# Optimistic Thompson Sampling-based Algorithms for Episodic Reinforcement Learning (Supplementary material)

Bingshan Hu<sup>1,2</sup>

Tianyue H. Zhang<sup>3</sup>

Nidhi Hegde<sup>1,4</sup>

Mark Schmidt<sup>3,4</sup>

<sup>1</sup>Department of Computing Science, University of Alberta, Edmonton, AB, Canada
 <sup>2</sup>Alberta Machine Intelligence Institute (Amii), Edmonton, AB, Canada
 <sup>3</sup>Department of Computer Science, University of British Columbia, Vancouver, BC, Canada,
 <sup>4</sup>Canada CIFAR AI Chair, Alberta Machine Intelligence Institute (Amii), Canada

### Abstract

We propose two Thompson Sampling-like, modelbased learning algorithms for episodic Markov decision processes (MDPs) with a finite time horizon. Our proposed algorithms are inspired by Optimistic Thompson Sampling (O-TS), empirically studied in Chapelle and Li [2011], May et al. [2012] for stochastic multi-armed bandits. The key idea for the original O-TS is to clip the posterior distribution in an optimistic way to ensure that the sampled models are always better than the empirical models. Both of our proposed algorithms are easy to implement and only need one posterior sample to construct an episode-dependent model. Our first algorithm, Optimistic Thompson Sampling for MDPs (O-TS-MDP), achieves a  $\widetilde{O}\left(\sqrt{AS^2H^4T}\right)$  regret bound, where S is the size of the state space, A is the size of the action space, H is the number of time-steps per episode and T is the number of episodes. Our second algorithm, Optimistic Thompson Sampling plus for MDPs (O-TS-MDP<sup>+</sup>), achieves the (near)-optimal  $\widetilde{O}\left(\sqrt{ASH^3T}\right)$  regret bound by taking a more aggressive clipping strategy. Since O-TS was only empirically studied previously, we derive regret bounds of O-TS for stochastic bandits. In addition, we propose, O-TS-Bandit<sup>+</sup>, a randomized version of UCB1 [Auer et al., 2002], for stochastic bandits. Both O-TS and O-TS-Bandit<sup>+</sup> achieve the optimal  $O\left(\frac{A\ln(T)}{\Delta}\right)$  problem-dependent regret bound, where  $\hat{\Delta}$  denotes the sub-optimality gap.

# **1 INTRODUCTION**

Reinforcement learning (RL) algorithms have been widely implemented in real-world applications such as autonomous driving, image processing, natural language processing, financial modeling, gaming, etc. Typically, an RL task can be formulated as a Markov decision process (MDP) with a state space, an action space, and a state transition function. In each time-step, the learning agent visits a state, plays an action, and transitions to the next state. In this paper, we consider the learning problem of episodic, non-stationary MDPs with S states, A actions, and a finite time horizon H. In each round  $t = 1, 2, \ldots, H$  belonging to episode  $k = 1, 2, \ldots, T$ , the learning agent visits a state and plays an action according to an action-sampling strategy. Then, the learning agent receives a random reward drawn from a fixed but unknown reward distribution and transitions to the next state sampled from a fixed but unknown transition probability distribution associated with the played action. The goal of the learning agent is to take actions wisely to maximize the cumulative reward over T episodes. The learning agent faces an exploitation-vs-exploration dilemma. In a single round, the learning agent can only choose an action that empirically performs the best so far to maximize the cumulative reward (exploitation) or choose an action that has not been played too often to learn the parameters of the associated unknown distributions (exploration).

Upper Confidence Bound (UCB)-based algorithms, inspired by the philosophy of optimism in the face of uncertainty (OFU), can achieve a balance between exploitation and exploration. The high-level idea behind this class of algorithms is to construct upper confidence bounds by adding an extra term to the empirical estimates. The additive term encourages the learning agent to play actions that have not been played too often. Many existing episodic MDP learning algorithms [Azar et al., 2017, Dann et al., 2017, Zanette and Brunskill, 2019, Dann et al., 2019, Zhang et al., 2020, Tiapkin et al., 2022b] are UCB-based. Notably, two modelbased algorithms, UCBVI [Azar et al., 2017] and Bayes-UCBVI [Tiapkin et al., 2022b], enjoy the (near)-optimal  $\widetilde{O}\left(\sqrt{ASH^3T}\right)$  regret bound.<sup>1</sup> UCB-based algorithms usu-

<sup>&</sup>lt;sup>1</sup>The  $\widetilde{O}(\cdot)$  notation only hides poly  $\log(ASHT)$  factors.

ally do not randomize the obtained data, and the exploration is driven by the additive terms.

Another class of algorithms perturb the obtained data in a certain way to encourage the learning agent to visit states and actions that have been less explored. The extra randomness can be achieved by injecting noise into the data. As shown in Osband et al. [2019], learning algorithms with random noise efficiently drive exploration. Many prominent state-of-the-art algorithms [Russo, 2019, Pacchiano et al., 2021, Xiong et al., 2022, Agrawal et al., 2021] for episodic MDPs are developed by adding calibrated Gaussian noise to the empirical estimates of the rewards. Although the transition probability distribution is unknown, the aforementioned learning algorithms do not add any noise to the empirical estimates of the transition probability distributions. Among them, a model-based algorithm, NARL-UCBVI [Pacchiano et al., 2021], and a model-free algorithm, C-RLSVI [Agrawal et al., 2021], achieve the same  $\widetilde{O}\left(\sqrt{AS^2H^4T}\right)$ regret bound. Very recently, SSR-Bernstein [Xiong et al., 2022], also a model-free learning algorithm, tightens the regret bound to  $\widetilde{O}\left(\sqrt{ASH^3T}\right)$ .

Different from adding noise directly to the data, extra randomness can also be achieved by drawing random samples from well-constructed data-dependent distributions. Interestingly, if the data-dependent distribution is designed to be the posterior distribution that models an unknown parameter, it coincides with the description of Thompson Sampling [Thompson, 1933, Chapelle and Li, 2011], one of the oldest randomized algorithms. For example, Gaussian distributions can be used to model the means of the reward distributions and Dirichlet distributions can be used to model the transition probability distributions in MDPs.

Thompson Sampling was originally invented for stochastic bandits, which can be viewed as a simple MDP with only one state, A actions, and one round per episode. Since there are no transitions between states, the only unknown parameters in a stochastic bandit problem are the means of the reward distributions. Conceptually, Thompson Sampling plays an action according to the posterior probability distribution of the optimal action. Empirically, it is not required to compute the exact posterior probability distribution of the optimal action. Instead, Thompson Sampling can draw a random sample from the posterior distribution associated with each action and then play the action with the highest posterior sample. The practical performance of Thompson Sampling has been studied extensively by Chapelle and Li [2011]. The theoretical performance of Thompson Sampling relies on the choice of the prior distributions. Thompson Sampling with Beta priors is asymptotically optimal [Agrawal and Goyal, 2017, Kaufmann et al., 2012], while Thompson Sampling with Gaussian priors is problem-dependent optimal [Agrawal and Goyal, 2017].

In reality, it is not necessary to restrict the data-dependent

distribution to the exact posterior distribution. If the datadependent distribution is designed to be the posterior distribution with some parameters modified, we term this type of algorithm as Thompson Sampling-like algorithms with posterior distribution reshaping. Optimistic Thompson Sampling (O-TS), a Thompson Sampling-like algorithm with posterior distribution reshaping, was first introduced and empirically evaluated by Chapelle and Li [2011], May et al. [2012].<sup>2</sup> The key idea of O-TS is to boost the random posterior sample to the mean of the posterior distribution (Gaussian distribution) if the random sample is smaller than the mean. In other words, O-TS reshapes the posterior distribution from a Gaussian distribution to a one-sided Gaussian distribution with the left side being clipped. There are other Thompson Sampling-like algorithms with reshaped posterior distributions. For stochastic bandits, Jin et al. [2021] devise MOTS, the first Thompson Sampling-like algorithm achieving minimax optimality. MOTS reshapes the posterior distribution by both clipping the upper tail and boosting the variance of the posterior distribution.

Different from stochastic bandits where the learning agent only needs to learn the means of the reward distributions, in episodic MDPs, the transition probability distributions are also unknown. Two Thompson Sampling-like, modelbased algorithms, SOS-OPS-RL [Agrawal and Jia, 2020] and OPSRL [Tiapkin et al., 2022a], use Dirichlet distributions to model the transition probability distributions. To drive exploration, they also boost the variance of the Dirichlet distributions. SOS-OPS-RL achieves a  $\tilde{O}\left(\sqrt{AS^2H^4T}\right)$ regret bound while SPSRL achieves the (near)-optimal  $\tilde{O}\left(\sqrt{ASH^3T}\right)$  regret bound.

Now, we list our key contributions in this paper.

(1) We propose O-TS-MDP, a computationally efficient and theoretically elegant model-based learning algorithm with randomized value functions, for episodic MDPs. O-TS-MDP only draws one random sample and enjoys a  $\widetilde{O}\left(\sqrt{AS^2H^4T}\right)$  regret bound. There are two key ingredients in O-TS-MDP. The first one is the usage of the boosted variance of the posterior distribution (a Gaussian distribution) to drive exploration. The second one is the usage of O-TS to clip the left side of the posterior distribution to simplify the theoretical analysis. Although the regret bound of O-TS-MDP is not as tight as OPSRL [Tiapkin et al., 2022a] and SSR-Bernstein [Xiong et al., 2022], OPSRL needs to draw O(1) random samples while SSR-Bernstein is a model-free algorithm. For our regret analysis of O-TS-MDP, we can avoid upper bounding the absolute value of the estimation error, thus simplifying the theoretical analysis as compared to the analysis of RLSVI-based algorithms [Russo, 2019, Agrawal et al., 2021, Xiong et al., 2022].

<sup>&</sup>lt;sup>2</sup>Originally, this learning algorithm was called Optimistic Bayesian Sampling (OBS) [May et al., 2012].

(2) We propose O-TS-MDP<sup>+</sup>, a model-based, OFU-inspired optimistic algorithm with randomized value functions.<sup>3</sup> O-TS-MDP<sup>+</sup> achieves the (near)-optimal  $\tilde{O}\left(\sqrt{ASH^3T}\right)$  regret bound. The key idea in O-TS-MDP<sup>+</sup> is a more aggressive clipping strategy of the posterior distribution. O-TS-MDP<sup>+</sup> boosts the value of the random sample to the upper confidence bound if the random sample is smaller than the upper confidence bound. The aggressive clipping contributes to reducing the variance of the reshaped posterior distribution as compared to O-TS-MDP. Consequently, the regret bound is tightened to be (near)-optimal. O-TS-MDP<sup>+</sup> can be viewed as a randomized version of UCB-VI [Azar et al., 2017].

(3) Although Chapelle and Li [2011], May et al. [2012] have demonstrated the empirical performance of O-TS for stochastic bandits, there is no theoretical analysis for it. We derive regret bounds for O-TS for bandits. In addition, we propose O-TS-Bandit<sup>+</sup>, an OFU-inspired learning algorithm, for stochastic bandits. Both O-TS and O-TS-Bandit<sup>+</sup> achieve the (order)-optimal  $O\left(\frac{A \ln(T)}{\Delta}\right)$  problem-dependent regret bound, where  $\Delta$  is the sub-optimality gap.

# 2 LEARNING PROBLEM

We consider an episodic non-stationary MDP problem which can be specified by  $M = \{S, A, H, P, \mu, p_0\}$ , where S is a finite state-space with size S, A is a finite action-space with size A, H is the finite number of rounds in each episode and  $p_0$  is the deterministic initial state distribution. Let Pand  $\mu$  denote the transition function and reward function, respectively. The learning agent interacts with the environment in an episodic way with the following learning protocol. In each round  $t \in [H]$  belonging to episode k, the learning agent observes a state  $s_t^k$  and plays an action  $a_t^k$ . Then, the learning agent receives a random reward  $X^k_{s^k_{*},a^k_{*},t} \in [0,1]$ that is drawn from a fixed reward distribution with mean  $\mu_{s_t^k, a_t^k, t} = \mu(s_t^k, a_t^k, t)$  and transitions to the next state  $s_{t+1}^k$ that is sampled from a fixed transition probability distribution  $P_{s_t^k, a_t^k, t} = \boldsymbol{P}(s_t^k, a_t^k, t)$ . The initial state  $s_1^k$  is sampled from  $p_0$ . The goal of the learning agent is to accumulate as much reward as possible over a finite number of T episodes, i.e., HT rounds in total.

A deterministic policy  $\pi = (\pi(\cdot, 1), \pi(\cdot, 2), \dots, \pi(\cdot, H))$  is a sequence of functions, where each  $\pi(\cdot, t) : S \to A$  takes a state as input and outputs an action that will be played if the learning agent visits that state. Let  $\Pi$  collect all such policies. The value function  $V_t^{\pi}(s)$  for state s of policy  $\pi$  in round t is defined as  $V_t^{\pi}(s) := \mu_{s,\pi(s,t),t} + P_{s,\pi(s,t),t}^{\pi}V_{t+1}^{\pi}$ . If we knew P and  $\mu$ , we could use backwards induction to compute the optimal policy  $\pi_*$ . Define  $V_{H+1}^{\pi_*} = \vec{0}$ . Then, for each round t = H, H - 1, ..., 1, for each state  $s \in S$ , we compute

$$\pi_*(s,t) = \arg \max_{a \in \mathcal{A}} \left\{ \mu_{s,a,t} + P_{s,a,t}^{\mathsf{T}} V_{t+1}^{\pi_*} \right\} V_t^{\pi_*}(s) = \mu_{s,\pi_*(s,t),t} + P_{s,\pi_*(s,t),t}^{\mathsf{T}} V_{t+1}^{\pi_*} .$$

The expected regret  $\mathcal{R}(T)$  over T episodes is defined as

$$\mathcal{R}(T) = \sum_{k=1}^{T} \mathbb{E}\left[ \left( V_1^{\pi_*}(s_1^k) - V_1^{\pi_k}(s_1^k) \right) \right] \quad , \qquad (1)$$

where  $\pi_k$  is random and the initial state  $s_1^k \sim p_0$ . If there exists (s,t) such that  $\pi_k(s,t) \neq \pi_*(s,t)$ , then regret may occur. Define  $\mathcal{F}_k = \left\{s_t^q, a_t^q, X_{s_t^q, a_t^q, t}^q, t \in [H], q \in [k]\right\}$  as the history trajectory by the end of episode k following policies  $\pi_1, \ldots, \pi_q, \ldots, \pi_k$  with the initial state in each episode independently drawn from  $p_0$ . Define  $\mathcal{F}_0 = \{\}$ .

### **3** O-TS-MDP AND O-TS-MDP<sup>+</sup>

### Algorithm 1 O-TS-MDP 1: Input: MDP instance M, number of episodes T2: Initialization: Set $\widehat{O}_{s,a,t} \leftarrow 0$ , $\widehat{P}_{s,a,t} \leftarrow \vec{0}$ , $\widehat{\mu}_{s,a,t} \leftarrow 0$ , $\forall (s,a,t)$ 3: for episode k = 1, 2, ..., T do Set $\widetilde{V'}_{H+1}^{\pi_k} = \vec{0}$ for $t = H, H - 1, \dots, 1$ do 4: 5: for $s \in S$ do 6: for $a \in \mathcal{A}$ do 7: Draw $\widetilde{\mu}_{s,a,t} \sim \mathcal{N}\left(\widehat{\mu}_{s,a,t}, \left(\sqrt{SH}\sigma_{s,a,t}^{k}\right)^{2}\right)$ Set $\widetilde{\mu}_{s,a,t}' \leftarrow \max\left\{\widetilde{\mu}_{s,a,t}, \widehat{\mu}_{s,a,t}\right\}$ Set $\widetilde{Q}_{s,a,t} \leftarrow \widetilde{\mu}_{s,a,t}' + \widehat{P}_{s,a,t}^{\mathsf{T}}\widetilde{V}_{t+1}^{\pi_{k}}$ 8: end for 9: Set $\pi_k(s,t) \leftarrow \arg \max_{a \in \mathcal{A}} \widetilde{Q}_{s,a,t}$ 10: Set $\widetilde{V'}_{t}^{\pi_{k}}(s) \leftarrow \widetilde{Q}_{s,\pi_{k}(s,t),t}$ end for 11: 12: end for Sample $s_1^k \sim p_0$ , run $\pi_k$ , and update $\widehat{\mu}_{s_t^k, \pi_k(s_t^k, t), t}$ , 13: $\widehat{O}_{s_{\star}^k,\pi_k(s_{\star}^k,t),t}$ , and $\widehat{P}_{s_{\star}^k,\pi_k(s_{\star}^k,t),t}$ for all $t \in [H]$ . 14: end for We first present some notations used by our proposed

We first present some notations used by our proposed algorithms O-TS-MDP and O-TS-MDP<sup>+</sup>. Let  $\hat{O}_{s,a,t}^k = \sum_{q=1}^k \mathbf{1}\left\{(s_t^q, a_t^q) = (s, a)\right\}$  denote the number of times that (s, a) has been visited in round t by the end of episode k. Let  $\hat{\mu}_{s,a,t}^k = \frac{1}{\hat{O}_{s,a,t}^k} \sum_{q=1}^k \mathbf{1}\left\{(s_t^q, a_t^q) = (s, a)\right\} X_{s,a,t}^q$  denote the empirical mean of (s, a, t) by the end of episode k. Let  $\hat{P}_{s,a,t}^k(s') = \frac{1}{\hat{O}_{s,a,t}^k} \sum_{q=1}^k \mathbf{1}\left\{(s_t^q, a_t^q) = (s, a), s_{t+1}^q = s'\right\}$  denote the empirical transition probability distribution. Let  $\sigma_{s,a,t}^k := 5\sqrt{H^2 \log^2\left(\frac{H}{\delta}\right)/\hat{O}_{s,a,t}^{k-1}}$ , where  $\delta = \frac{1}{ASH^2T^2}$ .

<sup>&</sup>lt;sup>3</sup>We say a learning algorithm is OFU-inspired and optimistic if the Optimism Decomposition [Pacchiano et al., 2021] can be used to decompose the regret.

For the case when (s, a, t) has not been visited yet by the end of episode k - 1, i.e.,  $\widehat{O}_{s,a,t}^{k-1} = 0$ , our algorithms set  $\sigma_{s,a,t}^k$  to a large constant.

# 3.1 O-TS-MDP

O-TS-MDP is presented in Algorithm 1. The key ingredients in O-TS-MDP are the boosted variance of the posterior distribution (a Gaussian distribution) to drive exploration and the usage of O-TS [May et al., 2012, Chapelle and Li, 2011] to clip a Gaussian distribution to a one-sided Gaussian distribution with the left side being truncated. The reshaping of the posterior distribution plays a crucial role in simplifying the algorithm and the theoretical analysis.

The same as other model-based algorithms, in episode k, O-TS-MDP constructs an episode-dependent model  $\tilde{M}'_k$  to simulate the true model. To construct  $\tilde{M}'_k$  with randomized value functions, O-TS-MDP draws a random sample  $\tilde{\mu}^k_{s,a,t} \sim \mathcal{N}\left(\hat{\mu}^{k-1}_{s,a,t}, SH\left(\sigma^k_{s,a,t}\right)^2\right)$  for each (s, a, t). If  $\tilde{\mu}^k_{s,a,t} < \hat{\mu}^{k-1}_{s,a,t}$ , O-TS-MDP boosts it to  $\hat{\mu}^{k-1}_{s,a,t}$ . Let  $\tilde{\mu}'_{s,a,t} := \max\left\{\hat{\mu}^{k-1}_{s,a,t}, \tilde{\mu}^k_{s,a,t}\right\}$ . Note that  $\tilde{\mu}'^k_{s,a,t}$  can be viewed as a random variable drawn from distribution  $\mathcal{N}'^k_{s,a,t}$  with the probability density function (PDF) f'(x) =

$$\begin{cases} 0, & x < \widehat{\mu}_{s,a,t}^{k-1}, \\ \phi\left(x; \widehat{\mu}_{s,a,t}^{k-1}, SH\left(\sigma_{s,a,t}^{k}\right)^{2}\right) + \frac{\delta\left(x - \widehat{\mu}_{s,a,t}^{k-1}\right)}{2}, & x \ge \widehat{\mu}_{s,a,t}^{k-1}, \end{cases}$$

where  $\phi(x; \mu, \sigma^2)$  denotes the PDF of  $\mathcal{N}(\mu, \sigma^2)$  and  $\delta(\cdot)$  denotes the Dirac delta function.<sup>4</sup> With  $\tilde{\mu'}_{s,a,t}^k$  for all (s, a, t) in hand, we construct  $\tilde{M}'_k = \left\{ \mathcal{S}, \mathcal{A}, H, \hat{P}^{k-1}, \tilde{\mu'}^k, p_0 \right\}$ , where  $\hat{P}^{k-1} = \left\{ \hat{P}^{k-1}_{s,a,t} \right\}$  collects all the empirical transition probability distributions by the end of episode k - 1 and  $\tilde{\mu'}^k = \left\{ \tilde{\mu'}^k_{s,a,t} \right\}$  collects all the random samples after the boosting. After constructing  $\tilde{M}'_k$ , O-TS-MDP uses backwards induction to find the optimal policy  $\pi_k$  for  $\tilde{M}'_k$  (shown in Line 4 to Line 12 in Algorithm 1). Let  $\tilde{V'}^{\pi}_t$  denote the value functions of a fixed policy  $\pi$  for  $\tilde{M}'_k$  in round t.

Now, we present a regret bound for Algorithm 1.

**Theorem 1.** The regret of Algorithm 1 is  $\widetilde{O}\left(\sqrt{AS^2H^4T}\right)$ .

O-TS-MDP is a *computationally efficient and space efficient* algorithm which only needs one random sample for each (s, a, t) to construct the episode-dependent model. Per episode, the time complexity is  $O(AS^2H)$  and the space

complexity is  $O(AS^2H)$ . In contrast, OPSRL [Tiapkin et al., 2022a] and SOS-OPS-RL [Agrawal and Jia, 2020] need multiple posterior samples to construct a model. The improvement of O-TS-MDP comes from the usage of  $\widehat{P}^{k-1}$ to construct the model. Instead, OPSRL and SOS-OPS-RL use Dirichlet random variables to construct the model. Although O-TS-MDP, OPSRL, and SOS-OPS-RL are all model-based algorithms with randomized value functions, O-TS-MDP is not an optimistic learning algorithm while OPSRL and SOS-OPS-RL are both optimistic algorithms. In other words, in O-TS-MDP, the value functions  $\widetilde{V'}_1^{\pi_*}(s)$  are not guaranteed to be greater than  $V_1^{\pi_*}(s)$  with high probability. As shown in the regret analysis, O-TS-MDP only achieves weak optimism. That is, each  $\widetilde{V'}_1^{\pi_*}(s)$  are only guaranteed to be greater than  $V_1^{\pi_*}(s)$  with a small constant probability. However, the strong optimism guarantee in OP-SRL and SOS-OPS-RL is at the cost of drawing multiple posterior samples. We believe that the regret bound of O-TS-MDP can also be tightened to  $\widetilde{O}\left(\sqrt{ASH^3T}\right)$  if drawing  $\tilde{O}(1)$  random samples.

The key idea behind SSR-Bernstein [Xiong et al., 2022] to achieve the optimal  $\tilde{O}\left(\sqrt{ASH^3T}\right)$  regret bound is to limit the amount of randomness within the learning algorithm. More specifically, in SSR-Bernstein, in each episode, all tuples (s, a, t) use the same random seed, which is a Gaussian random variable. In other words, for the entire learning algorithm across T episodes, the number of independent Gaussian random variables in SSR-Bernstein is exactly T. In contrast, in O-TS-MDP, each tuple (s, a, t) has its own random seed meaning that the total amount of independent Gaussian random variables is O(ASHT). As compared to O-TS-MDP, SSR-Bernstein does not fully randomize its obtained data.

Although O-TS-MDP and the RLSVI-based algorithms [Russo, 2019, Agrawal et al., 2021, Xiong et al., 2022] share in common an exploration mechanism, the introduce of O-TS to clip the left side of the posterior distribution simplifies the theoretical analysis in two ways. First, upper bounding the absolute value of the estimation error is not needed in the theoretical analysis of O-TS-MDP (Proof of Lemma 2 in the appendix presents more details). All the aforementioned RLSVI-based algorithms upper bound the absolute value of the estimation error, which is more complicated than upper bounding the one-sided error, as stated in Xiong et al. [2022]. Second, as compared to C-RLSVI of Agrawal et al. [2021] and SSR of Xiong et al. [2022], O-TS-MDP does not clip the randomized value functions to values in [0, H]. Consequently, the analysis of O-TS-MDP can reuse the value difference lemma (Lemma 16) directly.

Recall that  $\sigma_{s,a,t}^k = 5\sqrt{H^2 \log^2(T/\delta)/\widehat{O}_{s,a,t}^{k-1}}$ . To sketch the regret analysis, we first construct the empirical MDP  $\hat{M}_k = \{S, \mathcal{A}, H, \widehat{P}^{k-1}, \widehat{\mu}^{k-1}, p_0\}$ , where  $\widehat{\mu}^{k-1} =$ 

<sup>&</sup>lt;sup>4</sup>Note that from Algorithm 1 we can see that to implement O-TS-MDP, it is not required to compute f'(x). We simply draw a random sample from a Gaussian distribution and then compare the sample value with the mean of the Gaussian distribution.

 $\{\hat{\mu}_{s,a,t}^{k-1}\}$  collects all the empirical means. Let  $\hat{V}_t^{\pi}$  denote the value functions of a fixed policy  $\pi$  for  $\hat{M}_k$ . To decompose the regret, we define two high-probability events:

$$\mathcal{E}^{k} = \left\{ \left| \left( \widehat{P}_{s,a,t}^{k-1} - P_{s,a,t} \right)^{\mathsf{T}} V_{t+1}^{\pi_{k}} \right| \leq \sigma_{s,a,t}^{k}, \\ \left| \left( \widehat{\mu}_{s,a,t}^{k-1} - \mu_{s,a,t} \right) \right| \leq \sigma_{s,a,t}^{k}, \forall (s, a, t) \right\}, \\
\mathcal{E}^{k}_{\pi_{*}} = \left\{ \left| \left( P_{s,a,t} - \widehat{P}_{s,a,t}^{k-1} \right)^{\mathsf{T}} V_{t+1}^{\pi_{*}} \right| \leq \sigma_{s,a,t}^{k} \\ \left| \widehat{\mu}_{s,a,t}^{k-1} - \mu_{s,a,t} \right| \leq \sigma_{s,a,t}^{k}, \forall (s, a, t) \right\}.$$
(2)

We prepare three lemmas to prove Theorem 1. Recall  $V_1^{\pi_*}(s)$  is the value function of the optimal policy  $\pi_*$  for the true MDP M and  $\widetilde{V'}_1^{\pi_k}(s)$  is the value function of the optimal policy  $\pi_k$  for the episode-dependent MDP  $\widetilde{M'}_k$ . Our technical Lemma 2 upper bounds the expected performance gap between the optimal policy  $\pi_*$  over M and the optimal policy  $\pi_k$  over  $\widetilde{M'}_k$ .

**Lemma 2.** (*Optimism*). In episode k, we have

$$\mathbb{E}\left[\left(V_{1}^{\pi_{*}}(s_{1}^{k})-\widetilde{V'}_{1}^{\pi_{k}}(s_{1}^{k})\right)\mathbf{1}\left\{\mathcal{E}_{\pi_{*}}^{k}\right\}\right] \leq \sqrt{SH}\sum_{t=1}^{H}\mathbb{E}\left[O\left(\sigma_{s_{t}^{k},\pi_{k}(s_{t}^{k},t),t}^{k}\right)\right].$$
(3)

Recall that  $\hat{V}_1^{\pi_k}(s)$  is the value function of policy  $\pi_k$  over the empirical MDP  $\hat{M}_k$ . Lemma 3 upper bounds the expected performance gap for a single policy  $\pi_k$  over MDPs  $\tilde{M}'_k$  and  $\hat{M}_k$  and Lemma 4 upper bounds the expected performance gap for policy  $\pi_k$  over MDPs  $\hat{M}_k$  and M. Note that MDPs  $\hat{M}'_k$  and  $\hat{M}_k$  are constructed based on the same  $\hat{P}^{k-1}$  which is determined by  $\mathcal{F}_{k-1}$ .

**Lemma 3.** (*Posterior deviation*). In episode k, we have

$$\mathbb{E}\left[\widetilde{V'}_{1}^{\pi_{k}}(s_{1}^{k}) - \widehat{V}_{1}^{\pi_{k}}(s_{1}^{k})\right] \leq \sqrt{SH} \sum_{t=1}^{H} \mathbb{E}\left[\sigma_{s_{t}^{k},\pi_{k}(s_{t}^{k},t),t}^{k}\right].$$
(4)

Lemma 4. (Empirical deviation). In episode k, we have

$$\mathbb{E}\left[\left(\widehat{V}_{1}^{\pi_{k}}(s_{1}^{k})-V_{1}^{\pi_{k}}(s_{1}^{k})\right)\mathbf{1}\left\{\mathcal{E}^{k}\right\}\right] \leq 2\sum_{t=1}^{H}\mathbb{E}\left[\sigma_{s_{t},\pi_{k}}(s_{t},t),t\right].$$
(5)

*Proof of Theorem 1*. We have

$$\sum_{k=1}^{T} \mathbb{E} \left[ \left( V_{1}^{\pi_{*}}(s_{1}^{k}) - V_{1}^{\pi_{k}}(s_{1}^{k}) \right) \right]$$

$$\leq \sum_{k=1}^{T} \mathbb{E} \left[ \underbrace{\left( V_{1}^{\pi_{*}}(s_{1}^{k}) - \widetilde{V}_{1}^{\pi_{k}}(s_{1}^{k}) \right) \mathbf{1} \left\{ \mathcal{E}_{\pi_{*}}^{k} \right\}}_{\text{Lemma 2}} \right]$$

$$+ \sum_{k=1}^{T} \mathbb{E} \left[ \underbrace{\left( \widetilde{V}_{1}^{\pi_{k}}(s_{1}^{k}) - \widetilde{V}_{1}^{\pi_{k}}(s_{1}^{k}) \right)}_{\text{Lemma 3}} \right]$$

$$+ \sum_{k=1}^{T} \mathbb{E} \left[ \underbrace{\left( \widetilde{V}_{1}^{\pi_{k}}(s_{1}^{k}) - V_{1}^{\pi_{k}}(s_{1}^{k}) \right) \mathbf{1} \left\{ \mathcal{E}^{k} \right\}}_{\text{Lemma 4}} \right]$$

$$+ H \sum_{k=1}^{T} \mathbb{E} \left[ \underbrace{\left\{ \overline{\mathcal{E}^{k}} \right\}}_{\text{Lemma 18}} + \mathbb{E} \left\{ \overline{\mathcal{E}_{\pi_{*}}^{k}} \right\}}_{\text{Lemma 18}} \right]$$

$$\leq \sqrt{SH} \cdot \mathbb{E} \left[ \sum_{k=1}^{T} \sum_{t=1}^{H} O \left( \sigma_{s_{t}^{k}, \pi_{k}}(s_{t}^{k}, t), t \right) \right] + O(1)$$

$$\leq \widetilde{O} \left( \sqrt{AS^{2}H^{4}T} \right) , \qquad (6)$$

where the last inequality uses  $\sum_{k=1}^{T} \sum_{t=1}^{H} O\left(\sigma_{s_t^k, \pi_k(s_t^k, t), t}^k\right) \leq \widetilde{O}\left(\sqrt{ASH^3T}\right)$ , a well-known result in the MDP literature [Russo, 2019, Agrawal et al., 2021].

### **3.2 O-TS-MDP**<sup>+</sup>

Different from O-TS-MDP where only weak optimism is guaranteed, O-TS-MDP<sup>+</sup> is an OFU-inspired optimistic algorithm with randomized value functions. O-TS-MDP<sup>+</sup> takes a more aggressive clipping strategy to achieve strong optimism. O-TS-MDP<sup>+</sup> boosts the random sample to the upper confidence bound if it is smaller than the upper confidence bound. This aggressive clipping strategy contributes to reducing the variance of the posterior distribution as compared to O-TS-MDP, which, consequently, leads to tightening the regret bound to  $\tilde{O}(\sqrt{ASH^3T})$ .

Similar to Algorithm 1, in each episode, O-TS-MDP<sup>+</sup> also constructs a model  $\tilde{M}'_k = \left\{ S, A, H, \hat{P}^{k-1}, \tilde{\mu'}^k, p_0 \right\}$ . Now, we present how to construct  $\tilde{\mu'}^k$ . Let  $\overline{\mu}^k_{s,a,t} := \hat{\mu}^{k-1}_{s,a,t} + 2\sigma^k_{s,a,t}$  be the upper confidence bound for (s, a, t) which is determined by  $\mathcal{F}_{k-1}$ . At the beginning of episode k, for each (s, a, t), O-TS-MDP<sup>+</sup> draws a random sample  $\tilde{\mu}^k_{s,a,t} \sim \mathcal{N}\left(\hat{\mu}^{k-1}_{s,a,t}, \left(\sigma^k_{s,a,t}\right)^2\right)$ . Then, O-TS-MDP<sup>+</sup> boosts it to  $\overline{\mu}^k_{s,a,t}$  if  $\tilde{\mu}^k_{s,a,t} < \overline{\mu}^k_{s,a,t}$ . Let  $\tilde{\mu'}^k_{s,a,t} = \max\left\{\tilde{\mu}^k_{s,a,t}, \overline{\mu}^k_{s,a,t}\right\}$  denote the sample value after the boosting. The PDF for the distribution of  $\tilde{\mu'}^k_{s,a,t}$  can be defined as f'(x) = 0 if  $x < \overline{\mu}^k_{s,a,t}$ . Otherwise, f'(x) = 0  $\phi\left(x; \widehat{\mu}_{s,a,t}^{k-1}, (\sigma_{s,a,t})^2\right) + \Phi\left(\overline{\mu}_{s,a,t}^k; \widehat{\mu}_{s,a,t}^{k-1}, (\sigma_{s,a,t})^2\right) \delta(x - \overline{\mu}_{s,a,t}^k), \text{ where } \Phi(x; \mu, \sigma^2) \text{ denotes the cumulative distribution function (CDF) of } \mathcal{N}(\mu, \sigma^2). \text{ Let } \widetilde{\mu'}^k = \left\{\widetilde{\mu'}_{s,a,t}^k\right\} \text{ collect all the samples after the boosting. After constructing } \widetilde{M}'_k, \text{ O-TS-MDP}^+ \text{ computes the optimal policy } \pi_k \text{ for } \widetilde{M}'_k \text{ by using backwards induction. Algorithm 2 presents the pseudo-code of O-TS-MDP^+. The differences between O-TS-MDP and O-TS-MDP^+ are highlighted in Algorithm 1 and Algorithm 2, respectively.$ 

### Algorithm 2 O-TS-MDP<sup>+</sup>

1: **Input:** MDP instance M, number of episodes T 2: Initialization: Set  $\widehat{O}_{s,a,t} \leftarrow 0$ ,  $\widehat{P}_{s,a,t} \leftarrow \overrightarrow{0}$ ,  $\widehat{\mu}_{s,a,t} \leftarrow 0$ ,  $\forall (s, a, t)$ 3: **for** episode k = 1, 2, ..., T **do** Set  $\widetilde{V'}_{H+1}^{\pi_k} = \vec{0}$ for  $t = H, H-1, \dots, 1$  do 4: 5: for  $s \in \mathcal{S}$  do 6: 7: for  $a \in \mathcal{A}$  do Draw  $\widetilde{\mu}_{s,a,t} \sim \mathcal{N}\left(\widehat{\mu}_{s,a,t}, \left(\sigma_{s,a,t}^{k}\right)^{2}\right)$ 8: Set  $\overline{\mu}_{s,a,t} \leftarrow \widehat{\mu}_{s,a,t} + 2\sigma_{s,a,t}^k$ Set  $\widetilde{\mu}_{s,a,t}^{\prime} \leftarrow \max\left\{\widetilde{\mu}_{s,a,t}, \overline{\mu}_{s,a,t}\right\}$ Set  $\widetilde{Q}_{s,a,t} \leftarrow \widetilde{\mu}'_{s,a,t} + \widehat{P}_{s,a,t}^{\mathsf{T}} \widetilde{V'}_{t+1}^{\pi_k}$ end for 9: Set  $\pi_k(s,t) \leftarrow \arg \max_{a \in \mathcal{A}} \widetilde{Q}_{s,a,t}$ 10: Set  $\widetilde{V'}_t^{\pi_k}(s) \leftarrow \widetilde{Q}_{s,\pi_k(s,t),t}$ end for 11: 12: end for Sample  $s_1^k \sim p_0$ , run  $\pi_k$ , and update  $\widehat{\mu}_{s_t^k, \pi_k(s_t^k, t), t}$ , 13:  $\widehat{O}_{s_t^k,\pi_k(s_t^k,t),t}$  and  $\widehat{P}_{s_t^k,\pi_k(s_t^k,t),t}$  for all  $t \in [H]$ . 14: end for

Now, we present a regret bound for Algorithm 2.

**Theorem 5.** The regret of Algorithm 2 is  $\widetilde{O}\left(\sqrt{ASH^3T}\right)$ .

O-TS-MDP<sup>+</sup> achieves the same (near)-optimal regret bound as OPSRL of Tiapkin et al. [2022a] and SSR-Bernstein of Xiong et al. [2022]. O-TS-MDP<sup>+</sup> can be viewed as a randomized version of UCB-VI [Azar et al., 2017]. It is important to note that the O-TS-MDP<sup>+</sup> learning algorithm itself does not need a Bernstein-type bonus. However, the analysis of Theorem 5 relies on a concentration bound that is derived based on Bernstein's inequality (see Lemma 17 for more details).

Now, we sketch the regret analysis. Recall that  $\overline{\mu}_{s,a,t}^k = \widehat{\mu}_{s,a,t}^{k-1} + 2\sigma_{s,a,t}^k$ . We first construct a new MDP  $\overline{M}_k = \left\{ \mathcal{S}, \mathcal{A}, H, \widehat{P}^{k-1}, \overline{\mu}^k, p_0 \right\}$ , where  $\overline{\mu}^k = \left\{ \overline{\mu}_{s,a,t}^k \right\}$  collects all the upper confidence bounds. Let  $\overline{V}_t^{\pi}$  be the value functions of a fixed policy  $\pi$  for  $\overline{M}_k$ . Note that conditioned on history  $\mathcal{F}_{k-1}$ , although the constructed  $\overline{M}_k$  is deterministic,

 $\overline{V}_{1}^{\pi_{k}}(s)$  is still random as  $\pi_{k}$  is random. Recall that  $\pi_{k}$  is the optimal policy for  $\tilde{M}'_{k}$ . We still use  $\mathcal{E}^{k}$  and  $\mathcal{E}^{k}_{\pi_{*}}$ , the events that have been defined in (2), to decompose the regret. We prepare three lemmas for Theorem 5.

Lemma 6. (Optimism). In episode k, we have

$$\mathbb{E}\left[\left(V_1^{\pi_*}(s_1^k) - \widetilde{V'}_1^{\pi_k}(s_1^k)\right) \mathbf{1}\left\{\mathcal{E}_{\pi_*}^k\right\}\right] \le 0.$$
(7)

Lemma 7. (Posterior deviation). In episode k, we have

$$\mathbb{E}\left[\left(\widetilde{V'}_{1}^{\pi_{k}}(s_{1}^{k}) - \overline{V}_{1}^{\pi_{k}}(s_{1}^{k})\right)\right] \leq \sum_{t=1}^{H} \mathbb{E}\left[\sigma_{s_{t}^{k},\pi_{k}(s_{t}^{k},t),t}^{k}\right].$$
(8)

Lemma 8. (UCB-like). In episode k, we have

$$\mathbb{E}\left[\left(\overline{V}_{1}^{\pi_{k}}(s_{1}^{k})-V_{1}^{\pi_{k}}(s_{1}^{k})\right)\mathbf{1}\left\{\mathcal{E}^{k}\right\}\right] \\
\leq 2\sum_{t=1}^{H}\mathbb{E}\left[\sigma_{s_{t}^{k},\pi_{k}}(s_{t}^{k},t),t\right].$$
(9)

Proof of Theorem 5. We have

$$\sum_{k=1}^{T} \mathbb{E} \left[ \left( V_{1}^{\pi_{*}}(s_{1}^{k}) - V_{1}^{\pi_{k}}(s_{1}^{k}) \right) \right]$$

$$\leq \sum_{k=1}^{T} \mathbb{E} \left[ \underbrace{ \left( V_{1}^{\pi_{*}}(s_{1}^{k}) - \widetilde{V}_{1}^{\pi_{k}}(s_{1}^{k}) \right) \mathbf{1} \left\{ \mathcal{E}_{\pi_{*}}^{k} \right\} \right]$$

$$+ \sum_{k=1}^{T} \mathbb{E} \left[ \underbrace{ \left( \widetilde{V}_{1}^{\pi_{k}}(s_{1}^{k}) - \overline{V}_{1}^{\pi_{k}}(s_{1}^{k}) \right) \right] }_{\text{Posterior deviation, Lemma 7}} \right]$$

$$+ H \sum_{k=1}^{T} \mathbb{E} \left[ \underbrace{ \left( \overline{V}_{1}^{\pi_{k}}(s_{1}^{k}) - V_{1}^{\pi_{k}}(s_{1}^{k}) \right) \mathbf{1} \left\{ \mathcal{E}^{k} \right\} }_{\text{UCB-like, Lemma 8}} \right]$$

$$+ H \sum_{k=1}^{T} \mathbb{E} \left[ \underbrace{ \left\{ \overline{\mathcal{E}^{k}} \right\} + \mathbb{P} \left\{ \overline{\mathcal{E}_{\pi_{*}}^{k}} \right\} }_{\text{Lemma 18}} \right]$$

$$\leq \mathbb{E} \left[ \sum_{k=1}^{T} \sum_{t=1}^{H} O \left( \sigma_{s_{t}^{k}, \pi_{k}(s_{t}^{k}, t), t} \right) \right] + O(1)$$

$$\leq \tilde{O} \left( \sqrt{ASH^{3}T} \right).$$

# 4 O-TS AND O-TS-BANDIT<sup>+</sup>

Since a stochastic bandit problem can be viewed as a special MDP with S = 1, H = 1 and Chapelle and Li [2011] have already demonstrated the empirical performance of O-TS for stochastic bandits, to fill a gap in the stochastic bandit literature we present regret bounds of O-TS for stochastic bandits. In addition, we propose O-TS-Bandit<sup>+</sup>, an OFU-inspired, optimistic learning algorithm, for stochastic bandits. Note

that O-TS-Bandit<sup>+</sup> can be viewed as a randomized version of UCB1 [Auer et al., 2002].

Now, we present the learning problem of stochastic bandits with bounded rewards formally. In a stochastic bandit problem, we have an arm set  $\mathcal{A}$  with size A. At the beginning of each round t, the environment generates a reward vector  $X(t) = (X_1(t), X_2(t), \ldots, X_A(t))$  with each  $X_j(t) \in [0, 1]$  i.i.d. over time from a fixed but unknown probability distribution with mean  $\mu_j$ . Simultaneously, the learning agent pulls an arm  $J_t \in \mathcal{A}$ . At the end of round t, the learning agent observes and obtains  $X_{J_t}(t)$ , the reward associated with the pulled arm. The goal of the learning agent is to pull arms sequentially to accumulate as much reward as possible over a finite number of T rounds. Without loss of generality, we assume that the first arm is the unique optimal arm. In other words, we assume  $\mu_1 > \mu_j$  for all  $j \neq 1$ . Let  $\Delta_j := \mu_1 - \mu_j$  denote the mean reward gap.

We use regret to measure the performance of the learning agent's decisions. Similar to (1), the regret is defined as

$$\mathcal{R}(T) = T \cdot \mu_1 - \mathbb{E}\left[\sum_{t=1}^T \mu_{J_t}\right] ,$$
 (11)

where the expectation is taken over  $J_t$ . Different from episodic MDPs, where only the worst-case regret bounds are analyzed, for stochastic bandits we are interested in both problem-dependent regret bounds and problem-independent regret bounds. The difference between problem-dependent regret bounds and problem-independent regret bounds is the former one depends on the mean reward parameters  $\mu_1, \mu_2, \ldots, \mu_A$  while the latter one provides a regret bound for all the possible choices of mean reward parameters.

We introduce additional notation specific to stochastic bandits. Let  $O_j(t-1)$  denote the number of pulls of arm j by the end of round t-1 and  $\hat{\mu}_{j,O_j(t-1)}$  denote the empirical mean of arm j by the end of round t-1.

#### 4.1 O-TS

The learning algorithm of O-TS is presented in Algorithm 3. Similar to Algorithm 1, at the beginning of each round t, for each arm  $j \in \mathcal{A}$ , a random sample  $\tilde{\mu}_j(t)$  is drawn from  $\mathcal{N}\left(\hat{\mu}_{j,O_j(t-1)}, 1/O_j(t-1)\right)$ . If  $\tilde{\mu}_j(t)$  is smaller than  $\hat{\mu}_{j,O_j(t-1)}$ , it will be boosted to  $\hat{\mu}_{j,O_j(t-1)}$ . Let  $\tilde{\mu}'_j(t) = \max\left\{\tilde{\mu}_j(t), \hat{\mu}_{j,O_j(t-1)}\right\}$ . With all  $\tilde{\mu}'_j(t)$  in hand, the learning agent pulls arm  $J_t = \arg\max_{j\in\mathcal{A}}\tilde{\mu}'_j(t)$ .

Now, we present regret bounds for Algorithm 3.

**Theorem 9.** The problem-dependent regret bound of Algorithm 3 is  $\sum_{j \in \mathcal{A}: \Delta_j > 0} O\left(\frac{\ln(T)}{\Delta_j}\right)$ .

**Theorem 10.** The problem-independent regret bound of Algorithm 3 is  $O\left(\sqrt{AT \ln(A)}\right)$ .

Algorithm 3 O-TS (Optimistic Thompson Sampling [Chapelle and Li, 2011])

1: Input: an arm set  $\mathcal{A}$ 2: Pull each arm once to initialize  $O_j, \hat{\mu}_{j,O_j}$ 3: for round t = A + 1, A + 2, ... do 4: for  $a \in \mathcal{A}$  do 5: Draw  $\tilde{\mu}_j(t) \sim \mathcal{N}(\hat{\mu}_{j,O_j}, 1/O_j)$ Set  $\tilde{\mu}'_j(t) \leftarrow \max\{\tilde{\mu}_j(t), \hat{\mu}_{j,O_j}\}$ 6: end for 7: Pull arm  $J_t \leftarrow \arg\max_{j \in \mathcal{A}} \tilde{\mu}'_j(t)$ 8: Update  $O_{J_t}$  and  $\hat{\mu}_{J_t,O_{J_t}}$ .

9: end for

O-TS achieves the same problem-dependent and problemindependent regret bounds as Thompson Sampling with Gaussian priors (TS-Gaussian) (Algorithm 2 in Agrawal and Goyal [2017]). The key difference between O-TS and TS-Gaussian is TS-Gaussian uses normal distributions while O-TS uses one-sided Gaussian distributions with the left side being clipped. The problem-independent regret bound of O-TS is minimax optimal up to a  $\sqrt{\ln(A)}$  factor. Note that O-TS and TS-Gaussian are not optimistic learning algorithms.

# 4.2 O-TS-BANDIT<sup>+</sup>

Algorithm 1 O TS Pandit+

An OFU-inspired optimistic learning algorithm, O-TS-Bandit<sup>+</sup>, is presented in Algorithm 4. Similar to Algorithm 2, O-TS-Bandit<sup>+</sup> does the clipping aggressively to boost optimism and can be viewed as a randomized version of UCB1 [Auer et al., 2002]. Let  $\overline{\mu}_j(t) = \hat{\mu}_{j,O_j(t-1)} + \sqrt{1.5 \ln(t)/O_j(t-1)}$  be the upper confidence bound. O-TS-Bandit<sup>+</sup> boosts  $\tilde{\mu}_j(t)$  to  $\overline{\mu}_j(t)$  if it is smaller than  $\overline{\mu}_j(t)$ . Let  $\tilde{\mu}'_j(t) = \max\{\tilde{\mu}_j(t), \overline{\mu}_j(t)\}$  denote the value after the boosting. Then, O-TS-Bandit<sup>+</sup> pulls arm  $J_t = \arg \max_{j \in \mathcal{A}} \tilde{\mu}'_j(t)$ . The differences between O-TS and O-TS-Bandit<sup>+</sup> are highlighted in Algorithm 3 and Algorithm 4, respectively.

Algorium 4 O-1 S-Bandit
1: <b>Input:</b> an arm set $A$
2: Pull each arm once to initialize $O_j$ , $\hat{\mu}_{j,O_j}$
3: for round $t = A + 1, A + 2,$ do
4: for $j \in \mathcal{A}$ do
5: Draw $\widetilde{\mu}_j(t) \sim \mathcal{N}\left(\widehat{\mu}_{j,O_j}, 1/O_j\right)$
Set $\overline{\mu}_j \leftarrow \widehat{\mu}_{j,O_j} + \sqrt{1.5 \ln(t)/O_j}$
Set $\widetilde{\mu}'_{j}(t) \leftarrow \max\left\{\widetilde{\mu}_{j}(t), \overline{\mu}_{j}(t)\right\}$
6: end for
7: Pull arm $J_t \leftarrow \arg \max_{i \in \mathcal{A}} \widetilde{\mu}'_i(t)$
8: Update $O_{J_t}$ and $\widehat{\mu}_{J_t,O_{J_t}}$ .
9: end for

Now, we present regret bounds for Algorithm 4.

**Theorem 11.** The problem-dependent regret bound of Algorithm 4 is  $\sum_{j \in \mathcal{A}: \Delta_j > 0} O\left(\frac{\ln(T)}{\Delta_j}\right)$ .

**Theorem 12.** The problem-independent regret bound of Algorithm 4 is  $O\left(\sqrt{AT \ln(T)}\right)$ .

O-TS and O-TS-Bandit<sup>+</sup> have the same problem-dependent regret bound. For the problem-independent regret bound, O-TS-Bandit<sup>+</sup> is worse than O-TS. Note that O-TS-Bandit<sup>+</sup> is an optimistic algorithm. O-TS-Bandit<sup>+</sup> and MOTS [Jin et al., 2021] share in common that they both clip the Gaussian distributions based on the upper confidence bounds. The key difference lies in that MOTS clips the upper tail of Gaussian distributions to control the overestimation of the sub-optimal arms while O-TS-Bandit<sup>+</sup> keeps the upper tail of the Gaussian distributions to preserve optimism.

# **5 EXPERIMENTAL RESULTS**

In this section, we evaluate the empirical performance of our proposed algorithms O-TS-MDP and O-TS-MDP<sup>+</sup> for MDPs with S = [5, 20, 50], A = 3 and H = 10. For a fair performance comparison, our experimental set-up is fully adopted from Dann et al. [2017], where the empirical performance for several UCB-based algorithms was studied. For a specific (s, a, t), the random reward  $X_{s,a,t}$ in each episode is drawn from a Bernoulli distribution with parameter  $\mu_{s,a,t}$ . To ensure the sparsity of the random rewards, we set  $\mu_{s,a,t}\,=\,0$  with probability 0.85 and with probability 0.15, the value of  $\mu_{s,a,t}$  is drawn from a uniform distribution. The sparsity design is to control the occurrence that sub-optimal policies can obtain rewards by chance. We compare O-TS-MDP, O-TS-MDP<sup>+</sup>, SSR-Bernstein [Xiong et al., 2022], and TS-MDP, a Thompson Sampling-based learning algorithm without clipping the posterior distributions, i.e., constructing the episode-dependent model as  $\tilde{M} = \left\{ \mathcal{S}, \mathcal{A}, H, \widehat{P}^{k-1}, \widetilde{\mu}^k, p_0 \right\}$ . We set  $T = 10^7$  and compare the cumulative average rewards of each episode.

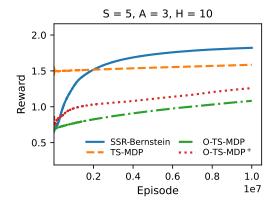


Figure 1: Empirical performance for 5 states

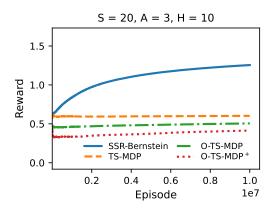


Figure 2: Empirical performance for 20 states

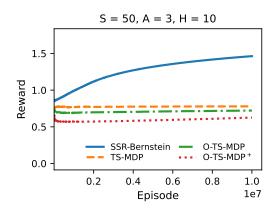


Figure 3: Empirical performance for 50 states

As shown in Figure 1, the rewards for all algorithms steadily increase as the learning agent gains a better estimation of the parameters of the true MDP over time. When the number of states is small (S = 5), O-TS-MDP<sup>+</sup> performs slightly better than O-TS-MDP. TS-MDP demonstrates a similar trend as O-TS-MDP since they are both Thompson Samplingbased algorithms. Despite the lack of theoretical analysis, TS-MDP does achieve better empirical performance. The gap between O-TS-MDP and TS-MDP comes from the fact that clipping the left side of the posterior distributions increases the chance to visit a sub-optimal (s, a, t), just as implied in the design of MOTS [Jin et al., 2021]. It is not surprising that SSR-Bernstein outperforms the remaining algorithms as it is theoretically optimal. Figure 2 and 3 show similar trends for Thomson-sampling-based methods in larger state space. SSR-Bernstein still performs the best.

It is important to note that SSR-Bernstein uses a single random seed for all (s, a, t) in each episode. In contrast, in our proposed algorithms, each (s, a, t) has its own randomness within an episode. In other words, our proposed algorithms inject more randomness than SSR-Bernstein. Additionally, SSR-Bernstein needs to construct confidence intervals to tune the magnitude of the variance, whereas our algorithms are simpler and easier to implement and enjoy good regret bounds. We also implement UCB-VI [Azar et al., 2017] and more experimental results can be found in Appendix H.

# 6 CONCLUSION AND FUTURE WORK

In this work, we have presented two Optimistic Thompson Sampling-based learning algorithms, O-TS-MDP and O-TS-MDP<sup>+</sup>, for episodic MDPs. The key feature that distinguishes our proposed learning algorithms from the existing RLSVI-based algorithms [Russo, 2019, Xiong et al., 2022, Agrawal et al., 2021] is the introduction of O-TS to avoid upper bounding the absolute value of the estimation error, thus simplifying the regret analysis. This work leaves two interesting open questions. Just as pointed out in Abeille and Lazaric [2017], Pacchiano et al. [2021], Agrawal et al. [2021], removing the extra  $\sqrt{SH}$  factor is challenging if the learning algorithms are Thompson Sampling-based. The first open question is whether the ideas in SSR of Xiong et al. [2022], i.e., controlling the amount of randomness within the learning algorithm, can be used to tighten the regret bound of O-TS-MDP to  $\widetilde{O}\left(\sqrt{ASH^3T}\right)$ . Our thought is that by reducing the amount of posterior random samples, a better regret bound for O-TS-MDP may be possible. The analysis of O-TS-MDP and RLSVI-based algorithms all rely on the property that the sum of multiple independent normal random variables is still normally distributed, and normal distributions have nice anti-concentration bounds. Although Tiapkin et al. [2022a] have proved a sharp anti-concentration bound for Dirichlet distributions, the distribution of the sum of multiple independent Dirichlet random variables is still less understood. The lack of understanding of Dirichlet distributions results in the need for multiple posterior samples in OPSRL of Tiapkin et al. [2022a]. The second interesting open question is whether we can reshape the Dirichlet posterior distribution in an optimistic way to improve the number of Dirichlet random variables in OPSRL to one.

# ACKNOWLEDGEMENTS

We thank Alan Milligan for helping with the experiments and providing comments on an early version of the manuscript. This work was partially supported by the Alberta Machine Intelligence Institute (Amii), the Canada CIFAR AI Program and the Natural Sciences and Engineering Research Council of Canada (NSERC) Discovery Grant RGPIN-2022-03669.

#### References

Marc Abeille and Alessandro Lazaric. Linear Thompson Sampling revisited. In *Artificial Intelligence and Statistics*, pages 176–184. PMLR, 2017.

Priyank Agrawal, Jinglin Chen, and Nan Jiang. Improved

worst-case regret bounds for randomized least-squares value iteration. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 35, pages 6566–6573, 2021.

- Shipra Agrawal and Navin Goyal. Near-optimal regret bounds for Thompson Sampling. http: //www.columbia.edu/~sa3305/papers/ j3-corrected.pdf, 2017.
- Shipra Agrawal and Randy Jia. Posterior sampling for reinforcement learning: Worst-case regret bounds. *arXiv* preprint arXiv:1705.07041, 2020.
- Peter Auer, Nicolo Cesa-Bianchi, and Paul Fischer. Finitetime analysis of the multi-armed bandit problem. *Machine learning*, 47:235–256, 2002.
- Mohammad Gheshlaghi Azar, Ian Osband, and Rémi Munos. Minimax regret bounds for reinforcement learning. In *International Conference on Machine Learning*, pages 263–272. PMLR, 2017.
- Olivier Chapelle and Lihong Li. An empirical evaluation of Thompson Sampling. *Advances in neural information processing systems*, 24, 2011.
- Christoph Dann, Tor Lattimore, and Emma Brunskill. Unifying PAC and regret: Uniform PAC bounds for episodic reinforcement learning. *Advances in Neural Information Processing Systems*, 30, 2017.
- Christoph Dann, Lihong Li, Wei Wei, and Emma Brunskill. Policy certificates: Towards accountable reinforcement learning. In *International Conference on Machine Learning*, pages 1507–1516. PMLR, 2019.
- Tianyuan Jin, Pan Xu, Jieming Shi, Xiaokui Xiao, and Quanquan Gu. MOTS: Minimax optimal Thompson Sampling. In *International Conference on Machine Learning*, pages 5074–5083. PMLR, 2021.
- Emilie Kaufmann, Nathaniel Korda, and Rémi Munos. Thompson Sampling: An asymptotically optimal finitetime analysis. In Algorithmic Learning Theory: 23rd International Conference, ALT 2012, Lyon, France, October 29-31, 2012. Proceedings 23, pages 199–213. Springer, 2012.
- Benedict C May, Nathan Korda, Anthony Lee, and David S Leslie. Optimistic Bayesian sampling in contextualbandit problems. *Journal of Machine Learning Research*, 13:2069–2106, 2012.
- Ian Osband, Benjamin Van Roy, Daniel J Russo, Zheng Wen, et al. Deep exploration via randomized value functions. *J. Mach. Learn. Res.*, 20(124):1–62, 2019.

- Aldo Pacchiano, Philip Ball, Jack Parker-Holder, Krzysztof Choromanski, and Stephen Roberts. Towards tractable optimism in model-based reinforcement learning. In *Uncertainty in Artificial Intelligence*, pages 1413–1423. PMLR, 2021.
- Daniel Russo. Worst-case regret bounds for exploration via randomized value functions. *Advances in Neural Information Processing Systems*, 32, 2019.
- William R Thompson. On the likelihood that one unknown probability exceeds another in view of the evidence of two samples. *Biometrika*, 25(3-4):285–294, 1933.
- Daniil Tiapkin, Denis Belomestny, Daniele Calandriello, Eric Moulines, Remi Munos, Alexey Naumov, Mark Rowland, Michal Valko, and Pierre MENARD. Optimistic posterior sampling for reinforcement learning with few samples and tight guarantees. In *Advances in Neural Information Processing Systems*, 2022a.
- Daniil Tiapkin, Denis Belomestny, Éric Moulines, Alexey Naumov, Sergey Samsonov, Yunhao Tang, Michal Valko, and Pierre Ménard. From Dirichlet to Rubin: Optimistic exploration in RL without bonuses. In *International Conference on Machine Learning*, pages 21380–21431. PMLR, 2022b.
- Zhihan Xiong, Ruoqi Shen, Qiwen Cui, Maryam Fazel, and Simon Shaolei Du. Near-optimal randomized exploration for tabular Markov decision processes. In *Advances in Neural Information Processing Systems*, 2022.
- Andrea Zanette and Emma Brunskill. Tighter problemdependent regret bounds in reinforcement learning without domain knowledge using value function bounds. In *International Conference on Machine Learning*, pages 7304–7312. PMLR, 2019.
- Zihan Zhang, Yuan Zhou, and Xiangyang Ji. Almost optimal model-free reinforcement learning via referenceadvantage decomposition. *Advances in Neural Information Processing Systems*, 33:15198–15207, 2020.

# APPENDIX

The appendix is organized as follows.

- 1. Appendix A presents proofs for Theorem 1;
- 2. Appendix B presents proofs for Theorem 5;
- 3. Appendix C presents other technical lemmas used in MDPs ;
- 4. Appendix D presents proofs for Theorem 9;
- 5. Appendix E presents proofs for Theorem 10;
- 6. Appendix F presents proofs for Theorem 11;
- 7. Appendix G presents proofs for Theorem 12;
- 8. Appendix H presents additional experimental results.

Since  $\mathbb{E}\left[\left(V_1^{\pi_*}(s_1^k) - V_1^{\pi_k}(s_1^k)\right)\right] = \mathbb{E}\left[\mathbb{E}\left[\left(V_1^{\pi_*}(s) - V_1^{\pi_k}(s)\right) \mid s_1^k = s\right]\right]$ , for the analysis in Appendix A and Appendix B, we upper bound the expected value difference conditioned on  $s_1^k = s$ . For ease of presentation, we drop the conditioning.

## A PROOFS FOR THEOREM 1

To prove Theorem 1, in episode k, we also construct another MDP  $\tilde{M}_k = \{S, A, H, \hat{P}^{k-1}, \tilde{\mu}^k, p_0\}$ , where  $\tilde{\mu}^k = \{\tilde{\mu}_{s,a,t}^k\}$  collects all the random samples that are initially drawn from Gaussian distributions (before doing the clippings). Note that  $\tilde{M}_k$  can be viewed as the "parental" MDP of  $\tilde{M}'_k$ . Let  $\tilde{V}_t^{\pi}$  denote the value functions of a fixed policy  $\pi$  for  $\tilde{M}_k$  in round t. We have the following facts.

- 1. The MDPs of  $\tilde{M}_k$  and  $\tilde{M}'_k$  use the same  $\widehat{P}^{k-1}$  to construct the models.
- 2. The learning algorithm of O-TS-MDP guarantees  $\tilde{\mu'}_{s,a,t}^k \ge \tilde{\mu}_{s,a,t}^k$  for all (s, a, t) hold simultaneously.
- 3. The learning algorithm of O-TS-MDP guarantees  $\tilde{\mu'}_{s,a,t}^k \ge \hat{\mu}_{s,a,t}^{k-1}$  for all (s, a, t) hold simultaneously.
- 4. The empirical estimates of  $\hat{\mu}^{k-1}$  and  $\hat{P}^{k-1}$ , the distributions for  $\tilde{\mu}^k$  and  $\tilde{\mu'}^k$ , and whether event  $\mathcal{E}_{\pi_*}^k$  is true or not are all determined by  $\mathcal{F}_{k-1}$ .
- Let  $c_0 = \frac{2e^{-2}}{5\sqrt{2\pi}}$  be a universal constant.

**Lemma 13.** (Weak optimism lemma). For any instantiation  $F_{k-1}$  of  $\mathcal{F}_{k-1}$  such that event  $\mathcal{E}_{\pi_*}^k$  is true, we have

$$\mathbb{P}\left\{\mathbf{1}\left\{\mathcal{E}_{\pi_{*}}^{k}\right\}\left(\widetilde{V}_{1}^{\pi_{*}}(s)-V_{1}^{\pi_{*}}(s)\right)\geq0\mid\mathcal{F}_{k-1}=F_{k-1}\right\}\geq c_{0}.$$
(12)

The proof of Lemma 2 uses the result stated in Lemma 13.

*Proof of Lemma 2 (Optimism lemma).* We use Markov's inequality and Lemma 13 to complete the proof. Some parts of the analysis use ideas presented in the proof of Lemma 6 in Russo [2019]. We would like to highlight that the introduce of O-TS simplifies the analysis avoiding upper bounding the absolute value of the estimation error.

We first rewrite the LHS in (3) as

LHS of (3) = 
$$\mathbb{E} \left[ \left( V_{1}^{\pi_{*}}(s) - \widetilde{V}_{1}^{\pi_{k}}(s) \right) \mathbf{1} \left\{ \mathcal{E}_{\pi_{*}}^{k} \right\} \right]$$
  

$$= \mathbb{E} \left[ \mathbb{E} \left[ \mathbf{1} \left\{ \mathcal{E}_{\pi_{*}}^{k} \right\} \left( V_{1}^{\pi_{*}}(s) - \widetilde{V}_{1}^{\pi_{k}}(s) \right) \mid \mathcal{F}_{k-1} \right] \right]$$
  

$$=^{(a)} \mathbb{E} \left[ \underbrace{\mathbb{E} \left[ \mathbf{1} \left\{ \mathcal{E}_{\pi_{*}}^{k} \right\} \left( V_{1}^{\pi_{*}}(s) - \max_{\pi \in \Pi} \widetilde{V}_{1}^{\pi}(s) \right) \mid \mathcal{F}_{k-1} \right] \right] , \qquad (13)$$

where equality (a) uses the fact that policy  $\pi_k$  is the optimal one for  $\tilde{M}'_k$ , i.e.,  $\tilde{V'}_1^{\pi_k}(s) = \max_{\pi \in \Pi} \tilde{V'}_1^{\pi}(s)$ . Since  $\lambda$  is determined by  $\mathcal{F}_{k-1}$ , we only need to consider all the instantiations  $F_{k-1}$  of  $\mathcal{F}_{k-1}$  such that  $\lambda > 0$ . Let  $\mathbb{E}_{k-1}[\cdot] = \mathbb{E}[\cdot | \mathcal{F}_{k-1} = F_{k-1}]$  and  $\mathbb{P}_{k-1}\{\cdot\} = \mathbb{P}\{\cdot | \mathcal{F}_{k-1} = F_{k-1}\}$ . Conditioned on such  $F_{k-1}$ , we use Markov's inequality and have

$$\lambda \leq \frac{\mathbb{E}_{k-1}\left[\max\left\{0, \mathbf{1}\left\{\mathcal{E}_{\pi_{*}}^{k}\right\}\left(\widetilde{V}_{1}^{\pi_{k}}(s) - \mathbb{E}_{k-1}\left[\max_{\pi\in\Pi}\widetilde{V}_{1}^{\pi}(s)\right]\right)\right\}\right]}{\mathbb{E}_{k-1}\left\{\max\left\{0, \mathbf{1}\left\{\mathcal{E}_{\pi_{*}}^{k}\right\}\left(\widetilde{V}_{1}^{\pi_{k}}(s) - \mathbb{E}_{k-1}\left[\max_{\pi\in\Pi}\widetilde{V}_{1}^{\pi}(s)\right]\right)\right\}\right\} \geq \lambda\right\}}{\mathbb{E}_{k-1}\left[\max\left\{0, \left(\widetilde{V}_{1}^{\pi_{k}}(s) - \mathbb{E}_{k-1}\left[\max_{\pi\in\Pi}\widetilde{V}_{1}^{\pi}(s)\right]\right)\right\}\right]}{\mathbb{E}_{k-1}\left\{\mathbf{1}\left\{\mathcal{E}_{\pi_{*}}^{k}\right\}\left(\widetilde{V}_{1}^{\pi_{k}}(s) - \mathbb{E}_{k-1}\left[\max_{\pi\in\Pi}\widetilde{V}_{1}^{\pi}(s)\right]\right)\geq\lambda\right\}}$$

$$(14)$$

**Construct a lower bound.** Now, we construct a lower bound for the denominator in the last step of (14) by using Lemma 13. We have

$$\mathbb{P}_{k-1} \left\{ \mathbf{1} \left\{ \mathcal{E}_{\pi_{*}}^{k} \right\} \left( \widetilde{V}_{1}^{\pi_{k}}(s) - \mathbb{E}_{k-1} \left[ \max_{\pi \in \Pi} \widetilde{V}_{1}^{\pi}(s) \right] \right) \geq \lambda \right\} \\
= \mathbb{P}_{k-1} \left\{ \mathbf{1} \left\{ \mathcal{E}_{\pi_{*}}^{k} \right\} \left( \widetilde{V}_{1}^{\pi_{k}}(s) - \mathbb{E}_{k-1} \left[ \max_{\pi \in \Pi} \widetilde{V}_{1}^{\pi}(s) \right] \right) \geq \mathbb{E}_{k-1} \left[ \mathbf{1} \left\{ \mathcal{E}_{\pi_{*}}^{k} \right\} \left( V_{1}^{\pi_{*}}(s) - \max_{\pi \in \Pi} \widetilde{V}_{1}^{\pi}(s) \right) \right] \right\} \\
= \mathbb{P}_{k-1} \left\{ \mathbf{1} \left\{ \mathcal{E}_{\pi_{*}}^{k} \right\} \left( \widetilde{V}_{1}^{\pi_{k}}(s) - V_{1}^{\pi_{*}}(s) \right) \geq 0 \right\} \\
\geq^{(a)} \mathbb{P}_{k-1} \left\{ \mathbf{1} \left\{ \mathcal{E}_{\pi_{*}}^{k} \right\} \left( \widetilde{V}_{1}^{\pi_{*}}(s) - V_{1}^{\pi_{*}}(s) \right) \geq 0 \right\} \\
\geq^{(b)} \mathbb{P}_{k-1} \left\{ \mathbf{1} \left\{ \mathcal{E}_{\pi_{*}}^{k} \right\} \left( \widetilde{V}_{1}^{\pi_{*}}(s) - V_{1}^{\pi_{*}}(s) \right) \geq 0 \right\} \\
\geq^{(c)} c_{0} ,$$
(15)

where inequality (a) uses the fact that  $\widetilde{V'}_{1}^{\pi_{k}}(s) \geq \widetilde{V'}_{1}^{\pi_{*}}(s)$  as policy  $\pi_{k}$  is the optimal one for  $\tilde{M}'_{k}$  and inequality (b) uses the fact that  $\widetilde{V'}_{1}^{\pi_{*}}(s) \geq \widetilde{V}_{1}^{\pi_{*}}(s)$  as MDPs  $\tilde{M}'_{k}$  and  $\tilde{M}_{k}$  are constructed based on the same  $\widehat{P}^{k-1}$  and O-TS-MDP guarantees that  $\widetilde{\mu'}_{s,a,t}^{k} \geq \widetilde{\mu}_{s,a,t}^{k}$  for all (s, a, t) hold simultaneously. Inequality (c) uses Lemma 13.

**Construct an upper bound.** To construct an upper bound for the numerator in the last step of (14), we introduce a new MDP  $\tilde{\tilde{M}}'_{k} = \left\{ S, A, H, \hat{P}^{k-1}, \tilde{\tilde{\mu}'}^{k}, p_0 \right\}$ , where  $\tilde{\tilde{\mu}'}_{s,a,t}^k \sim \mathcal{N}'_{s,a,t}^k$ . Note  $\tilde{\mu'}_{s,a,t}^k$  and  $\tilde{\tilde{\mu}'}_{s,a,t}^k$  are i.i.d. according to  $\mathcal{N}'_{s,a,t}^k$ , a distribution determined by  $\mathcal{F}_{k-1}$ . Let  $\tilde{\tilde{V}}_{t}^{\pi}$  denote the value functions of a fixed policy  $\pi$  for  $\tilde{M}'_{k}$ . Then, we have

$$\mathbb{E}_{k-1}\left[\widetilde{\widetilde{V}'}_{1}^{\pi_{k}}(s) \mid \pi_{k}\right] \leq \mathbb{E}_{k-1}\left[\max_{\pi \in \Pi}\widetilde{\widetilde{V}'}_{1}^{\pi}(s)\right] = \mathbb{E}_{k-1}\left[\max_{\pi \in \Pi}\widetilde{V'}_{1}^{\pi}(s)\right] \quad .$$
(16)

Now, we come back to constructing the upper bound for the numerator in the last step of (14). We have

where inequality (a) uses (16) and equality (b) uses the fact that conditioned on  $\mathcal{F}_{k-1} = F_{k-1}$  and  $\pi_k$ , we have  $I_1 \ge 0$  since MDPs  $\tilde{M}'_k$  and  $\hat{M}_k$  are constructed based on the same  $\hat{P}^{k-1}$  and O-TS-MDP guarantees  $\tilde{\mu}'_{s,a,t}^k \ge \hat{\mu}_{s,a,t}^{k-1}$  for all (s, a, t) hold simultaneously. Similarly, we have  $I_2 \le 0$ .

**Upper bound**  $\lambda$ . By plugging (15) and (17) into (14), we have

$$\lambda \leq \frac{1}{c_0} \cdot \left( \mathbb{E}_{k-1} \left[ \widetilde{V'}_1^{\pi_k}(s) - \widehat{V}_1^{\pi_k}(s) \right] + \mathbb{E}_{k-1} \left[ \widetilde{\widetilde{V'}}_1^{\pi_k}(s) - \widehat{V}_1^{\pi_k}(s) \right] \right) \\ = O \left( \mathbb{E}_{k-1} \left[ \widetilde{V'}_1^{\pi_k}(s) - \widehat{V}_1^{\pi_k}(s) \right] + \mathbb{E}_{k-1} \left[ \widetilde{\widetilde{V'}}_1^{\pi_k}(s) - \widehat{V}_1^{\pi_k}(s) \right] \right)$$
(18)

By plugging the upper bound of  $\lambda$  into (13), we have

$$\mathbb{E}\left[\mathbf{1}\left\{\mathcal{E}_{\pi_{*}}^{k}\right\}\cdot\left(V_{1}^{\pi_{*}}(s)-\widetilde{V'}_{1}^{\pi_{k}}(s)\right)\right] \leq O\left(\mathbb{E}\left[\widetilde{V'}_{1}^{\pi_{k}}(s)-\widehat{V}_{1}^{\pi_{k}}(s)\right]+\mathbb{E}\left[\widetilde{\widetilde{V'}}_{1}^{\pi_{k}}(s)-\widehat{V}_{1}^{\pi_{k}}(s)\right]\right) \quad .$$
(19)

Now, we use Lemma 3 to upper bound (19). We have

$$\mathbb{E}\left[\widetilde{V'}_{1}^{\pi_{k}}(s) - \widehat{V}_{1}^{\pi_{k}}(s)\right] \leq \sqrt{SH} \sum_{t=1}^{H} \mathbb{E}\left[\sigma_{s_{t},\pi_{k}}(s_{t},t),t\right] \quad .$$

$$(20)$$

Similarly, we have

$$\mathbb{E}\left[\widetilde{\widetilde{V}_{1}}^{\pi_{k}}(s) - \widehat{V}_{1}^{\pi_{k}}(s)\right] \leq \sqrt{SH} \sum_{t=1}^{H} \mathbb{E}\left[\sigma_{s_{t},\pi_{k}(s_{t},t),t}^{k}\right] \quad ,$$

$$(21)$$

which concludes the proof.

Before presenting the proof of Lemma 3, we present Lemma 14 first.

**Lemma 14.** Let  $\hat{\mu}$  be a constant in  $\mathbb{R}$  and  $\sigma > 0$  be a positive constant. Let  $\tilde{\mu}'$  be a random variable that is drawn from a distribution with probability density function f'(x) defined as the following.

$$f'(x) = \begin{cases} 0, & \text{if } x < \hat{\mu}; \\ \phi(x; \hat{\mu}, \sigma^2) + 0.5 \cdot \delta(x - \hat{\mu}), & \text{if } x \ge \hat{\mu}, \end{cases}$$
(22)

where  $\phi(x; \hat{\mu}, \sigma^2)$  denotes the PDF of  $\mathcal{N}(\hat{\mu}, \sigma^2)$  and  $\delta(x)$  denotes the Dirac delta function. Then, we have  $\mathbb{E}[\widetilde{\mu}'] - \widehat{\mu} \leq \sigma$ .

Proof of Lemma 14. We use the definition of expectation to complete the proof. We have

$$\mathbb{E}\left[\widetilde{\mu}'\right] = \int_{-\infty}^{+\infty} xf'(x)dx \\
= \int_{\widehat{\mu}}^{+\infty} xf'(x)dx \\
= \int_{\widehat{\mu}}^{+\infty} x \cdot \left(\phi\left(x;\widehat{\mu},\sigma^{2}\right) + 0.5 \cdot \delta(x-\widehat{\mu})\right)dx \\
= \int_{\widehat{\mu}}^{+\infty} (x-\widehat{\mu})\frac{1}{\sigma\sqrt{2\pi}}e^{-\frac{(x-\widehat{\mu})^{2}}{2\sigma^{2}}}dx + \int_{\widehat{\mu}}^{+\infty} \widehat{\mu}\frac{1}{\sigma\sqrt{2\pi}}e^{-\frac{(x-\widehat{\mu})^{2}}{2\sigma^{2}}}dx + 0.5\widehat{\mu} \\
\leq \sigma + \widehat{\mu} \quad .$$
(23)

Proof of Lemma 3 (Posterior deviation lemma). We have

$$\begin{split} \mathbb{E}\left[\widetilde{V'}_{1}^{\pi_{k}}(s) - \widehat{V}_{1}^{\pi_{k}}(s)\right] &= \mathbb{E}\left[\mathbb{E}\left[\underbrace{\widetilde{V'}_{1}^{\pi_{k}}(s) - \widehat{V}_{1}^{\pi_{k}}(s)}_{\text{LHS in Lemma 16}} \mid \mathcal{F}_{k-1}, \widetilde{M'_{k}}\right]\right] \\ &= \mathbb{E}\left[\mathbb{E}\left[\mathbb{E}\left[\underbrace{\mathbb{E}_{s_{2},...,s_{H}}\left[\sum_{t=1}^{H}\left(\widetilde{\mu'}_{s_{t},\pi_{k}(s_{t},t),t}^{k} - \widehat{\mu}_{s_{t},\pi_{k}(s_{t},t),t}^{k-1}\right) \mid \mathcal{F}_{k-1}, \widetilde{M'_{k}}\right]}_{\text{RHS in Lemma 16}} \mid \mathcal{F}_{k-1}, \widetilde{M'_{k}}\right]\right] \\ &= \mathbb{E}\left[\mathbb{E}_{s_{2},...,s_{H}}\left[\sum_{t=1}^{H}\left(\widetilde{\mu'}_{s_{t},\pi_{k}(s_{t},t),t}^{k} - \widehat{\mu}_{s_{t},\pi_{k}(s_{t},t),t}^{k-1}\right) \mid \mathcal{F}_{k-1}, \widetilde{M'_{k}}\right]\right] \\ &= \mathbb{E}\left[\mathbb{E}_{s_{2},...,s_{H}}\left[\sum_{t=1}^{H}\left(\widetilde{\mu'}_{s_{t},\pi_{k}(s_{t},t),t}^{k} - \widehat{\mu}_{s_{t},\pi_{k}(s_{t},t),t}^{k-1}\right)\right] \\ &= \mathbb{E}\left[\sum_{t=1}^{H}\left(\widetilde{\mu'}_{s_{t},\pi_{k}(s_{t},t),t}^{k} - \widehat{\mu}_{s_{t},\pi_{k}(s_{t},t),t}^{k-1}\right)\right] \\ &= \sum_{t=1}^{H}\mathbb{E}\left[\mathbb{E}\left[\left(\widetilde{\mu'}_{s_{t},\pi_{k}(s_{t},t),t}^{k} - \widehat{\mu}_{s_{t},\pi_{k}(s_{t},t),t}^{k}\right) \mid \mathcal{F}_{k-1}, s_{t}, \pi_{k}\right]\right] \\ &\leq \sum_{t=1}^{H}\mathbb{E}\left[\sqrt{SH} \cdot \sigma_{s_{t},\pi_{k}(s_{t},t),t}^{k}\right], \end{split}$$

where the second equality uses the fact that conditioned on  $\mathcal{F}_{k-1}$  and  $\tilde{M}'_k$ , the policy  $\pi_k$  is determined.

(24)

Proof of Lemma 4 (Empirical deviation lemma). We have

$$\mathbb{E}\left[\left(\widehat{V}_{1}^{\pi_{k}}(s) - V_{1}^{\pi_{k}}(s)\right) \cdot \mathbf{1}\left\{\mathcal{E}^{k}\right\}\right] \\
= \mathbb{E}\left[\mathbb{E}\left[\mathbb{E}\left[\left(\underbrace{\widehat{V}_{1}^{\pi_{k}}(s) - V_{1}^{\pi_{k}}(s)\right)}_{\text{LHS in Lemma 16}} \cdot \mathbf{1}\left\{\mathcal{E}^{k}\right\} | \pi_{k}, \mathcal{F}_{k-1}\right]\right] \\
= \mathbb{E}\left[\mathbb{E}\left[\mathbf{1}\left\{\mathcal{E}^{k}\right\}\underbrace{\mathbb{E}_{s_{2},...,s_{H}}\left[\sum_{t=1}^{H}\left(\widehat{\mu}_{s_{t},\pi_{k}(s_{t},t),t}^{k-1} - \mu_{s_{t},\pi_{k}(s_{t},t),t}\right) + \left(\widehat{P}_{s_{t},\pi_{k}(s_{t},t),t}^{k-1} - P_{s_{t},\pi_{k}(s_{t},t),t}\right)^{\mathsf{T}}V_{t+1}^{\pi_{k}} | \pi_{k}, \mathcal{F}_{k-1}\right] | \pi_{k}, \mathcal{F}_{k-1}\right] \\
\leq \mathbb{E}\left[\mathbb{E}\left[\mathbf{1}\left\{\mathcal{E}^{k}\right\}\mathbb{E}_{s_{2},...,s_{H}}\left[\sum_{t=1}^{H}\left|\widehat{\mu}_{s_{t},\pi_{k}(s_{t},t),t}^{k-1} - \mu_{s_{t},\pi_{k}(s_{t},t),t}\right| + \left|\left(\widehat{P}_{s_{t},\pi_{k}(s_{t},t),t}^{k-1} - P_{s_{t},\pi_{k}(s_{t},t),t}\right)^{\mathsf{T}}V_{t+1}^{\pi_{k}}\right| | \pi_{k}, \mathcal{F}_{k-1}\right] | \pi_{k}, \mathcal{F}_{k-1}\right] \\
\leq \mathbb{E}\left[\mathbb{E}\left[\mathbb{E}\left[\mathbb{E}_{s_{2},...,s_{H}}\left[\sum_{t=1}^{H}2\sigma_{s_{t},\pi_{k}(s_{t},t),t}^{k} | \pi_{k}, \mathcal{F}_{k-1}\right] | \pi_{k}, \mathcal{F}_{k-1}\right]\right] \\
= \mathbb{E}\left[\mathbb{E}_{s_{2},...,s_{H}}\left[\sum_{t=1}^{H}2\sigma_{s_{t},\pi_{k}(s_{t},t),t}^{k} | \pi_{k}, \mathcal{F}_{k-1}\right]\right] \\
= \mathbb{E}\left[\mathbb{E}_{s_{2},...,s_{H}}\left[\sum_{t=1}^{H}2\sigma_{s_{t},\pi_{k}(s_{t},t),t}^{k} | \pi_{k}, \mathcal{F}_{k-1}\right]\right] \\
= \mathbb{E}\left[\mathbb{E}_{s_{2},...,s_{H}}\left[\sum_{t=1}^{H}2\sigma_{s_{t},\pi_{k}(s_{t},t),t}^{k} | \pi_{k}, \mathcal{F}_{k-1}\right]\right] \\
= \sum_{t=1}^{H}\mathbb{E}\left[2\sigma_{s_{t},\pi_{k}(s_{t},t),t}^{k}\right] .$$
(25)

The last inequality uses the fact that if event  $\mathcal{E}^k$  is true, we have  $|(\hat{\mu}_{s,a,t}^{k-1} - \mu_{s,a,t})| \leq \sigma_{s,a,t}^k$  and  $|(\hat{P}_{s,a,t}^{k-1} - P_{s,a,t})^{\mathsf{T}} V_{t+1}^{\pi_k}| \leq \sigma_{s,a,t}^k$  for all (s, a, t) hold simultaneously.

*Proof of Lemma 13.* The proof is very similar to the proof of Lemma 5 in Russo [2019]. We use anti-concentration bounds of Gaussian distributions shown in Lemma 19. Let  $\mathbb{P}_{k-1} \{\cdot\} = \mathbb{P} \{\cdot \mid \mathcal{F}_{k-1} = F_{k-1}\}$  and  $\mathbb{E}_{k-1} [\cdot] = \mathbb{E} [\cdot \mid \mathcal{F}_{k-1} = F_{k-1}]$ . We first rewrite the LHS in (12) as

$$\mathbb{P}_{k-1}\left\{\mathbf{1}\left\{\mathcal{E}_{\pi_{*}}^{k}\right\}\left(\widetilde{V}_{1}^{\pi_{*}}(s)-V_{1}^{\pi_{*}}(s)\right)\geq0\right\}=\mathbb{P}_{k-1}\left\{\mathbf{1}\left\{\mathcal{E}_{\pi_{*}}^{k}\right\}\cdot\underbrace{\left(\widetilde{V}_{1}^{\pi_{*}}(s)-\widehat{V}_{1}^{\pi_{*}}(s)\right)}_{I_{2}}\geq\mathbf{1}\left\{\mathcal{E}_{\pi_{*}}^{k}\right\}\cdot\underbrace{\left(V_{1}^{\pi_{*}}(s)-\widehat{V}_{1}^{\pi_{*}}(s)\right)}_{I_{1}}\right\}.$$
(26)

Conditioned on  $\mathcal{F}_{k-1} = F_{k-1}$  such that event  $\mathcal{E}_{\pi_*}^k$  is true, we construct an upper bound on  $I_1$ . We have

$$I_{1} = \underbrace{V_{1}^{\pi_{*}}(s) - \widehat{V}_{1}^{\pi_{*}}(s)}_{\text{LHS in Lemma 16}} = \underbrace{\mathbb{E}_{s_{2},...,s_{H}} \left[ \sum_{t=1}^{H} \left( \mu_{s_{t},\pi_{*}(s_{t},t),t} - \widehat{\mu}_{s_{t},\pi_{*}(s_{t},t),t}^{k-1} \right) + \left( P_{s_{t},\pi_{*}(s_{t},t),t} - \widehat{P}_{s_{t},\pi_{*}(s_{t},t),t}^{k-1} \right)^{\mathsf{T}} V_{t+1}^{\pi_{*}} | \mathcal{F}_{k-1} = F_{k-1} \right]}_{\text{RHS in Lemma 16}}$$

$$\leq \mathbb{E}_{s_{2},...,s_{H}} \left[ \sum_{t=1}^{H} \left| \widehat{\mu}_{s_{t},\pi_{*}(s_{t},t),t}^{k-1} - \mu_{s_{t},\pi_{*}(s_{t},t),t}^{k} \right| + \left| \left( \widehat{P}_{s_{t},\pi_{*}(s_{t},t),t}^{k-1} - P_{s_{t},\pi_{*}(s_{t},t),t} \right)^{\mathsf{T}} V_{t+1}^{\pi_{*}} \right| | \mathcal{F}_{k-1} = F_{k-1} \right]$$

$$\leq \mathbb{E}_{s_{2},...,s_{H}} \left[ \sum_{t=1}^{H} 2\sigma_{s_{t},\pi_{*}(s_{t},t),t}^{k} | \mathcal{F}_{k-1} = F_{k-1} \right] ,$$

$$(27)$$

where the expectation is taken over the sampled trajectory  $s_2, \ldots, s_H$  drawn following  $\pi_*$  and  $\widehat{P}^{k-1}$  given s as the initial state. The last inequality uses the fact that if event  $\mathcal{E}_{\pi_*}^k$  is true, we have  $|\mu_{s,a,t} - \widehat{\mu}_{s,a,t}^{k-1}| \leq \sigma_{s,a,t}^k$  and  $|(P_{s,a,t} - \widehat{P}_{s,a,t}^{k-1})^{\mathsf{T}} V_{t+1}^{\pi_*}| \leq \sigma_{s,a,t}^k$  for all (s, a, t) hold simultaneously. By plugging the upper bound on  $I_1$  in (26), we have

$$\begin{aligned} (26) &= \mathbb{P}_{k-1} \left\{ \mathbf{1} \left\{ \mathcal{E}_{\pi_{*}}^{k} \right\} \cdot \underbrace{\left( \widetilde{V}_{1}^{\pi_{*}}(s) - \widehat{V}_{1}^{\pi_{*}}(s) \right)}_{I_{2}} \geq \mathbf{1} \left\{ \mathcal{E}_{\pi_{*}}^{k} \right\} \cdot \underbrace{\left( V_{1}^{\pi_{*}}(s) - \widehat{V}_{1}^{\pi_{*}}(s) \right)}_{I_{1}} \right\} \\ &\geq \mathbb{P}_{k-1} \left\{ \mathbf{1} \left\{ \mathcal{E}_{\pi_{*}}^{k} \right\} \cdot \left( \widetilde{V}_{1}^{\pi_{*}}(s) - \widehat{V}_{1}^{\pi_{*}}(s) \right) \geq \mathbf{1} \left\{ \mathcal{E}_{\pi_{*}}^{k} \right\} \cdot \underbrace{\left( \mathbb{E}_{s_{2},...,s_{H}} \left[ \sum_{t=1}^{H} 2\sigma_{s_{t},\pi_{*}(s_{t},t),t}^{k} \mid \mathcal{F}_{k-1} = F_{k-1} \right] \right)}_{\text{an upper bound on } I_{1}} \right\} \\ &= \mathbb{P}_{k-1} \left\{ \left( \widetilde{V}_{1}^{\pi_{*}}(s) - \widehat{V}_{1}^{\pi_{*}}(s) \right) \geq \mathbb{E}_{s_{2},...,s_{H}} \left[ \sum_{t=1}^{H} 2\sigma_{s_{t},\pi_{*}(s_{t},t),t}^{k} \mid \mathcal{F}_{k-1} = F_{k-1} \right] \right\} \\ &= \mathbb{E}_{k-1} \left[ \mathbf{1} \left\{ \left( \widetilde{V}_{1}^{\pi_{*}}(s) - \widehat{V}_{1}^{\pi_{*}}(s) \right) \geq \mathbb{E}_{s_{2},...,s_{H}} \left[ \sum_{t=1}^{H} 2\sigma_{s_{t},\pi_{*}(s_{t},t),t}^{k} \mid \mathcal{F}_{k-1} = F_{k-1} \right] \right\} \right] \\ &= \mathbb{E}_{k-1} \left[ \mathbb{E}_{k-1} \left[ \mathbf{1} \left\{ \left( \widetilde{V}_{1}^{\pi_{*}}(s) - \widehat{V}_{1}^{\pi_{*}}(s) \right) \geq \mathbb{E}_{s_{2},...,s_{H}} \left[ \sum_{t=1}^{H} 2\sigma_{s_{t},\pi_{*}(s_{t},t),t}^{k} \mid \mathcal{F}_{k-1} = F_{k-1} \right] \right\} \right] \right] \end{aligned}$$
(28)

Now, conditioned on  $\mathcal{F}_{t-1} = F_{t-1}$  and  $\tilde{M}_k$ , we rewrite  $I_2$  as

$$I_{2} = \widetilde{V}_{1}^{\pi_{*}}(s) - \widehat{V}_{1}^{\pi_{*}}(s) = \mathbb{E}_{s_{2},...,s_{H}} \left[ \sum_{t=1}^{H} \left( \widetilde{\mu}_{s_{t},\pi_{*}(s_{t},t),t}^{k} - \widehat{\mu}_{s_{t},\pi_{*}(s_{t},t),t}^{k-1} \right) \mid \mathcal{F}_{k-1} = F_{k-1}, \widetilde{M}_{k} \right] , \qquad (29)$$

where the expectation is still taken over the sampled trajectory  $s_2, \ldots, s_H$  drawn following  $\pi_*$  and  $\hat{P}^{k-1}$  given s as the initial state. Then, we have

$$(28) = \mathbb{E}_{k-1} \left[ \mathbb{E}_{k-1} \left[ \mathbf{1} \left\{ \underbrace{\left( \widetilde{V}_{1}^{\pi_{*}}(s) - \widehat{V}_{1}^{\pi_{*}}(s) \right)}_{I_{2}} \ge \mathbb{E}_{s_{2},...,s_{H}} \left[ \sum_{t=1}^{H} 2\sigma_{s_{t},\pi_{*}(s_{t},t),t}^{k} \mid \mathcal{F}_{k-1} = F_{k-1} \right] \right\} \mid \tilde{M}_{k} \right] \right]$$

$$= \mathbb{E}_{k-1} \left[ \mathbb{E}_{k-1} \left[ \mathbf{1} \left\{ \mathbb{E}_{s_{2},...,s_{H}} \left[ \sum_{t=1}^{H} \left( \widetilde{\mu}_{s_{t},\pi_{*}(s_{t},t),t}^{k} - \widehat{\mu}_{s_{t},\pi_{*}(s_{t},t),t}^{k-1} \right) \mid \mathcal{F}_{k-1} = F_{k-1}, \tilde{M}_{k} \right] \right]$$

$$= \mathbb{E}_{k-1} \left[ \mathbb{E}_{k-1} \left[ \mathbf{1} \left\{ \mathbb{E}_{s_{2},...,s_{H}} \left[ \sum_{t=1}^{H} 2\sigma_{s_{t},\pi_{*}(s_{t},t),t}^{k} \mid \mathcal{F}_{k-1} = F_{k-1} \right] \right\} \mid \tilde{M}_{k} \right] \right]$$

$$= \mathbb{E}_{k-1} \left[ \mathbb{E}_{k-1} \left[ \mathbf{1} \left\{ \mathbb{E}_{s_{2},...,s_{H}} \left[ \sum_{t=1}^{H} \left( \widetilde{\mu}_{s_{t},\pi_{*}(s_{t},t),t}^{k} - \widehat{\mu}_{s_{t},\pi_{*}(s_{t},t),t}^{k-1} \right) \mid \mathcal{F}_{k-1} = F_{k-1}, \tilde{M}_{k} \right] \right]$$

$$= \mathbb{E}_{k-1} \left[ \mathbb{E}_{k-1} \left[ \mathbf{1} \left\{ \mathbb{E}_{s_{2},...,s_{H}} \left[ \sum_{t=1}^{H} 2\sigma_{s_{t},\pi_{*}(s_{t},t),t}^{k} - \widehat{\mu}_{s_{t},\pi_{*}(s_{t},t),t}^{k-1} - F_{s_{t},\pi_{*}(s_{t},t),t}^{k} \right] \right] \left[ \tilde{M}_{k} \right] \right]$$

$$= \mathbb{E}_{k-1} \left[ \mathbb{E}_{k-1} \left[ \mathbf{1} \left\{ \mathbb{E}_{s_{2},...,s_{H}} \left[ \sum_{t=1}^{H} \left( \widetilde{\mu}_{s_{t},\pi_{*}(s_{t},t),t}^{k} - \widehat{\mu}_{s_{t},\pi_{*}(s_{t},t),t}^{k-1} - 2\sigma_{s_{t},\pi_{*}(s_{t},t),t}^{k} \right) \mid \mathcal{F}_{k-1} = F_{k-1}, \tilde{M}_{k} \right] \right]$$

$$= \mathbb{E}_{k-1} \left[ \mathbb{E}_{k-1} \left[ \mathbb{E}_{s_{2},...,s_{H}} \left[ \sum_{t=1}^{H} \left( \widetilde{\mu}_{s_{t},\pi_{*}(s_{t},t),t}^{k} - \widehat{\mu}_{s_{t},\pi_{*}(s_{t},t),t}^{k-1} - 2\sigma_{s_{t},\pi_{*}(s_{t},t),t}^{k} \right] \mid \mathcal{F}_{k-1} = F_{k-1}, \tilde{M}_{k} \right] \right]$$

$$= \mathbb{E}_{k-1} \left[ \mathbb{E}_{k-1} \left[ \mathbb{E}_{s_{2},...,s_{H}} \left[ \sum_{t=1}^{H} \left( \widetilde{\mu}_{s_{t},\pi_{*}(s_{t},t),t}^{k} - \widehat{\mu}_{s_{t},\pi_{*}(s_{t},t),t}^{k-1} - 2\sigma_{s_{t},\pi_{*}(s_{t},t),t}^{k} \right] \mid \mathcal{F}_{k-1} = F_{k-1}, \tilde{M}_{k} \right] \right]$$

$$= \mathbb{E}_{k-1} \left[ \mathbb{E}_{k-1} \left[ \mathbb{E}_{k-1} \left[ \mathbb{E}_{k-1} \left( \mathbb{E}_{k-1} \left[ \mathbb{E}_{k-1} \left( \widetilde{\mu}_{k-1} \left[ \mathbb{E}_{k-1} \left( \mathbb{E}_{k-1} \left[ \mathbb{E}_{k-1} \left( \mathbb{E}_{k-1} \left[ \mathbb{E$$

For each (s, a, t), let  $n_{s,a,t}^k := \tilde{\mu}_{s,a,t}^k - \hat{\mu}_{s,a,t}^{k-1}$  and  $\omega_{s,a,t}$  be the probability that (s, a) is visited in round t when following policy  $\pi_*$  and  $\hat{P}^{k-1}$  given s as the initial state. Now, we express  $I_3$  as

$$I_{3} = \underbrace{\sum_{t=1}^{H} \sum_{s \in S} \omega_{s,\pi_{*}(s,t),t} \cdot n_{s,\pi_{*}(s,t),t}^{k}}_{=:X} - \underbrace{\sum_{t=1}^{H} \sum_{s \in S} \omega_{s,\pi_{*}(s,t),t} \cdot 2\sigma_{s,\pi_{*}(s,t),t}^{k}}_{=:z} \quad .$$
(31)

Since  $\widetilde{\mu}_{s,a,t}^k \sim \mathcal{N}\left(\widehat{\mu}_{s,a,t}^{k-1}, SH\left(\sigma_{s,a,t}^k\right)^2\right)$ , we know  $n_{s,a,t}^k \sim \mathcal{N}\left(0, SH\left(\sigma_{s,a,t}^k\right)^2\right)$ , which future implies  $X \sim \left(0, \sum_{t=1}^{H} \sum_{s \in \mathcal{S}} SH \cdot \left(\omega_{s,\pi_*(s,t),t}\right)^2 \cdot \left(\sigma_{s,\pi_*(s,t),t}^k\right)^2\right)$ . Now, we construct an upper bound for z using Cauchy-Schwarz in-

equality. We have

$$z \leq \sqrt{\sum_{t=1}^{H} \sum_{s \in \mathcal{S}} 2^2} \sqrt{\sum_{t=1}^{H} \sum_{s \in \mathcal{S}} \left(\omega_{s, \pi_*(s, t), t}\right)^2 \left(\sigma_{s, \pi_*(s, t), t}^k\right)^2} \leq 2\sqrt{SH} \sqrt{\sum_{t=1}^{H} \sum_{s \in \mathcal{S}} \left(\omega_{s, \pi_*(s, t), t}\right)^2 \left(\sigma_{s, \pi_*(s, t), t}^k\right)^2}.$$
 (32)

Now, we come back to (30) and have

$$(30) = \mathbb{E}_{k-1} \left[ \mathbb{E}_{k-1} \left[ 1 \left\{ \underbrace{\sum_{t=1}^{H} \sum_{s \in S} \omega_{s,\pi_*(s,t),t} \cdot n_{s,\pi_*(s,t),t}^k - \sum_{t=1}^{H} \sum_{s \in S} \omega_{s,\pi_*(s,t),t} \cdot 2\sigma_{s,\pi_*(s,t),t}^k}_{=I_3} \ge 0 \right\} | \tilde{M}_k \right] \right]$$

$$= \mathbb{E}_{k-1} \left[ 1 \left\{ \underbrace{\sum_{t=1}^{H} \sum_{s \in S} \omega_{s,\pi_*(s,t),t} \cdot n_{s,\pi_*(s,t),t}^k - \sum_{t=1}^{H} \sum_{s \in S} \omega_{s,\pi_*(s,t),t} \cdot 2\sigma_{s,\pi_*(s,t),t}^k}_{z} \ge 0 \right\} \right]$$

$$= \mathbb{P}_{k-1} \left\{ \underbrace{\sum_{t=1}^{H} \sum_{s \in S} \omega_{s,\pi_*(s,t),t} \cdot n_{s,\pi_*(s,t),t}^k - \sum_{t=1}^{H} \sum_{s \in S} \omega_{s,\pi_*(s,t),t} \cdot 2\sigma_{s,\pi_*(s,t),t}^k \ge 0 \right\}$$

$$\geq \mathbb{P}_{k-1} \left\{ \underbrace{\sum_{t=1}^{H} \sum_{s \in S} \omega_{s,\pi_*(s,t),t} \cdot n_{s,\pi_*(s,t),t}^k}_{X} \ge 2 \cdot \sqrt{SH \sum_{t=1}^{H} \sum_{s \in S} (\omega_{s,\pi_*(s,t),t})^2 \cdot (\sigma_{s,\pi_*(s,t),t}^k)^2}_{X}} \right\}$$

$$\geq c_0 \quad ,$$

$$(33)$$

where the last inequality uses anti-concentration bounds of Gaussian distributions shown in Lemma 19.

### **B PROOFS FOR THEOREM 5**

Proof of Lemma 6 (Optimism lemma). As O-TS-MDP<sup>+</sup> guarantees  $\overline{V}_{1}^{\pi_{*}}(s) \leq \widetilde{V'}_{1}^{\pi_{*}}(s) \leq \widetilde{V'}_{1}^{\pi_{k}}(s)$ , we only need to show that if event  $\mathcal{E}_{\pi_{*}}^{k}$  is true, we have  $V_{1}^{\pi_{*}}(s) \leq \overline{V}_{1}^{\pi_{*}}(s)$  to complete the proof. We use backwards induction to prove this claim. Recall event  $\mathcal{E}_{\pi_{*}}^{k} = \left\{ \left| \mu_{s,a,t} - \widehat{\mu}_{s,a,t}^{k-1} \right| \leq \sigma_{s,a,t}^{k}, \left| \left( P_{s,a,t} - \widehat{P}_{s,a,t}^{k-1} \right)^{\mathsf{T}} V_{t+1}^{\pi_{*}} \right| \leq \sigma_{s,a,t}^{k}, \forall s, a, t \right\}$ . Define  $\overline{V}_{H+1}^{\pi_{*}} = V_{H+1}^{\pi_{*}} = \vec{0}$ . If event  $\mathcal{E}_{\pi_{*}}^{k}$  is true, we have the following.

When t = H, for any s, we have

$$V_{H}^{\pi_{*}}(s) = \mu_{s,\pi_{*}(s,H),H} + \underbrace{P_{s,\pi_{*}(s,H),H}^{\intercal}V_{H+1}^{\pi_{*}}}_{=0}$$

$$\leq \widehat{\mu}_{s,\pi_{*}(s,H),H}^{k-1} + \sigma_{s,\pi_{*}(s,H),H}^{k}$$

$$< \widehat{\mu}_{s,\pi_{*}(s,H),H}^{k-1} + 2\sigma_{s,\pi_{*}(s,H),H}^{k}$$

$$= \overline{\mu}_{s,\pi_{*}(s,H),H}^{k} + \underbrace{\langle \widehat{P}_{s,\pi_{*}(s,H),H}^{k-1}, \overline{V}_{H+1}^{\pi_{*}} \rangle}_{=0}$$

$$= \overline{V}_{H}^{\pi_{*}}(s) .$$
(34)

When t = H - 1, for any s, we have

$$V_{H-1}^{\pi_*}(s) = \mu_{s,\pi_*(s,H-1),H-1} + P_{s,\pi_*(s,H-1),H-1}^{\mathsf{T}} V_H^{\pi_*} \\ \leq \hat{\mu}_{s,\pi_*(s,H-1),H-1}^{k-1} + \sigma_{s,\pi_*(s,H-1),H-1}^k + \left\langle \hat{P}_{s,\pi_*(s,H-1),H-1}^{k-1}, V_H^{\pi_*} \right\rangle + \sigma_{s,\pi_*(s,H-1),H-1}^k \\ \leq \overline{\mu}_{s,\pi_*(s,H-1),H-1} + \left\langle \hat{P}_{s,\pi_*(s,H-1),H-1}^{k-1}, \overline{V}_H^{\pi_*} \right\rangle \\ = \overline{V}_{H-1}^{\pi_*}(s) \quad .$$
(35)

When t = 1, for any s, we have

$$\begin{aligned}
V_{1}^{\pi_{*}}(s) &= \mu_{s,\pi_{*}(s,1),1} + P_{s,\pi_{*}(s,1),1}^{\mathsf{T}}V_{2}^{\pi_{*}} \\
&\leq \widehat{\mu}_{s,\pi_{*}(s,1),1}^{k-1} + \sigma_{s,\pi_{*}(s,1),1}^{k} + \left\langle \widehat{P}_{s,\pi_{*}(s,1),1}^{k-1}, V_{2}^{\pi_{*}} \right\rangle + \sigma_{s,\pi_{*}(s,1),1}^{k} \\
&\leq \overline{\mu}_{s,\pi_{*}(s,1),1} + \left\langle \widehat{P}_{s,\pi_{*}(s,1),1}^{k-1}, \overline{V}_{2}^{\pi_{*}} \right\rangle \\
&= \overline{V}_{1}^{\pi_{*}}(s) , 
\end{aligned}$$
(36)

which concludes the proof.

Proof of Lemma 7 (Posterior deviation lemma). We have

$$\mathbb{E}\left[\widetilde{V}_{1}^{\pi_{k}}(s) - \overline{V}_{1}^{\pi_{k}}(s)\right] = \mathbb{E}\left[\mathbb{E}\left[\widetilde{V}_{1}^{\pi_{k}}(s) - \overline{V}_{1}^{\pi_{k}}(s)\right] + \mathcal{F}_{k-1}, \tilde{M}_{k}'\right]\right] \\
= \mathbb{E}\left[\mathbb{E}\left[\mathbb{E}\left[\underbrace{\widetilde{V}_{1}^{\pi_{k}}(s) - \overline{V}_{1}^{\pi_{k}}(s)}_{\text{LHS in Lemma 16}} + \mathcal{F}_{k-1}, \tilde{M}_{k}'\right] + \mathcal{F}_{k-1}, \tilde{M}_{k}'\right]\right] \\
= \mathbb{E}\left[\mathbb{E}\left[\mathbb{E}_{s_{2},...,s_{H}}\left[\sum_{t=1}^{H}\left(\widetilde{\mu}_{s_{t},\pi_{k}(s_{t},t),t}^{k} - \overline{\mu}_{s_{t},\pi_{k}(s_{t},t),t}^{k}\right) + \mathcal{F}_{k-1}, \tilde{M}_{k}'\right]\right] \\
= \mathbb{E}\left[\mathbb{E}_{s_{2},...,s_{H}}\left[\sum_{t=1}^{H}\left(\widetilde{\mu}_{s_{t},\pi_{k}(s_{t},t),t}^{k} - \overline{\mu}_{s_{t},\pi_{k}(s_{t},t),t}^{k}\right) + \mathcal{F}_{k-1}, \tilde{M}_{k}'\right]\right] \\
= \mathbb{E}\left[\mathbb{E}_{s_{2},...,s_{H}}\left[\sum_{t=1}^{H}\left(\widetilde{\mu}_{s_{t},\pi_{k}(s_{t},t),t}^{k} - \overline{\mu}_{s_{t},\pi_{k}(s_{t},t),t}^{k}\right) + \mathcal{F}_{k-1}, \tilde{M}_{k}'\right]\right] \\
= \mathbb{E}\left[\mathbb{E}\left[\left(\widetilde{\mu}_{s_{t},\pi_{k}(s_{t},t),t}^{k} - \overline{\mu}_{s_{t},\pi_{k}(s_{t},t),t}^{k}\right) + \pi_{k}, \mathcal{F}_{k-1}, s_{t}\right]\right] \\
\leq \sum_{t=1}^{H}\mathbb{E}\left[\mathcal{F}\left[\left(\widetilde{\mu}_{s_{t},\pi_{k}(s_{t},t),t}^{k}\right) - \overline{\mu}_{s_{t},\pi_{k}(s_{t},t),t}^{k}\right) + \pi_{k}, \mathcal{F}_{k-1}, s_{t}\right] \\
\leq \sum_{t=1}^{H}\mathbb{E}\left[\sigma_{s_{t},\pi_{k}(s_{t},t),t}^{k}\right], \quad (37)$$

where the first equality uses the fact that conditioned on  $\mathcal{F}_{k-1}$  and  $\tilde{M}'_k$ , MDP  $\bar{M}_k$  and policy  $\pi_k$  are determined. Note that  $\tilde{M}'_k$  and  $\bar{M}_k$  are constructed based on the same  $\hat{P}^{k-1}$ .

*Proof of Lemma 8 (UCB-like lemma).* The proof is very similar to the proofs for Lemma 4 and uses the result of Lemma 4. Note that  $\pi_k$  may not be the optimal policy for  $\overline{M}_k$ . We first do the following decomposition. We have

$$\mathbb{E}\left[\left(\overline{V}_{1}^{\pi_{k}}(s)-V_{1}^{\pi_{k}}(s)\right)\mathbf{1}\left\{\mathcal{E}^{k}\right\}\right] \leq \mathbb{E}\left[\left(\overline{V}_{1}^{\pi_{k}}(s)-\widehat{V}_{1}^{\pi_{k}}(s)\right)\right] + \underbrace{\mathbb{E}\left[\left(\widehat{V}_{1}^{\pi_{k}}(s)-V_{1}^{\pi_{k}}(s)\right)\mathbf{1}\left\{\mathcal{E}^{k}\right\}\right]}_{\leq \sum_{t=1}^{H}\mathbb{E}\left[2\sigma_{s_{t},\pi_{k}}^{k}(s_{t},a_{t}),t\right], \text{ Lemma 4}}$$

$$(38)$$

For the first term above, we have

$$\begin{aligned}
& \mathbb{E}\left[\left(\overline{V}_{1}^{\pi_{k}}(s) - \widehat{V}_{1}^{\pi_{k}}(s)\right)\right] \\
&= \mathbb{E}\left[\mathbb{E}\left[\left(\overline{V}_{1}^{\pi_{k}}(s) - \widehat{V}_{1}^{\pi_{k}}(s)\right) \mid \pi_{k}, \mathcal{F}_{k-1}\right]\right] \\
&= \mathbb{E}\left[\mathbb{E}\left[\mathbb{E}_{s_{2},...,s_{H}}\left[\sum_{t=1}^{H}\left(\overline{\mu}_{s_{t},\pi_{k}(s_{t},t),t}^{k} - \widehat{\mu}_{s_{t},\pi_{k}(s_{t},t),t}^{k-1}\right) \mid \pi_{k}, \mathcal{F}_{k-1}\right]\right] \mid \pi_{k}, \mathcal{F}_{k-1}\right] \\
&= \mathbb{E}\left[\mathbb{E}_{s_{2},...,s_{H}}\left[\sum_{t=1}^{H}\left(\overline{\mu}_{s_{t},\pi_{k}(s_{t},t),t}^{k} - \widehat{\mu}_{s_{t},\pi_{k}(s_{t},t),t}^{k-1}\right) \mid \pi_{k}, \mathcal{F}_{k-1}\right]\right] \\
&= \sum_{t=1}^{H}\mathbb{E}\left[\left(\overline{\mu}_{s_{t},\pi_{k}(s_{t},t),t}^{k} - \widehat{\mu}_{s_{t},\pi_{k}(s_{t},t),t}^{k-1}\right)\right] \\
&= \sum_{t=1}^{H}\mathbb{E}\left[\left(\overline{\mu}_{s_{t},\pi_{k}(s_{t},t),t}^{k}\right) - \widehat{\mu}_{s_{t},\pi_{k}(s_{t},t),t}^{k-1}\right)\right] .
\end{aligned}$$
(39)

Then, we have

$$(38) \leq \sum_{t=1}^{H} \mathbb{E}\left[O\left(\sigma_{s_t,\pi_k(s_t,a_t),t}^k\right)\right] \quad , \tag{40}$$

which concludes the proof.

**Lemma 15.** Let  $\hat{\mu}$  be a constant in  $\mathbb{R}$  and  $\sigma > 0$  be a positive constant. Let  $\overline{\mu} = \hat{\mu} + z\sigma$ , where constant z > 0. Let  $\tilde{\mu}'$  be a random variable that is drawn from a distribution with probability density function f'(x) defined as the following.

$$f'(x) = \begin{cases} 0, & \text{if } x < \overline{\mu}; \\ \phi(x; \widehat{\mu}, \sigma^2) + \Phi(\overline{\mu}; \widehat{\mu}, \sigma^2) \,\delta(x - \overline{\mu}), & \text{if } x \ge \overline{\mu}, \end{cases}$$
(41)

where  $\phi(x; \hat{\mu}, \sigma^2)$  and  $\Phi(x; \hat{\mu}, \sigma^2)$  denote the PDF and CDF of  $\mathcal{N}(\hat{\mu}, \sigma^2)$ , and  $\delta(x)$  denotes the Dirac delta function. Then, we have  $\mathbb{E}[\tilde{\mu}'] - \bar{\mu} \leq \sigma$ .

Proof of Lemma 15. We use the definition of expectation and have

$$\begin{split} & \mathbb{E}\left[\widetilde{\mu}'\right] \\ &= \int_{-\infty}^{+\infty} x f'(x) dx \\ &= \int_{\overline{\mu}}^{+\infty} x f'(x) dx \\ &= \int_{\overline{\mu}}^{+\infty} x \cdot \left(\phi\left(x;\widehat{\mu},\sigma^{2}\right) + \Phi\left(\overline{\mu};\widehat{\mu},\sigma^{2}\right)\delta(x-\overline{\mu}\right)\right) dx \\ &= \int_{\overline{\mu}}^{+\infty} (x-\widehat{\mu}) \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\widehat{\mu})^{2}}{2\sigma^{2}}} dx + \int_{\overline{\mu}}^{+\infty} \widehat{\mu} \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\widehat{\mu})^{2}}{2\sigma^{2}}} dx + \overline{\mu} \cdot \Phi\left(\overline{\mu};\widehat{\mu},\sigma^{2}\right) \\ &= \int_{\overline{\mu}}^{+\infty} (x-\widehat{\mu}) \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\widehat{\mu})^{2}}{2\sigma^{2}}} dx + \widehat{\mu} \cdot \left(1 - \int_{-\infty}^{\overline{\mu}} \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\widehat{\mu})^{2}}{2\sigma^{2}}} dx\right) + \overline{\mu} \cdot \Phi\left(\overline{\mu};\widehat{\mu},\sigma^{2}\right) \\ &\leq \int_{\widehat{\mu}}^{+\infty} (x-\widehat{\mu}) \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\widehat{\mu})^{2}}{2\sigma^{2}}} dx + \widehat{\mu} \cdot \left(1 - \Phi\left(\overline{\mu};\widehat{\mu},\sigma^{2}\right)\right) + \overline{\mu} \cdot \Phi\left(\overline{\mu};\widehat{\mu},\sigma^{2}\right) \\ &\leq \sigma + \widehat{\mu} + z\sigma \cdot \Phi\left(\overline{\mu};\widehat{\mu},\sigma^{2}\right) \\ &\leq \sigma + \overline{\mu} + z\sigma \end{aligned}$$

### C OTHER LEMMAS USED FOR MDPS

**Lemma 16.** (Value difference lemma, Lemma 3 in Russo [2019], Lemma E.15 in Dann et al. [2017]). Consider any fixed policy  $\pi$  and two MDPs  $M^{(1)} = (S, A, H, P^{(1)}, \mu^{(1)}, p_0)$  and  $M^{(2)} = (S, A, H, P^{(2)}, \mu^{(2)}, p_0)$ . Let  $V_t^{\pi,(1)}$  and  $V_t^{\pi,(2)}$  denote the respective value functions of  $\pi$  under  $M^{(1)}$  and  $M^{(2)}$ . Then, for any s, we have

$$V_{1}^{\pi,(1)}(s) - V_{1}^{\pi,(2)}(s) = \mathbb{E}_{s_{2},\dots,s_{H}} \left[ \sum_{t=1}^{H} \left( \mu_{s_{t},\pi(s_{t},t),t}^{(1)} - \mu_{s_{t},\pi(s_{t},t),t}^{(2)} \right) + \left( P_{s_{t},\pi(s_{t},t),t}^{(1)} - P_{s_{t},\pi(s_{t},t),t}^{(2)} \right)^{\mathsf{T}} V_{t+1}^{\pi,(2)} \mid s_{1} = s \right] \quad ,$$

$$(43)$$

where the expectation is over the sampled state trajectory  $s_2, \ldots, s_H$  drawn following  $\pi$  in  $M^{(1)}$  given s as the initial state.

**Lemma 17.** (Proposition 5.2 in Agrawal and Jia [2020]). For any fixed vector  $h \in [0, H]^S$ , let  $\hat{p} \in \Delta^S$  be the average of n independent multi-noulli trials with parameter  $p \in \Delta^S$ . Then, for any  $\delta \in (0, 1)$ , we have

$$\mathbb{P}\left\{ \left| (\widehat{p} - p)^{\mathsf{T}} h \right| > 5\sqrt{\frac{H^2 \log^2(T/\delta)}{n}} \right\} \le \delta \quad .$$
(44)

Proof of Lemma 17. Proposition 5.2 in Agrawal and Jia [2020] is derived based on Bernstein's inequality already. By setting  $c_i = H$  and using the fact that  $\gamma_i \leq p_i$  in Proposition 5.2, we have  $2\sqrt{\log(n/\delta)} \sum_{i < S} \frac{\gamma_i c_i^2}{n} < 2\sqrt{\frac{H^2 \log^2(T/\delta)}{n}}$  and the fast rate term  $3H \frac{\log(2/\delta)}{n} \leq 3H \frac{\log(T/\delta)}{n}$ . Combining both terms, we have the stated concentration bound.  $\Box$ 

**Lemma 18.** In any episode k, we have  $\mathbb{P}\left\{\overline{\mathcal{E}^k}\right\} \leq O(SAHT\delta)$  and  $\mathbb{P}\left\{\overline{\mathcal{E}^k_{\pi_*}}\right\} \leq O(SAHT\delta)$ .

Proof of Lemma 18. For each (s, a, t), we let  $\widehat{P}_{s,a,t}^{(n_{s,a,t})}$  denote the average of  $n_{s,a,t}$  independent multi-noulli trials with parameter  $P_{s,a,t}$  and  $\widehat{\mu}_{s,a,t}^{(n_{s,a,t})}$  denote the average of  $n_{s,a,t}$  independent Bernoulli trials with parameter  $\mu_{s,a,t}$ .

#### Proofs for the first claim. We have

$$\mathbb{P}\left\{\overline{\mathcal{E}^{k}}\right\} \leq \mathbb{P}\left\{\exists s, a, t: \left|\left(\widehat{P}_{s,a,t}^{k-1} - P_{s,a,t}\right)^{\mathsf{T}} V_{t+1}^{\pi_{k}}\right| > \sigma_{s,a,t}^{k}\right\} + \mathbb{P}\left\{\exists s, a, t: \left|\left(\widehat{\mu}_{s,a,t}^{k-1} - \mu_{s,a,t}\right)\right| > \sigma_{s,a,t}^{k}\right\}.$$
(45)

For the first term above, we use Lemma 17. For the second term above, we use Hoeffding's inequality. We have

$$\mathbb{P}\left\{\exists s, a, t: \left| \left( \widehat{P}_{s,a,t}^{k-1} - P_{s,a,t} \right)^{\mathsf{T}} V_{t+1}^{\pi_{k}} \right| > \sigma_{s,a,t}^{k} \right\} \\
\leq \sum_{s,a} \sum_{t=1}^{H} \mathbb{P}\left\{ \left| \left( \widehat{P}_{s,a,t}^{k-1} - P_{s,a,t} \right)^{\mathsf{T}} V_{t+1}^{\pi_{k}} \right| > \sigma_{s,a,t}^{k} \right\} \\
\leq \sum_{s,a} \sum_{t=1}^{H} \sum_{n_{s,a,t}=1}^{k-1} \mathbb{P}\left\{ \left| \left( \widehat{P}_{s,a,t}^{(n_{s,a,t})} - P_{s,a,t} \right)^{\mathsf{T}} V_{t+1}^{\pi_{k}} \right| > \sigma_{s,a,t}^{k} \right\} \\
= \sum_{s,a} \sum_{t=1}^{H} \sum_{n_{s,a,t}=1}^{k-1} \mathbb{E}\left[ \underbrace{\mathbb{P}\left\{ \left| \left( \widehat{P}_{s,a,t}^{(n_{s,a,t})} - P_{s,a,t} \right)^{\mathsf{T}} V_{t+1}^{\pi_{k}} \right| > \sigma_{s,a,t}^{k} \right| \pi_{k} \right\} \\
\leq O(SAHT\delta) ,$$
(46)

where the last inequality uses Lemma 17. Note that  $\pi_k$  is random as it is the optimal policy for  $\tilde{M}'_k$ . Conditioned on  $\pi_k$ , the value functions  $V_{t+1}^{\pi_k} \in [0, H]$  are determined.

Similarly, we have

$$\mathbb{P}\left\{\exists s, a, t: \left|\left(\widehat{\mu}_{s,a,t}^{k-1} - \mu_{s,a,t}\right)\right| > \sigma_{s,a,t}^{k}\right\} \\
\leq \sum_{s,a} \sum_{t=1}^{H} \sum_{n_{s,a,t}=1}^{k-1} \underbrace{\mathbb{P}\left\{\left|\left(\widehat{\mu}_{s,a,t}^{(n_{s,a,t})} - \mu_{s,a,t}\right)\right| > \sigma_{s,a,t}^{k}\right\}}_{\text{Hoeffding's inequality}} \\
\leq O(SAHT\delta) ,$$
(47)

which concludes the proof for the first claim.

#### Proofs for the second claim. We have

$$\mathbb{P}\left\{\overline{\mathcal{E}_{\pi_*}^k}\right\} \leq \mathbb{P}\left\{\exists (s,a,t) : \left| \left(P_{s,a,t} - \widehat{P}_{s,a,t}^{k-1}\right)^\mathsf{T} V_{t+1}^{\pi_*} \right| > \sigma_{s,a,t}^k\right\} + \mathbb{P}\left\{\exists (s,a,t) : \left|\mu_{s,a,t} - \widehat{\mu}_{s,a,t}^{k-1}\right| > \sigma_{s,a,t}^k\right\}$$

$$(48)$$

We only need to upper bound the first term above as the second term is exactly the same as (47). We have

$$\mathbb{P}\left\{\exists (s, a, t) : \left| \left( P_{s,a,t} - \widehat{P}_{s,a,t}^{k-1} \right)^{\mathsf{T}} V_{t+1}^{\pi_{*}} \right| > \sigma_{s,a,t}^{k} \right\} \\
\leq \sum_{s,a} \sum_{t=1}^{H} \mathbb{P}\left\{ \left| \left( \widehat{P}_{s,a,t}^{k-1} - P_{s,a,t} \right)^{\mathsf{T}} V_{t+1}^{\pi_{*}} \right| > \sigma_{s,a,t}^{k} \right\} \\
\leq \sum_{s,a} \sum_{t=1}^{H} \sum_{n_{s,a,t}=1}^{k-1} \mathbb{P}\left\{ \left| \left( \widehat{P}_{s,a,t}^{(n_{s,a,t})} - P_{s,a,t} \right)^{\mathsf{T}} V_{t+1}^{\pi_{*}} \right| > \sigma_{s,a,t}^{k} \right\} \\
\leq O(SAHT\delta) ,$$
(49)

which concludes the proof of the second claim.

For the case where (s, a, t) has not been visited yet by the of episode k - 1, i.e.,  $\widehat{O}_{s,a,t}^{k-1} = 0$ , based on the learning algorithm, we set  $\widehat{P}_{s,a,t}^{(k-1)} = \vec{0}$  and  $\widehat{\mu}_{s,a,t}^{k-1} = 0$ . Since  $\widehat{O}_{s,a,t}^{k-1} = 0$ , the learning algorithm can set  $\sigma_{s,a,t}^k = \widetilde{O}\left(\sqrt{\frac{H^2}{\widehat{O}_{s,a,t}^{k-1}}}\right)$  to an extremely large value. Then, we know events  $\left|\left(\widehat{P}_{s,a,t}^{(k-1)} - P_{s,a,t}\right)^{\mathsf{T}} V_{t+1}^{\pi_k}\right| > \sigma_{s,a,t}^k$ ,  $\left|\left(\widehat{P}_{s,a,t}^{(k-1)} - P_{s,a,t}\right)^{\mathsf{T}} V_{t+1}^{\pi_k}\right| > \sigma_{s,a,t}^k$  and  $\left|\widehat{\mu}_{s,a,t}^{(k-1)} - \mu_{s,a,t}\right| > \sigma_{s,a,t}^k$  cannot happen.

**Lemma 19.** (Concentration and anti-concentration bounds of Gaussian distributions). For a Gaussian distributed random variable Z with mean  $\mu$  and variance  $\sigma^2$ , for z > 0, we have

$$\mathbb{P}\{Z > \mu + z\sigma\} \le \frac{1}{2}e^{-\frac{z^2}{2}} \quad , \mathbb{P}\{Z < \mu - z\sigma\} \le \frac{1}{2}e^{-\frac{z^2}{2}} \quad ,$$
(50)

and

$$\mathbb{P}\left\{Z > \mu + z\sigma\right\} \ge \frac{1}{\sqrt{2\pi}} \frac{z}{z^2 + 1} e^{-\frac{z^2}{2}} \quad .$$
(51)

### **D PROOFS FOR THEOREM 9**

Proof of Theorem 9. Regret can be expressed as

$$\mathcal{R}(T) = \sum_{t=1}^{T} \mathbb{E}\left[\mu_1 - \mu_{J_t}\right] = \sum_{j \in \mathcal{A}: \Delta_j > 0} \underbrace{\sum_{t=1}^{T} \mathbb{E}\left[\mathbf{1}\left\{J_t = j\right\}\right]}_{\mathbb{E}[O_j(T)]} \cdot \Delta_j \quad .$$
(52)

We first define some events to decompose the regret. Let  $C_j(t-1) = \left\{ \left| \hat{\mu}_{j,O_j(t-1)} - \mu_j \right| \le \sqrt{\frac{0.5 \ln(T\Delta_j^2)}{O_j(t-1)}} \right\}$  be the event that the confidence interval of the empirical mean holds for an arm  $j \in \mathcal{A}$ . Let  $\tilde{\mu}_j(t)$  be the value of the random posterior sample of arm  $j \in \mathcal{A}$  before the boosting, i.e.,  $\tilde{\mu}_j(t) \sim \mathcal{N}\left(\hat{\mu}_{j,O_j(t-1)}, \frac{1}{O_j(t-1)}\right)$ . For any sub-optimal arm j, let  $y_j = \mu_j + \frac{1}{2}\Delta_j$ . Let  $\mathcal{E}'_j(t) = \{\tilde{\mu}'_j(t) \le y_j\}$  be the event that the random sample of the sub-optimal arm j after the boosting is near to the true mean  $\mu_j$ . Let  $\mathcal{F}_t = \{J_\tau, X_{J_\tau}(\tau), \tau = 1, 2, \dots, t\}$  collect all the history information by the end of round t. Now, for a fixed sub-optimal arm j, we upper bound the expected number of pulls of it by the end of round T. Let  $L_j = \frac{36 \ln(T\Delta_j^2)}{\Delta_j^2}$ . We have

**Upper bound**  $\omega_3$ . We only need to use Hoeffding's inequality here. Let  $\tau_s$  be the round when the *s*-th pull of arm *j* occurs. Define  $\tau_0 = 0$ . The definition of  $\tau_s$  means  $\mathbf{1} \{J_t = j\} = 0$  for all  $t \in \{\tau_s + 1, \dots, \tau_{s+1} - 1\}$ . We have

$$\begin{aligned}
\omega_{3} &= \sum_{t=1}^{T} \mathbb{E} \left[ \mathbf{1} \left\{ J_{t} = j, \overline{C_{j}(t-1)} \right\} \right] \\
&\leq \sum_{s=0}^{T} \mathbb{E} \left[ \sum_{t=\tau_{s}+1}^{\tau_{s+1}} \mathbf{1} \left\{ J_{t} = j, \overline{C_{j}(t-1)} \right\} \right] \\
&\leq \sum_{s=0}^{T} \mathbb{E} \left[ \mathbf{1} \left\{ J_{\tau_{s+1}} = j, \overline{C_{j}(\tau_{s+1}-1)} \right\} \right] \\
&\leq \sum_{s=0}^{T} \mathbb{E} \left[ \mathbf{1} \left\{ \overline{C_{j}(\tau_{s+1}-1)} \right\} \right] \\
&= \sum_{s=0}^{T} \mathbb{P} \left\{ \overline{C_{j}(\tau_{s+1}-1)} \right\} \\
&= \sum_{s=0}^{T} \mathbb{P} \left\{ |\hat{\mu}_{j,s} - \mu_{j}| > \sqrt{\frac{0.5 \ln(T\Delta_{j}^{2})}{s}} \right\} \\
&= O\left( \frac{1}{\Delta_{j}^{2}} \right) \\
&\leq O\left( \frac{1}{\Delta_{j}^{2}} \right) .
\end{aligned}$$
(54)

**Upper bound**  $\omega_2$  (**posterior deviation bound**). We have

$$\omega_{2} = \sum_{t=1}^{T} \mathbb{E} \left[ \mathbf{1} \left\{ J_{t} = j, \overline{\mathcal{E}_{j}'(t)}, C_{j}(t-1), O_{j}(t-1) > L_{j} \right\} \right] \\
= \sum_{t=1}^{T} \mathbb{E} \left[ \mathbf{1} \left\{ C_{j}(t-1), O_{j}(t-1) > L_{j} \right\} \cdot \mathbb{E} \left[ \mathbf{1} \left\{ J_{t} = j, \overline{\mathcal{E}_{j}'(t)} \right\} | \mathcal{F}_{t-1} \right] \right] \\
\leq \sum_{t=1}^{T} \mathbb{E} \left[ \mathbf{1} \left\{ C_{j}(t-1), O_{j}(t-1) > L_{j} \right\} \cdot \mathbb{P} \left\{ \overline{\mathcal{E}_{j}'(t)} | \mathcal{F}_{t-1} \right\} \right] \\
= \sum_{t=1}^{T} \mathbb{E} \left[ \underbrace{\mathbf{1} \left\{ C_{j}(t-1), O_{j}(t-1) > L_{j} \right\} \cdot \underbrace{\mathbb{P} \left\{ \widetilde{\mu}_{j}'(t) > y_{j} | \mathcal{F}_{t-1} \right\} }_{I_{2}}}_{I_{2}} \right] .$$
(55)

Note that the value of  $I_1$  is determined by  $\mathcal{F}_{t-1}$ . Now, we categorize all the possible instantiations  $F_{t-1}$  of  $\mathcal{F}_{t-1}$  into two types. For a particular instantiation  $F_{t-1}$  such that  $I_1 = 0$ , we have I = 0. For any instantiation  $F_{t-1}$  such that  $I_1 = 1$ , i.e.,  $\mathbf{1} \{C_j(t-1), O_j(t-1) > L_j\} = 1$ , we first construct a lower bound on  $y_j$ . From  $O_j(t-1) > L_j = \frac{36 \ln(T\Delta_j^2)}{\Delta_j^2}$ , we know  $\frac{\Delta_j}{2} > 3\sqrt{\frac{\ln(T\Delta_j^2)}{O_j(t-1)}}$ . Then, we have  $y_j = \mu_j + \frac{1}{2}\Delta_j \ge \hat{\mu}_{j,O_j(t-1)} - \sqrt{\frac{0.5 \ln(T\Delta_j^2)}{O_j(t-1)}} + \frac{1}{2}\Delta_j \ge \hat{\mu}_{j,O_j(t-1)} - \sqrt{\frac{0.5 \ln(T\Delta_j^2)}{O_j(t-1)}} + \frac{3\sqrt{\frac{\ln(T\Delta_j^2)}{O_j(t-1)}}}{D_j(t-1)}$ . Then, we have

$$\mathbb{P}\left\{\widetilde{\mu}_{j}'(t) > y_{j} \mid \mathcal{F}_{t-1} = F_{t-1}\right\} = 1 - \mathbb{P}\left\{\widetilde{\mu}_{j}'(t) \leq y_{j} \mid \mathcal{F}_{t-1} = F_{t-1}\right\} = 1 - \left(\int_{\widehat{\mu}_{j,O_{j}(t-1)}}^{y_{j}} \phi\left(x;\widehat{\mu}_{j,O_{j}(t-1)}, \frac{1}{O_{j}(t-1)}\right) dx + 0.5\right) = 1 - \left(0.5 - \int_{y_{j}}^{+\infty} \phi\left(x;\widehat{\mu}_{j,O_{j}(t-1)}, \frac{1}{O_{j}(t-1)}\right) dx + 0.5\right) = \int_{y_{j}}^{+\infty} \phi\left(x;\widehat{\mu}_{j,O_{j}(t-1)}, \frac{1}{O_{j}(t-1)}\right) dx = \mathbb{P}\left\{\widetilde{\mu}_{j}(t) > y_{j} \mid \mathcal{F}_{t-1} = F_{t-1}\right\} = \mathbb{P}\left\{\widetilde{\mu}_{j}(t) - \widehat{\mu}_{j,O_{j}(t-1)} > y_{j} - \widehat{\mu}_{j,O_{j}(t-1)} \mid \mathcal{F}_{t-1} = F_{t-1}\right\}$$

$$\leq \mathbb{P}\left\{\widetilde{\mu}_{j}(t) - \widehat{\mu}_{j,O_{j}(t-1)} > \sqrt{\frac{2\ln(T\Delta_{j}^{2})}{O_{j}(t-1)}} \mid \mathcal{F}_{t-1} = F_{t-1}\right\}$$
Gaussian concentration inequality
$$\leq O\left(\frac{1}{T\Delta_{j}^{2}}\right) ,$$

which gives us  $I \leq O\left(\frac{1}{T\Delta_j^2}\right)$ . The last inequality uses concentration bound of Gaussian distributions shown in Lemma 19. Then, we have  $\omega_2 \leq \sum_{t=1}^T O\left(\frac{1}{T\Delta_j^2}\right) \leq O\left(\frac{1}{\Delta_j^2}\right)$ .

Upper bound  $\omega_1$ . The proof is very similar to the proof for Lemma 2.14 in Agrawal and Goyal [2017]. Let  $L_{1,j} = \left[\frac{288 \ln(T\Delta_j^2 + e^{32})}{\Delta_j^2}\right]$ . Let  $\tau_s$  be the round when the *s*-th pull of arm 1 occurs. The definition of  $\tau_s$  means  $\mathbf{1} \{J_t = 1\} = 0$  for

all  $t \in \{\tau_s + 1, \dots, \tau_{s+1} - 1\}$ . Set  $\tau_0 = 0$ . We have

$$\begin{split} \omega_{1} &= \sum_{t=1}^{I} \mathbb{E} \left[ \mathbf{1} \left\{ J_{t} = j, \mathcal{E}_{j}'(t) \right\} \right] \\ &= \sum_{t=1}^{T} \mathbb{E} \left[ \frac{\mathbb{P} \left\{ J_{t} = j, \mathcal{E}_{j}'(t) \mid \mathcal{F}_{t-1} \right\}}{\mathrm{LHS in Lemma 22}} \right] \\ &\leq \sum_{t=1}^{T} \mathbb{E} \left[ \frac{\mathbb{P} \left\{ \tilde{\mu}_{1}(t) \leq y_{j} \mid \mathcal{F}_{t-1} \right\}}{\mathbb{P} \left\{ \tilde{\mu}_{1}(t) \geq y_{j} \mid \mathcal{F}_{t-1} \right\}} \mathbb{P} \left\{ J_{t} = 1, \mathcal{E}_{j}'(t) \mid \mathcal{F}_{t-1} \right\} \right] \\ &= \sum_{t=1}^{T} \mathbb{E} \left[ \frac{\mathbb{P} \left\{ \tilde{\mu}_{1}(t) \leq y_{j} \mid \mathcal{F}_{t-1} \right\}}{\mathbb{P} \left\{ \tilde{\mu}_{1}(t) \geq y_{j} \mid \mathcal{F}_{t-1} \right\}} \mathbf{1} \left\{ J_{t} = 1, \mathcal{E}_{j}'(t) \right\} \right] \\ &\leq \sum_{s=1}^{T} \mathbb{E} \left[ \sum_{t=\tau_{s}+1}^{T} \mathbb{P} \left\{ \tilde{\mu}_{1}(t) \leq y_{j} \mid \mathcal{F}_{t-1} \right\}} \mathbf{1} \left\{ J_{t} = 1, \mathcal{E}_{j}'(t) \right\} \right] \\ &= \sum_{s=1}^{T} \mathbb{E} \left[ \sum_{t=\tau_{s}+1}^{T} \mathbb{P} \left\{ \tilde{\mu}_{1}(t) \leq y_{j} \mid \mathcal{F}_{t-1} \right\}} \mathbf{1} \left\{ J_{t} = 1, \mathcal{E}_{j}'(t) \right\} \right] \\ &= \sum_{s=1}^{T} \mathbb{E} \left[ \sum_{t=\tau_{s}+1}^{T} \mathbb{P} \left\{ \tilde{\mu}_{1}(t) \leq y_{j} \mid \mathcal{F}_{t-1} \right\}} \mathbf{1} \left\{ J_{t} = 1, \mathcal{E}_{j}'(t) \right\} \right] \\ &= \sum_{s=1}^{T} \mathbb{E} \left[ \mathbb{P} \left\{ \tilde{\mu}_{1}(\tau_{s+1}) \geq y_{j} \mid \mathcal{F}_{r_{s+1}-1} \right\}} \mathbf{1} \left\{ J_{\tau_{s+1}} = 1, \mathcal{E}_{j}'(\tau_{s+1}) \right\} \right] \\ &= \sum_{s=1}^{T} \mathbb{E} \left[ \mathbb{P} \left\{ \tilde{\mu}_{1}(\tau_{s+1}) \geq y_{j} \mid \mathcal{F}_{\tau_{s+1}-1} \right\}} \mathbf{1} \left\{ J_{\tau_{s+1}} = 1, \mathcal{E}_{j}'(\tau_{s+1}) \right\} \right] \\ &= \sum_{s=1}^{T} \mathbb{E} \left[ \mathbb{P} \left\{ \tilde{\mu}_{1}(\tau_{s+1}) \geq y_{j} \mid \mathcal{F}_{\tau_{s+1}-1} \right\}} \mathbf{1} \left\{ J_{\tau_{s+1}} = 1, \mathcal{E}_{j}'(\tau_{s+1}) \right\} \right] \\ &= \sum_{s=1}^{T} \mathbb{E} \left[ \mathbb{P} \left\{ \tilde{\mu}_{1}(\tau_{s+1}) \geq y_{j} \mid \mathcal{F}_{\tau_{s+1}-1} \right\}} \right] \\ &= \sum_{s=1}^{T} \mathbb{E} \left[ \mathbb{P} \left\{ \tilde{\mu}_{1}(\tau_{s+1}) \geq y_{j} \mid \mathcal{F}_{\tau_{s+1}-1} \right\}} \right] \\ &= \sum_{s=1}^{T} \mathbb{E} \left[ \mathbb{P} \left\{ \tilde{\mu}_{1}(\tau_{s+1}) \geq y_{j} \mid \mathcal{F}_{\tau_{s+1}-1} \right\}} \right] \\ &= \sum_{s=1}^{T} \mathbb{E} \left[ \mathbb{P} \left\{ \tilde{\mu}_{1}(\tau_{s+1}) \geq y_{j} \mid \mathcal{F}_{\tau_{s+1}-1} \right\}} \right] \\ &= \sum_{s=1}^{T} \mathbb{E} \left[ \mathbb{E} \left\{ \tilde{\mu}_{1}(\tau_{s+1}) \geq y_{j} \mid \mathcal{F}_{\tau_{s+1}-1} \right\}} \right] \\ &= \sum_{s=1}^{T} \mathbb{E} \left[ \mathbb{E} \left\{ \tilde{\mu}_{1}(\tau_{s+1}) \geq y_{j} \mid \mathcal{F}_{\tau_{s+1}-1} \right\}} \right] \\ &= \sum_{s=1}^{T} \mathbb{E} \left\{ \tilde{\mu}_{1}(\tau_{s+1}) \geq y_{s} \mid \mathcal{F}_{\tau_{s+1}-1} \right\}} \right] \\ &= \sum_{s=1}^{T} \mathbb{E} \left\{ \mathbb{E} \left\{ \tilde{\mu}_{1}(\tau_{s+1}) \geq y_{s} \mid \mathcal{F}_{\tau_{s+1}-1} \right\}} \right\} \\ &= \sum_{s=1}^{T} \mathbb{E} \left\{ \mathbb{E} \left\{ \tilde{\mu}_{1}(\tau_{s+1}) \geq y_{s} \mid \mathcal{F}_{s+1}-1} \right\} \right\} \\ &= \sum_{s=1}^{T} \mathbb{E} \left\{ \mathbb$$

where the last inequality uses Lemma 20.

Now, we plug the upper bounds on  $\omega_1, \omega_2$  and  $\omega_3$  into (53). We have

$$\mathbb{E}\left[O_{j}(T)\right] \leq O\left(\frac{\ln(T\Delta_{j}^{2})}{\Delta_{j}^{2}}\right) + O\left(\frac{\ln\left(T\Delta_{j}^{2} + e^{32}\right)}{\Delta_{j}^{2}}\right) + O\left(\frac{1}{\Delta_{j}^{2}}\right) + O\left(\frac{1}{\Delta_{j}^{2}}\right) \leq O\left(\frac{\ln\left(T\Delta_{j}^{2} + e^{32}\right)}{\Delta_{j}^{2}}\right) \quad , \quad (58)$$
nich gives

which gives

$$\mathcal{R}(T) \leq \sum_{j \in \mathcal{A}: \Delta_j > 0} O\left(\frac{\ln(T\Delta_j^2 + e^{32})}{\Delta_j}\right) \\
\leq \sum_{j \in \mathcal{A}: \Delta_j > 0} O\left(\frac{\ln(T + e^{32})}{\Delta_j}\right) \\
\leq \sum_{j \in \mathcal{A}: \Delta_j > 0} O\left(\frac{\ln(2Te^{32})}{\Delta_j}\right) \\
= \sum_{j \in \mathcal{A}: \Delta_j > 0} O\left(\frac{\ln(T)}{\Delta_j}\right) + O\left(\frac{\ln(2e^{32})}{\Delta_j}\right) \\
= \sum_{j \in \mathcal{A}: \Delta_j > 0} O\left(\frac{\ln(T)}{\Delta_j}\right) ,$$
(59)

which concludes the proof of Theorem 9.

Lemma 20. (Lemma 2.13 in Agrawal and Goyal [2017]). We have

$$\mathbb{E}\left[\frac{\mathbb{P}\left\{\widetilde{\mu}_{1}(\tau_{s+1}) \leq y_{j} \mid \mathcal{F}_{\tau_{s+1}-1}\right\}}{\mathbb{P}\left\{\widetilde{\mu}_{1}(\tau_{s+1}) > y_{j} \mid \mathcal{F}_{\tau_{s+1}-1}\right\}}\right] \leq \begin{cases} e^{64} + 5, & \forall s \\ \frac{5}{T\Delta_{j}^{2}}, & s > L_{1,j} \end{cases}$$
(60)

**Lemma 21.** (Lemma 2.8 in Agrawal and Goyal [2017]). For all t and all instantiations  $F_{t-1}$  of  $\mathcal{F}_{t-1}$ , we have

$$\mathbb{P}\left\{J_{t}=j,\mathcal{E}_{j}'(t) \mid \mathcal{F}_{t-1}=F_{t-1}\right\} \leq \frac{\mathbb{P}\left\{\tilde{\mu}_{1}'(t) \le y_{j} \mid \mathcal{F}_{t-1}=F_{t-1}\right\}}{\mathbb{P}\left\{\tilde{\mu}_{1}'(t) > y_{j} \mid \mathcal{F}_{t-1}=F_{t-1}\right\}} \mathbb{P}\left\{J_{t}=1,\mathcal{E}_{j}'(t) \mid \mathcal{F}_{t-1}=F_{t-1}\right\}$$
(61)

**Lemma 22.** For all t and all instantiations  $F_{t-1}$  of  $\mathcal{F}_{t-1}$ , we have

$$\mathbb{P}\left\{J_{t}=j,\mathcal{E}_{j}'(t) \mid \mathcal{F}_{t-1}=F_{t-1}\right\} \leq \frac{\mathbb{P}\{\tilde{\mu}_{1}(t)\leq y_{j}|\mathcal{F}_{t-1}=F_{t-1}\}}{\mathbb{P}\{\tilde{\mu}_{1}(t)>y_{j}|\mathcal{F}_{t-1}=F_{t-1}\}} \mathbb{P}\left\{J_{t}=1,\mathcal{E}_{j}'(t) \mid \mathcal{F}_{t-1}=F_{t-1}\right\} .$$
(62)

Proof of Lemma 22. From Lemma 21, we have

$$\mathbb{P}\left\{J_{t}=j,\mathcal{E}_{j}'(t) \mid \mathcal{F}_{t-1}=F_{t-1}\right\} \leq \frac{\mathbb{P}\left\{\tilde{\mu}_{1}'(t) \le y_{j} \mid \mathcal{F}_{t-1}=F_{t-1}\right\}}{\mathbb{P}\left\{\tilde{\mu}_{1}'(t) > y_{j} \mid \mathcal{F}_{t-1}=F_{t-1}\right\}} \mathbb{P}\left\{J_{t}=1,\mathcal{E}_{j}'(t) \mid \mathcal{F}_{t-1}=F_{t-1}\right\}$$
(63)

Now, we construct a lower bound for  $\mathbb{P}\left\{\widetilde{\mu}'_1(t) > y_j \mid \mathcal{F}_{t-1} = F_{t-1}\right\}$  to complete the proof. We have

$$\mathbb{P} \left\{ \widetilde{\mu}'_{1}(t) > y_{j} \mid \mathcal{F}_{t-1} = F_{t-1} \right\}$$

$$= \mathbb{P} \left\{ \max \left\{ \widetilde{\mu}_{1}(t), \widehat{\mu}_{1,O_{1}(t-1)} \right\} > y_{j} \mid \mathcal{F}_{t-1} = F_{t-1} \right\}$$

$$\geq \mathbb{P} \left\{ \widetilde{\mu}_{1}(t) > y_{j} \mid \mathcal{F}_{t-1} = F_{t-1} \right\} ,$$

$$(64)$$

which implies

$$\frac{\mathbb{P}\left\{\tilde{\mu}_{1}'(t) \leq y_{j} | \mathcal{F}_{t-1} = F_{t-1}\right\}}{\mathbb{P}\left\{\tilde{\mu}_{1}'(t) > y_{j} | \mathcal{F}_{t-1} = F_{t-1}\right\}} \leq \frac{\mathbb{P}\left\{\tilde{\mu}_{1}(t) \leq y_{j} | \mathcal{F}_{t-1} = F_{t-1}\right\}}{\mathbb{P}\left\{\tilde{\mu}_{1}(t) > y_{j} | \mathcal{F}_{t-1} = F_{t-1}\right\}}$$
(65)

# E PROOFS FOR THEOREM 10

*Proof of Theorem 10.* Set  $\Delta = \sqrt{\frac{A \ln(A)}{T}}$ . Let set  $\Phi = \{j \in \mathcal{A} : 0 < \Delta_j < \Delta\}$  collect all the arms with the mean reward gap smaller than  $\Delta$ . Let  $\overline{\Phi} = \{j \in \mathcal{A} : \Delta_j \ge \Delta\}$ . Then, we have

$$\begin{aligned} \mathcal{R}(T) &= \sum_{t=1}^{T} \mathbb{E}\left[\mu_{1} - \mu_{J_{t}}\right] \\ &= \sum_{t=1}^{T} \mathbb{E}\left[\left(\mu_{1} - \mu_{J_{t}}\right) \mathbf{1}\left\{J_{t} \in \Phi\right\}\right] + \sum_{t=1}^{T} \mathbb{E}\left[\left(\mu_{1} - \mu_{J_{t}}\right) \mathbf{1}\left\{J_{t} \in \overline{\Phi}\right\}\right] \\ &\leq T \cdot \Delta + \sum_{j \in \mathcal{A}: \Delta_{j} \geq \Delta} \sum_{t=1}^{T} \mathbb{E}\left[\mathbf{1}\left\{J_{t} = j\right\}\right] \cdot \Delta_{j} \\ &\leq^{(a)} T \cdot \Delta + \sum_{j \in \mathcal{A}: \Delta_{j} \geq \Delta} O\left(\frac{\ln(T\Delta_{j}^{2} + e^{32})}{\Delta_{j}}\right) \\ &\leq^{(b)} T \cdot \Delta + \sum_{j \in \mathcal{A}: \Delta_{j} \geq \Delta} O\left(\frac{\ln(T\Delta_{j}^{2} + e^{32})}{\Delta_{j}}\right) \\ &= T \cdot \Delta + \sum_{j \in \mathcal{A}: \Delta_{j} \geq \Delta} O\left(\frac{\ln(T\Delta_{j}^{2} + e^{32})}{\Delta_{j}}\right) + \sum_{j \in \mathcal{A}: \Delta_{j} \geq \Delta} O\left(\frac{\ln(2 \cdot e^{30})}{\Delta_{j}}\right) \\ &\leq^{(c)} T \cdot \Delta + \sum_{j \in \mathcal{A}: \Delta_{j} \geq \Delta} O\left(\frac{\ln(T\Delta^{2} e^{2})}{\Delta}\right) + \sum_{j \in \mathcal{A}: \Delta_{j} \geq \Delta} O\left(\frac{\ln(2 \cdot e^{30})}{\Delta}\right) \\ &\leq T \cdot \Delta + A \cdot O\left(\frac{\ln(T\Delta^{2} e^{2})}{\sqrt{\frac{\Delta \ln(\Delta)}{\Delta}}}\right) + A \cdot O\left(\frac{\ln(2 \cdot e^{30})}{\sqrt{\frac{\Delta \ln(\Delta)}{\Delta}}}\right) \\ &\leq^{(d)} T \cdot \Delta + A \cdot O\left(\frac{\ln(A^{2} \cdot e^{2})}{\sqrt{\frac{\Delta \ln(\Delta)}{T}}}\right) + O\left(\sqrt{AT}\right) \\ &= T \cdot \Delta + A \cdot O\left(\frac{\ln(A^{2} \cdot e^{2})}{\sqrt{\frac{\Delta \ln(\Delta)}{T}}}\right) + A \cdot O\left(\frac{\ln(e^{2})}{\sqrt{\frac{\Delta \ln(\Delta)}{T}}}\right) + O\left(\sqrt{AT}\right) \\ &\leq \sqrt{AT \ln(A)} + O\left(\sqrt{AT \ln(A)}\right) + O\left(\sqrt{AT \ln(A)}\right) + O\left(\sqrt{AT}\right) + O\left(\sqrt{AT}\right) \\ &= O\left(\sqrt{AT \ln(A)}\right) \quad , \end{aligned}$$

which concludes the proof.

Inequality (a) uses (58) and Inequality (b) uses the fact that  $x + y \le 2xy$  when x, y > 1. Inequality (c) uses the fact that  $f(x) = \frac{\ln(Tx^2e^2)}{x}$  is a decreasing function when  $x > \sqrt{\frac{1}{T}}$ . Inequality (d) uses the fact that  $\ln(x) \le x$  when x > 1.

# F PROOFS FOR THEOREM 11

*Proof of Theorem 11.* Since O-TS-Bandit<sup>+</sup> is an optimistic learning algorithm, the regret analysis can be very similar to the proofs for UCB1 policy of Auer et al. [2002]. Regret can be expressed as

$$\mathcal{R}(T) = \sum_{t=1}^{T} \mathbb{E}\left[\mu_1 - \mu_{J_t}\right] = \sum_{j \in \mathcal{A}: \Delta_j > 0} \underbrace{\sum_{t=1}^{T} \mathbb{E}\left[\mathbf{1}\left\{J_t = j\right\}\right]}_{\mathbb{E}[O_j(T)]} \cdot \Delta_j \quad .$$
(67)

Now, for a fixed sub-optimal arm j, we let  $L_j = \frac{25 \ln(T)}{\Delta_j^2}$ . Then, we do the following decomposition. We have

$$\mathbb{E}[O_{j}(T)] = \sum_{t=1}^{T} \mathbb{E}[\mathbf{1}\{J_{t}=j\}] \\
\leq L_{j} + \sum_{t=1}^{T} \mathbb{E}[\mathbf{1}\{J_{t}=j, O_{j}(t-1) \ge L_{j}\}] \\
\leq L_{j} + \sum_{t=1}^{T} \mathbb{E}\left[\mathbf{1}\{\tilde{\mu}_{j}'(t) \ge \tilde{\mu}_{1}'(t), O_{j}(t-1) \ge L_{j}\}\right] \\
\leq L_{j} + \sum_{t=1}^{T} \mathbb{E}\left[\mathbf{1}\{\tilde{\mu}_{1}'(t) \le \mu_{1}\}\right] + \sum_{t=1}^{T} \mathbb{E}\left[\mathbf{1}\{\tilde{\mu}_{j}'(t) \ge \mu_{j} + \sqrt{\frac{24\ln(t)}{O_{j}(t-1)}}, O_{j}(t-1) \ge L_{j}\}\right] \\
+ \sum_{t=1}^{T} \mathbb{E}\left[\mathbf{1}\left\{\sqrt{\frac{24\ln(t)}{O_{j}(t-1)}} > \Delta_{j}, O_{j}(t-1) \ge L_{j}\right\}\right] \\ = 0$$
(68)

Under-estimation of the optimal arm. We have

$$\begin{aligned}
\omega_{1} &= \sum_{t=1}^{T} \mathbb{E} \left[ \mathbf{1} \left\{ \widetilde{\mu}_{1}'(t) \leq \mu_{1} \right\} \right] \\
&\leq \sum_{t=1}^{T} \mathbb{E} \left[ \mathbf{1} \left\{ \overline{\mu}_{1}(t) \leq \mu_{1} \right\} \right] \\
&= \sum_{t=1}^{T} \mathbb{E} \left[ \mathbf{1} \left\{ \widehat{\mu}_{1,O_{1}(t-1)} + \sqrt{\frac{1.5 \ln(t)}{O_{1}(t-1)}} \leq \mu_{1} \right\} \right] \\
&\leq \sum_{t=1}^{T} \sum_{s=1}^{t-1} \mathbb{E} \left[ \mathbf{1} \left\{ \widehat{\mu}_{1,s} + \sqrt{\frac{1.5 \ln(t)}{s}} \leq \mu_{1} \right\} \right] \\
&= \sum_{t=1}^{T} \sum_{s=1}^{t-1} \mathbb{P} \left\{ \widehat{\mu}_{1,s} + \sqrt{\frac{1.5 \ln(t)}{s}} \leq \mu_{1} \right\} \\
&\leq \sum_{t=1}^{T} \sum_{s=1}^{t-1} O\left( \frac{1}{t^{3}} \right) \\
&\leq O(1) \quad .
\end{aligned}$$
(69)

**Over-estimation of the sub-optimal arm.** Define event  $\mathcal{E}_j(t) := \left\{ \left| \widehat{\mu}_{j,O_j(t-1)} - \mu_j \right| \le \sqrt{\frac{1.5 \ln(t)}{O_j(t-1)}} \right\}$ . Let  $\mathcal{F}_{t-1}$  collect all the history information by the end of round t-1. Then, we have

$$\begin{split} \omega_{2} &= \sum_{t=1}^{T} \mathbb{E} \left[ \mathbf{1} \left\{ \widetilde{\mu}_{j}'(t) \ge \mu_{j} + \sqrt{\frac{24\ln(t)}{O_{j}(t-1)}}, O_{j}(t-1) \ge L_{j} \right\} \right] \\ &= \sum_{t=1}^{T} \mathbb{E} \left[ \mathbf{1} \left\{ \widetilde{\mu}_{j}'(t) - \overline{\mu}_{j}(t) \ge \mu_{j} + \sqrt{\frac{24\ln(t)}{O_{j}(t-1)}} - \overline{\mu}_{j}(t), O_{j}(t-1) \ge L_{j}, \mathcal{E}_{j}(t) \right\} \right] \\ &\leq \sum_{t=1}^{T} \mathbb{E} \left[ \mathbf{1} \left\{ \widetilde{\mu}_{j}'(t) - \overline{\mu}_{j}(t) \ge \mu_{j} + \sqrt{\frac{24\ln(t)}{O_{j}(t-1)}} - \overline{\mu}_{j}(t), O_{j}(t-1) \ge L_{j}, \mathcal{E}_{j}(t) \right\} \right] \\ &= \sum_{t=1}^{T} \mathbb{E} \left[ \mathbf{1} \left\{ \widetilde{\mu}_{j}'(t) - \overline{\mu}_{j}(t) \ge \mu_{j} + \sqrt{\frac{24\ln(t)}{O_{j}(t-1)}} - \left( \sqrt{\frac{1.5\ln(t)}{O_{j}(t-1)}} + \widehat{\mu}_{j,O_{j}(t-1)} \right), O_{j}(t-1) \ge L_{j}, \mathcal{E}_{j}(t) \right\} \right] \\ &= \sum_{t=1}^{T} \mathbb{E} \left[ \mathbf{1} \left\{ \widetilde{\mu}_{j}'(t) - \overline{\mu}_{j}(t) \ge \sqrt{\frac{24\ln(t)}{O_{j}(t-1)}} - 2\sqrt{\frac{1.5\ln(t)}{O_{j}(t-1)}}, O_{j}(t-1) \ge L_{j} \right\} \right] + \sum_{t=1}^{T} \mathbb{E} \left[ \mathbf{1} \left\{ \overline{\mathcal{E}_{j}(t)} \right\} \right] \\ &= \sum_{t=1}^{T} \mathbb{E} \left[ \mathbf{1} \left\{ \widetilde{\mu}_{j}'(t) - \overline{\mu}_{j}(t) \ge \sqrt{\frac{6\ln(t)}{O_{j}(t-1)}}} \right\} \right] + \sum_{t=1}^{T} \mathbb{E} \left[ \mathbf{1} \left\{ \overline{\mathcal{E}_{j}(t)} \right\} \right] \\ &= \sum_{t=1}^{T} \mathbb{E} \left[ \mathbf{1} \left\{ \widetilde{\mu}_{j}'(t) - \overline{\mu}_{j}(t) \ge \sqrt{\frac{6\ln(t)}{O_{j}(t-1)}}} \right] + \mathcal{F}_{t=1}^{T} \mathbb{E} \left[ \mathbf{1} \left\{ \overline{\mathcal{E}_{j}(t)} \right\} \right] \\ &= \sum_{t=1}^{T} \mathbb{E} \left[ \mathbb{E} \left\{ \widetilde{\mu}_{j}'(t) - \overline{\mu}_{j}(t) \ge \sqrt{\frac{6\ln(t)}{O_{j}(t-1)}}} \right] + \mathcal{F}_{t=1}^{T} \mathbb{E} \left[ \mathbf{1} \left\{ \overline{\mathcal{E}_{j}(t)} \right\} \right] \\ &= \sum_{t=1}^{T} \mathbb{E} \left[ \mathbb{E} \left\{ \widetilde{\mu}_{j}'(t) - \overline{\mu}_{j}(t) \ge \sqrt{\frac{6\ln(t)}{O_{j}(t-1)}} \right] + \mathcal{F}_{t=1}^{T} \mathbb{E} \left[ \mathbf{1} \left\{ \overline{\mathcal{E}_{j}(t)} \right\} \right] \\ &= O(1) \\ &= \sum_{t=1}^{T} \mathbb{E} \left[ \mathbb{E} \left\{ \widetilde{\mu}_{j}'(t) \ge \overline{\mu}_{j}(t) + \sqrt{\frac{6\ln(t)}{O_{j}(t-1)}} \right] + \mathcal{F}_{t-1} \right\} \right] + O(1) \\ &\leq O(1) \quad , \tag{70}$$

where the second last inequality uses concentration bound for Gaussian distributions and

$$\sum_{t=1}^{T} \mathbb{E}\left[\mathbf{1}\left\{\overline{\mathcal{E}_{j}(t)}\right\}\right] = \sum_{t=1}^{T} \mathbb{P}\left\{\left|\widehat{\mu}_{j,O_{j}(t-1)} - \mu_{j}\right| > \sqrt{\frac{1.5\ln(t)}{O_{j}(t-1)}}\right\} \le \sum_{t=1}^{T} \sum_{s=1}^{t-1} \mathbb{P}\left\{\left|\widehat{\mu}_{j,s} - \mu_{j}\right| > \sqrt{\frac{1.5\ln(t)}{s}}\right\} \le O(1).$$

Then, we have

$$\mathcal{R}(T) = \sum_{j \in \mathcal{A}: \Delta_j > 0} \underbrace{\sum_{t=1}^{T} \mathbb{E} \left[ \mathbf{1} \left\{ J_t = j \right\} \right] \cdot \Delta_j}_{\mathbb{E}[O_j(T)]}$$

$$\leq \sum_{\substack{j \in \mathcal{A}: \Delta_j > 0 \\ j \in \mathcal{A}: \Delta_j > 0}} O\left( \frac{\ln(T)}{\Delta_j} \right) , \qquad (71)$$

which concludes the proof.

## G PROOFS FOR THEOREM 12

*Proof of Theorem 12.* Set  $\Delta = \sqrt{\frac{A \ln(T)}{T}}$ . Let set  $\Phi = \{j \in \mathcal{A} : 0 < \Delta_j < \Delta\}$  collect all the arms with the mean reward gap smaller than  $\Delta$ . Let  $\overline{\Phi} = \{j \in \mathcal{A} : \Delta_j \ge \Delta\}$ . Then, we have

$$\mathcal{R}(T) = \sum_{t=1}^{T} \mathbb{E} \left[ \mu_1 - \mu_{J_t} \right]$$

$$= \sum_{t=1}^{T} \mathbb{E} \left[ (\mu_1 - \mu_{J_t}) \mathbf{1} \{ J_t \in \Phi \} \right] + \sum_{t=1}^{T} \mathbb{E} \left[ (\mu_1 - \mu_{J_t}) \mathbf{1} \{ J_t \in \overline{\Phi} \} \right]$$

$$\leq T \cdot \Delta + \sum_{j \in \mathcal{A}: \Delta_j \ge \Delta} \sum_{t=1}^{T} \mathbb{E} \left[ \mathbf{1} \{ J_t = j \} \right] \cdot \Delta_j$$

$$\leq T \cdot \Delta + \sum_{j \in \mathcal{A}: \Delta_j \ge \Delta} O\left(\frac{\ln(T)}{\Delta_j}\right)$$

$$\leq \sqrt{AT \ln(T)} + O\left(\frac{A \ln(T)}{\Delta}\right)$$

$$= O\left(\sqrt{AT \ln(T)}\right) ,$$
(72)

which concludes the proof.

### H ADDITIONAL EXPERIMENTAL RESULTS

We run additional experiments with different random seeds and state size S = [5, 20, 50], action size A = 3 and H = 10. We use the same way as described in Section 5 to generate the underlying parameters of the MDPs. All experimental results share similar trends. We also include the performance of UCB based method UCB-VI here. From Figure 4, 5 and 6, we can see that SSR-Bernstein still performs the best. All three Thompson Sampling-like algorithms perform similarly and better than UCB-VI.

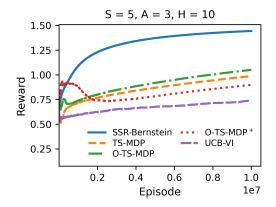


Figure 4: Empirical performance for 5 states, including UCB-VI

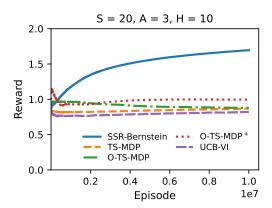


Figure 5: Empirical performance for 20 states, including UCB-VI

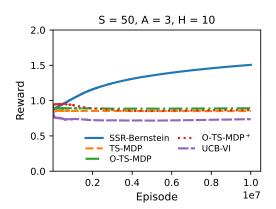


Figure 6: Empirical performance for 50 states, including UCB-VI