Abstract

Self-play, where the algorithm learns by playing against itself without requiring any direct supervision, has become the new weapon in modern Reinforcement Learning (RL) for achieving superhuman performance in practice. However, the majority of existing theory in reinforcement learning only applies to the setting where the agent plays against a fixed environment. It remains largely open whether self-play algorithms can be provably effective, especially when it is necessary to manage the exploration/exploitation tradeoff.

We study self-play in competitive reinforcement learning under the setting of Markov games, a generalization of Markov decision processes to the two-player case. We introduce a self-play algorithm—Value Iteration with Upper/Lower Confidence Bound (VI-ULCB), and show that it achieves regret $\tilde{O}(\sqrt{T})$ after playing $T$ steps of the game. The regret is measured by the agent’s performance against a fully adversarial opponent who can exploit the agent’s strategy at any step. We also introduce an explore-then-exploit style algorithm, which achieves a slightly worse regret of $\tilde{O}(T^{2/3})$, but is guaranteed to run in polynomial time even in the worst case. To the best of our knowledge, our work presents the first line of provably sample-efficient self-play algorithms for competitive reinforcement learning.

1 Introduction

This paper studies competitive reinforcement learning (competitive RL), that is, reinforcement learning with two or more agents taking actions simultaneously, but each maximizing their own reward. Competitive RL is a major branch of the more general setting of multi-agent reinforcement learning (MARL), with the specification that the agents have conflicting rewards (so that they essentially compete with each other) yet can be trained in a centralized fashion (i.e. each agent has access to the other agents’ policies) (Crandall and Goodrich, 2005).

There are substantial recent progresses in competitive RL, in particular in solving hard multi-player games such as GO (Silver et al., 2017), Starcraft (Vinyals et al., 2019), and Dota 2 (OpenAI, 2018). A key highlight in their approaches is the successful use of self-play for achieving super-human performance in absence of human knowledge or expert opponents. These self-play algorithms are able to learn a good policy for all players from scratch through repeatedly playing the current policies against each other and performing policy updates using these self-played game trajectories. The empirical success of self-play has challenged the conventional wisdom that expert opponents are necessary for achieving good performance, and calls for a better theoretical understanding.

In this paper, we take initial steps towards understanding the effectiveness of self-play algorithms in competitive RL from a theoretical perspective. We focus on the special case of two-player zero-sum Markov

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games (Shapley, 1953; Littman, 1994), a generalization of Markov Decision Processes (MDPs) to the two-player setting. In a Markov game, the two players share states, play actions simultaneously, and observe the same reward. However, one player aims to maximize the return while the other aims to minimize it. This setting covers the majority of two-player games including GO (there is a single reward of \{+1, −1\} at the end of the game indicating which player has won), and also generalizes zero-sum matrix games (von Neumann, 1928)—an important game-theoretic problem—into the multi-step (RL) case.

More concretely, the goal of this paper is to design low-regret algorithms for solving episodic two-player Markov games in the general setting (Kearns and Singh, 2002), that is, the algorithm is allowed to play the game for a fixed amount of episodes using arbitrary policies, and its performance is measured in terms of the regret. We consider a strong notion of regret for two-player zero-sum games, where the performance of the deployed policies in each episode is measured against the best response for that policy, which can be different in different episodes. Such a regret bound measures the algorithm’s ability in managing the exploration and exploitation tradeoff against fully adaptive opponents, and can directly translate to other types of guarantees such as the PAC sample complexity bound.

**Our contribution** This paper introduces the first line of provably sample-efficient self-play algorithms for zero-sum Markov game under no restrictive assumptions. Concretely,

- We introduce the first self-play algorithm with $\tilde{O}(\sqrt{T})$ regret for zero-sum Markov games. More specifically, it achieves $\tilde{O}(\sqrt{H^3S^2ABT})$ regret in the general case, where $H$ is the length of the game, $S$ is the number of states, $A, B$ are the number of actions for each player, and $T$ is the total number of steps played. In special case of turn-based games, it achieves $\tilde{O}(\sqrt{S(A + B)T})$ regret with guaranteed polynomial runtime.

- We also introduce an explore-then-exploit style algorithm. It has guaranteed polynomial runtime in the general setting of zero-sum Markov games, with a slightly worse $\tilde{O}(T^{2/3})$ regret.

- We raise the open question about the optimal dependency of the regret on $S,A,B$. We provide a lower bound $\Omega(\sqrt{S(A + B)T})$, and show that the lower bound can be achieved in simple case of two-step turn-based games by a mirror descent style algorithm.

Above results are summarized in Table 1.
1.1 Related Work

There is a fast-growing body of work on multi-agent reinforcement learning (MARL). Many of them achieve striking empirical performance, or attack MARL in the cooperative setting, where agents are optimizing for a shared or similar reward. We refer the readers to several recent surveys for these results (see e.g. Buşoniu et al., 2010; Nguyen et al., 2018; OroojlooyJadid and Hajinezhad, 2019; Zhang et al., 2019). In the rest of this section we focus on theoretical results related to competitive RL.

**Markov games** Markov games (or stochastic games) is proposed as a mathematical model for competitive RL back in the early 1950s (Shapley, 1953). There is a long line of classical work since then on solving this problem (see e.g. Littman, 1994, 2001; Hu and Wellman, 2003; Hansen et al., 2013). They design algorithms, possibly with runtime guarantees, to find optimal policies in Markov games when both the transition matrix and reward are known, or in the asymptotic setting where number of data goes to infinity. These results do not directly apply to the non-asymptotic setting where the transition and reward are unknown and only a limited amount of data are available for estimating them.

A few recent work tackles self-play algorithms for Markov games in the non-asymptotic setting, working under either structural assumptions about the game or stronger sampling oracles. Wei et al. (2017) propose an upper confidence algorithm for stochastic games and prove that a self-play style algorithm finds $\epsilon$-optimal policies in $\text{poly}(1/\epsilon)$ samples. Jia et al. (2019); Sidford et al. (2019) study turn-based stochastic games—a special case of general Markov games, and propose algorithms with near-optimal sample complexity. However, both lines of work make strong assumptions—on either the structure of Markov games or how we access data—that are not always true in practice. Specifically, Wei et al. (2017) assumes no matter what strategy one agent sticks to, the other agent can always reach all states by playing a certain policy, and Jia et al. (2019); Sidford et al. (2019) assume access to simulators (or generative models) which enable the agent to directly sample transition and reward information for any state-action pair. These assumptions greatly alleviate the challenge in exploration. In contrast, our results apply to general Markov games without further structural assumptions, and our algorithms have built-in mechanisms for solving the challenge in the exploration-exploitation tradeoff.

Finally, we note that classical R-MAX algorithm (Brafman and Tennenholtz, 2002) does not make restrictive assumptions. It also has provable guarantees even when playing against the adversarial opponent in Markov game. However, the theoretical guarantee in Brafman and Tennenholtz (2002) is weaker than the standard regret, and does not directly imply any self-play algorithm with regret bound in our setting (see Section E for more details).

**Adversarial MDP** Another line of related work focuses on provable algorithms against adversarial opponents in MDP. Most work in this line considers the setting with adversarial rewards (see e.g. Zimin and Neu, 2013; Rosenberg and Mansour, 2019; Jin et al., 2019). These results do not directly imply provable self-play algorithms in our setting, because the adversarial opponent in Markov games can affect both the reward and the transition. There exist a few works that tackle both adversarial transition functions and adversarial rewards (Yu and Mannor, 2009; Cheung et al., 2019; Lykouris et al., 2019). In particular, Lykouris et al. (2019) considers a stochastic problem with $C$ episodes arbitrarily corrupted and obtain $O(C\sqrt{T} + C^2)$ regret. When applying these results to Markov games with an adversarial opponent, $C$ can be $\Theta(T)$ without further assumptions, which makes the bound vacuous.

**Single-agent RL** There is an extensive body of research on the sample efficiency of reinforcement learning in the single agent setting (see e.g. Jaksch et al., 2010; Osband et al., 2014; Azar et al., 2017; Dann et al., 2017; Strehl et al., 2006; Jin et al., 2018), which are studied under the model of Markov decision process—a special case of Markov games. For the tabular episodic setting with nonstationary dynamics and no
simulators, the best regrets achieved by existing model-based and model-free algorithms are $O(\sqrt{HT^2\text{SAT}})$ (Azar et al., 2017) and $O(\sqrt{HT^3\text{SAT}})$ (Jin et al., 2018), respectively, where $S$ is the number of states, $A$ is the number of actions, $H$ is the length of each episode, and $T$ is the total number of steps played. Both of them (nearly) match the minimax lower bound $\Omega(\sqrt{HT^2\text{SAT}})$ (Jaksch et al., 2010; Osband and Van Roy, 2016; Jin et al., 2018).

2 Preliminaries

In this paper, we consider zero-sum Markov Games (MG) (Shapley, 1953; Littman, 1994), which also known as stochastic games in the literature. Zero-sum Markov games are generalization of standard Markov Decision Processes (MDP) into the two-player setting, in which the max-player seeks to maximize the total return and the min-player seeks to minimize the total return.

Formally, we consider tabular episodic zero-sum Markov games of the form $\text{MG}(H, S, A, B, P, r)$, where

- $H$ is the number of steps in each episode.
- $S = \cup_{h\in[H+1]}S_h$, and $S_h$ is the set of states at step $h$, with $\max_{h\in[H+1]}|S_h| \leq S$.
- $A = \cup_{h\in[H]}A_h$, and $A_h$ is the set of actions of the max-player at step $h$, with $\max_{h\in[H]}|A_h| \leq A$.
- $B = \cup_{h\in[H]}B_h$, and $B_h$ is the set of actions of the min-player at step $h$, with $\max_{h\in[H]}|B_h| \leq B$.
- $P = \{P_h\}_{h\in[H]}$ is a collection of transition matrices, so that $P_h(\cdot|s, a, b)$ gives the distribution over states if action pair $(a, b)$ is taken for state $s$ at step $h$.
- $r = \{r_h\}_{h\in[H]}$ is a collection of reward functions, and $r_h: S_h \times A_h \times B_h \to [0, 1]$ is the deterministic reward function at step $h$. Note that we are assuming that rewards are in $[0, 1]$ for normalization. $^1$

In each episode of this MG, an initial state $s_1$ is picked arbitrarily by an adversary. Then, at each step $h \in [H]$, both players observe state $s_h \in S_h$, pick the action $a_h \in A_h$, $b_h \in B_h$ simultaneously, receive reward $r_h(s_h, a_h, b_h)$, and then transition to the next state $s_{h+1} \sim P_h(\cdot|s_h, a_h, b_h)$. The episode ends when $s_{H+1}$ is reached.

Policy and value function A policy $\mu$ of the max-player is a collection of $H$ functions $\{\mu_h: S \to \Delta_{A_h}\}_{h\in[H]}$, where $\Delta_{A_h}$ is the probability simplex over action set $A_h$. Similarly, a policy $\nu$ of the min-player is a collection of $H$ functions $\{\nu_h: S \to \Delta_{B_h}\}_{h\in[H]}$. We use the notation $\mu_h(a|s)$ and $\nu_h(b|s)$ to present the probability of taking action $a$ or $b$ for state $s$ at step $h$ under policy $\mu$ or $\nu$ respectively. We use $V^\mu\nu_h: S_h \to \mathbb{R}$ to denote the value function at step $h$ under policy $\mu$ and $\nu$, so that $V^\mu\nu_h(s)$ gives the expected cumulative rewards received under policy $\mu$ and $\nu$, starting from $s_h = s$, until the end of the episode:

$$V^\mu\nu_h(s) := \mathbb{E}_{\mu, \nu} \left[ \sum_{h'=h}^{H} r_{h'}(s_{h'}, a_{h'}, b_{h'}) \mid s_h = s \right].$$

We also define $Q^\mu\nu_h: S_h \times A_h \times B_h \to \mathbb{R}$ to denote $Q$-value function at step $h$ so that $Q^\mu\nu_h(s, a)$ gives the cumulative rewards received under policy $\mu$ and $\nu$, starting from $s_h = s, a_h = a, b_h = b$, till the end of the

$^1$While we study deterministic reward functions for notational simplicity, our results generalize to randomized reward functions.
Therefore, the optimal strategies (\( \mu^\dagger, \nu^\dagger \)) satisfy \( V_{h,\mu^\dagger,\nu^\dagger}^\mu(s) = \inf_\nu V_{h,\mu^\dagger,\nu}(s) \) for any \((s, h)\). For simplicity, we can define the best response of the max-player \( \mu^\dagger(\nu) \), and define \( V_{h,\mu^\dagger}^\nu \). The value functions \( V_{h,\mu^\dagger}^\nu \) and \( V_{h,\mu^\dagger}^\mu \) satisfy the following Bellman optimality equations:

\[
V_{h,\mu^\dagger}^\nu(s) = \inf_{\nu \in \Delta_{B_h}} \sum_{a,b} \mu_h(a|s)\nu_h(b|s)Q_{h}^{\mu^\dagger,\nu}(s,a,b), \\
V_{h,\mu^\dagger}^\mu(s) = \sup_{\mu \in \Delta_{A_h}} \sum_{a,b} \mu(a)\nu_h(b|s)Q_{h}^{\mu,\nu}(s,a,b).
\]

(3) (4)

It is further known that there exist policies \( \mu^*, \nu^* \) that are optimal against the best responses of the opponent:

\[
V_{h,\mu^*,\nu^*}^\mu(s) = \sup_{\mu} V_{h,\mu^\dagger}^\mu(s), \quad V_{h,\mu^\dagger}^\nu(s) = \inf_{\nu} V_{h,\mu^\dagger}^\nu(s), \quad \text{for all } (s, h).
\]

It is also known that, for any \((s, h)\), the minimax theorem holds:

\[
\sup_{\mu} \inf_{\nu} V_{h,\mu^\dagger,\nu^\dagger}^\mu(s) = V_{h,\mu^*,\nu^*}^\mu(s) = \inf_{\nu} \sup_{\mu} V_{h,\mu^\dagger,\nu^\dagger}^\mu(s).
\]

Therefore, the optimal strategies \((\mu^*, \nu^*)\) are also the Nash Equilibrium for the Markov game. Based on this, it is sensible to measure the suboptimality of any pair of policies \((\hat{\mu}, \hat{\nu})\) using the gap between their performance and the performance of the optimal strategy when playing against the best responses respectively, i.e.,

\[
\left[ V_{h}^{\hat{\mu},\hat{\nu}}(s) - \inf_{\nu} V_{h,\mu^\dagger}^\nu(s) \right] + \left[ \sup_{\mu} V_{h,\mu^\dagger}^\mu(s) - V_{h,\mu^\dagger}^{\hat{\mu},\hat{\nu}}(s) \right] = V_{h,\mu^\dagger}^{\hat{\mu},\hat{\nu}}(s) - V_{h}^{\mu,\nu}(s).
\]

(5)

We make this formal in the following definition of the regret.

**Definition 1** (Regret). *For any algorithm that plays the Markov game for \( K \) episodes with (potentially adversarial) starting state \( s^k_1 \) for each episode \( k = 1, 2, \ldots, K \), the regret is defined as*

\[
\text{Regret}(K) = \sum_{k=1}^{K} \left[ V_{1,\mu^k,\nu^k}^{\mu^k,\nu^k}(s^k_1) - V_{1}^{\mu^k,\nu^k}(s^k_1) \right],
\]

*where \((\mu^k, \nu^k)\) denote the policies deployed by the algorithm in the \( k \)-th episode.*
We note that as a unique feature of self-play algorithms, the learner is playing against herself, and thus chooses strategies for both max-player and min-player at each episode.

2.1 Turn-based games

In zero-sum Markov games, each step involves the two players playing simultaneously and independently. It is a general framework, which constrains a very important special case—turn-based games. (Shapley, 1953; Jia et al., 2019).

The main feature of a turn-based game is that only one player is taking actions in each step; in other words, the max and min player take turns to play the game. Formally, a turn-based game can be defined through a partition of steps \([H]\) into two sets \(\mathcal{H}_{\text{max}}\) and \(\mathcal{H}_{\text{min}}\), where \(\mathcal{H}_{\text{max}}\) and \(\mathcal{H}_{\text{min}}\) denote the sets of steps the max-player and the min-player choose the actions respectively, which satisfies \(\mathcal{H}_{\text{max}} \cap \mathcal{H}_{\text{min}} = \emptyset\) and \(\mathcal{H}_{\text{max}} \cup \mathcal{H}_{\text{min}} = [H]\). As a special example, GO is a turn-based game in which the two players play in alternate turns, i.e.

\[
\mathcal{H}_{\text{max}} = \{1, 3, \ldots, H - 1\} \quad \text{and} \quad \mathcal{H}_{\text{min}} = \{2, 4, \ldots, H\}
\]

Mathematically, we can specialize general zero-sum Markov games to turn-based games by restricting \(\mathcal{A}_h = \{\hat{a}\}\) for all \(h \in \mathcal{H}_{\text{min}}\), and \(\mathcal{B}_h = \{\hat{b}\}\) for all \(h \in \mathcal{H}_{\text{max}}\), where \(\hat{a}\) and \(\hat{b}\) are special dummy actions. Consequently, in those steps, \(\mathcal{A}_h\) or \(\mathcal{B}_h\) has only a single action as its element, i.e. the corresponding player can not affect the game in those steps. A consequence of this specialization is that the Nash Equilibria for turn-based games are pure strategies (i.e. deterministic policies) (Shapley, 1953), similar as in one-player MDPs. This is not always true for general Markov games.

3 Main Results

In this section, we present our algorithm and main theorems. In particular, our algorithm is the first self-play algorithm that achieves \(\tilde{O}(\sqrt{T})\) regret in Markov Games. We describe the algorithm in Section 3.1, and present its theoretical guarantee for general Markov games in Section 3.2. In Section 3.3, we show that when specialized to turn-based games, the regret and runtime of our algorithm can be further improved.

3.1 Algorithm description

To solve zero-sum Markov games, the main idea is to extend the celebrated UCB (Upper Confidence Bounds) principle—an algorithmic principle that achieves provably efficient exploration in bandits (Auer et al., 2002) and single-agent RL (Azar et al., 2017; Jin et al., 2018)—to the two-player setting. Recall that in single-agent RL, the provably efficient UCBVI algorithm (Azar et al., 2017) proceeds as

**Algorithm** (UCBVI for single-player RL): Compute \(\{Q_{up}^h(s, a) : h, s, a\}\) based on estimated transition and optimistic (upper) estimate of reward, then play one episode with the greedy policy with respect to \(Q_{up}\).

Regret bounds for UCBVI is then established by showing and utilizing the fact that \(Q_{up}\) remains an optimistic (upper) estimate of the optimal \(Q^*\) throughout execution of the algorithm.

In zero-sum games, the two player have conflicting goals: the max-player seeks to maximize the return and the min-player seeks to minimize the return. Therefore, it seems natural here to maintain two sets of Q estimates, one upper bounding the true value and one lower bounding the true value, so that each player can play optimistically with respect to her own goal. We summarize this idea into the following proposal.
Proposal (Naive two-player extension of UCBVI): Compute \( \{Q_{h}^{up}(s, a, b), Q_{h}^{low}(s, a, b)\} \) based on estimated transition and \{upper, lower\} estimates of rewards, then play one episode where the max-player (\( \mu \)) is greedy with respect to \( Q^{up} \) and the min-player (\( \nu \)) is greedy with respect to \( Q^{low} \).

However, the above proposal is not yet a well-defined algorithm: a greedy strategy \( \mu \) with respect to \( Q^{up} \) requires the knowledge of how the other player chooses \( b \), and vice versa. Therefore, what we really want is not that “\( \mu \) is greedy with respect to \( Q^{up} \)”, but rather that “\( \mu \) is greedy with respect to \( Q_{h}^{up}(s, \cdot, \cdot) \)” when the other player uses \( \nu \), and vice versa. In other words, we rather desire that \( (\mu, \nu) \) are jointly greedy with respect to \( (Q^{up}, Q^{low}) \).

Our algorithm concretizes such joint greediness precisely, building on insights from one-step matrix games: we choose \( (\mu_{h}, \nu_{h}) \) to be the Nash equilibrium for the general-sum game in which the payoff matrix for the max player is \( Q_{h}^{up} \) and for the min player is \( Q_{h}^{low} \). In other words, both player have their own payoff matrix (and they are not equal), but they jointly determine their policies. Formally, we let \( (\mu, \nu) \) be determined as

\[
(\mu_{h}(\cdot|s), \nu_{h}(\cdot|s)) = \text{NASH\_GENERAL\_SUM}(Q_{h}^{up}(s, \cdot, \cdot), Q_{h}^{low}(s, \cdot, \cdot))
\]

for all \( (h, s) \), where NASH\_GENERAL\_SUM is a subroutine that takes two matrices \( P, Q \in \mathbb{R}^{A \times B} \), and returns the Nash equilibrium \( (\phi, \psi) \in \Delta_{A} \times \Delta_{B} \) for general sum game, which satisfies

\[
\phi^{\top}P\psi = \max_{\phi} \phi^{\top}P\psi, \quad \phi^{\top}Q\psi = \min_{\psi} \phi^{\top}Q\psi.
\]  \hspace{1cm} (6)

Such an equilibrium is guaranteed to exist due to the seminal work of Nash (1951), and is computable by algorithms such as the Lemke-Howson algorithm (Lemke and Howson, 1964). With the NASH\_GENERAL\_SUM subroutine in hand, our algorithm can be briefly described as

Our Algorithm (VI-ULCB): Compute \( \{Q_{h}^{up}(s, a, b), Q_{h}^{low}(s, a, b)\} \) based on estimated transition and \{upper, lower\} estimates of rewards, along the way determining policies \( (\mu, \nu) \) by running the NASH\_GENERAL\_SUM subroutine on \( (Q^{up}, Q^{low}) \). Play one episode according to \( (\mu, \nu) \).

The full algorithm is described in Algorithm 1.

### 3.2 Guarantees for General Markov Games

We are now ready to present our main theorem.

Theorem 2 (Regret bound for VI-ULCB). For zero-sum Markov games, Algorithm 1 (with choice of bonus \( \beta_{t} = c\sqrt{H^{2}S_{i}T_{i}/t} \) for large absolute constant \( c \)) achieves regret

\[
\text{Regret}(K) \leq O\left(\sqrt{H^{3}S^{2}\max_{h \in [H]} A_{h}B_{h}T_{i}}\right) \leq O\left(\sqrt{H^{3}S^{2}ABT_{i}}\right)
\]

with probability at least \( 1 - p \), where \( i = \log(SABT/p) \).

We defer the proof of Theorem 2 into Appendix A.1.
Algorithm 1 Value Iteration with Upper-Lower Confidence Bound (VI-ULCB)

1: Initialize: for any \((s, a, b, h)\), \(Q_h^{\text{up}}(s, a, b) \leftarrow H\), \(Q_h^{\text{low}}(s, a, b) \leftarrow 0\), \(N_h(s, a, b) \leftarrow 0\).
2: for episode \(k = 1, \ldots, K\) do
3:   Receive \(s_1\).
4:   for step \(h = H, H - 1, \ldots, 1\) do
5:      for \((s, a, b) \in S_h \times A_h \times B_h\) do
6:         \(t = N_h(s, a, b)\);
7:         if \(t = 0\) then
8:            \(Q_h^{\text{up}}(s, a, b) \leftarrow H\), \(Q_h^{\text{low}}(s, a, b) \leftarrow 0\).
9:         else
10:            \(Q_h^{\text{up}}(s, a, b) \leftarrow \min\{\hat{r}_h(s, a, b) + [\hat{P}_h V_{h+1}^{\text{up}}](s, a, b) + \beta_t, H\}\)
11:            \(Q_h^{\text{low}}(s, a, b) \leftarrow \max\{\hat{r}_h(s, a, b) + [\hat{P}_h V_{h+1}^{\text{low}}](s, a, b) - \beta_t, 0\}\)
12:      end for \(s \in S_h\) do
13:         \((\mu_h(\cdot|s), \nu_h(\cdot|s)) \leftarrow \text{NASHGENERALSUM}(Q_h^{\text{up}}(s, \cdot, \cdot), Q_h^{\text{low}}(s, \cdot, \cdot))\)
14:         \(V_h^{\text{up}}(s) \leftarrow \sum_{a, b} \mu_h(a|s) \nu_h(b|s) Q_h^{\text{up}}(s, a, b)\).
15:         \(V_h^{\text{low}}(s) \leftarrow \sum_{a, b} \mu_h(a|s) \nu_h(b|s) Q_h^{\text{low}}(s, a, b)\).
16:      end for step \(h = 1, \ldots, H\) do
17:         Take action \(a_h \sim \mu_h(s_h)\), \(b_h \sim \nu_h(s_h)\).
18:         Observe reward \(r_h\) and next state \(s_{h+1}\).
19:         \(N_h(s_h, a_h, b_h) \leftarrow N_h(s_h, a_h, b_h) + 1\).
20:         \(N_h(s_{h+1}, a_h, b_h, s_{h+1}) \leftarrow N_h(s_h, a_h, b_h, s_{h+1}) + 1\).
21:         \(\hat{P}_h(\cdot|s_h, a_h, b_h) \leftarrow N_h(s_h, a_h, b_h, \cdot)/N_h(s_h, a_h, b_h)\).
22:      \(\hat{r}_h(s_h, a_h, b_h) \leftarrow r_h\).

Optimism in the face of uncertainty and best response An implication of Theorem 2 is that a low regret can be achieved via self-play, i.e. the algorithm plays with itself and does not need an expert as its opponent. This is intriguing because the regret is measured in terms of the suboptimality against the worst-case opponent:

\[
\text{Regret}(K) = \sum_{k=1}^{K} \left[ V_1^{\mu^k}(s_1^k) - V_1^{\hat{\mu}^k}(s_1^k) \right] \\
= \sum_{k=1}^{K} \left[ \max_{\mu} V_1^{\mu^k}(s_1^k) - V_1^{\hat{\mu}^k}(s_1^k) \right] + \left[ V_1^{\hat{\mu}^k}(s_1^k) - \inf_{\nu} V_1^{\hat{\mu}^k}(s_1^k) \right].
\]

(Note that this decomposition of the regret has a slightly different form from (5).) Therefore, Theorem 2 demonstrates that self-play can protect against fully adversarial opponent even when such a strong opponent is not explicitly available.

The key technical reason enabling such a guarantee is that our \(Q\) estimates are optimistic in the face of both the uncertainty of the game, as well as the best response from the opponent. More precisely, we show that the \((Q^{\text{up}}, Q^{\text{low}})\) in Algorithm 1 satisfy with high probability

\[
Q_h^{\text{up}, k}(s, a, b) \geq \sup_{\mu} Q_h^{\mu, \nu}(s, a, b) \geq \inf_{\nu} Q_h^{\mu, \nu}(s, a, b) \geq Q_h^{\text{low}, k}(s, a, b)
\]

for all \((s, a, b, h, k)\), where \((Q^{\text{up}, k}, Q^{\text{low}, k})\) denote the running \((Q^{\text{up}}, Q^{\text{low}})\) at the beginning of the \(k\)-th episode (Lemma 11). In constrast, such a guarantee (and consequently the regret bound) is not achiev-
able if the upper and lower estimates are only guaranteed to \{upper, lower\} bound the values of the Nash equilibrium.

**Translation to PAC bound** Our regret bound directly implies a PAC sample complexity bound for learning near-equilibrium policies, based on an online-to-batch conversion. We state this in the following Corollary, and defer the proof to Appendix A.2.

**Corollary 3** (PAC bound for VI-ULCB). Suppose the initial state of Markov game is fixed at \(s_1\), then there exists a pair of (randomized) policies \((\hat{\mu}, \hat{\nu})\) derived through the VI-ULCB algorithm such that with probability at least \(1 - \rho\) over the randomness in the trajectories we have

\[
\mathbb{E}_{\hat{\mu}, \hat{\nu}}\left[V^{\hat{\mu}, \hat{\nu}}(s_1) - V^{\hat{\mu}, \hat{\nu}}(s_1)\right] \leq \epsilon,
\]

as soon as the number of episodes \(K \geq \Omega(H^4S^2AB\epsilon/\epsilon^2)\), where \(\epsilon = \log(HSAB/(p\epsilon))\), and the expectation is over the randomization in \((\hat{\mu}, \hat{\nu})\).

**Runtime of Algorithm 1** Algorithm 1 involves the \texttt{NASH\_GENERAL\_SUM} subroutine for computing the Nash equilibrium of a general sum matrix game. However, it is known that the computational complexity for approximating\(^2\) such an equilibrium is PPAD-complete (Daskalakis, 2013), a complexity class conjectured to not enjoy polynomial or quasi-polynomial time algorithms. Therefore, Algorithm 1 is strictly speaking not a polynomial time algorithm, despite of being rather sample-efficient.

We note however that there exists practical implementations of the subroutine such as the Lemke-Howson algorithm (Lemke and Howson, 1964) that can usually find the solution efficiently. We will further revisit the computational issue in Section 4, in which we design a computationally efficient algorithm for zero-sum games with a slightly worse \(\tilde{O}(T^{2/3})\) regret.

### 3.3 Guarantees for Turn-based Markov Games

We now instantiate Theorem 2 on turn-based games (introduced in Section 2.1), in which the same algorithm enjoys better regret guarantee and polynomial runtime. Recall that in turn-based games, for all \(h\), we have either \(A_h = 1\) or \(B_h = 1\), therefore given \(\max_h A_h \leq A\) and \(\max_h B_h \leq B\) we have

\[
\max_h A_h B_h \leq \max \{A, B\} \leq A + B,
\]

and thus by Theorem 2 the regret of Algorithm 1 on turn-based games is bounded by \(\tilde{O}(\sqrt{H^4S^2(A + B)T})\).

Further, since either \(A_h = 1\) or \(B_h = 1\), all the \texttt{NASH\_GENERAL\_SUM} subroutines reduce to vector games rather than matrix games, and can be trivially implemented in polynomial (indeed linear) time. Indeed, suppose the payoff matrices in (6) has dimensions \(P, Q \in \mathbb{R}^{A \times 1}\), then \texttt{NASH\_GENERAL\_SUM} reduces to finding \(\phi \in \Delta_A\) and \(\psi \equiv 1\) such that

\[
\phi^T P = \max_{\phi} \phi^T P
\]

(the other side is trivialized as \(\psi \in \Delta_1\) has only one choice), which is solved at \(\phi = e_{a^*}\) where \(a^* = \arg \max_{a \in [A]} P_a\). The situation is similar if \(P, Q \in \mathbb{R}^{1 \times B}\).

We summarize the above results into the following corollary.

**Corollary 4** (Regret bound for VI-ULCB on turn-based games). For turn-based zero-sum Markov games, Algorithm 1 has runtime \(\text{poly}(S, A, B, T)\) and achieves regret bound \(\tilde{O}(\sqrt{H^4S^2(A + B)T\epsilon})\) with probability at least \(1 - \rho\), where \(\epsilon = \log(SABT/p)\).

\(^2\)More precisely, our proof requires the subroutine to find a \((1 + 1/H)\)-multiplicative approximation of the equilibrium, that is, for payoff matrices \(P, Q \in \mathbb{R}^{A\times B}\) we desire vectors \(\phi \in \Delta_A\) and \(\psi \in \Delta_B\) such that \(\max_\phi \phi^T P \psi - \min_\psi \phi^T Q \psi \leq (1 + 1/H)\phi^T (P - Q) \psi\).
Algorithm 2 Value Iteration after Exploration (VI-Explore)

1: $(\hat{P}, \hat{r}) \leftarrow \text{REWARD\_FREE\_EXPLORATION}(\epsilon)$.
2: $V_{\hat{H}}(s) \leftarrow 0$ for any $s \in S_{\hat{H}}$.
3: for step $h = H - 1, \ldots, 1$ do
4:   for $(s, a, b) \in S \times A \times B$ do
5:     $Q_{\hat{H}}(s, a, b) \leftarrow \hat{r}(s, a, b) + [\hat{P}_{\hat{H}}V_{\hat{H}+1}](s, a, b)$.
6:   for $s \in S$ do
7:     $(\hat{\mu}_{\hat{H}}(\cdot|s), \hat{\nu}_{\hat{H}}(\cdot|s)) \leftarrow \text{NASH\_ZERO\_SUM}(Q_{\hat{H}}(s, \cdot, \cdot))$
8:     $V_{\hat{H}}(s) = \sum_{a,b} \hat{\mu}_{\hat{H}}(a|s)\hat{\nu}_{\hat{H}}(b|s)Q_{\hat{H}}(s, a, b)$.
9:   for all remaining episodes do
10:     Play the game with policy $(\hat{\mu}, \hat{\nu})$.

4 Computationally Efficient Algorithm

In this section, we show that the computational issue of Algorithm 1 is not intrinsic to the problem: there exists a sublinear regret algorithm for general zero-sum Markov games that has a guaranteed polynomial runtime, with regret scaling as $O(T^{2/3})$, slightly worse than that of Algorithm 1. Therefore, computational efficiency can be achieved if one is willing to trade some statistical efficiency (sample complexity). For simplicity, we assume in this section that the initial state $s_1$ is fixed.

Value Iteration after Exploration At a high level, our algorithm follows an explore-then-exploit approach. We begin by running a (polynomial time) reward-free exploration procedure $\text{REWARD\_FREE\_EXPLORATION}(\epsilon)$ on a small number of episodes, which queries the MDP and outputs an estimate $(\hat{P}, \hat{r})$. Then, we run value iteration on the empirical version of Markov game with transition $\hat{P}$ and reward $\hat{r}$, which finds its Nash equilibrium $(\hat{\mu}, \hat{\nu})$. Finally, the algorithm simply plays the policy $(\hat{\mu}, \hat{\nu})$ for the remaining episodes. The full algorithm is described in Algorithm 2 in the Appendix.

By “reward-free” exploration, we mean the procedure will not use any reward information to guide exploration. Instead, the procedure prioritize on visiting all possible states and gathering sufficient information about their transition and rewards, so that $(\hat{P}, \hat{r})$ are close to $(P, r)$ in the sense that the Nash equilibria of $\text{MG}(\hat{P}, \hat{r})$ and $\text{MG}(P, r)$ are close, where $\text{MG}(\hat{P}, \hat{r})$ denotes the Markov game with transition $\hat{P}$ and reward $\hat{r}$.

This goal can be achieved by the following algorithm. For any fixed state $s$, we can create an artificial reward $\hat{r}$ defined as $\hat{r}(s, a, b) = 1$ and $\hat{r}(s', a, b) = 0$ for any $s' \neq s, a$ and $b$. Then, we can treat $C = A \times B$ as a new action set for a single agent, and run any standard reinforcement learning algorithm with PAC or regret guarantees to find a near-optimal policy $\tilde{\pi}$ of MDP($H, S, C, P, r$). It can be shown that the optimal policy for this MDP is the policy that maximize the probability to reach state $s$. Therefore, by repeatedly playing $\tilde{\pi}$, we can gather transition and reward information at state $s$ as well as we can. Finally, we repeat the routine above for all state $s$. See Appendix B for more details.

In this paper, we adapt the sharp treatments in Jin et al. (2020) which studies reward-free exploration in the single-agent MDP setting, and provide following guarantees for the $\text{REWARD\_FREE\_EXPLORATION}$ procedure.

Theorem 5 (PAC bound for VI-Explore). With probability at least $1 - p$, $\text{REWARD\_FREE\_EXPLORATION}(\epsilon)$ runs for $c(H^3S^2AB_1/\epsilon^2 + H^7S^4AB_3/\epsilon)$ episodes with some large constant $c$, and $t = \log(HSAB/(pe))$, and outputs $(\hat{P}, \hat{r})$ such that the Nash equilibrium $(\hat{\mu}, \hat{\nu})$ of $\text{MG}(\hat{P}, \hat{r})$ satisfies

$$\left[ V^{+, \hat{\nu}}(s_1) - V^{\hat{\mu}, +}(s_1) \right] \leq \epsilon.$$
Importantly, such Nash equilibrium \((\hat{\mu}, \hat{\nu})\) of MG\((\hat{p}, \hat{r})\) can be computed by Value Iteration (VI) using \(\hat{p}\) and \(\hat{r}\). VI only calls NASH_ZERO_SUM subroutine, which takes a matrix \(Q \in \mathbb{R}^{A \times B}\) and returns the Nash equilibrium \((\phi, \psi) \in \Delta_A \times \Delta_B\) for zero-sum game, which satisfies

\[
\max_{\phi} \phi^\top Q \psi = \phi^\top Q \psi = \min_{\psi} \phi^\top Q \psi.
\] (7)

This problem can be solved efficiently (in polynomial time) by many existing algorithms designed for convex-concave optimization (see, e.g. (Koller, 1994)), and does not suffer from the PPAD-completeness that NASH_GENERAL_SUM does.

The PAC bound in Theorem 5 can be easily converted into a regret bound, which is presented as follows.

**Corollary 6** (Polynomial time algorithm via explore-then-exploit). For zero-sum Markov games, with probability at least \(1 - p\), Algorithm 2 runs in \(\text{poly}(S, A, B, H, T)\) time, and achieves regret bound

\[
\mathcal{O}\left((H^5 S^2 A B T^2 \iota) + \sqrt{H^7 S^4 A B T \iota^3}\right),
\]

where \(\iota = \log(S A B T / p)\).

## 5 Towards the Optimal Regret

We investigate the tightness of our regret upper bounds in Theorem 2 and Corollary 4 through raising the question of optimal regret in two-player Markov games, and making initial progresses on it by providing lower bounds and new upper bounds in specific settings. Specifically, we ask an

**Open question:** What is the optimal regret for general Markov games (in terms of dependence on \((H, S, A, B)\))?

It is known that the (tight) regret lower bound for single-player MDPs is \(\Omega(\sqrt{SAT \cdot \text{poly}(H)})\) (Azar et al., 2017). By restricting two-player games to a single-player MDP (making the other player dummy), we immediately have

**Corollary 7** (Regret lower bound, corollary of Jaksch et al. (2010), Theorem 5). The regret\(^3\) for any algorithm on turn-based games (and thus also general zero-sum games) is lower bounded by \(\Omega(\sqrt{H^2 S(A + B)T})\).

Comparing this lower bound with the upper bound in Theorem 2 \((\tilde{O}(\sqrt{S^2 A B T \cdot \text{poly}(H)})\) regret for general games and \(\tilde{O}(\sqrt{S^2 (A + B)T \cdot \text{poly}(H)})\) regret for turn-based games), there are gaps in both the S-dependence and the \((A, B)\)-dependence.

**Matching the lower bound on short-horizon games** Towards closing the gap between lower and upper bounds, we develop alternative algorithms in the special case where *each player only plays once*, i.e. one-step general games with \(H = 1\) and two-step turn-based games. In these cases, we show that there exists mirror descent type algorithms that achieve an improved regret \(\tilde{O}(\sqrt{S(A + B)T})\) (and thus matching the lower bounds), provided that we consider a weaker notion of the regret defined as

**Definition 8** (Weak Regret). The weak regret for any algorithm that deploys policies \((\mu^k, \nu^k)\) in episode \(k\) is defined as

\[
\text{WeakRegret}(K) := \max_{\mu} \sum_{k=1}^{K} V^{\mu, \nu^k}(x_k^k) - \min_{\nu} \sum_{k=1}^{K} V^{\mu^k, \nu}(x_k^k).
\] (8)

\(^3\)This also applies to the weak regret defined in (8).
The difference in the weak regret is that it uses fixed opponents—as opposed to adaptive opponents—for measuring the performance gap: the max is taken with respect to a fixed \( \mu \) for all episodes \( k = 1, \ldots, K \), rather than a different \( \mu \) for each episode. By definition, we have for any algorithm that \( \text{WeakRegret}(K) \leq \text{Regret}(K) \).

With the definition of the weak regret in hand, we now present our results for one-step games. Their proofs can be found in Appendix C.

**Theorem 9** (Weak regret for one-step simultaneous game, adapted from Rakhlin and Sridharan (2013)).

For one-step simultaneous games \( (H = 1) \), there exists a mirror descent type algorithm that achieves weak regret bound \( \text{WeakRegret}(T) \leq \tilde{O}(\sqrt{SA + B}T) \) with high probability.

**Theorem 10** (Weak regret for two-step turn-based game).

For one-step turn-based games \( (H = 2) \), there exists a mirror descent type algorithm that achieves weak regret bound \( \text{WeakRegret}(T) \leq \tilde{O}(\sqrt{SA + B}T) \) with high probability.

**Proof insights; bottleneck in multi-step case**

The improved regret bounds in Theorem 9 and 10 are possible due to availability of unbiased estimates of counterfactual \( Q \) values, which in turn can be used in mirror descent type algorithms with guarantees. Such unbiased estimates are only achievable in one-step games as the two policies are “not intertwined” in a certain sense. In contrast, in multi-step games (where each player plays more than once), such unbiased estimates of counterfactual \( Q \) values are no longer available, and it is unclear how to construct a mirror descent algorithm there. We believe it would be an important open question to close the gap in multi-step games (as well as the gap between regret and weak regret) for a further understanding of exploration in games.

6 Conclusion

In this paper, we studied the sample complexity of finding the equilibrium policy in the setting of competitive reinforcement learning, i.e. zero-sum Markov games with two players. We designed a self-play algorithm for zero-sum games and showed that it can efficiently find the Nash equilibrium policy in the exploration setting through establishing a regret bound. Our algorithm—Value Iteration with Upper and Lower Confidence Bounds—builds on a principled extension of UCB/optimism into the two-player case by constructing upper and lower bounds on the value functions and iteratively solving general sum subgames.

Towards investigating the optimal runtime and sample complexity in two-player games, we provided accompanying results showing that (1) the computational efficiency of our algorithm can be improved by explore-then-exploit type algorithms, which has a slightly worse regret; (2) the state and action space dependence in the regret can be reduced in the special case of one-step games via alternative mirror descent type algorithms.

We believe this paper opens up many interesting directions for future work. For example, can we design a computationally efficient algorithms that achieves \( \tilde{O}(\sqrt{T}) \) regret? What are the optimal dependence of the regret on \( (S, A, B) \) in multi-step games? Also, the present results only work in tabular games, and it would be of interest to investigate if similar results can hold in presence of function approximation.

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A Proofs for Section 3

A.1 Proof of Theorem 2

Notation: To be clear from the context, we denote the upper bound and lower bound $Q^{up}$ and $Q^{low}$ computed at the $k$-th episode as $Q^{up,k}$ and $Q^{low,k}$, and policies computed and used at the $k$-th episode as $\mu$ and $\nu$.

Choice of bonus: $\beta_t = c \sqrt{SH^2t/t}$ for sufficient large absolute constant $c$.

Lemma 11 (UCLB). With probability at least $1 - p$, we have following bounds for any $(s, a, b, h, k)$:

\begin{align*}
V^{up,k}_h(s) &\geq \sup_{\mu} V^{\mu,k}_h(s), & Q^{up,k}_h(s, a, b) &\geq \sup_{\mu} Q^{\mu,k}_h(s, a, b) \quad (9) \\
V^{low,k}_h(s) &\leq \inf_{\nu} V^{\mu,k}_h(s), & Q^{low,k}_h(s, a, b) &\leq \inf_{\nu} Q^{\mu,k}_h(s, a, b) \quad (10)
\end{align*}

Proof. By symmetry, we only need to prove the statement (9). For each fixed $k$, we prove this by induction from $h = H + 1$ to $h = 1$. For base case, we know at the $(H + 1)$-th step, $V^{up,k}_{H+1}(s) = \sup_{\mu} V^{\mu,k}_{H+1}(s) = 0$.

Now, assume the left inequality in (9) holds for $(h + 1)$-th step, for the $h$-th step, we first recall the updates for $Q$ functions respectively:

\begin{align*}
Q^{up,k}_h(s, a, b) &= \min_{\mu} \left\{ r_h(s, a, b) + [\hat{P}^{k}_{h} V^{up,k}_{h+1}](s, a, b) + \beta_t, H \right\} \\
\sup_{\mu} Q^{\mu,k}_h(s, a, b) &= r_h(s, a, b) + [\mathbb{P}_h \sup_{\mu} V^{\mu,k}_{h+1}](s, a, b)
\end{align*}
In case of \( Q_{h}^{\text{up},k}(s, a, b) = H \), the right inequality in (9) clearly holds. Otherwise, we have:

\[
Q_{h}^{\text{up},k}(s, a, b) - \sup_{\mu} Q_{h}^{\mu,\nu,k}(s, a, b) = (\hat{P}_{h}^{k} - P_{h}) \sup_{\mu} V_{h+1}^{\text{up},k}(s, a, b) + \beta_{t}
\]

\[
= (\hat{P}_{h}^{k}(V_{h+1}^{\text{up},k}) - \sup_{\mu} V_{h+1}^{\mu,\nu,k})(s, a, b) + \beta_{t}
\]

Since \( \hat{P}_{h}^{k} \) preserves the positivity, by induction assumption, we know the first term is positive. By Lemma 12, we know the second term \( \geq -\beta_{t} \). This finishes the proof of the right inequality in (9).

To prove the left inequality in (9), again recall the updates for \( V \) functions respectively:

\[
V_{h+1}^{\text{up},k}(s) = \mu_{h}^{k}(s)\top Q_{h}^{\text{up},k}(s, \cdot, \cdot) \nu_{h}^{k}(s) = \max_{\phi \in \Delta_{A}} \phi\top Q_{h}^{\text{up},k}(s, \cdot, \cdot) \nu_{h}^{k}(s)
\]

\[
\sup_{\mu} V_{h+1}^{\mu,\nu,k}(s) = \max_{\phi \in \Delta_{A}} \phi\top \sup_{\mu} Q_{h}^{\mu,\nu,k}(s, \cdot, \cdot) \nu_{h}^{k}(s)
\]

where the first equation is by the definition of policy \( \mu^{k} \) the algorithm picks. Therefore:

\[
V_{h+1}^{\text{up},k}(s) - \sup_{\mu} V_{h+1}^{\mu,\nu,k}(s) \geq \max_{\phi \in \Delta_{A}} \phi\top (\sup_{\mu} Q_{h}^{\mu,\nu,k}(s, \cdot, \cdot) \nu_{h}^{k}(s) - \sup_{\mu} Q_{h}^{\mu,\nu,k}(s, \cdot, \cdot) \nu_{h}^{k}(s)) \geq 0.
\]

This finishes the proof. \( \square \)

**Lemma 12 (Uniform Concentration).** Consider value function class

\[
\mathcal{V}_{h+1} = \{ V : S_{h+1} \to \mathbb{R} \mid V(s) \in [0, H] \text{ for all } s \in S_{h+1} \}.
\]

There exists an absolute constant \( c \), with probability at least \( 1 - p \), we have:

\[
\left| \left[ (\hat{P}_{h}^{k} - P_{h}) V \right](s, a, b) \right| \leq c \sqrt{SH^{2}t/N_{h}^{k}(s, a, b)} \quad \text{for all } (s, a, b, k, h) \text{ and all } V \in \mathcal{V}_{h+1}.
\]

**Proof.** We show this for one \( (s, a, b, k, h) \); the rest follows from a union bound over these indices (and results in a larger logarithmic factor.) Throughout this proof we let \( c > 0 \) to be an absolute constant that may vary from line to line.

Let \( \mathcal{V}_{\epsilon} \) be an \( \epsilon \)-covering of \( \mathcal{V}_{h+1} \) in the \( \infty \) norm (that is, for any \( V \in \mathcal{V}_{h+1} \) there exists \( \hat{V} \in \mathcal{V}_{\epsilon} \) such that \( \sup_{s} |V(s) - \hat{V}(s)| \leq \epsilon \). We have \( |\mathcal{V}_{\epsilon}| \leq (1/\epsilon)^{S} \), and by Hoeffding inequality and a union bound, we have with probability at least \( 1 - p \) that

\[
\left| \sup_{\hat{V} \in \mathcal{V}_{\epsilon}} \left[ (\hat{P}_{h}^{k} - P_{h}) \hat{V} \right] \right| \leq \sqrt{\frac{H^{2}(S \log(1/\epsilon) + \log(1/p))}{N_{h}^{k}(s, a, b)}}.
\]

Taking \( \epsilon = c \sqrt{H^{2}S_{t}/N_{h}^{k}(s, a, b)} \), the above implies that

\[
\left| \sup_{\hat{V} \in \mathcal{V}_{\epsilon}} \left[ (\hat{P}_{h}^{k} - P_{h}) \hat{V} \right] \right| \leq c \sqrt{\frac{H^{2}S_{t}}{N_{h}^{k}(s, a, b)}}.
\]

Meanwhile, with this choice of \( \epsilon \), for any \( V \in \mathcal{V}_{h+1} \), there exists \( \hat{V} \in \mathcal{V}_{\epsilon} \) such that \( \sup_{s} |V(s) - \hat{V}(s)| \leq \epsilon \), and therefore

\[
\left| \left[ (\hat{P}_{h}^{k} - P_{h}) V \right] - \left[ (\hat{P}_{h}^{k} - P_{h}) \hat{V} \right] \right| \leq 2\epsilon = c \sqrt{\frac{H^{2}S_{t}}{N_{h}^{k}(s, a, b)}}.
\]

Combining the preceding two bounds, we have that the desired concentration holds for all \( V \in \mathcal{V}_{h+1} \). \( \square \)
Proof of Theorem 2. By Lemma 11, we know the regret,

\[ \text{Regret}(K) = \sum_{k=1}^{K} \left[ \sup_{\mu} V_1^{\mu,k}(s_k) - \inf_{\nu} V_1^{\nu,k}(s_k) \right] \leq \sum_{k=1}^{K} \left[ V_1^{\text{up},k}(s_k) - V_1^{\text{low},k}(s_k) \right] \]

On the other hand, by the updates in Algorithm 1, we have:

\[
\begin{align*}
[V_1^{\text{up},k} - V_1^{\text{low},k}](s_k) &= \mu_h(s_k) \top \left[ Q_h^{\text{up},k} - Q_h^{\text{low},k} \right](s_k, \cdot, b) \nu_h(s_k), \\
&= [Q_h^{\text{up},k} - Q_h^{\text{low},k}](s_k, a_h^k, b_h^k) + \xi_h^k \\
&\leq [\xi_h^k + \xi_h^k](V_1^{\text{up},k} - V_1^{\text{low},k})(s_k, a_h^k, b_h^k) + 2\beta_h + \zeta_h^k \\
&\leq [\xi_h^k + \xi_h^k](V_1^{\text{up},k} - V_1^{\text{low},k})(s_k, a_h^k, b_h^k) + 4\beta_h^k + \zeta_h^k \\
&= [\xi_h^k + \xi_h^k](s_k, a_h^k, b_h^k) + 4\beta_h^k + \zeta_h^k \\
\end{align*}
\]

the last inequality is due to Lemma 12. \(\xi_h^k\) and \(\zeta_h^k\) are defined as

\[
\begin{align*}
\xi_h^k &= \mathbb{E}_{a \sim \mu_h^k(s_k), b \sim \nu_h^k(s_k)} [Q_h^{\text{up},k} - Q_h^{\text{low},k}](s_k, a, b) - [Q_h^{\text{up},k} - Q_h^{\text{low},k}](s_k, a_h^k, b_h^k), \\
\zeta_h^k &= \mathbb{E}_{s \sim \pi_h(s \mid s_h, a_h^k, b_h^k)} [V_1^{\text{up},k} - V_1^{\text{low},k}](s) - [V_1^{\text{up},k} - V_1^{\text{low},k}](s_{h+1}) \\
\end{align*}
\]

Both \(\xi_h^k\) and \(\zeta_h^k\) are martingale difference sequence, therefore by the Azuma-Hoeffding inequality we have with probability \(1 - p\) that

\[
\sum_{k, h} \xi_h^k \leq O(\sqrt{HTt}) \quad \text{and} \quad \sum_{k, h} \zeta_h^k \leq O(\sqrt{HTt}).
\]

Therefore, by our choice of bonus \(\beta_t\) and the Pigeonhole principle, we have

\[
\begin{align*}
\sum_{k=1}^{K} \left[ V_1^{\text{up},k}(s_1) - V_1^{\text{low},k}(s_1) \right] &\leq \sum_{k, h} \left( 4\beta_h^k + \xi_h^k + \zeta_h^k \right) \\
&\leq \sum_{h, s \in S_h, a \in A_h, b \in B_h} \left[ N_h^K(s, a, b) \right] \sqrt{\frac{H^2 S \cdot K}{t}} + O(\sqrt{HTt}) \\
&= \sum_{h, s \in S_h, a \in A_h, b \in B_h} O\left( \sqrt{H^2 S \cdot N_h^K(s, a, b)} \right) + O(\sqrt{HTt}) \\
&\leq \sum_{h \in \mathcal{H}} O\left( \sqrt{H^2 S^2 A_h B_h K t} \right) \leq O\left( \sqrt{H^4 S^2 \left[ \max_h A_h B_h \right] K t} \right) = O\left( \sqrt{H^3 S^2 \left[ \max_h A_h B_h \right] T^t} \right).
\end{align*}
\]

This finishes the proof. \(\square\)

A.2 Proof of Corollary 3

The proof is based on a standard online-to-batch conversion (e.g. (Section 3.1, Jin et al., 2018).) Let \((\hat{\mu}^k, \hat{\nu}^k)\) denote the policies deployed by the VI-ULCB algorithm in episode \(k\). We sample \(\hat{\mu}, \hat{\nu}\) uniformly as

\[
\hat{\mu} \sim \text{Unif}\{\mu^1, \ldots, \mu^K\} \quad \text{and} \quad \hat{\nu} \sim \text{Unif}\{\nu^1, \ldots, \nu^K\}.
\]
Taking expectation with respect to this sampling gives

\[
\mathbb{E}_{\hat{\mu}, \hat{\nu}} \left[ V_{\hat{\mu}, \hat{\nu}}^t(s_1) - V_{\hat{\mu}, \hat{\nu}}^{t+1}(s_1) \right] = \frac{1}{K} \sum_{k=1}^{K} \left[ V_{\hat{\mu}, \hat{\nu}}^t(s_1) - V_{\mu, \nu}^{t+1}(s_1) \right] = \frac{1}{K} \text{Regret}(K)
\]

\[
\leq \tilde{O}\left( \frac{\sqrt{H^3S^2ABT}}{K} \right) \leq \tilde{O}\left( \frac{\sqrt{H^4S^2AB}}{K} \right),
\]

where we have applied Theorem 2 to bound the regret with high probability. Choosing \( K \geq \tilde{O}(H^4S^2AB/\epsilon^2) \), the right hand side is upper bounded by \( \epsilon \), which finishes the proof.

## B Proofs for Section 4

In this section, we prove Theorem 5 and Corollary 6 based on the following lemma about subroutine REWARD-FREE EXPLORATION. We will defer the proof of this Lemma to Appendix D.

**Lemma 13.** Under the preconditions of Theorem 5, with probability at least \( 1 - p \), for any policy \( \mu, \nu \), we have:

\[
|\hat{V}_{1}^{\mu, \nu}(s_1) - V_{1}^{\mu, \nu}(s_1)| \leq \epsilon/2
\]

(11)

where \( \hat{V}, V \) are the value functions of \( MG(\hat{P}, \hat{r}) \) and \( MG(P, r) \).

### B.1 Proof of Theorem 5

Since both inf and sup are contractive maps, by Lemma 13, we have:

\[
|\inf_{\nu} V_{1}^{\hat{\mu}, \nu}(s_1) - \inf_{\nu} \hat{V}_{1}^{\hat{\mu}, \nu}(s_1)| \leq \epsilon/2
\]

\[
|\sup_{\mu} V_{1}^{\mu, \hat{\nu}}(s_1) - \sup_{\mu} \hat{V}_{1}^{\mu, \hat{\nu}}(s_1)| \leq \epsilon/2
\]

Since \((\hat{\mu}, \hat{\nu})\) are the Nash Equilibria for \( MG(\hat{P}, \hat{r}) \), we have \( \inf_{\nu} \hat{V}_{1}^{\hat{\mu}, \nu}(s_1) = \sup_{\mu} \hat{V}_{1}^{\mu, \hat{\nu}}(s_1) \). This gives:

\[
\sup_{\mu} V_{1}^{\mu, \hat{\nu}}(s_1) - \inf_{\nu} V_{1}^{\hat{\mu}, \nu}(s_1) \leq |\sup_{\mu} V_{1}^{\mu, \hat{\nu}}(s_1) - \sup_{\mu} \hat{V}_{1}^{\mu, \hat{\nu}}(s_1)| + |\sup_{\mu} \hat{V}_{1}^{\mu, \hat{\nu}}(s_1) - \inf_{\nu} V_{1}^{\hat{\mu}, \nu}(s_1)|
\]

\[+ |\inf_{\nu} \hat{V}_{1}^{\hat{\mu}, \nu}(s_1) - \inf_{\nu} V_{1}^{\hat{\mu}, \nu}(s_1)| \leq \epsilon.
\]

which finishes the proof.

### B.2 Proof of Corollary 6

Recall that Theorem 5 requires \( T_0 = c(H^5S^2AB\epsilon/\epsilon^2 + H^7S^4AB\epsilon^3/\epsilon) \) episodes to obtain an \( \epsilon \)-optimal policies in the sense:

\[
\sup_{\mu} V_{1}^{\mu, \hat{\nu}}(s_1) - \inf_{\nu} V_{1}^{\hat{\mu}, \nu}(s_1) \leq \epsilon.
\]

Therefore, if the agent plays the Markov game for \( T \) episodes, it can use first \( T_0 \) episodes to explore to find \( \epsilon \)-optimal policies \((\hat{\mu}, \hat{\nu})\), and use the remaining \( T - T_0 \) episodes to exploit (always play \((\hat{\mu}, \hat{\nu})\)). Then, the total regret will be upper bounded by:

\[
\text{Regret}(K) \leq T_0 \times 1 + (T - T_0) \times \epsilon
\]
Finally, choose
\[ \epsilon = \max \left\{ \left( \frac{H^5 S^2 AB_t}{T} \right)^{\frac{1}{4}}, \left( \frac{H^7 S^4 AB_t^3}{T} \right)^{\frac{1}{2}} \right\} \]
we finishes the proof.

C Proofs for Section 5

C.1 Proof of Theorem 9

The theorem is almost an immediate consequence of the general result on mirror descent (Rakhlin and Sridharan, 2013). However, for completeness, we provide a self-contained proof here. The main ingredient in our proof is to show that a “natural” loss estimator satisfies desirable properties—such as unbiasedness and bounded variance—for the standard analysis of mirror descent type algorithms to go through.

Special case of \( S = 1 \) We first deal with the case of \( S = 1 \). As the game only has one step \((H = 1)\), it reduces to a zero-sum matrix game with a noisy bandit feedback, i.e. there is an unknown payoff matrix \( R \in [0, 1]^{A \times B} \), the algorithm playes policies \((\mu_k, \nu_k) \in \Delta_A \times \Delta_B\), observes feedback \( r(a_k, b_k) = R_{a_k b_k} \) where \((a_k, b_k) \sim \mu_k \times \nu_k\), and the weak regret has form
\[
\text{WeakRegret}(T) = \max_{\mu} \sum_{k=1}^{T} \mu^\top R \nu_k - \min_{\nu} \sum_{k=1}^{K} \mu_k^\top R \nu.
\]

Note that this regret can be decomposed as
\[
\text{WeakRegret}(T) = \max_{\mu} \sum_{k=1}^{T} \mu^\top R \nu_k - \sum_{k=1}^{T} \mu_k^\top R \nu_k + \sum_{k=1}^{T} \mu_k^\top R \nu_k - \min_{\nu} \sum_{k=1}^{T} \mu_k^\top R \nu.
\]

We now describe the mirror descent algorithm for the max-player and show that it achieves bound \( I \leq \tilde{O}(\sqrt{AT}) \) regardless of the strategy of the min-player. A similar argument on the min-player will yield a regret bound \( II \leq \tilde{O}(\sqrt{BT}) \) on the second part of the above regret and thus show \( \text{WeakRegret}(T) \leq \tilde{O}(\sqrt{(A+B)T}) \).

For all \( k \in [T] \), define the loss vector \( \ell_k \in \mathbb{R}^A \) for the max-player as
\[
\ell_k(a) := e_a^\top R \nu_k, \quad \text{for all } a \in A.
\]

With this definition the regret \( I \) can be written as
\[
I = \max_{a} \sum_{k=1}^{T} \ell_k(a) - \sum_{k=1}^{T} \mu_k(a) \ell_k(a).
\]

Now, define the loss estimate \( \tilde{\ell}_k(a) \) as
\[
\tilde{\ell}_k(a) := 1 - \frac{1}{\mu_k(a)} \left[ 1 - r(a, b_k) \right].
\]

We now show that this loss estimate satisfies the following properties:
Computable: the reward \( r(a, b^k) \) is seen when \( a = a^k \), and the loss estimate is equal to 1 for all \( a \neq a^k \).

Bounded: we have \( \tilde{\ell}_k(a) \leq 1 \) almost surely for all \( k \) and \( a \).

Unbiased estimate of \( \ell_k(a) \). For any fixed state \( a \in A \), we have

\[
\mathbb{E} \left[ \tilde{\ell}_k(a) \mid F_{k-1} \right] = 1 - \mu_k(a) \cdot \frac{1}{\mu_k(a)} \mathbb{E}_{q_k \sim \nu_k} \left[ 1 - r(a, b^k) \right]
\]

\[= 1 - \left( 1 - \mathbb{E}_{q_k \sim \nu_k} [r(a, b^k)] \right) = E_{q_k \sim \nu_k}[r(a, b^k)] = e_a^T R \nu_k = \ell_k(a).\]

Bounded variance: one can check that

\[
\mathbb{E} \left[ \sum_{a \in A} \mu_k(a) \tilde{\ell}_k(a)^2 \mid F_{k-1} \right]
\]

\[= E_{q_k \sim \nu_k} \left[ \sum_{a \in A} \mu_k(a) \left( 1 - 2 \left( 1 - r(a, b^k) \right) \right) + \sum_{a \in A} (1 - r(a, b^k))^2 \right].\]

Letting \( y_a := 1 - r(a, b^k) \), we have \( y_a \in [0, 1] \) almost surely (though it is random), and thus

\[
\sum_a \mu_k(a)(1 - 2y_a) + \sum_a y_a^2 \leq 1 - 2 \min_a y_a + \sum_a y_a^2 = \sum_{a \neq a^*} y_a^2 + (y_{a^*} - 1)^2 \leq A,
\]

where \( a^* = \arg \min_{a \in A} y_a \).

Therefore, adapting the proof of standard regret-based bounds for the mirror descent (EXP3) algorithm (e.g. (Lattimore and Szepesvári, 2018, Theorem 11.1)), using the loss estimate \( \tilde{\ell}_k(a) \) and taking the step-size to be \( \eta_+ \equiv \sqrt{\log A/AT} \), we have the regret bound

\[\text{WeakRegret}_+ \leq C \cdot \sqrt{AT \log A},\]

where \( C > 0 \) is an absolute constant. This shows the desired bound \( \tilde{O}(\sqrt{AT}) \) for term I in the regret, and a similar bound \( \tilde{O}(\sqrt{BT}) \) holds for term II by using the same algorithm on the min-player.

Case of \( S > 1 \) The case of \( S > 1 \) can be viewed as \( S \) independent zero-sum matrix games. We can let both players play the each matrix game independently using an adaptive step-size sequence (such as the EXP3++ algorithm of Seldin and Slivkins (2014)) so that on the game with initial state \( s \in S \) they achieve regret bound

\[\tilde{O}(\sqrt{(A + B)T_s}),\]

where \( T_s \) denotes the number of games that has context \( s \). Summing the above over \( s \in S \) gives the regret bound

\[\text{WeakRegret}(T) \leq \sum_s \tilde{O}(\sqrt{(A + B)T_s}) \leq \tilde{O}(\sqrt{S(A + B)T}),\]

as \( \sum_s T_s = T \) and thus \( \sum_s \sqrt{T_s} \leq \sqrt{ST} \) by Cauchy-Schwarz.
We begin by decomposing the weak regret into two parts: 

\[ \text{WeakRegret}(T) = \max_{\mu} \sum_{k=1}^{K} V^{\mu, \nu} \left( s_{1}^{k} \right) - \min_{\nu} \sum_{k=1}^{K} V_{1}^{\mu, \nu} \left( s_{1}^{k} \right) \]

\[ = \max_{\mu} \sum_{k=1}^{K} V_{1}^{\mu, \nu} \left( s_{1}^{k} \right) - \sum_{k=1}^{K} V_{1}^{\mu, \nu} \left( s_{1}^{k} \right) + \sum_{k=1}^{K} V_{1}^{\mu, \nu} \left( s_{1}^{k} \right) - \min_{\nu} \sum_{k=1}^{K} V_{1}^{\mu, \nu} \left( s_{1}^{k} \right). \]

\[ \text{WeakRegret}_+ \quad \text{WeakRegret}_- \]

In the following, we show that both \( \text{WeakRegret}_+ \leq O(\sqrt{SAT}) \) and \( \text{WeakRegret}_- \leq O(\sqrt{SBT}) \), which when combined gives the desired result.
We now show that this loss estimate satisfies the following properties:

Above, the last equality follows by the fact the max player will not play again after the initial action in one-step games, i.e. \( Q_1^{\mu,\nu}((s,a))\) does not depend on \( \mu \). Applying the above expression, \( \text{WeakRegret}_{+} \) can be rewritten as

\[
\text{WeakRegret}_{+} = \max_{\mu} \sum_{k=1}^{K} \left( Q_1^{\mu,\nu}(s_1, \cdot), \mu(\cdot|s_1) \right) _a - \sum_{k=1}^{K} \left( Q_1^{\mu,\nu}(s_1, \cdot), \mu^k(\cdot|s_1) \right) _a,
\]

Therefore, bounding \( \text{WeakRegret}_{+} \) reduces to solving an online linear optimization problem over \( \Delta_A \) with bandit feedback, where at each step we play \( \mu^k \) and then suffer a linear loss with loss vector \( \{ Q_1^{\mu,\nu}(s_1, \cdot) \} _{a \in A} \).

Now, recall that our loss estimate in (12), adapted to the setting that \( s_1^k \equiv s_1 \) can be written as:

\[
\tilde{Q}_1^k(s_1, a) = 2 - \frac{1 \{ a^k = a \} }{\mu^k(a|s_1)} \cdot \left[ 2 - (r(s_1, a) + r(s_2^k, b^k)) \right].
\]

We now show that this loss estimate satisfies the following properties:

1. Computable: the reward \( r(s_1, a) \) is seen when \( a = a^k \), and the loss estimate is equal to 2 for all other \( a \neq a^k \).

2. Bounded: we have \( \tilde{Q}_1^k(s_1, a) \leq 2 \) for all \( k \) and \( a \).

3. Unbiased estimate of \( Q_1^{\mu,\nu}(s_1, \cdot) \). For any fixed state \( a \), when \( a^k = a \) happens, \( s_2^k \) is drawn from the MDP transition \( \mathbb{P}_1(\cdot|s_1, a) \). Therefore, letting \( \mathcal{F}_{k-1} \) be the \( \sigma \)-algebra that encodes all the information observed at the end of episode \( k - 1 \), we have that

\[
\tilde{Q}_1^k(s_1, a) | \mathcal{F}_{k-1} \overset{d}{=} 2 - \frac{1 \{ a^k = a \} }{\mu^k(a|s_1)} \cdot \left[ 2 - (r(s_1, a) - r(s_2^k, b^k)) \right],
\]

where \( d \) denotes equal in distribution, \( s_2^a \sim \mathbb{P}_1(\cdot|s_1, a) \) is an “imaginary” state had we played action \( a \) at step 1, and \( b^a \sim \nu^k(\cdot|s_2^a) \). Therefore we have

\[
\mathbb{E} \left[ \tilde{Q}_1^k(s_1, a) | \mathcal{F}_{k-1} \right] = \mathbb{E}_{a \sim \mu^k(\cdot|s_1)} \left[ 2 - \frac{1 \{ a^k = a \} }{\mu^k(a|s_1)} \mathbb{E}_{s_2^a, b^a} \left[ 2 - (r(s_1, a) - r(s_2^a, b^a)) \right] \right] = \mathbb{E}_{s_2^a, b^a} \left[ 2 - (r(s_1, a) + r(s_2^a, b^a)) \right] = Q_1^{\mu,\nu}(s_1, a).
\]

4. Bounded variance: one can check that

\[
\mathbb{E} \left[ \sum_{a \in A} \mu^k(a|s_1) \tilde{Q}_1^k(s_1, a)^2 | \mathcal{F}_{k-1} \right] = 4 \sum_{a \in A} \mu^k(a|s_1) \left( 1 - \mathbb{E}_{s_2^a, b^a} \left[ 2 - (r(s_1, a) - r(s_2^a, b^a)) \right] \right) + \sum_{a \in A} \mathbb{E}_{s_2^a, b^a} \left[ (2 - r(s_1, a) - r(s_2^a, b^a))^2 \right]
\]

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Letting $p_a := \mu^K(a|s_1)$ and $y_a := 2 - r(s_1, a) - r(s_2^{(a)}, b_2^{(a)})$, we have $y_a \in [0, 2]$ almost surely (though it is random), and thus

$$4 \sum_a p_a(1 - y_a) + \sum_a y_a^2 \leq 4(1 - \min_a y_a) + \sum_a y_a^2 = \sum_{a \neq a^*} y_a^2 + (y_{a^*} - 2)^2 \leq 4A,$$

where $a^* = \arg\min_{a \in A} y_a$.

Therefore, adapting the proof of standard regret-based bounds for the mirror descent (EXP3) algorithm (e.g. (Lattimore and Szepesvári, 2018, Theorem 11.1)), taking $\eta_+ \equiv \sqrt{\log A/AT}$, we have the regret bound

$$\text{WeakRegret}_+ \leq C \cdot \sqrt{AT \log A},$$

where $C > 0$ is an absolute constant.

In the general case where $s_1^k$ are not fixed and can be (in the worst case) adversarial, the design of Algorithm 3 guarantees that for any $s \in S$, $\mu(\cdot|s)$ gets updated after the $k$-th episode only if $s_1^k = s$; otherwise the $\mu(\cdot|s)$ is left unchanged. Therefore, the algorithm behaves like solving $S$ bandit problems independently, so we can sum up all the one-state regret bounds of the above form and obtain that

$$\text{WeakRegret}_+ \leq \sum_{s \in S} C \sqrt{AT_s \log A} \leq C \sqrt{SAT \log A} = O(\sqrt{SAT \log T}).$$

where $T_s := \#\{k : s_1^k = s\}$ denotes the number of occurrences of $s$ among all the initial states, and (i) uses that $\sum_s T_s = T$ and the Cauchy-Schwarz inequality (or pigeonhole principle). Note that we do not know $\{T_s\}_{s \in S}$ before the algorithm starts to play and thus cannot use $\eta_+(s) = \sqrt{\log A/AT_s}$. We instead use the EXP3++ algorithm (Seldin and Slivkins, 2014) whose step-size $\eta_{+,k}(s) = \sqrt{\log A/AN_k(s)}$ is computable at each episode $k$.

**Bounding WeakRegret** For any $\nu$ define $r(s_2, \nu(s_2)) := \mathbb{E}_{b \sim \nu(\cdot|s_2)}[r(s_2, b)]$ for convenience. We have

$$\text{WeakRegret}_- = \sum_{k=1}^K V^\mu_k,\nu_k(s_1^k) - \min_\nu \sum_{k=1}^K V^\mu_k,\nu(s_1^k)$$

$$= \sum_{k=1}^K \mathbb{E}_{a \sim \mu_k(\cdot|s_1)}[r(s_1^k, a) + \mathbb{P}_1[r(s_2, \nu_k(s_2))](s_1^k, a)]$$

$$- \min_\nu \sum_{k=1}^K \mathbb{E}_{a \sim \mu_k(\cdot|s_1)}[r(s_1^k, a) + \mathbb{P}_1[r(s_2, \nu(s_2))](s_1^k, a)]$$

$$= \sum_{k=1}^K \mathbb{E}_{a \sim \mu_k(\cdot|s_1)}[r(s_1^k, a) + \mathbb{P}_1[r(s_2, \nu_k(s_2))](s_1^k, a)]$$

$$- \sum_{k=1}^K \mathbb{E}_{a \sim \mu_k(\cdot|s_1)}[r(s_1^k, a) + \mathbb{P}_1[r(s_2, \nu^*(s_2))](s_1^k, a)]$$

$$= \sum_{k=1}^K \mathbb{E}_{a \sim \mu_k(\cdot|s_1), s_2 \sim \mathbb{P}_1(\cdot|s_1^k,a)}[r(s_2, \nu_k(s_2)) - r(s_2, \nu^*(s_2))],$$

where (i) follows from the fact that if we define $\nu^*(s_2) = \arg\min_\nu r(s_2, b')$, then $\nu^*$ is optimal at every state $s_2$ and thus also attains the minimum outside. Defining $f_k(s_2) = r(s_2, \nu_k(s_2)) - r(s_2, \nu^*(s_2))$, we have that $f_k(s_2) \in [0, 1]$ and is a fixed function of $s_2$ before playing episode $k$. Thus, if we define

$$\Delta_k = \mathbb{E}_{a,s_2}[f_k(s_2)] - f_k(s_2^k),$$

...
then $\Delta_k$ is a bounded martingale difference sequence adapted to $\mathcal{F}_{k-1}$, so by the Azuma-Hoeffding inequality we have with probability at least $1 - \delta$ that
\[
\left| \sum_{k=1}^{K} \Delta_k \right| \leq C \sqrt{K \log(1/\delta)} = C \sqrt{T \log(1/\delta)}.
\]
On this event, we have
\[
\text{WeakRegret}_- = \sum_{k=1}^{K} f_k(s_k^2) + \sum_{k=1}^{K} \Delta_k \\
\leq \sum_{k=1}^{K} \left[ r(s_k^2, \nu^k(s_2)) - r(s_2, \nu^*(s_2)) \right] + C \sqrt{K \log(1/\delta)}.
\]
The first term above is the regret for the contextual bandit problem (with context $s_2$) that the min player faces. Further, the min player in Algorithm 3 plays the mirror descent (EXP3) algorithm independently for each context $s_2$. Therefore, by standard regret bounds for mirror descent (e.g. Theorem 11.1, (Lattimore and Szepesvári, 2018)) we have (choosing $\eta_\epsilon \equiv \sqrt{\log B/T}$ in the fixed $s_2$ case, and using the EXP3++ scheduling (Seldin and Slivkins, 2014)) for the contextual case), we have
\[
I \leq \sum_{s \in \mathcal{S}_2} C \sqrt{B T_s \log B} \leq C \sqrt{S B T \log B},
\]
which combined with the above bound gives that with high probability
\[
\text{WeakRegret}_- \leq O(\sqrt{S B T \iota}),
\]
where $\iota = \log(S A B T / \delta)$. 

\section{Subroutine REWARD\_FREE\_EXPLORATION}

In this section, we present the REWARD\_FREE\_EXPLORATION algorithm, as well as the proofs for Lemma 13. The algorithm and results presented in this section is simple adaptation of the algorithm in Jin et al. (2020), which studies reward-free exploration in the single-agent MDP setting.

Since the guarantee of Lemma 13 only involves the evaluation of the value under fixed policies, it does not matter whether players try to maximize the reward or minimize the reward. Therefore, to prove Lemma 13 in this section, with out loss of generality, we will treat this Markov game as a single player MDP, where the agent take control of both players’ actions in MG. For simplicity, prove for the case $\mathcal{S}_1 = \mathcal{S}_2 = \cdots = \mathcal{S}_H$, $\mathcal{A}_1 = \mathcal{A}_2 = \cdots = \mathcal{A}_H = \mathcal{A}$. It is straightforward to extend the proofs in this section to the setting where those sets are not equal.

The algorithm is described in Algorithm 4, which consists of three loops. The first loop computes a set of policies $\Psi$. By uniformly sampling policy within set $\Psi$, one is guaranteed visit all “significant” states with reasonable probabilities. The second loop simply collecting data from such sampling procedure for $N$ episodes. The third loop computes empirical transition and empirical reward by averaging the observation data collected in the second loop. We note Algorithm 4 use subroutine EULER, which is the algorithm presented in Zanette and Brunskill (2019).

We can prove the following lemma, where Lemma 13 is a direct consequence of Lemma 14.
Algorithm 4 REWARD\_FREE\_EXPLORATION

1: **Input:** iteration number $N_0, N$
2: set policy class $\Psi \leftarrow \emptyset$, and dataset $D \leftarrow \emptyset$.
3: for all $(s, h) \in S \times [H]$ do
4:  $r_h(s', a') \leftarrow 1[s' = s \text{ and } h' = h]$ for all $(s', a', h') \in S \times A \times [H]$.
5:  $\Phi(s, h) \leftarrow \text{EULER}(r, N_0)$.
6:  $\pi_h(\cdot | s) \leftarrow \text{Uniform}(A)$ for all $\pi \in \Phi(s, h)$.
7:  $\Psi \leftarrow \Psi \cup \Phi(s, h)$.
8: for $n = 1 \ldots N$ do
9:  sample policy $\pi \sim \text{Uniform}(\Psi)$.
10: play $\mathcal{M}$ using policy $\pi$, and observe the trajectory $z_n = (s_1, a_1, \ldots, s_H, a_H, r_H, s_{H+1})$.
11: $D \leftarrow D \cup \{z_n\}$
12: for all $(s, a, h) \in S \times A \times [H]$ do
13:  $N_h(s, a) \leftarrow \sum_{(s_h, a_h) \in D} \mathbb{1}[s_h = s, a_h = a]$.
14:  $R_h(s, a) \leftarrow \sum_{(s_h, a_h) \in D} r_h \mathbb{1}[s_h = s, a_h = a]$.
15:  $\hat{\mu}_h(s, a) \leftarrow R_h(s, a)/N_h(s, a)$.
16: for all $s' \in S$ do
17:  $N_h(s, a, s') \leftarrow \sum_{(s_h, a_h, s_{h+1}) \in D} \mathbb{1}[s_h = s, a_h = a, s_{h+1} = s']$
18:  $\hat{P}_h(s'|s, a) \leftarrow N_h(s, a, s')/N_h(s, a)$.
19: **Return:** empirical transition $\hat{P}$, empirical reward $\hat{r}$.

Lemma 14. There exists absolute constant $c > 0$, for any $\epsilon > 0$, $p \in (0, 1)$, if we set $N_0 \geq cS^3AH^6\epsilon^3/\epsilon$, and $N \geq cH^3S^2A/\epsilon^2$ where $\epsilon := \log(SAH/(pe))$, then with probability at least $1 - p$, for any policy $\pi$:

$$|\hat{V}^\pi_1(s_1) - V^\pi_1(s_1)| \leq \epsilon/2$$

where $\hat{V}, V$ are the value functions of $\text{MG}(\hat{P}, \hat{r})$ and $\text{MG}(P, r)$, and $(\hat{P}, \hat{r})$ is the output of the algorithm 4.

Proof: The proof is almost the same as the proof of Lemma 3.6 in Jin et al. (2020) except that there is no error in estimating $r$ in Jin et al. (2020). We note the error introduced by the difference of $\hat{r}$ and $r$ is a same or lower order term compared to the error introduced by the difference of $\hat{P}$ and $P$. We can bound the former error using the similar treatment as in bounding the latter error. This finishes the proof. \hfill $\square$

E Connection to Algorithms against Adversarial Opponents and R-MAX

Similar to the standard arguments in online learning, we can use any algorithm with low regret against adversarial opponent in Markov games to design a provable self-play algorithm with low regret.

Formally, suppose algorithm $\mathcal{A}$ has the following property. The max-player runs algorithm $\mathcal{A}$ and has following guarantee:

$$\max_{\mu} \sum_{k=1}^{K} V^{\mu, \nu_k}_{1}(s^k_1) - \sum_{k=1}^{K} V^{\mu, \nu_k}_{1}(s^k_1) \leq f(S, A, B, T)$$

(14)

where $\{\mu_k\}_{k=1}^{K}$ are strategies played by the max-player, $\{\nu_k\}_{k=1}^{K}$ are the possibly adversarial strategies played by the opponent, and function $f$ is a regret bound depends on $S, A, B, T$. Then, by symmetry, we can also let min-player runs the same algorithm $\mathcal{A}$ and obtain following guarantee:

$$\sum_{k=1}^{K} V^{\mu, \nu_k}_{1}(s^k_1) - \min_{\nu} \sum_{k=1}^{K} V^{\mu, \nu}_{1}(s^k_1) \leq f(S, B, A, T).$$

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This directly gives a self-play algorithm with following regret guarantee

\[
\text{WeakRegret}(T) = \max_{\mu} \sum_{k=1}^{K} V^{\mu, \nu^k}_1(s^k_1) - \min_{\nu} \sum_{k=1}^{K} V^{\mu^k, \nu}_1(s^k_1)
\]

\[
= \max_{\mu} \sum_{k=1}^{K} V^{\mu, \nu^k}_1(s^k_1) - \sum_{k=1}^{K} V^{\mu^k, \nu^k}_1(s^k_1) + \sum_{k=1}^{K} V^{\mu^k, \nu^k}_1(s^k_1) - \min_{\nu} \sum_{k=1}^{K} V^{\mu^k, \nu}_1(s^k_1) \leq f(S, A, B, T) + f(S, B, A, T)
\]

However, we note there are two notable cases, despite they are also results with guarantees against adversarial opponent, their regret are not in the form (14), thus can not be used to give self-play algorithm, and obtain regret bound in our setting.

The first case is R-MAX algorithm (Brafman and Tennenholtz, 2002), which studies Markov games, with guarantees in the following form.

\[
\sum_{k=1}^{K} V^{\mu^k, \nu^k}_1(s^k_1) - \sum_{k=1}^{K} V^{\mu^k, \nu^k}_1(s^k_1) \leq g(S, A, B, T)
\]

where \(\{\mu_k\}^K_{k=1}\) are strategies played by the max-player, \(\{\nu_k\}^K_{k=1}\) are the adversarial strategies played by the opponent, \((\mu^*, \nu^*)\) are the Nash equilibrium of the Markov game, \(g\) is a bound depends on \(S, A, B, T\). We note this guarantee is weaker than (14), and thus can not be used to obtain regret bound in the setting of this paper.

The second case is algorithms designed for adversarial MDP (see e.g. Zimin and Neu, 2013; Rosenberg and Mansour, 2019; Jin et al., 2019), whose adversarial opponent can pick adversarial reward function. We note in Markov games, the action of the opponent not only affects the reward received but also affects the transition to the next state. Therefore, these results for adversarial MDP with adversarial rewards do not directly apply to the setting of Markov game.