(0)}$

policy of $\tilde{M}$ is equivalent to the optimal policy of M. Therefore, a solution for $\tilde{M}$ can readily be obtained by solving M with existing MDP solvers, as shown in Figure 1. In the following, we formalize these ideas.

Definition 1. *Given an NCMDP $\tilde{M}$ with rewards $\tilde{r}_t$, states $\tilde{s}_t$, actions a_t, the Markovian state transition probability distribution $\tilde{p}(\tilde{r}_t, \tilde{s}_{t+1}|\tilde{s}_t, a_t)$, and non-cumulative objective function f, we define a corresponding MDP M with rewards r_t, states s_t, the same actions a_t, and state transition probability distribution $p(r_t, s_{t+1}|s_t, a_t)$ with functions ρ and u, and vectors h_t with initial values h_0 such that*

$$r_t = f(\tilde{r}_0, \ldots, \tilde{r}_t) - f(\tilde{r}_0, \ldots, \tilde{r}_{t-1}) = \rho(h_t, \tilde{r}_t), \tag{3}$$

$$s_t = (\tilde{s}_t, h_t) \text{ with } h_{t+1} = u(h_t, \tilde{r}_t), \tag{4}$$

$$p\big(r_t, s_{t+1}{=}(\tilde{s}_{t+1}, h_{t+1})|s_t{=}(\tilde{s}_t, h_t), a_t\big) = \sum_{\tilde{r}_t} \tilde{p}(\tilde{r}_t, \tilde{s}_{t+1}|\tilde{s}_t, a_t)\delta_{h_{t+1}, u(h_t, \tilde{r}_t)}\delta_{r_t, \rho(h_t, \tilde{r}_t)}, \tag{5}$$

where δ is the Kronecker delta. For continuous probability distributions, the sum should be replaced by an integral and the δ by Dirac delta functions.

We now provide some intuition for this definition: Equation (3) ensures that the return of M, i.e. $\sum_{t=0}^{T-1} r_t$, is equal to the return of $\tilde{M}$, i.e. $f(\tilde{r}_0, \ldots, \tilde{r}_{T-1})$. To compute the immediate rewards r_t of M in a purely Markovian manner, we need access to information about the previous rewards of the trajectory. This can be achieved by extending the state space with h_t, which preserves all necessary information about the reward history. The function u in Equation (4) updates this information at each time step. Finally, the Kronecker deltas in Equation (5) 'pick' all the possible $\tilde{r}_t$ that result in the same h_{t+1} and r_t. For example, for $f(\tilde{r}_0, \ldots, \tilde{r}_t) = \min(\tilde{r}_0, \ldots, \tilde{r}_t)$, we can choose $r_0 = h_1 = \tilde{r}_0$ followed by $h_{t+1} = u(h_t, \tilde{r}_t) = \min(h_t, \tilde{r}_t)$, and $r_t = \rho(h_t, \tilde{r}_t) = \min(0, \tilde{r}_t - h_t)$. More examples are shown in Table 1.

Due to Definition 1, there is a mapping between trajectories of NCMDPs and corresponding MDPs, which we will exploit to use the same policy for both decision processes:

Definition 2. *A trajectory $\tilde{\mathcal{T}} = (\tilde{s}_0, a_0, \tilde{r}_0, \dots)$ of an NCMDP $\tilde{M}$ is mapped onto a trajectory $\mathcal{T} = \text{map}\left(\tilde{\mathcal{T}}\right) = (s_0, a_0, r_0, \dots)$ of a corresponding MDP M by calculating r_t according to Equation* (3), *setting $s_t = (\tilde{s}_t, h_t)$ with h_t calculated according to Equation* (4), *and keeping the actions a_t the same.*

Note that multiple $\tilde{\mathcal{T}}$ potentially map to the same $\mathcal{T}$ since ρ and u, and, therefore, the map operation are not necessarily injective. We can now state the main result of this manuscript:

Theorem 1. *Consider an NCMDP $\tilde{M}$ and a corresponding MDP M, both defined as in Definition 1. Then, given a policy $\pi(a_t|s_t)$ of M, the expected return of M is equal to the expected return of $\tilde{M}$, i.e.*

$$\mathbb{E}_\pi \left[\sum_{t=0}^{T-1} r_t \right] = \mathbb{E}_\pi \left[f(\tilde{r}_0, \dots, \tilde{r}_{T-1}) \right], \tag{6}$$

if $\pi(a_t|s_t)$ is used to interact with $\tilde{M}$ as follows: At each time step t, map the current trajectory $\tilde{\mathcal{T}}$ of $\tilde{M}$ to a trajectory $\mathcal{T} = \text{map}\left(\tilde{\mathcal{T}}\right)$ of M as described in Definition 2, thereby finding s_t. Then choose an action according to $\pi(a_t|s_t)$.

For a proof of this theorem see Appendix A1. Since M is a standard MDP, we can find its optimal policy using standard methods and are guaranteed that it will also be the ideal policy of $\tilde{M}$. More generally, also non-ideal policies will yield the same return for both decision processes. By mapping the NCMDP to an MDP, all guarantees available for MDP solvers, e.g. convergence proofs for Q-learning (Watkins & Dayan, 1992), or the policy gradient theorem for policy-based methods (Sutton et al., 1999), directly apply also to NCMDPs.

We demonstrate the need for the additional state information h_t in the two-step NCMDP depicted in Figure 2, which captures the main conceptual difficulties in solving NCMDPs: A non-cumulative objective in a stochastic environment. Here, the goal is to maximize the expected minimum of the rewards, i.e. $\min(\tilde{r}_0, \tilde{r}_1)$. If $\tilde{r}_0 = 1$ in the first step, the ideal policy is to choose a_1 in the second step, while if $\tilde{r}_0 = -1$ the agent should choose a_0. Therefore, the choice of the ideal action depends on information contained in the past rewards, which is captured by $h_1 = \tilde{r}_0$. We show the MDP constructed from the NCMDP as described above in the Appendix in Figure A6 and its state-action value function found by value iteration in Table A5. Our method finds the optimal policy, while previous methods for solving NCMDPs fail even in this simple example because they neglect the extra state information (see Table A4).

The question remains how to find the functions u and ρ given a new objective f. There is always at least one MDP corresponding to a given NCMDP since we can take $h_t = [\tilde{r}_0, \dots, \tilde{r}_{t-1}]$ with $u(h_t, \tilde{r}_t) = [h_t, \tilde{r}_t]$ and $\rho(h_t, \tilde{r}_t) = f([h_t, \tilde{r}_t]) - f(h_t)$. However, this is not ideal because it leads to a state size that grows linearly with the trajectory length. In Appendix A2.1, we provide a necessary and sufficient condition for objectives f with constant size additional state information h_t. Moreover, we also provide a sufficient, but not necessary, condition that is easier to verify and covers a large class of functions, e.g. all functions in Table 1. For functions in this class, we also provide an explicit construction of u, ρ, and h_t (see Appendix A2.2). In practice, we have empirically observed that a simple analytical consideration leads to h_t of a small and constant size for each of the objectives f considered in this manuscript, which is desirable for efficient learning and integration with standard function estimators such as neural networks.

Figure 2: Two-step decision process with non-cumulative objective. In the first step, the agent has only one action available and receives a probabilistic reward. In the second step, the agent can choose between two actions.

Limitation: Our method may result in a significantly increased state space, which might pose challenges for tabular reinforcement learning methods and dynamic programming techniques. However, deep reinforcement learning techniques are well equipped to address these challenges, as they can effectively handle exponentially large and continuous state spaces.

From an implementation perspective, our scheme of mapping NCMDPs to MDPs requires minimal effort, since we can treat both the NCMDP and the used MDP solver as black boxes by simply adding a layer between them, as shown in Figure 1. In addition, our treatment facilitates online learning and does not require any computationally expensive preprocessing of the NCMDP. This opens the door for researchers with specific domain knowledge, who are not necessarily experts in reinforcement learning, to use standard libraries such as `stable-baselines3` (Raffin et al., 2021) to solve their non-cumulative problems. Conversely, it allows reinforcement learning experts to quickly tackle existing environments using our method.

3 Experiments

There are three kinds of experiments presented in this manuscript:

1. We show that our method, in conjunction with dynamic programming, can find the optimal policy in a proof-of-principle stochastic NCMDPs where previous methods fail (see previous section, Figure 2).

2. In Appendix A3, we compare our method with the only previous approach for solving NCMDPs with objectives other than the max function, which was introduced by Cui & Yu (2023), and is only applicable with more restrictive objectives f, in deterministic environments, and in conjunction with Q-learning methods. Our experiments indicate that even in this restricted setting, our more general method performs similar overall and may even outperform the previous method in terms of final performance.

3. In the following sections, we show applications in real-world tasks where previous methods used for solving special cases of NCMDPs cannot be applied. In lack of a general method for solving NCMDPs, prior reinforcement learning based approaches to these real-world problems have so far relied on standard MDPs and approximate solutions which we use as a baseline to compare our method to.

Figure 3: Average return in the lunar lander environment (inset) against the velocity penalty coefficient c defined in Equation (7) for the non-cumulative MAXVELPPO and the cumulative FINALPPO algorithm.

If not otherwise specified, shaded regions in plots and uncertainties in tables denote a 95% bootstrap confidence interval calculated over multiple seeds of the experiment. We provide details on hyperparameters, compute resources, and training curves for all experiments in Appendix A4.

3.1 Classical Control

As a first use case of our method, we train a reinforcement learning agent in the lunar lander environment of the `gymnasium` (Towers et al., 2023) library. The agent controls a spacecraft with four discrete actions corresponding to different engines while being pushed by a stochastic wind. Immediate positive rewards r_t are given for landing the spacecraft safely with small negative rewards given for using the engines. A

realistic goal when landing a spacecraft is to not let the spacecraft get too fast, e.g. to avoid excessive frictional heating. Therefore, we define an objective where the agent is penalized for its maximum speed during a trajectory, i.e. we try to maximize

$$\mathbb{E}_\pi \left[\sum_{t=0}^{T-1} r_t - c \max\left(v_0, \ldots, v_{T-1}\right) \right], \tag{7}$$

where v_t is the speed of the agent at time t and c defines a trade-off between minimizing the maximum speed and the other goals of the agent. We train RL agents using Proximal Policy Optimization (PPO) (Schulman et al., 2017) on the MDP constructed from the NCMDP as described above (MAXVELPPO) for different values of c. We compare our results to an RL agent where the velocity penalty $-c \max\left(v_0, \ldots, v_{T-1}\right)$ is added to the final reward resulting in a cumulative objective (FINALPPO). As shown in Figure 3, the non-cumulative MAXVELPPO agent can find a better trade-off than the cumulative FINALPPO agent.

The reward function of the FINALPPO agent is non-Markovian. Therefore, we also tested adding the extra state information h_t, i.e. the past maximum velocity, to the FINALPPO agent's observations to restore Markovianity. However, this did not result in a performance gain (see Figure A3). All experiments were performed with 5 agents using different seeds.

Our method presented here could be applied to similar use cases in other classical control problems, such as teaching a robot to reach a goal while minimizing the maximum impact forces on its joints or the forces its motors need to apply.

3.2 Portfolio Optimization with Sharpe Ratio as Objective

Next, we consider the task of portfolio optimization where an agent decides how to best invest its assets across different possibilities. A common measure for a successful investment strategy is its Sharpe ratio (Sharpe, 1966)

$$\frac{\text{MEAN}(\tilde{r}_0, \ldots, \tilde{r}_{T-1})}{\text{STD}(\tilde{r}_0, \ldots, \tilde{r}_{T-1})}, \tag{8}$$

where $\tilde{r}_t = (P_{t+1} - P_t)/P_t$ are the simple returns and P_t is the portfolio value at time t. By dividing through the standard deviation of the simple returns, the agent is discouraged from risky strategies with high volatility. As the Sharpe ratio is non-cumulative, reinforcement learning strategies so far needed to fall back on the approximate differential Sharpe ratio as a reward (Moody et al., 1998; Moody & Saffell, 2001). However, using the methods developed in this paper we can directly maximize the exact Sharpe ratio. We perform experiments on an environment as described by Sood et al. (2023) where an agent trades on the 11 different S&P500 sector indices between 2006 and 2021. The states contain a history of returns of each index and different volatility measures. Actions are the continuous relative

Figure 4: Portfolio optimization. Sharpe ratio during 10 different training periods for algorithms maximizing either the cumulative differential Sharpe ratio (DIFFSHARPE) or the exact Sharpe ratio by using our non-cumulative method (SHARPE) or by giving the Sharpe ratio as a single final reward (FINALSHARPE).

portfolio allocations for each day. The experiment described by Sood et al. (2023) consists of training 5 agents with different seeds on 10 overlapping periods spanning 5 years each. We re-implement this experiment by training agents using PPO with the cumulative differential Sharpe ratio (DIFFSHARPE) or the exact Sharpe ratio as their objective. For the agents maximizing the exact Sharpe ratio, we either phrase the problem as an NCMDP and use our method described above (SHARPE), or we provide a single reward at the end of the trajectory (FINALSHARPE). As depicted in Figure 4, the SHARPE algorithm outperforms

the other algorithms. As in Section 3.1, restoring Markovianity in the FINALSHARPE algorithm by adding h_t to the states did not improve performance.

Limitation: After training, all of the considered algorithms do not generalize well to new, unseen periods indicating over-fitting of the agents' policies to the years they are trained on. Therefore, the experiments presented here should be understood as showing improved performance of the SHARPE agent only in the environment it was trained in. This limitation could potentially be offset by generating more data to train on, e.g. by using realistic stock-market simulators which are for example being developed using Generative Adversarial Networks (Li et al., 2020).

While the Sharpe ratio is most widely adopted in finance, our method opens up the possibility to maximize it also in other scenarios where risk-adjusted rewards are desirable, i.e. all problems where consistent rewards with low variance are more important than a higher cumulative reward. For example, in chronic disease management, maintaining stable health metrics is preferable to sporadic improvements. In emergency or customer service, ensuring predictable response times is often more important than occasional fast responses mixed with slow ones.

3.3 Discrete Optimization Problems

Next, we consider a large class of applications where RL is commonly used: Problems where the agent iteratively transforms a state by its actions to find a state with a lower associated cost. These problems are common in scientific applications such as physics, e.g. to reduce the length of quantum logic circuits (Fösel et al., 2021), or chemistry, e.g. for molecular discovery (Zhou et al., 2019). Another prominent example is the discovery of new algorithms (Mankowitz et al., 2023). Intuitively, these problems can be understood as searching for the state with the lowest cost within an equivalence class defined by all states that can be reached from the start state by the agent's actions.

Concretely, we consider the class of discrete optimization problems equipped with a scalar cost function $c(\tilde{s}_t)$ and the immediate rewards $\tilde{r}_t = c(\tilde{s}_t) - c(\tilde{s}_{t+1})$. Additionally, we are interested in the state with the lowest cost found during a trajectory, i.e. the goal is to maximize

$$\mathbb{E}_\pi \left[c(\tilde{s}_0) - \min_{k \in [0, T-1]} c(\tilde{s}_k) \right] = \mathbb{E}_\pi \left[\max_{k \in [-1, T-1]} \sum_{t=0}^{k} \tilde{r}_t \right]. \tag{9}$$

In the deterministic settings we study in the following experiments, the ideal policy for maximizing the cumulative reward $\mathbb{E}_\pi \left[\sum_{t=0}^{T-1} \tilde{r}_t \right]$ maximizes also Equation (9). We conjecture that directly maximizing Equation (9) by formulating the problem as an NCMDP will yield better results due to the following reasons:

1. The agent does not need to learn an optimal stopping point.

2. Considering only the rewards up to the minimum found cost might decrease the variance of the gradient estimate.

3. The agent does not receive negative rewards for trying to escape a local cost minimum during a trajectory and is therefore not discouraged from exploring. This leads to learning difficult optimization strategies requiring an intermittent cost increase more easily.

3.3.1 Peak environment

To facilitate an in-depth analysis, we first consider a toy environment with the cost function depicted in the inset of Figure 5 (a). The cost function was chosen to be simple while still requiring intermittently cost-increasing actions of the optimal policy. Each trajectory lasts 10 steps and the agent's actions are stepping to the left, right, or doing nothing. To minimize the number of hyperparameters, we use the REINFORCE algorithm (Williams, 1992) with a linear policy network and one-hot state encoding. We compare agents trained with the non-cumulative objective Equation (9) (MAXREINFORCE) with agents that maximize the

Figure 5: Peak environment. (a) Cost improvement during the trajectory against training episodes for the cumulative REINFORCE agent and the MAXREINFORCE agent maximizing Equation (9). The inset shows the cost function of the environment. (b) Difference between the empirical variance of MAXREINFORCE and REINFORCE against training progress (negative values indicate lower variance of MAXREINFORCE). (c) Estimated dot product of the average gradient of both agents against training progress.

cumulative rewards (REINFORCE). As shown in Figure 5 (a), the MAXREINFORCE agent trains much faster. Two possible sources of this speed-up are a different, more advantageous direction of the gradient updates and a reduced variance when estimating these gradients. To investigate which is the case, we periodically stop training and run $n = 1000$ trajectories with a fixed policy. We then compute the empirical variance of the gradient update inspired by Kaledin et al. (2022) as

$$\text{VAR} = \frac{1}{n} \sum_{i=0}^{n-1} \|\vec{g}_i\|_2^2 - \left\| \frac{1}{n} \sum_{i=0}^{n-1} \vec{g}_i \right\|_2^2, \tag{10}$$

where $\vec{g}_i$ is the gradient from a single trajectory derived either by the MAXREINFORCE or the REINFORCE algorithm. As this variance scales with the squared magnitude of the average gradients, we normalize it by this value to ensure a fair comparison between the two algorithms. In Figure 5 (b), we show that the MAXREINFORCE algorithm reduces variance in the initial phase of training. To compare the direction of the gradients we use the same data to compute the normalized average gradients of both algorithms and show their dot product in Figure 5 (c). We find that the gradients are correlated (i.e. the dot product is bigger than zero) but not the same. Therefore, we conclude that the training speed-up is likely derived both from lower variance and a better true gradient direction. All results reported are averaged over 10 seeds.

3.3.2 Quantum error correction

As a first real-world use case, we focus on optimization problems where the initial state is always the same and the optimal stopping point is known. The specific task we consider is the search for quantum programs to prepare logical states of a given quantum error correction code - critical for the eventual realization of quantum computation (Terhal, 2015). The agent iteratively adds elementary quantum logic gates until the program delivers the desired result. The agents' policies are encoded by standard multilayer perceptrons and they are trained on five different sized problems. For details on the used environment, see Zen et al. (2024). We use PPO to train agents to maximize either Equation (9) (MAXPPO) or the cumulative reward (PPO). To obtain a single performance measure encompassing both final performance and training speed, we continuously evaluate the mean cost improvement of the agents and average it over the training process as suggested by Andrychowicz et al. (2020b). Intuitively, this measure can be understood as the area under the agent's training curve. In Table 2, we report the quotient of this performance measure of the MAXPPO algorithm and the PPO algorithm for both the best of 10 and the mean of 10 trained agents. The different tasks are denoted by three integers, as customary in the quantum error correction community. We find that the MAXPPO algorithm performs better.

Table 2: Results for quantum error correction environments.

Task	Area under training curve $\frac{\text{MAXPPO}}{\text{PPO}}$	
	Best of 10	Mean of 10
$[[5, 1, 3]]$	1.04	$1.07\,(1.04, 1.09)$
$[[7, 1, 3]]$	1.18	$1.21\,(1.17, 1.25)$
$[[9, 1, 3]]$	1.01	$1.09\,(1.04, 1.17)$
$[[15, 1, 3]]$	1.14	$1.03\,(0.98, 1.08)$
$[[17, 1, 5]]$	1.47	$1.62\,(1.52, 1.78)$

We also trained MAXPPO for a second quantum circuit discovery task [for details see Olle et al. (2024)]. In this case, PPO and MAXPPO performed equally well. We argue that the large degeneracy present in the solution space of this second discovery task diverts the more exploratory MAXPPO, lowering its performance to the level of PPO.

3.3.3 ZX-diagrams

As another real-world discrete optimization problem, we consider the simplification of ZX-diagrams, which are graph representations of quantum processes (Coecke & Kissinger, 2017) with applications e.g. in the compilation of quantum programs (Duncan et al., 2020; Riu et al., 2023). An example of a typical ZX-diagram is shown in the inset of Figure 6 (b). We consider the environment described by Nägele & Marquardt (2024), where the cost function of a diagram is given by its node number, the start states are randomly sampled ZX-diagrams, and the actions are a set of local graph transformations. In total, there are 6 actions per node and 6 actions per edge in the diagram. This is a challenging reinforcement learning task that requires the use of graph neural networks to accommodate the changing size of the state and action space. As shown in Figure 6 (a) the MAXPPO agent initially trains faster than the PPO agent (left inset). This is likely due to the reduced variance and different gradient direction as described above. The PPO agent then shortly catches up, but ultimately requires about twice as many training steps to reach optimal performance as the MAXPPO agent (right inset). We argue that this is because the MAXPPO agent is better at exploring and therefore learning difficult optimization strategies (reason 3 in Section 3.3). This is captured by the entropy of the MAXPPO agent's policy staying much higher than the entropy of the PPO agent, as shown in Figure 6 (b). The reported results are averaged over 5 seeds.

Limitation: When applying MAXPPO to discrete optimization problems with long trajectories in the many hundreds of steps, we empirically observed an initially slow learning speed. This could be due to the agent initially mostly increasing cost and therefore receiving zero reward for almost the entire trajectory. A possible solution could be to dynamically adjust the trajectory length in these problems going from shorter to longer trajectories during the training process.

4 Related Work

A special case of NCMDPs is first considered by Quah & Quek (2006), who adapt Q-learning to the max objective by redefining the temporal difference error of their learning algorithms and demonstrate their algorithms on an optimal stopping problem. However, they do not adapt state space and do not provide theoretical convergence guarantees. Gottipati et al. (2020) rediscover the same algorithm, apply it to molecule generation, and provide convergence guarantees for their method, while Eyckerman et al. (2022) consider the same algorithm for application placement in fog environments. Cui & Yu (2023) finally show a shortcoming of the method used in the above papers: It is guaranteed to converge to the optimal policy only in deterministic settings. Additionally, they provide convergence guarantees of Q-learning in deterministic environments for a larger class of functions f, focusing on the min function for network routing applications. In Appendix A2.1 we show that the class of objectives f considered by Cui & Yu (2023) is a subclass of all objectives that lead to constant size extra state information h_t using our method. Independently, the max function is also used in the field of safety reinforcement learning in deterministic environments both for Q-learning (Fisac et al., 2015;

Figure 6: ZX environment. (a) Cost improvement during the trajectory against total steps taken in the environment for the cumulative PPO agent and the MAXPPO agent maximizing Equation (9). Left inset: Zoom-in to the initial training phase. Right inset: Zoom-in to the final training phase. (b) Entropy of the agents' policies against total steps taken in the environment. Inset: A typical ZX-diagram.

2019; Hsu et al., 2021) and policy-based reinforcement learning (Yu et al., 2022). Moflic & Paler (2023) use a reward function with parameters that depend on the past rewards of the trajectory to tackle quantum circuit optimization problems that require large intermittent negative rewards, albeit without providing theoretical convergence guarantees. Additionally, Wang et al. (2020) investigate planning problems with non-cumulative objectives within deterministic settings. They provide provably efficient planning algorithms for a large class of functions f by discretizing rewards and appending them to the states. Recently, Veviurko et al. (2024) showed how to use the max objective also in probabilistic settings by augmenting state space and provide convergence guarantees for both Q-learning and policy-based methods. They then show experiments with their algorithm yielding improvements in MDPs with shaped rewards. However, they do not redefine the rewards, which requires adaptation of the implementation of their MDP solvers. Our method described above reduces to an effectively equivalent algorithm to theirs in the special case of the max objective.

A limitation of all works discussed above is that they require a potentially complicated adaptation of their reinforcement learning algorithms and only consider specific MDP solvers or specific non-cumulative objectives. They are also limited to deterministic settings, except for Veviurko et al. (2024), which consider only the max objective.

5 Discussion & Conclusion

In this work, we described a mapping from a decision process with a general non-cumulative objective (NCMDP) to a standard Markov decision process (MDP) applicable in deterministic and probabilistic settings. As our method is agnostic to the algorithm used to solve the resulting MDP, it works for arbitrary action spaces and in conjunction with both off- and on-policy algorithms. Its implementation is straightforward and directly enables solving NCMDPs with state-of-the-art MDP solvers, allowing us to show improvements in a diverse set of tasks such as classical control problems, portfolio optimization, and discrete optimization problems. Note that these improvements are achieved without adding a single additional hyperparameter to the solving algorithms. Moreover, the computational overhead of our method is typically negligible, since it requires only the evaluation of a few elementary mathematical expressions per time step in the environment (see Table 1).

In further theoretical work, a full constructive classification of objective functions f with constant-size extra state information h_t would be desirable. From an applications perspective, there are a lot of interesting objectives with non-cumulative f that could not be maximized so far. For example, the geometric mean could be used to maximize average growth rates, or the function $f(\tilde{r}_0, \ldots, \tilde{r}_t) = \delta^t \sum_{k=0}^{t} \tilde{r}_k, \delta \in (0, 1)$ could be used to define an exponential trade-off between trajectory length and cumulative reward in settings where long trajectories are undesirable. We believe that a multitude of other applications with non-cumulative objectives

are still unknown to the reinforcement learning (RL) community, and conversely, that researchers working on non-cumulative problems are not aware of RL, simply because these two concepts could not straightforwardly be unified so far. This manuscript offers the exciting possibility of discovering and addressing this class of problems still unexplored by reinforcement learning.

6 Code Availability

Anonymized code including exact hyperparameters and random seeds, generated data, trained agent weights, and instructions for running the code for all presented experiments are available for download at `https://osf.io/ajwmk/?view_only=38b116ac6633496a83657aeff43db34a`. Upon acceptance, we will make the code and data publicly available.

References

Marcin Andrychowicz, Bowen Baker, Maciek Chociej, Rafal Józefowicz, Bob McGrew, Jakub Pachocki, Arthur Petron, Matthias Plappert, Glenn Powell, Alex Ray, Jonas Schneider, Szymon Sidor, Josh Tobin, Peter Welinder, Lilian Weng, and Wojciech Zaremba. Learning dexterous in-hand manipulation. *The International Journal of Robotics Research*, 39(1):3–20, 2020a. doi: 10.1177/0278364919887447. URL `https://journals.sagepub.com/doi/10.1177/0278364919887447`.

Marcin Andrychowicz, Anton Raichuk, Piotr Stańczyk, Manu Orsini, Sertan Girgin, Raphaël Marinier, Leonard Hussenot, Matthieu Geist, Olivier Pietquin, and Marcin Michalski. What matters for on-policy deep actor-critic methods? A large-scale study. In *International conference on learning representations*, 2020b. doi: 10.48550/arXiv.2006.05990. URL `https://openreview.net/forum?id=nIAxjsniDzg`.

Bob Coecke and Aleks Kissinger. *Picturing Quantum Processes: A First Course in Quantum Theory and Diagrammatic Reasoning.* Cambridge University Press, 2017. ISBN 9781107104228.

Wei Cui and Wei Yu. Reinforcement learning with non-cumulative objective. *IEEE Transactions on Machine Learning in Communications and Networking*, 1:124–137, 2023. doi: 10.1109/TMLCN.2023.3285543. URL `https://ieeexplore.ieee.org/document/10151914`.

Ross Duncan, Aleks Kissinger, Simon Perdrix, and John Van De Wetering. Graph-theoretic simplification of quantum circuits with the ZX-calculus. *Quantum*, 4:279, 2020. doi: 10.22331/q-2020-06-04-279. URL `http://quantum-journal.org/papers/q-2020-06-04-279/`.

Reinout Eyckerman, Phil Reiter, Steven Latré, Johann Marquez-Barja, and Peter Hellinckx. Application placement in fog environments using multi-objective reinforcement learning with maximum reward formulation. In *NOMS 2022-2022 IEEE/IFIP Network Operations and Management Symposium*, pp. 1–6, 2022. doi: 10.1109/NOMS54207.2022.9789757. URL `https://ieeexplore.ieee.org/document/9789757`.

Jaime F Fisac, Mo Chen, Claire J Tomlin, and S Shankar Sastry. Reach-avoid problems with time-varying dynamics, targets and constraints. In *Proceedings of the 18th international conference on hybrid systems: computation and control*, pp. 11–20, 2015. doi: 10.1145/2728606.2728612. URL `https://dl.acm.org/doi/10.1145/2728606.2728612`.

Jaime F. Fisac, Neil F. Lugovoy, Vicenç Rubies-Royo, Shromona Ghosh, and Claire J. Tomlin. Bridging Hamilton-Jacobi safety analysis and reinforcement learning. In *2019 International Conference on Robotics and Automation (ICRA)*, pp. 8550–8556, 2019. doi: 10.1109/ICRA.2019.8794107. URL `https://ieeexplore.ieee.org/document/8794107`.

Thomas Fösel, Murphy Yuezhen Niu, Florian Marquardt, and Li Li. Quantum circuit optimization with deep reinforcement learning. *arXiv*, 2021. doi: 10.48550/arXiv.2103.07585. URL `https://arxiv.org/abs/2103.07585`.

Sai Krishna Gottipati, Yashaswi Pathak, Rohan Nuttall, Raviteja Chunduru, Ahmed Touati, Sriram Ganapathi Subramanian, Matthew E Taylor, and Sarath Chandar. Maximum reward formulation in reinforcement learning. *arXiv*, 2020. doi: 10.48550/arXiv.2010.03744. URL `https://arxiv.org/abs/2010.03744`.

Kai-Chieh Hsu, Vicenç Rubies-Royo, Claire J Tomlin, and Jaime F Fisac. Safety and liveness guarantees through reach-avoid reinforcement learning. In *Proceedings of Robotics: Science and Systems*, July 2021. doi: 10.15607/RSS.2021.XVII.077. URL https://www.roboticsproceedings.org/rss17/p077.pdf.

Maxim Kaledin, Alexander Golubev, and Denis Belomestny. Variance reduction for policy-gradient methods via empirical variance minimization. *arXiv*, 2022. doi: 10.48550/arXiv.2206.06827. URL https://arxiv.org/abs/2206.06827.

Junyi Li, Xintong Wang, Yaoyang Lin, Arunesh Sinha, and Michael Wellman. Generating realistic stock market order streams. *Proceedings of the AAAI Conference on Artificial Intelligence*, 34:727–734, 2020. doi: 10.1609/aaai.v34i01.5415. URL https://ojs.aaai.org/index.php/AAAI/article/view/5415.

Chris Lu, Jakub Kuba, Alistair Letcher, Luke Metz, Christian Schroeder de Witt, and Jakob Foerster. Discovered policy optimisation. *Advances in Neural Information Processing Systems*, 35:16455–16468, 2022. doi: 10.48550/arXiv.2210.05639. URL https://proceedings.neurips.cc/paper_files/paper/2022/hash/688c7a82e31653e7c256c6c29fd3b438-Abstract-Conference.html.

Daniel J. Mankowitz, Andrea Michi, Anton Zhernov, Marco Gelmi, Marco Selvi, Cosmin Paduraru, Edouard Leurent, Shariq Iqbal, Jean-Baptiste Lespiau, Alex Ahern, Thomas Köppe, Kevin Millikin, Stephen Gaffney, Sophie Elster, Jackson Broshear, Chris Gamble, Kieran Milan, Robert Tung, Minjae Hwang, Taylan Cemgil, Mohammadamin Barekatain, Yujia Li, Amol Mandhane, Thomas Hubert, Julian Schrittwieser, Demis Hassabis, Pushmeet Kohli, Martin Riedmiller, Oriol Vinyals, and David Silver. Faster sorting algorithms discovered using deep reinforcement learning. *Nature*, 618(7964):257–263, 2023. doi: 10.1038/s41586-023-06004-9. URL https://doi.org/10.1038/s41586-023-06004-9.

Volodymyr Mnih, Koray Kavukcuoglu, David Silver, Andrei A. Rusu, Joel Veness, Marc G. Bellemare, Alex Graves, Martin Riedmiller, Andreas K. Fidjeland, Georg Ostrovski, Stig Petersen, Charles Beattie, Amir Sadik, Ioannis Antonoglou, Helen King, Dharshan Kumaran, Daan Wierstra, Shane Legg, and Demis Hassabis. Human-level control through deep reinforcement learning. *Nature*, 518(7540):529–533, 2015. doi: 10.1038/nature14236. URL https://doi.org/10.1038/nature14236.

Ioana Moflic and Alexandru Paler. Cost explosion for efficient reinforcement learning optimisation of quantum circuits. In *2023 IEEE International Conference on Rebooting Computing (ICRC)*, pp. 1–5. IEEE, 2023. doi: 10.1109/ICRC60800.2023.10386864. URL https://www.computer.org/csdl/proceedings-article/icrc/2023/10386864/1TJmieJCklW.

J. Moody and M. Saffell. Learning to trade via direct reinforcement. *IEEE Transactions on Neural Networks*, 12(4):875–889, 2001. doi: 10.1109/72.935097. URL https://ieeexplore.ieee.org/document/935097.

John Moody, Lizhong Wu, Yuansong Liao, and Matthew Saffell. Performance functions and reinforcement learning for trading systems and portfolios. *Journal of Forecasting*, 17(5-6):441–470, 1998. doi: https://doi.org/10.1002/(SICI)1099-131X(1998090)17:5/6<441::AID-FOR707>3.0.CO;2-\#. URL https://onlinelibrary.wiley.com/doi/10.1002/%28SICI%291099-131X%281998090%2917%3A5/6%3C441%3A%3AAID-FOR707%3E3.0.CO%3B2-%23.

Maximilian Nägele and Florian Marquardt. Optimizing ZX-diagrams with deep reinforcement learning. *Machine Learning: Science and Technology*, 5(3):035077, 2024. doi: 10.1088/2632-2153/ad76f7. URL https://iopscience.iop.org/article/10.1088/2632-2153/ad76f7.

Jan Olle, Remmy Zen, Matteo Puviani, and Florian Marquardt. Simultaneous discovery of quantum error correction codes and encoders with a noise-aware reinforcement learning agent. *npj Quantum Information*, 10(1):126, 2024. doi: 10.1038/s41534-024-00920-y. URL https://doi.org/10.1038/s41534-024-00920-y.

K.H. Quah and Chai Quek. Maximum reward reinforcement learning: A non-cumulative reward criterion. *Expert Systems with Applications*, 31(2):351–359, 2006. doi: 10.1016/j.eswa.2005.09.054. URL https://www.sciencedirect.com/science/article/pii/S0957417405002228.

Antonin Raffin. Rl baselines3 zoo. https://github.com/DLR-RM/rl-baselines3-zoo, 2020.

Antonin Raffin, Ashley Hill, Adam Gleave, Anssi Kanervisto, Maximilian Ernestus, and Noah Dormann. Stable-baselines3: Reliable reinforcement learning implementations. *Journal of Machine Learning Research*, 22(268):1–8, 2021. URL http://jmlr.org/papers/v22/20-1364.html.

Jordi Riu, Jan Nogué, Gerard Vilaplana, Artur Garcia-Saez, and Marta P Estarellas. Reinforcement learning based quantum circuit optimization via ZX-calculus. *arXiv*, 2023. doi: 10.48550/arXiv.2312.11597. URL https://arxiv.org/abs/2312.11597.

John Schulman, Filip Wolski, Prafulla Dhariwal, Alec Radford, and Oleg Klimov. Proximal policy optimization algorithms. *arXiv*, 2017. doi: 10.48550/arXiv.1707.06347. URL https://arxiv.org/abs/1707.06347.

William F. Sharpe. Mutual fund performance. *The Journal of Business*, 39(1):119–138, 1966. ISSN 00219398, 15375374. URL http://www.jstor.org/stable/2351741.

Srijan Sood, Kassiani Papasotiriou, Marius Vaiciulis, and Tucker Balch. Deep reinforcement learning for optimal portfolio allocation: A comparative study with mean-variance optimization. *International Conference on Automated Planning and Scheduling*, pp. 21, 2023. URL https://icaps23.icaps-conference.org/papers/finplan/FinPlan23_paper_4.pdf.

Richard S. Sutton and Andrew G. Barto. *Reinforcement Learning: An Introduction, Second edition.* The MIT Press, 2018. ISBN 9780262039246. URL http://incompleteideas.net/book/RLbook2020.pdf.

Richard S Sutton, David McAllester, Satinder Singh, and Yishay Mansour. Policy gradient methods for reinforcement learning with function approximation. *Advances in neural information processing systems*, 12, 1999. URL https://papers.nips.cc/paper_files/paper/1999/hash/464d828b85b0bed98e80ade0a5c43b0f-Abstract.html.

Barbara M. Terhal. Quantum error correction for quantum memories. *Rev. Mod. Phys.*, 87:307–346, 2015. doi: 10.1103/RevModPhys.87.307. URL https://link.aps.org/doi/10.1103/RevModPhys.87.307.

Mark Towers, Jordan K. Terry, Ariel Kwiatkowski, John U. Balis, Gianluca de Cola, Tristan Deleu, Manuel Goulão, Andreas Kallinteris, Arjun KG, Markus Krimmel, Rodrigo Perez-Vicente, Andrea Pierré, Sander Schulhoff, Jun Jet Tai, Andrew Tan Jin Shen, and Omar G. Younis. Gymnasium, 2023. URL https://zenodo.org/record/8127025.

Grigorii Veviurko, Wendelin Boehmer, and Mathijs de Weerdt. To the max: Reinventing reward in reinforcement learning. In *41st International Conference on Machine Learning (ICML)*, 2024. doi: 10.48550/arXiv.2402.01361. URL https://openreview.net/forum?id=4KQ0VwqPg8.

Ruosong Wang, Peilin Zhong, Simon S Du, Russ R Salakhutdinov, and Lin Yang. Planning with general objective functions: Going beyond total rewards. In H. Larochelle, M. Ranzato, R. Hadsell, M.F. Balcan, and H. Lin (eds.), *Advances in Neural Information Processing Systems*, volume 33, pp. 14486–14497, 2020. URL https://proceedings.neurips.cc/paper_files/paper/2020/file/a6a767bbb2e3513233f942e0ff24272c-Paper.pdf.

Christopher JCH Watkins and Peter Dayan. Q-learning. *Machine learning*, 8:279–292, 1992. doi: 10.1007/BF00992698. URL https://link.springer.com/article/10.1007/BF00992698.

Ronald J. Williams. Simple statistical gradient-following algorithms for connectionist reinforcement learning. *Machine Learning*, 8(3):229–256, 1992. doi: 10.1007/BF00992696. URL https://doi.org/10.1007/BF00992696.

Dongjie Yu, Haitong Ma, Shengbo Li, and Jianyu Chen. Reachability constrained reinforcement learning. In *Proceedings of the 39th International Conference on Machine Learning*, volume 162, pp. 25636–25655, 2022. doi: 10.48550/arXiv.2205.07536. URL https://proceedings.mlr.press/v162/yu22d.html.

Remmy Zen, Jan Olle, Luis Colmenarez, Matteo Puviani, Markus Müller, and Florian Marquardt. Quantum circuit discovery for fault-tolerant logical state preparation with reinforcement learning. *arXiv*, 2024. doi: 10.48550/arXiv.2402.1776. URL https://arxiv.org/abs/2402.17761.

Zhenpeng Zhou, Steven Kearnes, Li Li, Richard N. Zare, and Patrick Riley. Optimization of molecules via deep reinforcement learning. *Scientific Reports*, 9:10752, 2019. doi: 10.1038/s41598-019-47148-x. URL https://www.nature.com/articles/s41598-019-47148-x.

A1 Proof of Theorem 1

First, we find that the probability $p(\mathcal{T})$ of a trajectory $\mathcal{T}$ occurring in M is the sum of the probabilities $p(\tilde{\mathcal{T}})$ of all possible trajectories $\tilde{\mathcal{T}}$ occurring in $\tilde{M}$ that map to $\mathcal{T}$ if π is used as a policy for $\tilde{M}$ as described above:

$$
\begin{aligned}
p(\mathcal{T}) &= p(s_0) \prod_{t=0}^{T-1} \pi(a_t|s_t) p(r_t, s_{t+1}|s_t, a_t) \\
&= p(\tilde{s}_0) \prod_{t=0}^{T-1} \pi(a_t|s_t) \sum_{\tilde{r}_t} \tilde{p}(\tilde{r}_t, \tilde{s}_{t+1}|\tilde{s}_t, a_t) \delta_{h_{t+1}, u(h_t, \tilde{r}_t)} \delta_{r_t, \rho(h_t, \tilde{r}_t)} \\
&= \sum_{\mathrm{map}(\tilde{\mathcal{T}})=\mathcal{T}} p(\tilde{s}_0) \prod_{t=0}^{T-1} \pi(a_t|s_t) \tilde{p}(\tilde{r}_t, \tilde{s}_{t+1}|\tilde{s}_t, a_t) = \sum_{\mathrm{map}(\tilde{\mathcal{T}})=\mathcal{T}} p(\tilde{T}),
\end{aligned}
\tag{A1}
$$

where $\sum_{\mathrm{map}(\tilde{\mathcal{T}})=\mathcal{T}}$ is the sum over all trajectories of $\tilde{M}$ that map to $\mathcal{T}$. The second to last step can be shown through induction. Therefore, we find

$$
\begin{aligned}
\mathbb{E}_\pi \left[\sum_{t=0}^{T-1} r_t \right] &= \sum_{\mathcal{T}} p(\mathcal{T}) \sum_{t=0}^{T-1} r_t = \sum_{\mathcal{T}} \sum_{\mathrm{map}(\tilde{\mathcal{T}})=\mathcal{T}} p(\tilde{\mathcal{T}}) f(\tilde{r}_0, \ldots, \tilde{r}_{T-1}) \\
&= \sum_{\tilde{\mathcal{T}}} p(\tilde{\mathcal{T}}) f(\tilde{r}_0, \ldots, \tilde{r}_{T-1}) = \mathbb{E}_\pi \left[f(\tilde{r}_0, \ldots, \tilde{r}_{T-1}) \right],
\end{aligned}
\tag{A2}
$$

where in the second step we used Equations (3) and (A1), and in the third step that each $\tilde{\mathcal{T}}$ maps to a unique $\mathcal{T}$. ∎

A2 Objectives f with Constant Size Extra State Information h_t

A2.1 Necessary and sufficient condition for constant size extra state information h_t

First, note that if we can predict $f(\tilde{r}_0, \ldots, \tilde{r}_t)$ in a Markovian manner, we can also predict $f(\tilde{r}_0, \ldots, \tilde{r}_t) - f(\tilde{r}_0, \ldots, \tilde{r}_{t-1})$ in a Markovian manner by adding just one more dimension to our state h_t, i.e. $f(\tilde{r}_0, \ldots, \tilde{r}_{t-1})$. Therefore, we focus on predicting $f(\tilde{r}_0, \ldots, \tilde{r}_t)$ in the following. Rewriting Definition 1, we find using

$$
f(\tilde{r}_0, \ldots, \tilde{r}_t) - f(\tilde{r}_0, \ldots, \tilde{r}_{t-1}) = \rho\left(\tilde{r}_t, u\left(\tilde{r}_{t-1}, u\left(\tilde{r}_{t-2}, \ldots\right)\right)\right)
\tag{A3}
$$

or equivalently

$$
f(\tilde{r}_0, \ldots, \tilde{r}_t) = \rho'\left(\tilde{r}_t, u'\left(\tilde{r}_{t-1}, u'\left(\tilde{r}_{t-2}, \ldots\right)\right)\right),
\tag{A4}
$$

with

$$
u'(\tilde{r}_t, h_t') = u'\left(\tilde{r}_t, (h_t, f_{t-1})\right) = \left[u(\tilde{r}_t, h_t), f_{t-1} + \rho(\tilde{r}_t, h_t)\right],
\tag{A5}
$$

and

$$
\rho'(\tilde{r}_t, h_t') = \rho(\tilde{r}_t, h_t) + f_{t-1}.
\tag{A6}
$$

Given these definitions $f_t = f(\tilde{r}_0, \ldots, \tilde{r}_t)$. If f admits a representation of the form Equation (A4) with u' of constant output dimension, additional state information h_t of the same constant size is possible. Cui & Yu (2023) find a condition of similar form to Equation (A4) for the objectives f which their method can optimize:

$$
f(\tilde{r}_0, \ldots, \tilde{r}_t) = g\left(\tilde{r}_t, g\left(\tilde{r}_{t-1}, g\left(\tilde{r}_{t-2}, \ldots\right)\right)\right), g : \mathbb{R}^2 \to \mathbb{R}.
\tag{A7}
$$

Table A1: Objectives f in the form of Equation (A8). All f except $\max_{k\in[-1,t]}\sum_{i=0}^{k}\tilde{r}_i$ are permutation invariant resulting in associative $\mathbb{B}_j$.

$f(\tilde{r}_0,\ldots,\tilde{r}_t)$	$F(t,b_0,\ldots,b_{k-1})$	$[\mathbb{B}_j]$	$[\varphi_j(t,\tilde{r}_t)]$
$\max(\tilde{r}_0,\ldots,\tilde{r}_t)$	$h_t^{(0)}$	$\mathbb{B}_0 = \max$	$\varphi_0(\tilde{r}_t) = \tilde{r}_t$
$\min(\tilde{r}_0,\ldots,\tilde{r}_t)$	$h_t^{(0)}$	$\mathbb{B}_0 = \min$	$\varphi_0(\tilde{r}_t) = \tilde{r}_t$
Sharpe ratio $\frac{\text{MEAN}(\tilde{r}_0,\ldots,\tilde{r}_t)}{\text{STD}(\tilde{r}_0,\ldots,\tilde{r}_t)}$	$\dfrac{h_t^{(0)}/t}{\sqrt{h_t^{(1)}/t-\left(h_t^{(0)}/t\right)^2}}$	$\mathbb{B}_0 = \mathbb{B}_1 = +$	$\varphi_0(\tilde{r}_t) = \tilde{r}_t,$ $\varphi_1(\tilde{r}_t) = \tilde{r}_t^2$
$\max_{k\in[-1,t]}\sum_{i=0}^{k}\tilde{r}_i$	$h_t^{(1)} + h_t^{(0)}$	$\mathbb{B}_0\left(\varphi_0(\tilde{r}_t), h_t^{(0)}\right) =$ $\max\left(0, h_t^{(0)} - \varphi_0(\tilde{r}_t)\right),$ $\mathbb{B}_1 = +$	$\varphi_0(\tilde{r}_t) = \tilde{r}_t,$ $\varphi_1(\tilde{r}_t) = \tilde{r}_t$
$\tilde{r}_0\tilde{r}_1\ldots\tilde{r}_t$	$h_t^{(0)}$	$\mathbb{B}_0 = \times$	$\varphi_0(\tilde{r}_t) = \tilde{r}_t$
Harmonic mean $\frac{1}{\frac{1}{\tilde{r}_0}+\cdots+\frac{1}{\tilde{r}_t}}$	$\frac{1}{h_t^{(0)}}$	$\mathbb{B}_0 = +$	$\varphi_0(\tilde{r}_i) = \frac{1}{\tilde{r}_t}$
$\delta^t \sum_{t=0}^{t}\tilde{r}_t,$ $\delta \in (0,1)$	$\delta^t h_t^{(0)}$	$\mathbb{B}_0 = +$	$\varphi_0(\tilde{r}_t) = \tilde{r}_t$
$\frac{1}{t+1}\sum_{k=0}^{t}\tilde{r}_k$	$\frac{1}{t}h_t^{(0)}$	$\mathbb{B}_0 = +$	$\varphi_0(\tilde{r}_t) = \tilde{r}_t$

In this sense, our method can be seen as extending the class of objectives f with constant size extra state information by allowing for $\rho \neq u$ and by allowing a multidimensional update function $u : \mathbb{R}^{k+1} \to \mathbb{R}^k$ instead of g. Also, note that the method of Cui & Yu (2023) only works in deterministic environments in conjunction with Q-learning based methods.

A2.2 Sufficient condition for constant size extra state information h_t

While Equation (A4) provides a complete categorization of functions with constant size h_t, in practice it may be difficult to check whether a given function satisfies this property. In the following, we consider a smaller set of functions including all of the functions in Table 1, and provide an explicit construction of u, constant size h_t, and ρ for functions of this class. Specifically, we consider function families that can be written with a constant $k \in \mathbb{N}$ as

$$f(\tilde{r}_0,\ldots,\tilde{r}_t) = F(t, b_0,\ldots,b_{k-1}),\tag{A8}$$

where $F : \mathbb{R}^{k+1} \to \mathbb{R}$,

$$b_j = b_j(\tilde{r}_0,\ldots,\tilde{r}_t) = \mathbb{B}_j\big(\varphi_j(0,\tilde{r}_0),\ldots,\varphi_j(t,\tilde{r}_t)\big),\tag{A9}$$

where $\varphi_j : \mathbb{R}^2 \to \mathbb{R}$, and $\mathbb{B}_j$ is an arbitrary binary operation, such as $+, \times, \max, \min$, and

$$\mathbb{B}_j(x_0,\ldots,x_t) = \mathbb{B}_j(x_t, \mathbb{B}_j(x_{t-1}, \mathbb{B}_j(\ldots))).\tag{A10}$$

For example, if $\mathbb{B}_j$ is the multiplication operation, $\mathbb{B}_j(x_0,\ldots,x_t) = \prod_{i=0}^{t} x_i$. As we show by construction below, all objectives f of this form have extra state information h_t of maximum dimension $k+1$. Since we are dealing with function families, Equation (A8) introduces a notion of consistency for different sizes of inputs $(\tilde{r}_0,\ldots,\tilde{r}_t)$, since it requires the use of the same φ_j for all input sizes. Note that for permutation invariant f, φ_j is independent of the time step, i.e. $\varphi_j(i,\tilde{r}_i) = \varphi_j(\tilde{r}_i)$, and $\mathbb{B}_j$ is associative. All but one of the objectives f we consider in this manuscript are permutation invariant.

Given Equation (A8), we can directly construct the update function

$$h_{t+1}^{(j)} = u^{(j)}(\tilde{r}_t, h_t) = \mathbb{B}_j\left(\varphi_j\left(h_t^{(k)}, \tilde{r}_t\right), h_t^{(j)}\right), 0 \leq j < k,\tag{A11}$$

Figure A1: Example of a grid environment for the min objective with $N = 5$. Orange arrows indicate the ideal policy.

where superscript (j) indicates the jth entry of a vector. Additionally,

$$h_{t+1}^{(k)} = h_t^{(k)} + 1$$

is keeping track of the time step. In this case, each $b_j(\tilde{r}_0, \dots, \tilde{r}_{t-1})$ is a dimension of h_t. Finally,

$$\rho(\tilde{r}_t, h_t) = F\left(h_{t+1}^{(k)}, \left\{h_{t+1}^{(j)}\right\}_{j=0}^{j=k-1}\right) - F\left(h_t^{(k)}, \left\{h_t^{(j)}\right\}_{j=0}^{j=k-1}\right). \tag{A12}$$

We show in Table A1 how all functions in Table 1 can be written in this form.

A3 Grid Environment: Experiments Comparing to Cui & Yu (2023)

In this section, we compare our method to the more specialized method for solving NCMDPs introduced by Cui & Yu (2023), which can only be applied in deterministic environments in conjunction with Q-learning methods. We want to answer the question of whether our more general method can be competitive even in this specialized scenario. To this end, we consider the min objective in a grid environment, where each tile is associated with a deterministic reward sampled uniformly from $[-1, 1]$ when initializing the grid. At each step, the agent can choose to move forward and left, forward and right, or forward and straight, and an episode terminates when the agent has crossed from one side of the grid to the other (see Figure A1). We perform experiments on grid sizes $N = 3, 4, 5$ with 10 random grids per size. For each grid and training method, we train 5 agents with different initializations. To facilitate a fair comparison between both methods, we use a vanilla deep Q-learning algorithm with minimal hyperparameters for training (for details see Appendix A4). We either extend the states and adjust the rewards as specified in Table 1 for the minimum objective and use the standard Q-function update of Q-learning (ours), or we only change the Q-function update as specified by Cui & Yu (2023) to $Q(s_t, a_t) \leftarrow \min(r_t, \underset{a}{\operatorname{argmax}} Q(s_{t+1}, a))$. Our results indicate that the overall performance of the two algorithms is similar. While our method may yield a higher final return (see Table A2), it may train slightly slower (see Table A3). The prediction loss of the Q-function is also similar for both methods (see Figure A2).

A4 Details on Experiments

Lunar lander: For training, we use the PPO implementation of `stables-baselines3` (Raffin et al., 2021). The hyperparameters and network architecture of both algorithms were chosen as by Raffin (2020) (which are optimized to give good performance without the velocity penalty), only increasing the batch size and the total training steps to ensure convergence. Training a single agent takes around one hour on a Quadro RTX 6000 GPU with the environment running in parallel on 32 CPUs.

Portfolio optimization: For training, we use the PPO implementation of `stables-baselines3` (Raffin et al., 2021). The hyperparameters and network architecture of all algorithms were chosen as by Sood et al. (2023)

where they were optimized to give a good performance of the DIFFSHARPE algorithm. Training a single agent takes around one hour on a Quadro RTX 6000 GPU with the environment running in parallel on 10 CPUs.

Peak environment: For training, we use a custom REINFORCE implementation with a tabular policy to keep the number of hyperparameters minimal, updating the agent's policy after each completed trajectory. We use a learning rate of 2^{-10} but also performed experiments scanning the learning rate which leaves qualitative results similar. Training a single agent takes around 20 minutes on a Quadro RTX 6000 GPU with the environment running on a single CPU.

ZX-diagrams: For training, we use the PPO implementation of Nägele & Marquardt (2024) to facilitate the changing observation and action space. The hyperparameters and network architecture were chosen as by Nägele & Marquardt (2024) who originally chose them to give good performance of the PPO algorithm. This is the most compute-intensive experiment reported in this work with one training run lasting for 12 hours using two Quadro RTX 6000 GPUs and 32 CPUs.

Quantum error correction For training, we use the PPO implementation of `PureJaxRL` (Lu et al., 2022). The hyperparameters have been chosen to be the optimal ones reported in Zen et al. (2024), which were optimized for performance of the PPO algorithm. All of the training is done on a single Quadro RTX 6000 GPU. Training 10 agents to complete the code discovery task takes 1 to 2 minutes, depending on the target code parameters. For the logical state preparation task, it takes around 100 seconds for $[[5, 1, 3]]_l$ and around 2500 seconds for $[[17, 1, 5]]_l$ to train 10 agents in parallel.

Grid environment: For training, we use a vanilla Q-learning algorithm. Per training run, we take a total of 10^5 steps in the environment. After a warmup phase of 1000 steps, we train after every 100 steps taken in the environment on a batch consisting of the last 1000 experiences of the agent. For exploration, we use an ϵ-greedy strategy with $\epsilon = 0.1$. We use the Adam optimizer with the learning rate linearly annealed from 10^{-2} to 10^{-7}. For the Q-network, we use a multilayer perceptron with 2 hidden layers of dimension 128 with tanh activations. One training run takes around 30 seconds on a single CPU.

Total compute resources: We estimate the total compute time to reproduce the results of this manuscript to be around 1250 GPU hours and 25000 CPU hours.

Table A2: Final return in the grid environment using our method or the method described by Cui & Yu (2023). Statistically significant differences between the algorithms are highlighted.

Grid seed	Final return, this work	Final return, Cui et al.
Grid size $N = 3$		
0	**0.46** (**0.46**, **0.46**)	0.16 (0.09, 0.31)
1	0.66 (0.66, 0.66)	0.66 (0.66, 0.66)
2	-0.45 (-0.45, -0.45)	-0.45 (-0.45, -0.45)
3	-0.04 (-0.04, -0.04)	-0.06 (-0.10, -0.04)
4	0.21 (0.21, 0.21)	0.21 (0.21, 0.21)
5	-0.43 (-0.43, -0.43)	-0.43 (-0.43, -0.43)
6	**0.36** (**0.36**, **0.36**)	0.28 (0.27, 0.32)
7	0.63 (0.61, 0.64)	0.63 (0.61, 0.64)
8	-0.12 (-0.12, -0.12)	-0.12 (-0.12, -0.12)
9	**0.83** (**0.83**, **0.83**)	0.59 (0.48, 0.72)
mean	0.21	0.15
Grid size $N = 4$		
0	**0.44** (**0.21**, **0.66**)	0.09 (0.09, 0.09)
1	0.13 (-0.13, 0.39)	-0.09 (-0.09, -0.09)
2	**0.31** (**0.31**, **0.31**)	0.20 (0.12, 0.28)
3	-0.21 (-0.44, -0.06)	-0.08 (-0.12, -0.04)
4	0.60 (0.60, 0.60)	0.60 (0.59, 0.60)
5	-0.18 (-0.18, -0.18)	-0.18 (-0.18, -0.18)
6	0.32 (0.28, 0.35)	0.33 (0.30, 0.35)
7	-0.11 (-0.11, -0.11)	-0.10 (-0.11, -0.08)
8	-0.43 (-0.51, -0.28)	-0.23 (-0.36, -0.14)
9	-0.03 (-0.03, -0.03)	-0.05 (-0.09, -0.03)
mean	0.08	0.05
Grid size $N = 5$		
0	0.09 (-0.03, 0.19)	-0.08 (-0.15, 0.07)
1	-0.09 (-0.09, -0.09)	-0.17 (-0.32, -0.09)
2	-0.52 (-0.59, -0.45)	-0.45 (-0.45, -0.45)
3	-0.00 (-0.20, 0.23)	-0.18 (-0.31, -0.08)
4	**0.60** (**0.60**, **0.60**)	0.06 (-0.00, 0.20)
5	-0.18 (-0.18, -0.18)	-0.18 (-0.18, -0.18)
6	**0.36** (**0.36**, **0.36**)	-0.14 (-0.14, -0.14)
7	-0.62 (-0.81, -0.51)	-0.35 (-0.55, -0.13)
8	-0.52 (-0.52, -0.52)	**-0.49** (**-0.49**, **-0.49**)
9	-0.03 (-0.03, -0.03)	-0.03 (-0.03, -0.03)
mean	-0.09	-0.20

Table A3: Area under the training curve in the grid environment using our method or the method described by Cui & Yu (2023). Statistically significant differences between the algorithms are highlighted.

Grid seed	Area under training curve, this work	Area under training curve, Cui et al.
	Grid size $N = 3$	
0	$\mathbf{0.44}\,(\mathbf{0.42}, \mathbf{0.45})$	$0.15\,(0.13, 0.17)$
1	$\mathbf{0.65}\,(\mathbf{0.64}, \mathbf{0.65})$	$0.63\,(0.63, 0.63)$
2	$-0.46\,(-0.47, -0.46)$	$\mathbf{-0.46}\,(\mathbf{-0.47}, \mathbf{-0.46})$
3	$-0.06\,(-0.06, -0.06)$	$-0.07\,(-0.11, -0.05)$
4	$0.18\,(0.16, 0.19)$	$\mathbf{0.20}\,(\mathbf{0.20}, \mathbf{0.21})$
5	$-0.44\,(-0.44, -0.44)$	$\mathbf{-0.44}\,(\mathbf{-0.44}, \mathbf{-0.44})$
6	$0.34\,(0.33, 0.35)$	$0.29\,(0.25, 0.33)$
7	$0.59\,(0.57, 0.60)$	$\mathbf{0.57}\,(\mathbf{0.56}, \mathbf{0.58})$
8	$-0.13\,(-0.14, -0.13)$	$\mathbf{-0.13}\,(\mathbf{-0.14}, \mathbf{-0.13})$
9	$0.79\,(0.78, 0.81)$	$0.55\,(0.53, 0.56)$
mean	0.19	0.13
	Grid size $N = 4$	
0	$0.12\,(0.05, 0.21)$	$0.05\,(0.02, 0.10)$
1	$-0.05\,(-0.15, 0.08)$	$-0.15\,(-0.17, -0.13)$
2	$0.22\,(0.17, 0.27)$	$0.23\,(0.20, 0.26)$
3	$-0.15\,(-0.16, -0.15)$	$\mathbf{-0.12}\,(\mathbf{-0.15}, \mathbf{-0.09})$
4	$\mathbf{0.56}\,(\mathbf{0.54}, \mathbf{0.58})$	$0.48\,(0.45, 0.52)$
5	$-0.26\,(-0.28, -0.23)$	$\mathbf{-0.21}\,(\mathbf{-0.22}, \mathbf{-0.20})$
6	$0.13\,(0.05, 0.21)$	$\mathbf{0.21}\,(\mathbf{0.15}, \mathbf{0.26})$
7	$-0.20\,(-0.24, -0.16)$	$\mathbf{-0.14}\,(\mathbf{-0.16}, \mathbf{-0.13})$
8	$-0.50\,(-0.51, -0.49)$	$\mathbf{-0.34}\,(\mathbf{-0.42}, \mathbf{-0.28})$
9	$-0.12\,(-0.14, -0.10)$	$\mathbf{-0.06}\,(\mathbf{-0.07}, \mathbf{-0.05})$
mean	-0.02	0.0
	Grid size $N = 5$	
0	$\mathbf{-0.03}\,(\mathbf{-0.13}, \mathbf{0.07})$	$-0.16\,(-0.18, -0.14)$
1	$-0.11\,(-0.12, -0.10)$	$-0.12\,(-0.12, -0.11)$
2	$-0.55\,(-0.59, -0.52)$	$\mathbf{-0.48}\,(\mathbf{-0.48}, \mathbf{-0.47})$
3	$-0.24\,(-0.32, -0.14)$	$-0.21\,(-0.25, -0.16)$
4	$0.35\,(0.15, 0.50)$	$0.20\,(0.07, 0.33)$
5	$-0.22\,(-0.22, -0.21)$	$\mathbf{-0.20}\,(\mathbf{-0.20}, \mathbf{-0.20})$
6	$-0.02\,(-0.14, 0.10)$	$-0.14\,(-0.16, -0.10)$
7	$-0.69\,(-0.76, -0.61)$	$\mathbf{-0.57}\,(\mathbf{-0.65}, \mathbf{-0.49})$
8	$-0.53\,(-0.53, -0.53)$	$\mathbf{-0.52}\,(\mathbf{-0.52}, \mathbf{-0.51})$
9	$-0.13\,(-0.21, -0.08)$	$\mathbf{-0.07}\,(\mathbf{-0.08}, \mathbf{-0.06})$
mean	-0.09	-0.20

Figure A2: Square error when predicting the Q-function in the grid environment using our method (orange) and the method of Cui & Yu (2023) (blue) against the training step. N indicates the grid size with 10 different random grids per size (only 5 shown). The prediction loss of the Q-function is similar for both methods but our method may lead to a higher final return (see Table A2).

Figure A3: Training progress of the cumulative FINALPPO algorithm (with and without added state information h_t) and of the non-cumulative MAXVELPPO algorithm in the lunar lander environment.

Figure A4: Training progress in the portfolio optimization task.

Figure A5: Training progress in the quantum error correction tasks. The best and worst performance of 10 seeds is shaded.

Figure A6: Markov decision process constructed from the non-cumulative Markov decision process depicted in Figure 2.

Table A4: Q-function Q' of the MDP depicted in Figure 2 found by value iteration using the method of Cui & Yu (2023). The resulting policy is not optimal and results in an expected return of -0.5.

State s	Action a	$Q(s, a)$
$\tilde{s}_0$	-	-0.15
$(\tilde{s}_1, 1)$	a_0	-1
$(\tilde{s}_1, 1)$	a_1	-0.3
$(\tilde{s}_1, -1)$	a_0	0
$(\tilde{s}_1, -1)$	a_1	-0.1

State $\tilde{s}$	Action a	$Q'(\tilde{s}, a)$
$\tilde{s}_0$	-	-0.5
$\tilde{s}_1$	a_0	0
$\tilde{s}_1$	a_1	-0.2

Table A5: Q-function Q of the MDP depicted in Figure A6 (which corresponds to the NCMDP of Figure 2) found by value iteration using our method. The resulting policy is optimal and results in an expected return of -0.15.