Provably Efficient Maximum Entropy Exploration

Elad Hazan$^{12}$ Sham M. Kakade$^{134}$ Karan Singh$^{12}$ Abby Van Soest$^2$

$^1$ Google AI Princeton
$^2$ Department of Computer Science, Princeton University
$^3$ Allen School of Computer Science and Engineering, University of Washington
$^4$ Department of Statistics, University of Washington
{ehazan,karans,asoest}@princeton.edu, sham@cs.washington.edu,

Abstract

Suppose an agent is in a (possibly unknown) Markov Decision Process in the absence of a reward signal, what might we hope that an agent can efficiently learn to do? One natural, intrinsically defined, objective problem is for the agent to learn a policy which induces a distribution over state space that is as uniform as possible, which can be measured in an entropic sense. Despite the corresponding mathematical program being non-convex, our main result provides a provably efficient method, both in terms of sample size and computational complexity, to construct such a maximum-entropy exploratory policy. Key to our algorithmic methodology is utilizing the conditional gradient method (a.k.a. the Frank-Wolfe algorithm) which utilizes an approximate MDP solver.

1 Introduction

In the reinforcement learning (RL) problem, an agents seeks to learn a policy (a mapping from states to actions) which maximizes some notion of long term reward, potentially in a setting where the agent does not know the environment. Direct optimization approaches to this problem (such as the common policy gradient methods used in deep learning) tend to perform favorably when random sequences of actions lead the agent to some reward, but tend to fail when the rewards may be difficult to find by random search (such as cases where the reward function is sparse in the state space). Thus far, the most practical approaches to address this have either been through some carefully constructed reward shaping (e.g. [NHR99] where dense reward functions are provided to make the optimization problem more tractable) or through inverse reinforcement learning and imitation learning [AN04, RGB11] (where an expert demonstrates to the agent how to act).

In theory, for the case of tabular Markov decision processes, the balance of exploration and exploitation has been addressed in that there are a number of methods which utilize confidence based reward bonuses to encourage exploration in order to ultimately behave near optimally [KS02, Kak03, SLW+06, LH14, DB15, SS10, AOM17]. There are a host of recent empirical success using deep RL methods which encourage exploration in some form [MKS+15, SHM+16]. The approaches which encourage exploration are based on a few related ideas: that of encouraging encouraging exploration through state visitation frequencies (e.g. [OBvdOM17, BSO+16, THF+17]) and those based on a intrinsic reward signal derived from novelty or prediction error [LLTyO12, PAED17, SRM+18, FCRL17, MLR15, HCC+16, SRM+18, WRR+17], aligning an intrinsic reward to the target objective [Kae93, CBS05, SLBS10, SLB09, ZOS18], or sample based approaches to tracking of value function uncertainty [OBPVR16, OAC18].

More generally, there may be value in understanding how to focus the learning such that the agent can master how to manipulate the environment in a sense that is more general than just optimizing a single scalar reward function. In particular, it may be insightful to understand if there are intrinsic learning problems to focus on in the absence of any extrinsic scalar reward signal, where this intrinsic learning
problem encourages the agent to find policies which can manipulate its environment. Works in [CBS05, SLB09, SLBS10] established computational theories of intrinsic reward signals (and how it might help with downstream learning of tasks) and other works also showed how to incorporate intrinsic rewards (in the absence of any true reward signal) [WdWK+18, BESK18, BEP+18, NPD+18]. The potential benefit is that such learning may help the agent reach a variety of achievable goals and do well on other extrinsically defined tasks, not just the task under which it was explicitly trained for under one specific reward function (e.g. see [CBS05, SLB09, WdWK+18, NPD+18]).

The majority of provably efficient methods for reinforcement learning are restricted to the setting where the underlying objective is that of maximizing the (long term) expected reward. In the absence of an extrinsic reward signal, it may be natural to understand if there are other provably efficient methods for which an agent can learn to manipulate its environment based on an intrinsic optimization objective. This is the focus of this work, where we consider a wider class of objective functions based on entropic measures of the visitation distribution of the state space (as opposed to focusing on maximization of a scalar reward function).

Concretely, this work focuses on the problem of learning a (possibly non-stationary) policy which induces a distribution over the state space that is as uniform as possible, which can be measured in an entropic sense. Although we show the corresponding mathematical program is non-convex, our main contribution is in providing an efficient learning algorithm for computing an ($\epsilon$-approximate) maximum entropy policy, in settings where the model is either known or unknown. Key to our algorithmic methodology is utilizing the conditional gradient method\footnote{For detailed description of the Frank-Wolfe method as well as its online variant see [Haz16] chapter 7.} (a.k.a. the Frank-Wolfe algorithm [FW56]) in order to solve a certain sub-problem. While we focus on this particular entropic measure, generalizations are possible.

## 2 Preliminaries

**Markov decision process:** An infinite-horizon discounted Markov Decision Process is a tuple $\mathcal{M} = (S, A, r, P, \gamma, d_0)$, where $S$ is the set of states, $A$ is the set of actions, and $d_0$ is the distribution of the initial state $s_0$. At each timestep $t$, upon observing the state $s_t$, the execution of an action $a_t$ triggers an observable reward of $r_t = r(s_t, a_t)$ and a transition to a new state $s_{t+1} \sim P(\cdot|s_t, a_t)$. The performance on an infinite sequence of states & actions (hereafter, referred to as a trajectory) is judged through the (discounted) cumulative reward it accumulates, defined as

$$V(\tau = (s_0, a_0, s_1, a_1, \ldots)) = (1 - \gamma) \sum_{t=0}^{\infty} \gamma^t r(s_t, a_t).$$

**Policies:** A policy is a (randomized) mapping from a history, say $(s_0, a_0, r_0, s_1, a_1, r_1, \ldots s_{t-1}, a_{t-1}, r_{t-1})$, to an action $a_t$. A stationary policy $\pi$ is a (randomized) function which maps a state to an action in a time-independent manner, i.e. $\pi : S \rightarrow \Delta(A)$. When a policy $\pi$ is executed on some MDP $\mathcal{M}$, it produces a distribution over infinite-length trajectories $\tau = (s_0, a_0, s_1, a_1 \ldots)$ as specified below.

$$P(\tau|\pi) = P(s_0) \prod_{i=0}^{\infty} \left( \pi(a_i|s_i)P(s_{i+1}|s_i, a_i) \right)$$

The (discounted) value $V_\pi$ of a policy $\pi$ is the expected cumulative reward an action sequence sampled from the policy $\pi$ gathers.

$$V_\pi = \mathbb{E}_{\tau \sim P(\cdot|\pi)} V(\tau) = (1 - \gamma) \sum_{t=0}^{\infty} \gamma^t r(s_t, a_t)$$

**Induced state distributions:** The $t$-step state distribution and the (discounted) state distribution of
a policy $\pi$ that result are
\begin{equation}
    d_{t,\pi}(s) = P(s_t = s|\pi) = \sum_{\tau \text{ with } s_t = s} P(\tau|\pi),
\end{equation}
\begin{equation}
    d(\pi)(s) = (1 - \gamma) \sum_{t=1}^{\infty} \gamma^t d_{t,\pi}(s).
\end{equation}
The latter distribution can be viewed as the analogue of the stationary distribution in the infinite horizon setting.

**Mixtures of stationary policies:** Given a sequence of $k$ policies $C = (\pi_0, \ldots, \pi_{k-1})$, and $\alpha \in \Delta_k$, we define $\pi_{\text{mix}} = (\alpha, C)$ to be a mixture over stationary policies. The (non-stationary) policy $\pi_{\text{mix}}$ is one where, at the first timestep $t = 0$, we sample policy $\pi_i$ with probability $\alpha_i$ and then use this policy for all subsequent timesteps. In particular, the behavior of a mixture $\pi_{\text{mix}}$ with respect to an MDP is that it induces infinite-length trajectories $\tau = (s_0, a_0, s_1, a_1, \ldots)$ with the probability law:
\begin{equation}
    P(\tau|\pi_{\text{mix}}) = \sum_{i=0}^{k-1} \alpha_i P(\tau|\pi_i)
\end{equation}
and the induced state distribution is:
\begin{equation}
    d_{\pi_{\text{mix}}}(s) = \sum_{i=0}^{k-1} \alpha_i d_{\pi_i}(s).
\end{equation}
Note that such a distribution over policies need not be representable as a stationary stochastic policy (even if the $\pi_i$’s are stationary) due to that the sampled actions are no longer conditionally independent given the states.

3 **The Objective: MaxEnt Exploration**

As each policy induces a distribution over states, we can associate an entropy with this induced distribution:
\begin{equation}
    H(d(\pi)) = -\mathbb{E}_{s \sim d(\pi)} \log d(\pi)(s).
\end{equation}
We say that a policy $\pi^*$ is a maximum-entropy exploration policy, also to referred to as the max-ent policy, if the corresponding induced state distribution has the maximum possible entropy among the class of all policies.
\begin{equation}
    \pi^* \in \arg \max_{\pi} H(d(\pi)).
\end{equation}
Our goal is to find a policy that induces a state distribution with comparable entropy.

3.1 **Other entropic measures**

The same techniques we derive can also be used to optimize other entropic measures. For example, we may be interested in maximizing:
\begin{equation}
    \arg \max_{\pi} \left\{ -\text{KL}(d(\pi)\|Q) = \mathbb{E}_{s \sim d(\pi)} \log \frac{Q(s)}{d(\pi)(s)} \right\}
\end{equation}
for some given distribution $Q(s)$. Alternatively, we may seek to minimize a cross entropy measure:
\begin{equation}
    \arg \min_{\pi} \left\{ \mathbb{E}_{s \sim Q} \log \frac{1}{d(\pi)(s)} = \text{KL}(Q\|d(\pi)) + H(Q) \right\}
\end{equation}
where the expectation is now under $Q$. For uniform $Q$, this latter measure may be more aggressive in forcing $\pi$ to have more uniform coverage than the MaxEnt policy.
3.2 Non-convexity of the objective function

We establish that the entropy of the state distribution is not a concave function of the policy. Despite the concavity of the entropy functional, our overall maximization problem is not concave due to that the state distribution is not an affine function of the policy. This is made precise in the following lemma.

Lemma 1. $H(d_x)$ is not concave in $\pi$.

Proof. Figure 1 demonstrates the behavior of $\pi_0, \pi_1, \pi_2$ on a 6-state MDP with binary actions. Note that for sufficiently large $\gamma \rightarrow 1$ and any policy $\pi$, the discounted state distribution converges to the distribution on the states at the second timestep, or formally $d_{\pi} \rightarrow d_{2,\pi}$. Now with the realization $\pi_0 = \frac{\pi_1 + \pi_2}{2}$, observe that $d_{2,\pi_0}$ is not uniform on $\{s_{2,0}, s_{2,1}, s_{2,2}\}$, implying that $H(d_{2,\pi_0}) < \frac{H(d_{2,\pi_1}) + H(d_{2,\pi_2})}{2}$.

Lemma 2. For any policy $\pi$ and MDP $M$, define the matrix $P_\pi \in \mathbb{R}^{|S| \times |S|}$ so that

$$P_\pi(s', s) = \sum_{a \in A} \pi(a|s)P(s'|s, a).$$

Then it is true that

1. $P_\pi$ is linear in $\pi$,
2. $d_{t,\pi} = P_\pi^td_{0}$ for all $t \geq 0$,
3. $d_{\pi} = (1 - \gamma)(I - \gamma P_\pi)^{-1}d_{0}$.

Proof. Linearity of $P_\pi$ is evident from the definition. (2,3) may be verified by calculation.

4 Algorithms & Main Results

The algorithm maintains a distribution over policies, and proceeds by adding a new policy to the support of the mixture and reweighing the components. To describe the algorithm, we will utilize access to two kinds of oracles. The constructions for these are detailed in later sections.

1. **Approximate planning oracle:** Given a reward function (on states) $r : S \rightarrow \mathbb{R}$ and a sub-optimality gap $\varepsilon_1$, the planning oracle returns a stationary policy $\pi = \Pi(r, \varepsilon_1)$ with the guarantee that $V_\pi \geq \max_{\pi} V_\pi - \varepsilon_1$.

2. **State distribution estimate oracle:** A state distribution oracle estimates the state distribution $d_x = D(\pi, \varepsilon_0)$ of any given (non-stationary) policy $\pi$, guaranteeing that $\|d_x - \hat{d}_\pi\|_{\infty} \leq \varepsilon_0$.

\[\text{As the oracle is solving a discounted problem, we know the optimal value is achieved by a stationary policy.}\]
Algorithm 1 Maximum-entropy policy computation.

1: **Input:** Step size \( \eta \), number of iterations \( T \), planning oracle error tolerance \( \varepsilon_1 > 0 \), state distribution oracle error tolerance \( \varepsilon_0 > 0 \), smoothing parameter \( \beta \).
2: Set \( C_0 = \{ \pi_0 \} \) where \( \pi_0 \) is an arbitrary policy.
3: Set \( \alpha_0 = 1 \).
4: for \( t = 0, \ldots, T - 1 \) do
5: Call the state distribution oracle on \( \pi_{\text{mix},t} = (\alpha_t, C_t) \) to get:
\[
\hat{d}_{\pi_{\text{mix},t}} = D(\pi_{\text{mix},t}, \varepsilon_0).
\]
6: Define the reward function \( r_t \) as
\[
r_t(s) := (\nabla H_\beta(\hat{d}_{\pi_{\text{mix},t}}))_s = -\left( \log(\hat{d}_{\pi_{\text{mix},t}}(s) + \beta) + \frac{\hat{d}_{\pi_{\text{mix},t}}(s)}{\hat{d}_{\pi_{\text{mix},t}}(s) + \beta} \right).
\]
7: Compute the (approximately) optimal policy on \( r_t \) as:
\[
\pi_{t+1} = \Pi(r_t, \varepsilon_1).
\]
8: Update \( \pi_{\text{mix},t+1} = (\alpha_{t+1}, C_{t+1}) \) to be
\[
C_{t+1} = (\pi_0, \ldots, \pi_t, \pi_{t+1}), \tag{5}
\]
\[
\alpha_{t+1} = ((1 - \eta)\alpha_t, \eta). \tag{6}
\]
9: end for
10: **return** \( \pi_{\text{mix},T} = (\alpha_T, C_T) \).

Algorithm 1 also makes use of a smoothed version of the entropy function, \( H_\beta \), which is defined to be
\[
H_\beta(P) := -\mathbb{E}_{s \sim P} \log(P(s) + \beta)
\]
where \( \beta \geq 0 \) is a smoothing parameter that is set appropriately in the following theorem.

**Theorem 3.** For any \( \varepsilon > 0 \), set \( \beta = \frac{0.1 \varepsilon}{2|S|} \), \( \varepsilon_1 = 0.1 \varepsilon \), \( \varepsilon_0 = \frac{0.1 \varepsilon^2}{80|S|} \), and \( \eta = \frac{0.1 \varepsilon^2}{40|S|} \). When Algorithm 1 is run for \( T \) iterations where:
\[
T \geq \frac{40|S|}{0.1 \varepsilon^2} \log \frac{|S|}{0.1 \varepsilon},
\]
we have that:
\[
H(\pi_{\text{mix},T}) \geq \max_\pi H(d_\pi) - \varepsilon.
\]

Before we begin the proof, it is helpful to establish a few properties about \( H_\beta \) in Lemma 4, deferring their proof to the end of this subsection.

**Lemma 4.** For any two distributions \( P, Q \in \Delta_d \), for all \( i < d \), we have
\[
(A) \ (\nabla H_\beta(P))_i = -\left( \log(P_i + \beta) + \frac{P_i}{P_i + \beta} \right),
\]
\[
(B) H_\beta(P) \text{ is concave in } P,
\]
(C) $H_\beta(P)$ is $2\beta^{-1}$ smooth, i.e. $-2\beta^{-1}d \leq \nabla^2 H_\beta(P) \leq 2\beta^{-1}d$,

(D) $|H(P) - H_\beta(P)| \leq d\beta$,

(E) $\|\nabla H_\beta(P) - \nabla H_\beta(Q)\|_\infty \leq 2\beta^{-1}\|P - Q\|_\infty$.

Proof of Theorem 3. Let $\pi^*$ be a maximum-entropy policy, i.e. $\pi^* \in \arg\max_{\pi} H(d_\pi)$. The proof strategy is to argue that $\pi_{mix,T}$ and $\pi^*$ are close in terms of the value they attain on $H_\beta$. Subsequently, we utilize the fact that functions $H$ and $H_\beta$ are close point-wise. For any $t < T$, we note that

$$H_\beta(d_{\pi_{mix,t+1}}) = H_\beta((1 - \eta)d_{\pi_{mix,t}} + \eta d_{\pi_{t+1}})$$

Equation [3]

$$\geq H_\beta(d_{\pi_{mix,t}}) + \eta \langle d_{\pi_{t+1}} - d_{\pi_{mix,t}}, \nabla H_\beta(d_{\pi_{mix,t}}) \rangle - \eta^2 \beta^{-1}\|d_{\pi_{t+1}} - d_{\pi_{mix,t}}\|^2_2$$

Lemma 4(C)

The second inequality follows from the smoothness of $H_\beta$. (See Section 2.1 in [B+15] for equivalent definitions of smoothness in terms of the function value and the Hessian.)

To incorporate the error due to the two oracles, observe

$$\langle d_{\pi_{t+1}}, \nabla H_\beta(d_{\pi_{mix,t}}) \rangle \geq \langle d_{\pi_{t+1}}, \nabla H_\beta(d_{\pi_{mix,t}}) \rangle - 2\beta^{-1}\|d_{\pi_{mix,t}} - \hat{\nabla} d_{\pi_{mix,t}}\|_\infty$$

Lemma 4(E)

$$\geq \langle d_{\pi^*}, \nabla H_\beta(d_{\pi_{mix,t}}) \rangle - 2\beta^{-1}\|d_{\pi^*} - d_{\pi_{mix,t}}\|_\infty$$

Lemma 4(E)

Note that the second inequality above follows from the defining character of the planning oracle, i.e. with respect to the reward vector $r_t = \nabla H_\beta(d_{\pi_{mix,t}})$, for any policy $\pi'$, it holds true that

$$V_{\pi_{mix}} = \langle d_{\pi_{mix}}, r_t \rangle \geq V_{\pi'} - \epsilon_1 = \langle d_{\pi^*}, r_t \rangle - \epsilon_1$$

In particular, this statement holds for the choice $\pi' = \pi^*$. This argument does not rely on $\pi^*$ being a stationary policy, since $\pi_{t+1}$ is an optimal policy for the reward function $r_t$ among the class of all policies.

Using the above fact and continuing on

$$H_\beta(d_{\pi_{mix,t+1}}) \geq H_\beta(d_{\pi_{mix,t}}) + \eta \langle d_{\pi^*} - d_{\pi_{mix,t}}, \nabla H_\beta(d_{\pi_{mix,t}}) \rangle - 4\eta\beta^{-1}\|d_{\pi^*} - d_{\pi_{mix,t}}\|_\infty$$

Lemma 4(B)

Now, with the aid of the above, we observe the following inequality.

$$H_\beta(d_{\pi^*}) - H_\beta(d_{\pi_{mix,t+1}}) \leq (1 - \eta)(H_\beta(d_{\pi^*}) - H_\beta(d_{\pi_{mix,t}})) + 4\eta\beta^{-1}\|d_{\pi^*} - d_{\pi_{mix,t}}\|_\infty + \eta\epsilon_1 + 2\eta^2\beta^{-1}.$$}

Telecopying the inequality and using Lemma 4(D), this simplifies to

$$H(d_{\pi^*}) - H(d_{\pi_{mix,T}}) \leq 2|S|\beta + (1 - \eta)^T(H(d_{\pi^*}) - H_\beta(d_{\pi_{mix,0}})) + 4\beta^{-1}\|d_{\pi^*} - d_{\pi_{mix,0}}\| + \epsilon_1 + 2\eta\beta^{-1}$$

$$\leq 2|S|\beta + e^{-T\eta}\log|S| + 4\beta^{-1}\epsilon_0 + \epsilon_1 + 2\eta\beta^{-1}.\text{setting } \beta = \frac{0.1\epsilon}{2|S|}, \epsilon_1 = 0.1\epsilon, \epsilon_0 = \frac{0.1\epsilon^2}{80|S|}, \eta = \frac{0.1\epsilon}{40|S|}, T = \frac{40|S|}{0.1\epsilon^2}\log\frac{\log|S|}{0.1\epsilon}\text{ suffices.}\square$$

Proof of Lemma 4. (A) may be verified by explicit calculation. Observe $\nabla^2 H_\beta(P)$ is a diagonal matrix with entries

$$\langle \nabla^2 H_\beta(P) \rangle_{i,i} = -\frac{P_i + 2\beta}{(P_i + \beta)^2}.$$
The last inequality follows from \( \log x \leq x - 1, \forall x > 0 \). Finally, to see (E), using Taylor’s theorem, observe

\[
\|\nabla H_\beta(P) - \nabla H_\beta(Q)\|_\infty \leq \max_{i,\alpha \in [0,1]} \|\nabla^2 H_\beta(\alpha P + (1 - \alpha)Q)_{i,i}\| P - Q\|_\infty \\
\leq 2\beta^{-1}\|P - Q\|_\infty.
\]

\[\square\]

4.1 The known MDP case

With the knowledge of the transition matrix \( P \) of a MDP \( M \) in the form of an explicit tensor, the planning oracle can be implemented via any of the exact solution methods [Ber05], e.g. value iteration, linear programming. The state distribution oracle can be efficiently implemented as Lemma 2 suggests.

**Corollary 5.** When the MDP \( M \) is known explicitly, with the oracles described in Section 4, Algorithm 7 runs in \( \text{poly}(|S|, |A|, \frac{1}{1-\gamma}, \frac{1}{\epsilon}) \) time to guarantee \( H(d_{\pi_{\text{mix},T}}) \geq \max_\pi H(d_\pi) - \epsilon \).

4.2 The unknown MDP case

For the case of an unknown MDP, a sample-based algorithm must successively try to learn about the MDP through its interactions with the environment. Here, we assume a \( \gamma \)-discounted episodic setting, where the agent can act in the environment starting from \( s_0 \sim d_0 \) for some number of steps, and is then able to reset.

Our measure of sample complexity in this setting is the number of \( \tilde{O} \left( \frac{1}{1-\gamma} \right) \)-length episodes the agent must sample to achieve a \( \epsilon \)-suboptimal performance guarantee. The algorithm outlined below makes a distinction between the set of states it is (relatively) sure about and the set of states that have not been visited enough number of times yet. The algorithm and the analysis is similar to the \( E^3 \) algorithm [KS02].

**Theorem 6.** For an unknown MDP, with Algorithm 2 as the planning oracle and Algorithm 3 as the distribution estimate oracle, Algorithm 1 runs in \( \text{poly}(|S|, |A|, \frac{1}{1-\gamma}, \frac{1}{\epsilon}) \) time and executes \( \tilde{O} \left( \frac{|S|^2|A|}{\epsilon^2(1-\gamma)^2} + \frac{|S|^3}{\epsilon^3} \right) \) episodes of length \( \tilde{O} \left( \frac{\log \frac{|S|}{\epsilon \log \gamma}}{\log \frac{\log \frac{|S|}{\epsilon \log \gamma}}{\log \gamma}} \right) \) to guarantee that

\[
H(d_{\pi_{\text{mix},T}}) \geq \max_\pi H(d_\pi) - \epsilon.
\]

Before we state the proof, we note the following lemmas. The first is an adaptation of the analysis of the \( E^3 \) algorithm. The second is standard. We only include the second for completeness. The proof of these follow that of the main theorem.

**Lemma 7.** For any reward function \( r \), \( \epsilon > 0 \), with \( \epsilon_1 = 0.1\epsilon \), \( m = \frac{32|S|\log|S|}{(1-\gamma)^2(0.1\epsilon)^2} \), \( n = \frac{32|S|^2|A|\log|S|}{(1-\gamma)^2|A|^2(0.1\epsilon)^2} \), \( t_0 = \frac{\log \frac{|S|}{\epsilon \log \gamma}}{\log \frac{\log \frac{|S|}{\epsilon \log \gamma}}{\log \gamma}} \), Algorithm 6 guarantees with probability \( 1 - \delta \)

\[
V_\pi \geq \max_\pi V_\pi - \epsilon_1.
\]

Furthermore, note that if Algorithm 6 is invoked \( T \) times (on possibly different reward functions), the total number of episodes sampled across all the invocations is \( n(T + m|S||A|) = \tilde{O} \left( \frac{T}{\epsilon^2} + \frac{|S|^2|A|}{\epsilon^2(1-\gamma)^2} \right) \), each episode being of length \( t_0 \).

**Lemma 8.** For any \( \epsilon_0, \delta > 0 \), when Algorithm 3 is run with \( m = \frac{200l_0\log|S|\log 0.1\epsilon}{\delta \log \gamma} \), \( t_0 = \frac{\log 0.1\epsilon}{\log \gamma} \), \( \hat{d}_\pi \) satisfies \( \|\hat{d}_\pi - d_\pi\|_\infty \leq \epsilon_0 \) with probability at least \( 1 - \delta \). In this process, the algorithm samples \( m \) episodes of length \( t_0 \).
**Algorithm 2** Sample-based planning for an unknown MDP.

1. **Input:** Reward $r$, error tolerance $\varepsilon > 0$, exact planning oracle tolerance $\varepsilon_1 > 0$, oversampling parameter $m$, number of rollouts $n$, rollout length $t_0$.
2. Initialize a persistent data structure $C \in \mathbb{R}^{\vert S \vert^2 \times |A|}$, which is maintained across different calls to the planning algorithm to keep transition counts, to $C(s'|s,a) = 0$ for every $(s', s,a) \in S^2 \times A$.
3. **repeat**
   4. Declare $K = \{ s : \min_{a \in A} \sum_{s' \in S} C(s'|s,a) \geq m \}$, $\hat{P}(s'|s,a) = \begin{cases} \frac{C(s'|s,a)}{\sum_{s' \in S} C(s'|s,a)}, & \text{if } s \in K \\ 1, & \text{otherwise.} \end{cases}$
   5. Define the reward function as $r_K(s) = \begin{cases} r(s), & \text{if } s \in K \\ \log |S|, & \text{otherwise.} \end{cases}$
   6. Compute an (approximately) optimal policy on the MDP induced by $\hat{P}$ and reward $r_K$. This task is purely computational, and can be done as indicated in Section 4.1. Also, modify the policy so that on every state $s \in S - K$, it chooses the least performed action.
   7. Run $\pi$ on the true MDP $M$ to obtain $n$ independently sampled $t_0$-length trajectories $(\tau_1, \ldots, \tau_n)$, and increment the corresponding counts in $C(s'|s,a)$.
   8. If and only if no trajectory $\tau_i$ contains a state $s \in S - K$, mark $\pi$ as stable.
9. **until** $\pi$ is stable.
10. **return** $\pi$.

**Algorithm 3** Sample-based estimate of the state distribution.

1. **Input:** A policy $\pi$, termination length $t_0$, oversampling parameter $m$.
2. Sample $m$ trajectories $(\tau_0, \ldots, \tau_{m-1})$ of length $t_0$ following the policy $\pi$.
3. For every $t < t_0$, calculate the empirical state distribution $d_{t,\pi}$.

$$d_{t,\pi}(s) = \frac{\vert \{ i < m : \tau_i = (s_0,a_0,\ldots) \text{ with } s_t = s \} \vert}{m}$$

4. **return** $\hat{d}_\pi = \frac{1-\gamma}{1-\gamma^{t_0}} \sum_{t=0}^{t_0-1} \gamma^t d_{t,\pi}$

**Proof of Theorem 6** As parameter settings in Theorem 3 indicate, $T = \frac{40|S|}{0.1 \varepsilon_1^2} \log \frac{\log |S|}{0.1 \varepsilon_1} \varepsilon_1 = 0.1 \varepsilon_1 \varepsilon_0 = \frac{0.1 \varepsilon_2^2}{20|S|}$ suffices. This setting requires Algorithm 2 to be sample $\hat{O} \left( \frac{|S|^3}{\varepsilon_1^2} + \frac{|S|^2 |A|}{\varepsilon_1 (1-\gamma)^2} \right) = \hat{O} \left( \frac{|S|^2 |A|}{\varepsilon_1 (1-\gamma)^2} \right)$ episodes across all invocations, and Algorithm 3 to sample $\hat{O} \left( \frac{|S|^3}{\varepsilon_1^2} \right)$ episodes. \square

The following notions & lemmas are helpful in proving Lemma 7. We shall call a state $s \in K$ $m$-known if, for all actions $a \in A$, action $a$ has been executed at state $s$ at least $m$ times. For any MDP $M = (S,A,r,P,\gamma)$ and a set of $m$-known states $K \subseteq S$, define an induced MDP $M_K = (S,A,r_K,P_K,\gamma)$ so that the states absent from $K$ are absorbing and maximally rewarding.

$$r_K(s,a) = \begin{cases} r(s,a), & \text{if } s \in K, \\ \log |S|, & \text{otherwise,} \end{cases} \quad P_K(s'|s,a) = \begin{cases} P(s'|s,a), & \text{if } s \in K, \\ 1, & \text{otherwise.} \end{cases}$$

The state distribution induced by a policy $\pi$ on $M_K$ shall be denoted by $d_{M_K,\pi}$. Often, in absence of an exact knowledge of the transition matrix $P$, the policy $\pi$ may be executed on an estimated transition matrix...
Lemma 9. (Lemma 8.4.4$^{[Kak03]}$) For any policy $\pi$, the later, supported on a domain of size $d$, we shall use $d_{M,K,\pi}$ to denote the state distribution of the policy $\pi$ executed on the MDP with the transition matrix $\hat{P}$. Also, define the following.

$$P_{K}(\text{escape}|\pi) = \mathbb{E}_{\tau \sim P(\cdot|\pi)} 1_{\exists t < t_0: \tau \notin K, t = (s_0, a_0, \ldots)},$$

$$P_{K,\gamma}(\text{escape}|\pi) = (1 - \gamma) \mathbb{E}_{\tau \sim P(\cdot|\pi)} \sum_{t=0}^{\infty} \gamma^t 1_{s_n \in K \forall u < t \text{ and } s_t \notin K, t = (s_0, a_0, \ldots)}.$$

Note that $P_{K}(\text{escape}|\pi) \geq P_{K,\gamma}(\text{escape}|\pi) - \gamma^0$.

Lemma 9. (Lemma 8.4.4$^{[Kak03]}$) For any policy $\pi$, the following statements are valid.

$$\langle d_{\pi}, r \rangle \geq \langle d_{M_{K,\pi}, r_{K}} \rangle - P_{K,\gamma}(\text{escape}|\pi)\|r_{K}\|_{\infty},$$

$$\langle d_{M_{K,\pi}, r_{K}} \rangle \geq \langle d_{\pi}, r \rangle.$$

Lemma 10. (Lemma 8.5.4$^{[Kak03]}$) If, for all $(s,a) \in S \times A$, $\|\hat{P}(\cdot|s,a) - P_{K}(\cdot|s,a)\|_{1} \leq \varepsilon$, then for any reward $r$, policy $\pi$, it is true that

$$\|\langle d_{M_{K,\pi}, r_{K}} \rangle - \langle d_{M_{K,\pi}, r_{K}} \rangle\|_{1} \leq \frac{\varepsilon}{1 - \gamma}.$$

Lemma 11. (Folklore, eg. Lemma 8.5.5$^{[Kak03]}$) When $m$ samples $\{x_1, \ldots, x_m\}$ are drawn from a distribution $P$, supported on a domain of size $d$, to construct an empirical distribution $\hat{P}(x) = \frac{\sum_{i=1}^{m} 1_{x_i = x}}{m}$, it is guaranteed that with probability $1 - \delta$.

$$\|P - \hat{P}\|_{1} \leq \sqrt{\frac{8d \log \frac{2d}{\delta}}{m}}.$$

Proof of Lemma 10. The key observation in dealing with an unknown MDP is: either $\pi$, computed on the the transition $\hat{P}$, is (almost) optimal for the given reward signal on the true MDP, or it escapes the set of known states $K$ quickly. If the former occurs, the requirement on the output of the algorithm is met. In case of the later, $\pi$ serves as a good policy to quickly explore new states — this can happen only a finite number of times.

Let $\pi^{*} = \arg \max_{\pi} V_{\pi}$. First, note that for any $\pi$ chosen in the Line 6, we have

$$V_{\pi} = \langle d_{\pi}, r \rangle$$

$$\geq \langle d_{M_{K,\pi}, r_{K}} \rangle - (\gamma^t_0 + P_{K}(\text{escape}|\pi)) \log |S|$$

$$\geq \langle d_{M_{K,\pi}, r_{K}} \rangle - \frac{1}{1 - \gamma} \sqrt{\frac{8|S| \log \frac{2|S|}{\delta}}{m}} - (\gamma^t_0 + P_{K}(\text{escape}|\pi)) \log |S|$$

$$\geq \langle d_{M_{K,\pi}, r_{K}} \rangle - \varepsilon_1 - \frac{1}{1 - \gamma} \sqrt{\frac{8|S| \log \frac{2|S|}{\delta}}{m}} - (\gamma^t_0 + P_{K}(\text{escape}|\pi)) \log |S|$$

$$\geq \langle d_{M_{K,\pi}, r_{K}} \rangle - \varepsilon_1 - \frac{2}{1 - \gamma} \sqrt{\frac{8|S| \log \frac{2|S|}{\delta}}{m}} - (\gamma^t_0 + P_{K}(\text{escape}|\pi)) \log |S|$$

If $P_{K}(\text{escape}|\pi) > \Delta$, then the probability that $\pi$ doesn’t escape $K$ in $n$ trials is $e^{-n\Delta}$. Accounting for the failure probabilities with a suitable union bound, Line 8 ensures that $\pi$ is marked stable only if $P_{K}(\text{escape}|\pi) \leq \frac{\log(N\delta^{-1})}{n}$, where $N$ is the total number of times the inner loop is executed.

To observe the truth of the second part of the claim, note that every reiteration of the inner loop coincides with the exploration of some action at a $m$-unknown state. There can be at most $m|S||A|$ such exploration steps. Finally, each run of the inner loop samples $n$ episodes.


MountainCar

(a) Entropy of the policy evolving with the number of epochs.

(b) The log-probability of occupancy of the two-dimensional state space visualized at different epochs.

Pendulum

(c) Entropy of the policies evolving with the number of epochs.

(d) The log-probability of occupancy of the two-dimensional state space visualized at different epochs.

Figure 2: Results of the preliminary experiments. In each plot, blue represents the MaxEnt agent, and orange represents the random baseline.

Proof of Lemma 8. First note that it suffices to ensure for all $t < t_0$ simultaneously, it happens $\|d_{t, \pi} - \hat{d}_{t, \pi}\|_\infty \leq 0.1\varepsilon_0$. This is because

$$\|d_\pi - \hat{d}_\pi\|_\infty \leq \frac{1 - \gamma}{(1 - \gamma^{t_0})} \sum_{t=0}^{t_0-1} \gamma^t \|\hat{d}_{t, \pi} - (1 - \gamma^{t_0})d_{t, \pi}\|_\infty + \gamma^{t_0}$$

$$\leq \frac{1 - \gamma}{(1 - \gamma^{t_0})} \sum_{t=0}^{t_0-1} \gamma^t \|\hat{d}_{t, \pi} - d_{t, \pi}\| + 0.3\varepsilon_0 \leq \varepsilon_0. \tag{8}$$

Since the trajectories are independently, $|\hat{d}_{t, \pi}(s) - d_{t, \pi}(s)| \leq \sqrt{\frac{2}{m} \log \frac{2}{\delta}}$ for each $t < t_0$ and state $s \in \mathcal{S}$ with probability $1 - \delta$, by Hoeffding’s inequality. A union bound over states and $t$ concludes the proof. \qed

5 Experimental Validation

We report the results from a preliminary set of experiments. In each case, the MaxEnt agent learns to access the set of reachable states within a fairly small number of iterations, while (almost) monotonically increasing the entropy of the induced state distribution. We detail the setup below.

Environments: The 2-dimensional state spaces for MountainCar and Pendulum (from BCP+16) were discretized evenly to grids of size $10 \times 9$ and $8 \times 8$, respectively. For Pendulum, the maximum torque and velocity were capped at 1.0 and 7.0, respectively.
Algorithmic Details: In each experiment, the planning oracle is a REINFORCE agent, where the output policy from the previous iteration is used as the initial policy for the next iteration. The policy class is a neural net with a single hidden layer consisting of 128 units. The agent is trained on 400 and 200 episodes every epoch for MountainCar and Pendulum, respectively. The baseline agent chooses its action randomly at every timestep.

References

[AN04] Pieter Abbeel and Andrew Y. Ng. Apprenticeship learning via inverse reinforcement learning. In ICML, 2004.

[AOM17] Mohammad Gheshlaghi Azar, Ian Osband, and Rémi Munos. Minimax regret bounds for reinforcement learning. arXiv preprint arXiv:1703.05449, 2017.

[B+15] Sébastien Bubeck et al. Convex optimization: Algorithms and complexity. Foundations and Trends in Machine Learning, 8(3-4):231–357, 2015.

[BCP+16] Greg Brockman, Vicki Cheung, Ludwig Pettersson, Jonas Schneider, John Schulman, Jie Tang, and Wojciech Zaremba. Openai gym. arXiv preprint arXiv:1606.01540, 2016.

[BEP+18] Yuri Burda, Harri Edwards, Deepak Pathak, Amos Storkey, Trevor Darrell, and Alexei A. Efros. Large-scale study of curiosity-driven learning. In arXiv:1808.04355, 2018.

[Ber05] Dimitri P Bertsekas. Dynamic programming and optimal control, volume 1. Athena Scientific, 2005.

[BESK18] Yuri Burda, Harrison Edwards, Amos Storkey, and Oleg Klimov. Exploration by random network distillation. arXiv preprint arXiv:1810.12894, 2018.

[BSO+16] Marc G. Bellemare, Sriram Srinivasan, Georg Ostrovski, Tom Schaul, David Saxton, and Rémi Munos. Unifying count-based exploration and intrinsic motivation. In Advances in Neural Information Processing Systems 29: Annual Conference on Neural Information Processing Systems 2016, December 5-10, 2016, Barcelona, Spain, pages 1471–1479, 2016.

[CBS05] Nuttapong Chentanez, Andrew G. Barto, and Satinder P. Singh. Intrinsically motivated reinforcement learning. In L. K. Saul, Y. Weiss, and L. Bottou, editors, Advances in Neural Information Processing Systems 17, pages 1281–1288. MIT Press, 2005.

[DB15] Christoph Dann and Emma Brunskill. Sample complexity of episodic fixed-horizon reinforcement learning. In Advances in Neural Information Processing Systems, pages 2818–2826, 2015.

[FCRL17] Justin Fu, John Co-Reyes, and Sergey Levine. Ex2: Exploration with exemplar models for deep reinforcement learning. In I. Guyon, U. V. Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett, editors, Advances in Neural Information Processing Systems 30, pages 2577–2587. Curran Associates, Inc., 2017.

[FW56] Marguerite Frank and Philip Wolfe. An algorithm for quadratic programming. Naval Research Logistics (NRL), 3(1-2):95–110, 1956.

[Haz16] Elad Hazan. Introduction to online convex optimization. Foundations and Trends in Optimization, 2(3-4):157–325, 2016.

[HCC+16] Rein Houthooft, Xi Chen, Xi Chen, Yan Duan, John Schulman, Filip De Turck, and Pieter Abbeel. Vime: Variational information maximizing exploration. In D. D. Lee, M. Sugiyama, U. V. Luxburg, I. Guyon, and R. Garnett, editors, Advances in Neural Information Processing Systems 29, pages 1109–1117. Curran Associates, Inc., 2016.
[Kae93] Leslie Pack Kaelbling. Learning to achieve goals. In Proceedings of the Thirteenth International Joint Conference on Artificial Intelligence, Chambery, France, 1993. Morgan Kaufmann.

[Kak03] Sham Machandranath Kakade. On the sample complexity of reinforcement learning. PhD thesis, University of London London, England, 2003.

[KS02] Michael Kearns and Satinder Singh. Near-optimal reinforcement learning in polynomial time. Machine learning, 49(2-3):209–232, 2002.

[LH14] Tor Lattimore and Marcus Hutter. Near-optimal pac bounds for discounted mdp's. Theoretical Computer Science, 558:125–143, 2014.

[LLTyO12] Manuel Lopes, Tobias Lang, Marc Toussaint, and Pierre yves Oudeyer. Exploration in model-based reinforcement learning by empirically estimating learning progress. In F. Pereira, C. J. C. Burges, L. Bottou, and K. Q. Weinberger, editors, Advances in Neural Information Processing Systems 25, pages 206–214. Curran Associates, Inc., 2012.

[MJR15] Shakir Mohamed and Danilo Jimenez Rezende. Variational information maximisation for intrinsically motivated reinforcement learning. In C. Cortes, N. D. Lawrence, D. D. Lee, M. Sugiyama, and R. Garnett, editors, Advances in Neural Information Processing Systems 28, pages 2125–2133. Curran Associates, Inc., 2015.

[NHR99] Andrew Y. Ng, Daishi Harada, and Stuart J. Russell. Policy invariance under reward transformations: Theory and application to reward shaping. In ICML, 1999.

[NPD+18] Ashvin Nair, Vitchyr Pong, Murtaza Dalal, Shikhar Bahl, Steven Lin, and Sergey Levine. Visual reinforcement learning with imagined goals. CoRR, abs/1807.04742, 2018.

[OAC18] Ian Osband, John Aslanides, and Albin Cassirer. Randomized prior functions for deep reinforcement learning. In S. Bengio, H. Wallach, H. Larochelle, K. Grauman, N. Cesa-Bianchi, and R. Garnett, editors, Advances in Neural Information Processing Systems 31, pages 8625–8637. Curran Associates, Inc., 2018.

[OBPVR16] Ian Osband, Charles Blundell, Alexander Pritzel, and Benjamin Van Roy. Deep exploration via bootstrapped dqn. In D. D. Lee, M. Sugiyama, U. V. Luxburg, I. Guyon, and R. Garnett, editors, Advances in Neural Information Processing Systems 29, pages 4026–4034. Curran Associates, Inc., 2016.

[OBvdOM17] Georg Ostrovski, Marc G. Bellemare, Aäron van den Oord, and Rémi Munos. Count-based exploration with neural density models. In Proceedings of the 34th International Conference on Machine Learning, ICML 2017, Sydney, NSW, Australia, 6-11 August 2017, pages 2721–2730, 2017.

[PAED17] Deepak Pathak, Pulkit Agrawal, Alexei A. Efros, and Trevor Darrell. Curiosity-driven exploration by self-supervised prediction. In ICML, 2017.

[RGB11] Stéphane Ross, Geoffrey J. Gordon, and J. Andrew Bagnell. A reduction of imitation learning and structured prediction to no-regret online learning. In AISTATS, 2011.

[SHM+16] David Silver, Aja Huang, Chris J Maddison, Arthur Guez, Laurent Sifre, George Van Den Driessche, Julian Schrittwieser, Ioannis Antonoglou, Veda Panneershelvam, Marc Lanctot, et al. Mastering the game of go with deep neural networks and tree search. nature, 529(7587):484, 2016.
[SLB09] Satinder Singh, Richard L. Lewis, and Andrew G. Barto. Where do rewards come from? Proceedings of the Annual Conference of the Cognitive Science Society (CogSci), 2009.

[SLBS10] Satinder P. Singh, Richard L. Lewis, Andrew G. Barto, and Jonathan Sorg. Intrinsically motivated reinforcement learning: An evolutionary perspective. IEEE Transactions on Autonomous Mental Development, 2:70–82, 2010.

[SLW+06] Alexander L Strehl, Lihong Li, Eric Wiewiora, John Langford, and Michael L Littman. Pac model-free reinforcement learning. In Proceedings of the 23rd international conference on Machine learning, pages 881–888. ACM, 2006.

[SMMS00] Richard S Sutton, David A McAllester, Satinder P Singh, and Yishay Mansour. Policy gradient methods for reinforcement learning with function approximation. In Advances in neural information processing systems, pages 1057–1063, 2000.

[SRM+18] Nikolay Savinov, Anton Raichuk, Raphaël Marinier, Damien Vincent, Marc Pollefeys, Timothy P. Lillicrap, and Sylvain Gelly. Episodic curiosity through reachability. CoRR, abs/1810.02274, 2018.

[SS10] István Szita and Csaba Szepesvári. Model-based reinforcement learning with nearly tight exploration complexity bounds. In Proceedings of the 27th International Conference on Machine Learning (ICML-10), pages 1031–1038, 2010.

[THF+17] Haoran Tang, Rein Houthooft, Davis Foote, Adam Stooke, OpenAI Xi Chen, Yan Duan, John Schulman, Filip DeTurck, and Pieter Abbeel. #exploration: A study of count-based exploration for deep reinforcement learning. In I. Guyon, U. V. Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett, editors, Advances in Neural Information Processing Systems 30, pages 2753–2762. Curran Associates, Inc., 2017.

[WdWK+18] David Warde-Farley, Tom Van de Wiele, Tejas Kulkarni, Catalin Ionescu, Steven Hansen, and Volodymyr Mnih. Unsupervised control through non-parametric discriminative rewards. CoRR, abs/1811.11359, 2018.

[WRR+17] Théophane Weber, Sébastien Racanière, David P Reichert, Lars Buesing, Arthur Guez, Danilo Jimenez Rezende, Adria Puigdomenech Badia, Oriol Vinyals, Nicolas Heess, Yujia Li, et al. Imagination-augmented agents for deep reinforcement learning. arXiv preprint arXiv:1707.06203, 2017.

[ZOS18] Zeyu Zheng, Junhyuk Oh, and Satinder Singh. On learning intrinsic rewards for policy gradient methods. CoRR, abs/1804.06459, 2018.