INSTANCE-DEPENDENT FIXED-BUDGET PURE EXPLORATION IN REINFORCEMENT LEARNING

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Paper under double-blind review

ABSTRACT

We study the problem of fixed budget pure exploration in reinforcement learning. The goal is to identify a near-optimal policy, given a fixed budget on the number of interactions with the environment. Unlike the standard PAC setting, we do not require the target error level ε and failure rate δ as input. We propose novel algorithms and provide, to the best of our knowledge, the first instance-dependent ε-uniform guarantee, meaning that the probability that ε-correctness is ensured can be obtained simultaneously for all ε above a budget-dependent threshold. It characterizes the budget requirements in terms of the problem-specific hardness of exploration. As a core component of our analysis, we derive a ε-uniform guarantee for the multiple bandit problem—solving multiple multi-armed bandit instances simultaneously—which may be of independent interest. To enable our analysis, we also develop tools for reward-free exploration under the fixed-budget setting, which we believe will be useful for future work.

1 INTRODUCTION

Reinforcement Learning (RL) theory Agarwal et al. (2019) has been studied under two main objectives: regret minimization and policy identification, also known as pure exploration. While the former focuses on maximizing cumulative reward during learning, the latter aims to identify a near-optimal policy without concern for rewards gained during learning. A substantial body of work on policy identification has focused on the fixed-confidence setting Kearns and Singh (2002). This line of research, often referred to as Probably Approximately Correct (PAC) RL, requires the algorithm to spend as many samples as possible until it can find an ε-optimal policy with probability at least $1 - \delta$. Specifically, the algorithm is required to *verify* itself that the returned arm is indeed ε-optimal policy – otherwise, it is not a fixed confidence algorithm. Due to the verification requirement, both ε and δ are input to the algorithm. Thus, the analysis must be done for the correctness of the *verification* (i.e., proving that the returned arm is indeed an ε-optimal policy) as well as the sample complexity (i.e., proving how many samples are taken before stopping).

However, the fixed-confidence setting is not the only way to perform policy identification. The fixed-budget setting has been popular in multi-armed bandits (Even-Dar et al., 2006; Bubeck et al., 2009). In this setting, the learner is given a fixed number of interactions with the environment as a budget and is required to output a good policy after exhausting the budget. This setting has numerous merits. First, this setting is arguably more practical because the user of the algorithm can control the budget explicitly. In contrast, the fixed confidence setting assumes that the algorithm can use as many samples as possible (though less is preferred). When stopped forcefully to satisfy practical constraints, it is hard to guarantee the quality of the returned policy. Second, the fixed budget setting has potential to guarantee a better sample complexity because there is no verification requirement (i.e., the algorithm itself certifies that the returned policy is ε-optimal). This was true for multi-armed bandits where instant-dependent accelerated rates can be obtained as a function of how many good arms there are, and also a data-poor regime guarantee can be obtained, meaning that where a nontrivial performance guarantee is obtained even if the sampling budget is smaller than the number of arms, depending on the problem instance Zhao et al. (2023). These bounds are not likely to be obtained in the fixed confidence setting due to the verification requirement unless extra knowledge about the best arm is known such as Chaudhuri and Kalyanakrishnan (2017). While the ε-correctness verification from the fixed-confidence setting can be necessary in mission-critical applications, there are many

applications that do not require such a guarantee, in which case the parameters ε and δ becomes a cumbersome hyperparameter.

Despite the desirable properties of the fixed-budget setting in bandit problems, its counterpart in MDPs remains largely unexplored to our knowledge. In this paper, we take the first step at studying fixed-budget policy identification in MDPs, providing new theoretical insights and algorithms that bridge this gap. Specifically, a fixed budget algorithm is required to take in a episode budget B and return a policy $\hat{\pi}$ at the end of B-th episode. Our central interest is to upper bound the probability that the algorithm fails to return an ε-optimal policy as an exponentially decaying function of the budget B and instance-dependent quantities, *simultaneously for all* $\varepsilon \geq \varepsilon'$ for some budget dependent threshold ε'. We refer to this type of theoretical guarantee as an *ε-uniform guarantee*. In other words, the degree of suboptimality of the learned policy $\hat{\pi}$ is a random variable, and we are characterizing its distribution, in particular its tail behavior.

Contributions. Our main contributions are as follows:

- We propose a novel algorithm, **BREA** (Backward Reachability Estimation and Action elimination), which is, to the best of our knowledge, the first fixed-budget pure exploration algorithm for episodic MDPs with instance-dependent ε-uniform guarantees. The algorithm only requires the episode budget B as an input, and does not assume the uniqueness of the optimal action.
- For the first time, we establish an ε-uniform guarantee for the SAR algorithm (Bubeck et al., 2013) for the muliple bandit problem. This may be of independent interest.
- We develop algorithmic and analytical tools for fixed-budget reward-free exploration by carefully adapting a fixed-confidence reward-free exploration algorithm, L2E (Wagenmaker et al., 2022), to the fixed-budget setting. We prove an ε-uniform guarantee for our fixed-budget reward-free algorithms.

2 PRELIMINARIES

Finite-horizon MDP. We consider a finite-horizon non-stationary Markov Decision Process (MDP) defined by the tuple $\mathcal{M} = (\mathcal{S}, \mathcal{A}, H, \{P_h\}_{h=0}^{H-1}, \{R_h\}_{h=1}^{H})$, where $\mathcal{S}$ is a finite set of states of size S, $\mathcal{A}$ is a finite set of actions of size A, $H \in \mathbb{N}$ is the horizon, $P_0 \in \Delta(\mathcal{S})$ is the initial distribution, $P_h : \mathcal{S} \times \mathcal{A} \to \Delta(\mathcal{S})$ is the transition kernel, and $R_h : \mathcal{S} \times \mathcal{A} \to \Delta([0,1])$ is the random rewards with $\mathbb{E}[R_h(s,a)] = r_h(s,a)$. $\{P_h\}_{h=0}^{H-1}$ and $\{R_h\}_{h=1}^{H}$ are unknown to the learner.

The initial state s_1 is drawn from the initial distribution P_0. At each step h, taking action a_h in state s_h results in a next state s_{h+1} sampled from the transition kernel $P_h(\cdot \mid s_h, a_h)$. A trajectory $\{(s_h, a_h, R_h(s_h, a_h))\}_{h=1}^{H}$ is called an *episode*, and when the learner reaches the end of the episode, a new episode begins.

A *policy* $\pi = (\pi_1, \ldots, \pi_H)$ is a sequence of decision rules $\pi_h : \mathcal{S} \to \Delta(\mathcal{A})$ for each step $h \in [H]$. The Q-value function of a policy π at step $h \in [H]$ is defined as

$$Q_h^\pi(s,a) := \mathbb{E}_\pi[\sum_{h'=h}^{H} R_{h'}(s_{h'}, a_{h'}) | s_h = s, a_h = a]$$

and it represents the expected reward obtained by choosing action a in state s at step h and choosing the subsequent actions according to the policy π. The value function of π at step h is defined as

$$V_h^\pi(s) = \mathbb{E}_\pi[Q_h^\pi(s, \pi_h(s))]$$

and it represents the expected reward obtained by choosing actions according to the policy π starting in state s at step h. We also define $V_0^\pi := \mathbb{E}_{s\sim P_0}[V_1^\pi(s)]$. The optimal Q-value function, optimal value function are defined as

$$Q_h^*(s,a) = \sup_\pi Q_h^\pi(s,a), \quad V_h^*(s) = \sup_\pi V_h^\pi(s), \quad V_0^* = \sup_\pi V_0^\pi.$$

Throughout the paper, we do not assume that the optimal action or policy is unique.

Pure exploration under the fixed budget setting. In pure exploration under the fixed budget setting, the goal is to identify an optimal policy π^* (or near-optimal) based on a limited interaction budget. Specifically, the learner is allowed to execute a total of B episodes and must return a single policy $\hat{\pi}$ at the end. The performance is measured by the simple regret, which is defined as

$$V_0^* - V_0^{\hat{\pi}}.$$

A policy $\hat{\pi}$ is called *ε-good* if $V_0^* - V_0^{\hat{\pi}} \leq \varepsilon$. In this paper, we propose an algorithm and prove their performance guarantee by showing some instance-dependent upper bounds of the failure probability

$$\mathbb{P}(V_0^* - V_0^{\hat{\pi}} > \varepsilon).$$

Instance-dependent quantities. To capture the instance-dependent complexity of the problem, we need the notion of *suboptimality gaps* defined as

$$\Delta_h(s,a) := V_h^*(s) - Q_h^*(s,a),$$
$$\Delta_h^\pi(s,a) := \max_{a'} Q_h^\pi(s,a') - Q_h^\pi(s,a).$$

For our analysis, we also denote

$$\bar{\Delta}_h(s,a) := \begin{cases} \Delta_h(s,a), & \text{if } Q_h^*(s,a) < V_h^*(s) \\ \Delta_h(s,a'), & \text{if } Q_h^*(s,a) = V_h^* \text{ and } a' \text{ is the second best action,} \end{cases}$$

$$\bar{\Delta}_h^\pi(s,a) := \begin{cases} \Delta_h^\pi(s,a), & \text{if } Q_h^\pi(s,a) < \max_{a'} Q_h^\pi(s,a') \\ \Delta_h^\pi(s,\tilde{a}), & \text{if } Q_h^\pi(s,a) = \max_{a'} Q_h^\pi(s,a') \text{ and } \tilde{a} \text{ is the second best action with respect to } \pi. \end{cases}$$

Thus, if the optimal action in $s \in \mathcal{S}$ at step h is unique, $\bar{\Delta}_h(s,a) > 0$ for all $a \in \mathcal{A}$. In contrast, if there are multiple optimal actions in $s \in \mathcal{S}$ at step h, $\bar{\Delta}_h(s,a) = 0$ for all optimal actions a. Similar results hold for $\bar{\Delta}_h(s,a)$ as well.

In MDP, the probability of reaching each state or action is important. Let π be a policy, $s \in \mathcal{S}, a \in \mathcal{A}, h \in [H], \mathcal{Z} \subset \mathcal{S} \times \mathcal{A}$, we use the following notations:

$$w_h^\pi(s) = \mathbb{P}_\pi[s_h = s], \qquad w_h^\pi(s,a) = \mathbb{P}_\pi[s_h = s, a_h = a], \qquad w_h^\pi(\mathcal{Z}) = \mathbb{P}_\pi[(s_h, a_h) \in \mathcal{Z}],$$
$$W_h(s) = \sup_\pi w_h^\pi(s) = \sup_\pi w_h^\pi(s,a), \qquad W_h(\mathcal{Z}) = \sup_\pi w_h^\pi(\mathcal{Z}).$$

We refer to $w_h^\pi(\cdot)$ as the *occupancy measure* and $W_h(\cdot)$ as the *reachability*. Using these notions, we define the *controllability* of MDP at step h as

$$C_h := \sup_\pi \sum_{s, W_h(s) > 0} \frac{w_h^\pi(s)}{W_h(s)}.$$

Then, we have

$$1 = \sup_\pi \sum_{s, W_h(s) > 0} w_h^\pi(s) \leq C_h = \sup_\pi \sum_{s, W_h(s) > 0} \frac{w_h^\pi(s)}{W_h(s)} \leq \sum_{s, W_h(s) > 0} \sup_\pi \frac{w_h^\pi(s)}{W_h(s)} \leq S.$$

We can see that $C_h = 1$ if $W_h(s) = 0$ or 1 for any state s i.e. the learner can reach $s_h = s$ with probability 1 by some policy for any reachable state s. On the other hand, $C_h = S$ if $w_h^\pi(s) = W_h(s) > 0$ for any state $s \in \mathcal{S}$, any policy π i.e. the learner cannot control the occupancy measure by varying policy and all states are reachable. Therefore, intuitively, a larger C_h indicates that the MDP is more difficult to control at step h.

3 THE BREA ALGORITHM

There are inherent difficulties in achieving instance-dependent ε-uniform guarantee for fixed budget setting. First, while it is relatively straightforward to analyze algorithms in the fixed confidence setting using concentration bounds such as Hoeffding or Bernstein bound with a prespecified confidence level δ, it is much more challenging in the fixed budget setting, where neither the confidence level δ nor the accuracy level ε is known in advance. Second, whereas the fixed-confidence setting typically

allows for a potentially excessive number of samples before termination (depending on the confidence level), the fixed-budget setting strictly limits the algorithm to a finite number of samples. Third, it is hard to simply convert the fixed-confidence algorithms since it requires the knowledge of nontrivial instance-dependent terms. Even if it is possible, the conversion of fixed-confidence algorithm would require not only the budget B but also one of the confidence δ and the accuracy ε. Also, theoretical guarantee of this conversion would only applies to prespecified ε (or δ), which is much weaker than ε-uniform guarantee. In this section, we present how we design and analyze our algorithm to overcome the aforementioned difficulties.

At step h, each state s can be treated as a bandit problem, where the expected reward of each action a is given by $Q_h^*(s,a)$. If we aim to learn the exact optimal policy maximizing $Q_h^*(s,a)$, we need to sample trajectories $s_{h+1}, a_{h+1}, \ldots, s_H, a_H$ generated under the optimal policy $\{\pi^*_{h'}\}_{h'=h+1}^H$, which is unknown. Fortunately, since our goal is to learn an approximately optimal policy, the following proposition shows that it suffices to use a suitably accurate policy $\{\hat{\pi}_{h'}\}_{h'=h+1}^H$ for sampling in order to learn $\hat{\pi}_h$.

Proposition 1. *(Wagenmaker et al., 2022, Lemma B.1) Assume that some deterministic policy $\hat{\pi}$ satisfies $\Delta_h^{\hat{\pi}}(s, \hat{\pi}_h(s)) \le \varepsilon_h(s)$ for any $h' \le h \le H$ and any $s \in \mathcal{S}$. Then, for any policy π',*

$$\sum_s w_{h'}^{\pi'}(s) \left(V_{h'}^*(s) - V_{h'}^{\hat{\pi}}(s) \right) \le \sum_{h=h'}^{H} \sup_{\pi} \sum_s w_h^{\pi}(s) \varepsilon_h(s).$$

Note that $\Delta_h^{\hat{\pi}}(s,a)$ depends only on the future policies $\{\hat{\pi}_{h'}\}_{h'=h+1}^H$, implying that we must determine them before learning $\hat{\pi}_h(s)$. By this observation, our learning proceeds backward from H to 1.

If we assume that the hypothesis of the previous proposition holds with $h' = 1$ and $\varepsilon_h(s) := \frac{\varepsilon}{C_h H W_h(s)}$, then the proposition says

$$\begin{aligned} V_0^* - V_0^{\hat{\pi}} &\le \sum_{h=1}^{H} \sup_{\pi} \sum_s w_h^{\pi}(s) \varepsilon_h(s) \\ &= \sum_{h=1}^{H} \sup_{\pi} \sum_s w_h^{\pi}(s) \frac{\varepsilon}{C_h H W_h(s)} \\ &= \sum_{h=1}^{H} \frac{\varepsilon}{H} && \text{(definition of } C_h\text{)} \\ &= \varepsilon. \end{aligned}$$

Therefore, we design our algorithm to identify a $\Theta(\frac{\varepsilon}{C_h H W_h(s)})$-good action for each relevant state s. The precise definition of "relevant state" will be given in the analysis. We again emphasize that ε is not an input to our algorithm and can be chosen arbitrarily for the purpose of analysis. Our algorithm consists of two key components: estimating the reachability $W_h(s)$ and eliminating actions. We introduce the following notation, which will be used in the statements of upcoming results.

$$\varepsilon_B := (1 + \frac{\log(2) B}{c(B)})^{-0.6321}$$

denotes an error threshold that depends on the budget B. The factor

$$C_{\mathrm{L2E}}(B) = \tilde{O}(\mathrm{poly}(S, A, H)),$$

is formally defined in Appendix C, equation 5. We denote $C_{\mathrm{L2E}}(B) = SH^2 c(B)$.

3.1 Reachability estimation

The first part of our algorithm is greatly influenced by Wagenmaker et al. (2022). Through the first part, we estimate the reachability $W_h(s)$ of each state s at step h. To this end, we execute a fixed-budget reward-free exploration. One notable benefit of reward-free exploration is that it only needs to be run once, after which the collected data can be applied to a variety of downstream reward

Algorithm 1 **F**ixed **B**udget **L**earn to **E**xplore (FB-L2E)

function FB-L2E($\mathcal{X} \subseteq \mathcal{S} \times \mathcal{A}$, step h, budget B)
  if $|\mathcal{X}| = 0$ **then**
    return $\{(\emptyset, \emptyset, 0)\}$
  end if
  $J \leftarrow \lceil 0.6321 \log_2(1 + \frac{\log(2)B}{c(B)}) \rceil$ ($c(B)$ is defined in Appendix C)
  for $j = 1$ to J **do**
    $L_j \leftarrow 2^{J-j}, \quad \delta_j \leftarrow (\frac{1}{8SAH})^{0.6321 L_j \log\log(8SAH)}$
    $K_j \leftarrow K_j(\delta_j, SAH\delta_j)$ (K_j is defined in Appendix C)
    $N_j \leftarrow K_j / (4|\mathcal{X}| \cdot 2^j)$
    $(\mathcal{X}_j, \Pi_j) \leftarrow$ FINDEXPLORABLESETS($\mathcal{X}, h, \delta, K_j, N_j$)
    $\mathcal{X} \leftarrow \mathcal{X} \setminus \mathcal{X}_j$
  end for
  return $\{(\mathcal{X}_j, \Pi_j, N_j)\}_{j=1}^{J}$
end function

function FINDEXPLORABLESETS($\mathcal{X} \subseteq \mathcal{S} \times \mathcal{A}$, step h, confidence δ, epochs K, samples N)
  $r_h^1(s,a) \leftarrow 1$ if $(s,a) \in \mathcal{X}$, else 0
  $N(s,a,h) \leftarrow 0, \mathcal{Y} \leftarrow \emptyset, \Pi \leftarrow \emptyset, j \leftarrow 1$
  for $k = 1$ to K **do**
    // StrongEuler is as defined in Simchowitz and Jamieson (2019)
    Run STRONGEULER(δ) on reward r_h^j to get trajectory $\{(s_h^k, a_h^k, h)\}_{h=1}^{H}$ and policy π_k
    $N(s_h^k, a_h^k) \leftarrow N(s_h^k, a_h^k) + 1, \quad \Pi \leftarrow \Pi \cup \{\pi_k\}$
    if $N(s_h^k, a_h^k) \geq N$, $(s_h^k, a_h^k) \in \mathcal{X}$ and $(s_h^k, a_h^k) \notin \mathcal{Y}$ **then**
      $\mathcal{Y} \leftarrow \mathcal{Y} \cup (s_h^k, a_h^k)$
      $r_h^{j+1}(s,a) \leftarrow 1$ if $(s,a) \in \mathcal{X} \setminus \mathcal{Y}$, else 0
      $j \leftarrow j + 1$
      Restart STRONGEULER(δ)
    end if
  end for
  return $\mathcal{Y}, \Pi$
end function

functions. More specifically, we reset the reward as $R_{h'}(s', a') = \begin{cases} 1, & \text{if } (s', a', h') = (s, 1, h), \\ 0, & \text{otherwise.} \end{cases}$,
where we arbitrarily fix an action and denote it by 1. With this reset reward, an optimal policy maximizes the visitation probability of $(s, 1)$ at step h. Therefore, $V_0^* = W_h(s, 1) = W_h(s)$. To approximate such an optimal policy, we employ STRONGEULER (Simchowitz and Jamieson, 2019).

More generally, the reachability $W_h(\mathcal{X})$ of any subset $\mathcal{X} \subset \mathcal{S} \times \mathcal{A}$ can be estimated in the same manner. We formalize this in Algorithm 1, which we refer to as **FB-L2E**, short for *Fixed-Budget Learn2Explore*. It is a careful adaptation of Learn2Explore algorithm introduced in Wagenmaker et al. (2022), which itself is inspired by Zhang et al. (2021); Brafman and Tennenholtz (2003).

Algorithm 1 satisfies the following guarantee:

Theorem 3.1. *Consider running Algorithm 1 with $B \geq c(B)$. Then, the following statements hold.*

1. *The total budget used is at most B.*
2. *For any $\varepsilon \geq 2SH^2\varepsilon_B$, with probability at least $1 - \exp\left(-\tilde{\Theta}\left(\frac{\varepsilon B}{C_{\mathrm{L2E}}(B)}\right)\right)$,*

   (1) The reachability of each set $\mathcal{X}_i$ satisfies

$$\frac{|\mathcal{X}_i|}{|\mathcal{X}|} \cdot 2^{-i-3} \leq W_h(\mathcal{X}_i) \leq 2^{-i+1} \quad \textit{for all } i \leq i_\varepsilon := \left\lceil \log_2\left(\frac{2SH^2}{\varepsilon}\right) \right\rceil,$$

(2) The remaining elements, $\bar{\mathcal{X}} := \mathcal{X} \setminus \cup_{i=1}^{i_\varepsilon} \mathcal{X}_i$ satisfy

$$\sup_{\pi} \sum_{(s,a)\in\bar{\mathcal{X}}} w_h^\pi(s,a) \le \frac{\varepsilon}{2SH^2}.$$

(3) Moreover, for any $i \le i_\varepsilon$, if each policy in Π_i is executed A times, then every state-action pair $(s,a) \in \mathcal{X}_i$ is visited at least $\frac{1}{8}AN_i$ times.

Here, the probability accounts for both the randomness in execution and resampling.

The proof of Theorem 3.1 is deferred to Appendix C.

Remark 2. *Theorem 3.1 crucially relies on the fact that* StrongEuler *(Simchowitz and Jamieson, 2019) achieves a high probability regret bound with $\log\frac{1}{\delta}$ dependence. However, when the target set is $\mathcal{X} = \{(s,a)\}$, similar results can be obtained by applying a boosting technique even if we use other algorithms with worse dependence. Although we only present Algorithm 1 in the main text for the simplicity, the algorithm with boosting technique is described in Appendix C, Algorithm 0.*

3.2 Action elimination

In the second part of our algorithm, we iteratively sample trajectories, compute empirical Q-function of state-action pairs, and eliminate suboptimal actions. For the purpose of efficient elimination, we employ a multiple bandit algorithm, *Successive Accepts and Rejects* (**SAR**), proposed by Bubeck et al. (2013), and, for the first time, provide an ε-correctness guarantee for this algorithm. By employing this algorithm to our main algorithm, we are able to reduce the dependency on S compared to applying its multi-armed bandit counterpart. For a more detailed explanation, see Appendix D, Remark 27.

Multiple bandit problem. Consider M instances of multi-armed bandit problems, each with K arms. Each arm i in instance m yields stochastic rewards supported on $[0,\sigma]$, with mean $\mu_{m,i}$, ordered such that $\mu_{m,1} \ge \cdots \ge \mu_{m,K}$. We denote each bandit-arm pair by (m,i), where $m \in [M]$ and $i \in [K]$. The objective is to identify a good arm in each instance $m \in [M]$ under a total budget of B pulls.

We now define some notations. Let $\widehat{\mu}_{m,i}(n)$ denote the empirical mean reward of arm i in instance m after n pulls. Define the suboptimality gap as

$$\bar{\Delta}_{m,i} := \begin{cases} \mu_{m,1} - \mu_{m,2}, & \text{if } i = 1, \\ \mu_{m,1} - \mu_{m,i}, & \text{if } i \in \{2,\dots,K\}. \end{cases}$$

We enumerate all gaps $\bar{\Delta}_{m,i}$ over all $(m,i) \in [M]\times[K]$ in increasing order as

$$\bar{\Delta}_{(1)} \le \bar{\Delta}_{(2)} \le \cdots \le \bar{\Delta}_{(MK)}.$$

Let

$$g(\varepsilon) := \left|\left\{(m,i) \in [M]\times[K] : \mu_{m,1} - \mu_{m,i} \le \varepsilon\right\}\right|$$

for any $\varepsilon > 0$, and define the harmonic log term

$$\overline{\log}(MK) := \frac{1}{2} + \sum_{i=2}^{MK} \frac{1}{i}.$$

For each $k \in [MK-1]$, define

$$n_k(B,M,K) := \left\lceil \frac{1}{\overline{\log}(MK)} \cdot \frac{B - MK}{MK + 1 - k} \right\rceil. \tag{1}$$

The SAR algorithm (Bubeck et al., 2013) is summarized in Algorithm 2. By leveraging the ranking of empirical gaps, SAR adaptively distributes the budget across bandit instances, solving the multiple bandit problem efficiently. We present a theoretical guarantee for its ability to identify ε-good arms.

Theorem 3.2. *If we run Algorithm 2 with $B \ge MK$, then the total number of budget used is at most B and*

$$\mathbb{P}(\exists m \in [M] : \mu_{m,1} - \mu_{m,J(m)} > \varepsilon) \le 2M^2K^2 \exp\left(-\frac{B - MK}{128\sigma^2\,\overline{\log}(MK)\cdot\sum_{i\in[MK]}(\bar{\Delta}_{(i)} \vee \varepsilon)^{-2}}\right).$$

for any $\varepsilon \ge 0$.

The proof of Theorem 3.2 is deferred to Appendix D.

Algorithm 2 **S**uccessive **A**ccept and **R**eject (SAR) for the multiple bandit

input: Budget B
$A_1 \leftarrow \{(1,1),\ldots,(M,K)\}$, $n_0 \leftarrow 0$
for $k = 1$ to $MK-1$ **do**
  $n_k \leftarrow n_k(B,M,K)$ (as defined in equation 1)
  $\forall (m,i) \in A_k$, pull (m,i) for $n_k - n_{k-1}$ times
  $\forall m$, $\hat{1}_m \leftarrow \arg\max_{i:(m,i)\in A_k} \hat{\mu}_{m,i}(n_k)$ (Break ties arbitrarily)
  if $\exists m$ such that $\hat{1}_m$ is the last active arm in m **then**
    $J_m = \hat{1}_m$ (Accept)
    $A_{k+1} \leftarrow A_k \setminus \{(m,\hat{1}_m)\}$ (Deactivate)
  else
    $(m_k,i_k) \leftarrow \arg\max_{(m,i)\in A_k} \left(\hat{\mu}_{m,\hat{1}_m}(n_k) - \hat{\mu}_{m,i}(n_k)\right)$ (Break ties arbitrarily)
    $A_{k+1} \leftarrow A_k \setminus \{(m_k,i_k)\}$ (Reject and deactivate)
  end if
end for
$J_m \leftarrow i$ for $A_{MK} = \{(m,i)\}$
return $\{(m,J_m)\}_{m=1}^M$

3.3 Overview of the BREA algorithm

We combine the two mechanisms described above to construct our main algorithm. The algorithm proceeds in a backward manner over steps $h = H, H-1, \ldots, 1$. At each step h, the first half of the budget is devoted to estimating the reachability $W_h(s)$ for each state s, while the second half applies the SAR mechanism to eliminate suboptimal actions. Although the logic by which our algorithm eliminates actions is entirely different, the structure of eliminating actions after reward-free exploration was also used in the fixed-confidence algorithm, MOCA (Wagenmaker et al., 2022).

In general MDPs, the stochasticity of the transition kernel prevents us from freely collecting arbitrary state-action samples. However, Theorem 3.1 ensures that, with high probability, the policies stored during the reachability estimation phase yield sufficient samples for each relevant state-action pair. Under this event, the SAR mechanism is expected to perform reliably. We now present our main theorem and its corollary; their proofs are provided in Appendix E.

Theorem 3.3. *If we run Algorithm 3 with*

$$B \geq \max\{2SHc(\frac{B}{2SH}), 2SA\varepsilon_{\frac{B}{2SH}} \log_2 \frac{1}{\varepsilon_{\frac{B}{2SH}}}\},$$

then the total number of budget used is at most B. Moreover, for any $\varepsilon \geq 2SH^2\varepsilon_{\frac{B}{2SH}}$,

$$\mathbb{P}\left(V_0^* - V_0^{\hat{\pi}} > \varepsilon\right) \leq \exp\left(-\tilde{\Theta}\left(\frac{\varepsilon B}{C_{\mathrm{L2E}}(\frac{B}{2SH})}\right)\right) + \exp\left(-\tilde{\Theta}\left(\frac{B}{H^5 \max_{h\in[H]} C_h^2 \sum_{s\in\mathcal{S}} W_h(s)^{-1} \sum_{a\in\mathcal{A}} (\bar{\Delta}_h(s,a) \vee \frac{\varepsilon}{W_h(s)})^{-2}}\right)\right).$$

Corollary 3. *In addition to the hypothesis of Theorem 3.3, assume further that $2SH^2\varepsilon_{\frac{B}{2SH}} < \varepsilon^* := \min\{\min^+_{s,h} W_h(s), 2H \min^+_{s,a,h} C_h W_h(s)\bar{\Delta}_h(s,a)\}$ and the optimal action in each state s at each step h is unique. Then, we obtain a guarantee of the best policy identification, given by*

$$\mathbb{P}\left(V_0^* - V_0^{\hat{\pi}} > 0\right) \leq \exp\left(-\tilde{\Theta}\left(\frac{\varepsilon^* B}{C_{\mathrm{L2E}}(\frac{B}{2SH})}\right)\right) + \exp\left(-\tilde{\Theta}\left(\frac{B}{H^3 \max_{h\in[H]} \sum_{s\in\mathcal{S}} W_h(s)^{-1} \sum_{a\in\mathcal{A}} \bar{\Delta}_h(s,a)^{-2}}\right)\right).$$

Remark 4. *From Theroem 3.3, we can derive the sample complexity required by BREA to identify an ε-correct policy with probability at least $1-\delta$, given by*

$$\tau_{\varepsilon,\delta} = \tilde{\Theta}\left(\frac{C_{\mathrm{L2E}}\left(\frac{B}{2SH}\right)}{\varepsilon} + H^5 \max_{h\in[H]} C_h^2 \sum_{s\in\mathcal{S}} \frac{1}{W_h(s)} \sum_{a\in\mathcal{A}} \frac{1}{\left(\bar{\Delta}_h(s,a) \vee \frac{\varepsilon}{W_h(s)}\right)^2}\right) \log\frac{1}{\delta}.$$

Algorithm 3 **B**ackward **R**eachability **E**stimation and **A**ction elimination (BREA)

input: Budget B
$B' \leftarrow \lfloor \frac{B}{2SH} \rfloor, \quad J \leftarrow \lceil 0.6321 \log_2(1 + \frac{\log(2)B'}{c(B')}) \rceil$
$B'' \leftarrow \frac{B}{2HJ}$
for $h = H, H-1, \ldots, 1$ **do**
  $\mathcal{Z}_h \leftarrow \emptyset$
  for $s \in \mathcal{S}$ **do** $\{(\mathcal{X}_j^{sh}, \Pi_j^{sh}, N_j^{sh})\}_{j=1}^{J} \leftarrow$ FB-L2E$(\{(s,1)\}, h, B')$ (1 is an arbitrary action)
    if $\mathcal{X}_h^{sh} = \{(s,1)\}$ for some $j \in [J]$ **then**
      $\widehat{W}_h(s) \leftarrow 2^{-j+1}, \quad \mathcal{Z}_h \leftarrow \mathcal{Z}_h \cup \{s\}$
    end if
  end for
  for $i = 1$ to J **do**
    $\mathcal{Z}_{hi} \leftarrow \{s \in \mathcal{Z}_h : \widehat{W}_h(s) = 2^{-i+1}\}, \quad A_1 \leftarrow \mathcal{Z}_{hi} \times \mathcal{A},$
    $\forall (s,a) \in A_1, \quad N(s,a) \leftarrow 0, \quad T(s,a) \leftarrow 0, \quad T_0(s,a) = 0, \quad Q(s,a) \leftarrow 0$
    for $k = 1$ to $|\mathcal{Z}_{hi}|A - 1$ **do**
      $n_k \leftarrow n_k(\lfloor B'' 2^{-i-2} \rfloor, |\mathcal{Z}_{hi}|, A)$ (as defined in equation 1)
      for $(s,a) \in A_k$ **do**
        $T_k(s,a) \leftarrow \lfloor \frac{n_k}{N_i^{sh}} \rfloor$
        Rerun each policy in Π_i^{sh} for $T_k(s,a) - T_{k-1}(s,a)$ times
        for each time $t = T(s,a) + 1$ to $T_k(s,a)$ **do**
          if (s,a) is visited at step h **then**
            Take action a and extend a trajectory using $\{\hat{\pi}_{h'}\}_{h'=h+1}^{H}$
            $N(s,a) \leftarrow N(s,a) + 1$
            $Q(s,a) \leftarrow Q(s,a) + \sum_{h'=h}^{H} R_{h'}^t(s_{h'}^t, a_{h'}^t)$
          end if
        end for
        $\hat{Q}_h^{\hat{\pi}}(s,a) \leftarrow Q(s,a)/N(s,a)$ **if** $N(s,a) > 0$ **else** 0
        $T(s,a) \leftarrow T(s,a) + T_k(s,a)$
      end for
      if $\exists$ state s with unique surviving pair (s,a) in A_k **then**
        $\hat{\pi}_h(s) \leftarrow a, \quad A_{k+1} \leftarrow A_k \setminus \{(s,a)\}$
      else
        $\forall (s,a) \in A_k, \quad \widehat{\Delta}_h^{\hat{\pi}}(s,a) \leftarrow \max_{a:(s,a)\in A_k} \hat{Q}_h^{\hat{\pi}}(s,a) - \hat{Q}_h^{\hat{\pi}}(s,a)$
        $(s', a') \leftarrow \arg\max_{(s,a)\in A_k} \widehat{\Delta}_h^{\hat{\pi}}(s,a)$ (Break ties arbitrarily)
        $A_{k+1} \leftarrow A_k \setminus \{(s', a')\}$
      end if
    end for
    $\hat{\pi}(s) \leftarrow a$ for $A_{|\mathcal{Z}_{hi}|A} = \{(s,a)\}$
  end for
  For each $s \in \mathcal{S} \setminus \mathcal{Z}_h$, set $\hat{\pi}_h(s)$ as any action
end for
return $\hat{\pi}$

The first term inside $\tilde{\Theta}$ is a lower-order term. The second term inside $\tilde{\Theta}$ becomes $\sum_{a\in\mathcal{A}} \frac{1}{(\tilde{\Delta}(a)\vee\varepsilon)^2}$ for multi-armed bandits ($S = H = 1$). This is consistent with known results in the bandit literature ((Even-Dar et al., 2006; Audibert et al., 2010; Karnin et al., 2013)). It is also noteworthy that our sample complexity is deterministic while the sample complexity of PAC RL algorithm typically is guaranteed with probability at least $1 - \delta$.

Remark 5. *Our sample complexity involves $H^5 \max_h$ term, in contrast to the $H^4 \sum_h$ dependence that appear in PAC RL literature ((Wagenmaker et al., 2022; Wagenmaker and Jamieson, 2022; Tirinzoni et al., 2023)). This difference stems from the inherent difficulty of the fixed budget setting, where the algorithm does not know in advance how to distribute the budget across different h. A similar issue regarding the dependency on S could be resolved by employing a multiple bandit algorithm instead of a multi-armed bandit algorithm.*

3.4 INCORPORATING TARGET ACCURACY

If an accuracy level ε is provided as input, we can modify Algorithm 3 to include a third part and obtain a different form of probabilistic guarantee. While Algorithm 3 allocates $\frac{B}{4}$ budget to each of its two parts, the modified algorithm assigns $\frac{B}{4}$ to the first and the second part and assgins $\frac{B}{2}$ to the last part.

In the third part, for each multiple-bandit instance $\mathcal{Z}_{hi}$, let $\hat{g}_{hi}^{\hat{\pi}}(\varepsilon)$ denote the number of pairs $(s,a) \in \mathcal{Z}_{hi}$ such that $\widehat{\Delta}_h^{\hat{\pi}}(s,a) \leq \frac{\varepsilon}{\widehat{W}_h(s)}$. After the second part, we gather the last $\hat{g}_{hi}^{\hat{\pi}}(\varepsilon)$ surviving pairs and perform an additional refinement step.

Theoretical guarantees for this variant are presented in the next theorem. The full algorithm and its analysis are provided in Appendix F.

Theorem 3.4. *(Informal) There exists a variant of Algorithm 3 that, when given a sufficiently large budget B and an accuracy level $\varepsilon \geq 2SH^2\varepsilon_{\frac{B}{2SH}}$ as input, it uses at most budget B and satisfies the following:*

$$\mathbb{P}\left(V_0^* - V_0^{\hat{\pi}} > \varepsilon\right) \leq \exp\left(-\tilde{\Theta}\left(\frac{\varepsilon B}{\mathrm{poly}(S,A,H,\log B)}\right)\right) + \exp\left(-\tilde{\Theta}\left(\frac{B}{H^3 \max_{h\in[H]} \sum_{s\in\mathcal{S}} W_h(s)^{-1} \sum_{a\in\mathcal{A}} (\bar{\Delta}_h(s,a) \vee \frac{\varepsilon}{W_h(s)})^{-2}}\right)\right) + \exp\left(-\tilde{\Theta}\left(\frac{\varepsilon^2 B}{H^5 \max_{h\in[H]} |\,\mathrm{OPT}_h(\varepsilon)|}\right)\right),$$

where $\mathrm{OPT}_h(\varepsilon) = \{(s,a) \in \mathcal{S}\times\mathcal{A} : \Delta_h(s,a) W_h(s) \leq \varepsilon\}$.

Remark 6. *From Theorem 3.4, we can derive the sample complexity required by the modified algorithm to identify an ε-correct policy with probability at least $1-\delta$, given by*

$$\tau_{\varepsilon,\delta} = \tilde{\Theta}\left(\frac{\mathrm{poly}(S,A,H,\log B)}{\varepsilon} + H^3 \max_{h\in[H]} \sum_{s\in\mathcal{S}} \frac{1}{W_h(s)} \sum_{a\in\mathcal{A}} \frac{1}{\left(\bar{\Delta}_h(s,a) \vee \frac{\varepsilon}{W_h(s)}\right)^2} + \frac{H^5 \max_{h\in[H]} |\,\mathrm{OPT}_h(\varepsilon)|}{\varepsilon^2}\right) \log\frac{1}{\delta}.$$

It is interesting that even though the logic of action elimination is very different, this expression is closely aligned with the sample complexity

$$\tau_{\varepsilon,\delta} = \frac{C_{\mathrm{LOT}}(\varepsilon)}{\varepsilon} + \tilde{\Theta}\left(H^2 \sum_{h\in[H]} \sum_{s\in\mathcal{S}} \frac{1}{W_h(s)} \sum_{a\in\mathcal{A}} \frac{1}{\left(\bar{\Delta}_h(s,a) \vee \frac{\varepsilon}{W_h(s)}\right)^2} + \frac{H^4 \sum_{h\in[H]} |\,\mathrm{OPT}_h(\varepsilon)|}{\varepsilon^2}\right) \log\frac{1}{\delta}$$

of MOCA algorithm (Wagenmaker et al., 2022), where $C_{\mathrm{LOT}} = \mathrm{poly}(S,A,H,\log\frac{1}{\varepsilon},\log\frac{1}{\delta})$.

4 CONCLUSION

In this paper, we have explored the fixed-budget setting of the pure exploration MDP, which is surprisingly underexplored in RL theory. While our results establish the first fully instance-dependent guarantee in the fixed budget setting, these are just beginning. First, it would be great to see what kind of instance-dependent acceleration can be proven in MDP, which should be possible given that accelerated rates were possible in bandits as a function of the number of good arms Katz-Samuels and Jamieson (2020); Zhao et al. (2023). Second, similarly, it would be interesting to explore what kind of data-poor regime guarantees are attainable – again, such bounds are available in the bandit setting Katz-Samuels and Jamieson (2020); Zhao et al. (2023). Third, we believe the factor H^2 in the sample complexity may be improved by leveraging variance-dependent concentration bounds. Finally, it would be interesting to extend our setting to the function approximation setting.

REPRODUCIBILITY STATEMENT

We have carefully specified all details of the algorithms presented in this paper. Moreover, we clearly state all assumptions required for the theoretical guarantees of our methods. We believe that this level of detail ensures the reproducibility of our results.

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Notation. For a positive integer n, we write $[n] := \{1, 2, \ldots, n\}$. We use $f = \tilde{\Theta}(g)$ to denote that the ratio $\frac{f}{g}$ is bounded both above and below by polylogarithmic functions. We define $\min^+_{x \in X} f(x) := \min_{x \in X : f(x) > 0} f(x)$. We use $\text{poly}(\cdot)$ to denote a polynomial in the variables inside the parentheses. We write $\log$ for natural logarithm and $\log_2$ for binary logarithm.

A Related work

Given the breadth of the literature on each topic, we focus on introducing only the most recent and relevant works.

Instance-dependent regret minimization in episodic MDPs. Zanette and Brunskill (2019) proposed the EULER algorithm and proved a regret bound of $\sqrt{SAK \min\{\mathbb{Q}_\star H, \mathcal{G}^2\}}$, where $\mathbb{Q}_\star, \mathcal{G}$ are instance dependent term. Soon after, Simchowitz and Jamieson (2019) proposed StrongEuler algorithm and proved a gap-dependent regret bound for episodic tabular MDPs, showing that optimistic algorithms can achieve $O\big(\sum_{s,a,h} \frac{\log T}{\Delta_h(s,a)}\big)$ regret. This result, obtained via a novel "clipped" regret decomposition, smoothly interpolates between instance-dependent $O(\log T)$ growth and the worst-case $O(\sqrt{T})$ rate, without requiring simplifying assumptions like a bounded mixing time. Dann et al. (2021) further refined these bounds by defining value-function gaps that ignore states never visited by an optimal policy. Finally, we note that any low-regret algorithm can be converted into a high-probability guarantee on near-optimal performance via an online-to-batch conversion. For detailed explanations, see Jin et al. (2018). However, recent studies ((Wagenmaker et al., 2022; Tirinzoni et al., 2023)) suggest that algorithms for minimizing regret cannot be instance-optimal for identifying good policies, motivating specialized algorithms that explore more strategically than standard optimism.

Instance-dependent episodic PAC RL. The history of instance-dependent episodic PAC RL is not very long. Wagenmaker et al. (2022) proposed a planning-based algorithm, MOCA, and analyzed its instance-dependent sample complexity. Tirinzoni et al. (2022) provided an instance-dependent lower bound for deterministic MDPs and proposed the EPRL algorithm, which has an upper bound of sample complexity matching the lower bound up to a H^2 factor and logarithmic terms. Wagenmaker and Jamieson (2022) considered finite horizon linear MDPs, a superset of tabular MDPs. They proposed the PEDEL algorithm, which takes a policy set as an input, and analyzed its sample complexity. Tirinzoni et al. (2023) proved, for the first time, an instance-dependent sample complexity of an optimistic algorithm, BPI-UCRL.

Instance-dependent pure exploration in multi-armed bandits. The problem of pure exploration in multi-armed bandits (a special case of RL with $S = H = 1$) has a rich history and is typically studied in two frameworks: the fixed-confidence ((ε, δ)-PAC) setting and the fixed-budget setting.

In the fixed-confidence setting, the goal is to identify an arm whose mean reward is within ε of the optimal arm's mean with probability at least $1 - \delta$, while minimizing the number of samples (pulls). Even-dar et al. (2002) initiated this line of work by proposing the Successive Elimination algorithm, which guarantees an optimal arm with probability $1 - \delta$ using distribution-dependent samples ((ε, δ)-sample complexity). Mannor and Tsitsiklis (2004) later provided a distribution-dependent lower bound on the (ε, δ)-sample complexity. Kalyanakrishnan et al. (2012) proposed the LUCB algorithm and analyzed their sample complexity. Karnin et al. (2013) introduced the Exponential-Gap Elimination algorithm, removed unnecessary log factors and attained near-optimal sample complexity in the fixed-confidence regime. Garivier and Kaufmann (2016) gave a tighter lower bound and proposed an algorithm, Track and Stop, which exactly hits the lower bound asymptotically.

In the fixed-budget setting, the learner is given a total sampling budget T and aims to maximize the probability of identifying the best arm by time T. Here, the results are often characterized by the exponential rate at which the failure probability decays with T. Audibert et al. (2010) studied this setting and proposed the Successive Rejects algorithm, proving that its error probability decays at an optimal rate, up to logarithmic factors in the number of arms. Karnin et al. (2013) proposed the Sequential Halving algorithm, proving that its error probability has an improved rate, which is optimal up to doubly logarithmic factors in the number of arms. Zhao et al. (2023) provided a tighter analysis of the Sequential Halving algorithm and obtained an accelerated decay rate of ε-error probability.

B PROPERTIES OF MDP

Although the statements and proofs of the lemmas in this section are nearly identical to those in the appendix of Wagenmaker et al. (2022), we include them here for completeness.

Lemma 7. *Assume that some deterministic policy $\hat{\pi}$ satisfies $\Delta_h^{\hat{\pi}}(s, \hat{\pi}_h(s)) \le \varepsilon_h(s)$ for any $h' \le h \le H$ and any $s \in \mathcal{S}$. Then, for any policy π',*

$$\sum_s w_{h'}^{\pi'}(s) \left(V_{h'}^*(s) - V_{h'}^{\hat{\pi}}(s) \right) \le \sum_{h=h'}^{H} \sup_\pi \sum_s w_h^\pi(s) \varepsilon_h(s).$$

Proof. The proof proceeds by backward induction on h'. When $h' = H$, the statement trivially holds. Assume that

$$\sum_s w_{h'}^{\pi'}(s) \left(V_{h'}^*(s) - V_{h'}^{\hat{\pi}}(s) \right) \le \sum_{h=h'}^{H} \sup_\pi \sum_s w_h^\pi(s) \varepsilon_h(s)$$

holds for step $h' > 1$ and any policy π. Assume further that

$$\Delta_{h'-1}^{\hat{\pi}}(s, \hat{\pi}(s)) \le \varepsilon_{h'-1}(s).$$

By definition,

$$\begin{aligned} V_{h'-1}^*(s) - V_{h'-1}^{\hat{\pi}}(s) &= Q_{h'-1}^*(s, \pi_{h'-1}^*(s)) - Q_{h'-1}^{\hat{\pi}}(s, \hat{\pi}_{h'-1}(s)) \\ &= \underbrace{Q_{h'-1}^*(s, \pi_{h'-1}^*(s)) - Q_{h'-1}^{\hat{\pi}}(s, \pi_{h'-1}^*(s))}_{(1)} + \underbrace{Q_{h'-1}^{\hat{\pi}}(s, \pi_{h'-1}^*(s)) - \max_a Q_{h'-1}^{\hat{\pi}}(s, a)}_{(2)} \\ &\quad + \underbrace{\max_a Q_{h'-1}^{\hat{\pi}}(s, a) - Q_{h'-1}^{\hat{\pi}}(s, \hat{\pi}_{h'-1}(s))}_{(3)}. \end{aligned}$$

It is obvious that $(2) \le 0$ and $(3) = \Delta_{h'-1}^{\hat{\pi}}(s, \hat{\pi}_{h'-1}(s)) \le \varepsilon_{h'-1}(s)$ by our assumption. Furthermore,

$$(1) = \sum_{s'} P_{h'-1}(s'|s, \pi_{h'-1}^*(s))(V_{h'}^*(s') - V_{h'}^{\hat{\pi}}(s')).$$

Then, for any policy π',

$$\begin{aligned} \sum_s w_{h'-1}^{\pi'}(s)(V_{h'-1}^*(s) - V_{h'-1}^{\hat{\pi}}(s)) &\le \sum_s \sum_{s'} w_{h'-1}^{\pi'}(s) P_{h'-1}(s'|s, \pi_{h'-1}^*(s))(V_{h'}^*(s') - V_{h'}^{\hat{\pi}}(s')) \\ &\quad + \sum_s w_{h'-1}^{\pi'}(s) \varepsilon_{h'-1}(s) \\ &= \sum_s w_{h'}^{\pi''}(s)(V_{h'}^*(s) - V_{h'}^{\hat{\pi}}(s)) + \sum_s w_{h'-1}^{\pi''}(s) \varepsilon_{h'-1}(s) \\ &\le \sum_{h=h'-1}^{H} \sup_\pi \sum_s w_h^\pi(s) \varepsilon_h(s), \end{aligned}$$

where π'' is a policy that is equal to π' in step $1, \dots, h'-2$ and equal to π^* in step $h'-1, \dots, H$, the last inequality follows by the induction hypothesis. □

Lemma 8. *Assume* $\sup_\pi \sum_s w_{h+1}^\pi(s) \left(V_{h+1}^*(s) - V_{h+1}^{\hat{\pi}}(s) \right) \le \varepsilon$. *Then*

$$|\Delta_h(s, a) - \Delta_h^{\hat{\pi}}(s, a)| \le \varepsilon / W_h(s).$$

Proof.

$$\begin{aligned} |\Delta_h(s, a) - \Delta_h^{\hat{\pi}}(s, a)| &= |V_h^*(s) - Q_h^*(s, a) - (\max_{a'} Q_h^{\hat{\pi}}(s, a') - Q_h^{\hat{\pi}}(s, a))| \\ &\le \max\{|V_h^*(s) - \max_{a'} Q_h^{\hat{\pi}}(s, a')|, |Q_h^{\hat{\pi}}(s, a) - Q_h^*(s, a)|\}, \end{aligned}$$

where the last inequality follows since

$$V_h^*(s) - Q_h^*(s,a) - (\max_{a'} Q_h^{\hat{\pi}}(s,a') - Q_h^{\hat{\pi}}(s,a)) \le V_h^*(s) - \max_{a'} Q_h^{\hat{\pi}}(s,a')$$

and

$$-(V_h^*(s) - Q_h^*(s,a) - (\max_{a'} Q_h^{\hat{\pi}}(s,a') - Q_h^{\hat{\pi}}(s,a))) \le Q_h^*(s,a) - Q_h^{\hat{\pi}}(s,a).$$

We can write

$$Q_h^*(s,a) = r_h(s,a) + \sum_{s'} P_h(s'|s,a) V_{h+1}^*(s'),$$
$$Q_h^{\hat{\pi}}(s,a) = r_h(s,a) + \sum_{s'} P_h(s'|s,a) V_{h+1}^{\hat{\pi}}(s').$$

Then we have

$$\begin{aligned} Q_h^*(s,a) - Q_h^{\hat{\pi}}(s,a) &= \sum_{s'} P_h(s'|s,a)(V_{h+1}^*(s') - V_{h+1}^{\hat{\pi}}(s')) \\ &= \frac{1}{W_h(s)} \sum_{s'} W_h(s) P_h(s'|s,a)(V_{h+1}^*(s') - V_{h+1}^{\hat{\pi}}(s')) \\ &\le \frac{1}{W_h(s)} \sup_{\pi} \sum_{s'} w_{h+1}^{\pi}(s')(V_{h+1}^*(s') - V_{h+1}^{\hat{\pi}}(s')) \le \frac{\varepsilon}{W_h(s)}. \end{aligned} \tag{2}$$

Let $a_1 := \arg\max_a Q_h^*(s,a)$. Then

$$\begin{aligned} V_h^*(s) - \max_{a'} Q_h^{\hat{\pi}}(s,a') &= \max_{a'} Q_h^*(s,a') - \max_{a'} Q_h^{\hat{\pi}}(s,a') = Q_h^*(s,a_1) - \max_{a'} Q_h^{\hat{\pi}}(s,a') \\ &= Q_h^*(s,a_1) - Q_h^{\hat{\pi}}(s,a_1) + Q_h^{\hat{\pi}}(s,a_1) - \max_{a'} Q_h^{\hat{\pi}}(s,a') \le \frac{\varepsilon}{W_h(s)}. \end{aligned} \tag{3}$$

By (2), (3), the lemma follows. □

C Analysis of FB-L2E

C.1 Analysis of FindExplorableSets

The overall analysis is similar to that of Wagenmaker et al. (2022). However, the details should be changed as we use StrongEuler instead of Euler. We begin with a regret bound of StrongEuler. Throughout this section, let $M := (SAH^2)^2$.

Lemma 9. *If we run* StrongEuler *with confidence parameter δ for K episodes, with probability at least $1-\delta$,*

$$\sum_{k=1}^{K} V_0^* - \sum_{k=1}^{K} V_0^{\pi_k} \le c_{\mathrm{se}} \sqrt{SAH^2 V_0^* K \log(HK) \log(\frac{MHK}{\delta})} + c_{\mathrm{se}} S^2 A H^6 \log(HK) \log(\frac{MHK}{\delta}),$$

where $M = (SAH^2)^2$ and c_{se} is a universal constant.

Proof. In Simchowitz and Jamieson (2019, Theorem 2.4), the regret bound up to a universal constant is presented as

$$\sqrt{SA\bar{H}_T T \log(\frac{mT}{\delta})} + SAH^4(S \vee H) \log(\frac{mT}{\delta}) \min\{\log(\frac{mT}{\delta}), \log(\frac{mH}{\Delta_{\min}})\},$$

where $\Delta_{\min} = \min^+_{s,a,h} \Delta_h(s,a)$, $T = HK$, $m = (SAH)^2$, and $\bar{H}_T \le \frac{\mathcal{G}^2}{H} \log(T)$. Here, $\mathcal{G}$ is a constant such that the reward of one episode of our MDP is bounded by $\mathcal{G}$. We can reduce this $\frac{\mathcal{G}^2}{H}$ term to $\frac{V_0^*}{4H}$ by using the argument used in the proof of Jin et al. (2020, Lemma 3.4) and Wagenmaker et al. (2022, Lemma D.4). Thus, the regret bound (up to a universal constant) of StrongEuler is given as

$$\sqrt{SAV_0^* T \log(T) \log(\frac{mT}{\delta})} + SAH^4(S \vee H) \log(\frac{mT}{\delta}) \min\{\log(\frac{mT}{\delta}), \log(\frac{mH}{\Delta_{\min}})\},$$

The second term is derived from their Simchowitz and Jamieson (2019, Claim C.3). In the proof of Simchowitz and Jamieson (2019, Claim C.3), we can just bound

$$\log(1 + \frac{N \wedge n_{\mathrm{end}}}{n_0}) \leq \log(1 + T)$$

since $N \leq T, n_0 \geq 1$. By using this bound, we get a regret bound of

$$\sqrt{SAV_0^* T \log(T) \log(\frac{mT}{\delta})} + SAH^4(S \vee H) \log(\frac{mT}{\delta}) \log(T).$$

Although this bound only applies to stationary MDPs, stationary MDPs can represent non-stationary MDPs by augmenting states s to (s, h). In this case, the effective number of states is SH. Thus, by substituting SH in to S, HK into T, the lemma follows. □

We now define the important quantities

$$\begin{aligned} C_K(\delta, \delta_{\mathrm{samp}}, i) := \max \Bigg\{ & 432 c_{\mathrm{se}}^2 S^3 A^2 H^6 (i+6)^2 \log^2(2 \cdot 2 \cdot 432 c_{\mathrm{se}}^2 S^3 A^2 H^7 M(i+6)), \\ & 432 c_{\mathrm{se}}^2 S^3 A^2 H^6 \log(\frac{1}{\delta})(i+3) \log(2 \cdot 432 c_{\mathrm{se}}^2 S^3 A^2 H^7 \log(\frac{1}{\delta})(i+3)), \\ & 24 \log(\frac{4}{\delta}), \quad 2^{11} S^2 A^2 \log(\frac{4SAH}{\delta_{\mathrm{samp}}}) \Bigg\}, \\ K_i(\delta, \delta_{\mathrm{samp}}) := & \lceil 2^i C_K(\delta, \delta_{\mathrm{samp}}, i) \rceil. \end{aligned} \tag{4}$$

and prove the following property.

Lemma 10. *Let* $C_{\mathcal{R}} := 2c_{\mathrm{se}} S^3 A^2 H^6 \log(HK_i) \log(\frac{2MHK_i}{\delta}) + 2 \log \frac{4}{\delta}$ *and* $K_i = K_i(\delta, \delta_{\mathrm{samp}})$. *Then,*

$$K_i \geq 2^i \max\{4C_{\mathcal{R}}, 144 c_{\mathrm{se}}^2 S^2 A^2 H^2 \log(HK_i) \log(\frac{2MHK_i}{\delta})\}.$$

Proof. For any $i, j > 0$ and $C > 0$, if $x \geq C^i (i+3j)^j \log^j(C(i+3j))$, then $x \geq C^i \log^j x$ since

$$\begin{aligned} C^i \log^j x = C^i \log^j [C^i (i+3j)^j \log^j (C(i+3j))] &\leq C^i \log^j [C^{i+j} (i+3j)^{2j}] \\ &\leq C^i (i+3j)^j \log^j [C(i+3j)] \\ &= x \end{aligned}$$

Since

$$2MHK_i \geq 2^i \cdot 2 \cdot 432 c_{\mathrm{se}}^2 S^3 A^2 H^7 M(i+6)^2 \log^2(2 \cdot 2 \cdot 432 c_{\mathrm{se}}^2 S^3 A^2 H^7 M(i+6)),$$

we have

$$K_i \geq 2^i \cdot 2 \cdot 432 c_{\mathrm{se}}^2 S^3 A^2 H^6 \log^2(2MHK_i).$$

Since

$$HK_i \geq 2^i \cdot 432 c_{\mathrm{se}}^2 S^3 A^2 H^7 \log(\frac{1}{\delta})(i+3) \log(2 \cdot 432 c_{\mathrm{se}}^2 S^3 A^2 H^7 \log(\frac{1}{\delta})(i+3)),$$

we have

$$K_i \geq 2^i \cdot 432 c_{\mathrm{se}}^2 S^3 A^2 H^6 \log(HK_i) \log(\frac{1}{\delta}).$$

We also have $K_i \geq 2^i \cdot 24 \log(\frac{4}{\delta})$. Combining these three, we have

$$K_i \geq 2^i \left(144 c_{\mathrm{se}}^2 S^3 A^2 H^6 (\log^2(2MHK_i) + \log(HK_i) \log(\frac{1}{\delta}) + 8 \log(\frac{4}{\delta}) \right),$$

which easily implies

$$\begin{aligned} K_i &\geq 2^i \cdot 144 c_{\mathrm{se}}^2 S^2 A^2 H^2 \log(HK_i) \log(\frac{2MHK_i}{\delta}), \\ K_i &\geq 8^i \left(2c_{\mathrm{se}} S^3 A^2 H^6 \log(HK_i) \log(\frac{2MHK_i}{\delta}) + 8 \log(\frac{4}{\delta}) \right) = 4C_{\mathcal{R}}. \end{aligned}$$

□

Throughout the rest of this subsection, we consider running

$$\text{FINDEXPLORABLESETS}(\mathcal{X}, h, \delta, K_i := K_i(\delta, \delta_{\text{samp}}), N_i := \frac{K_i}{4|\mathcal{X}|2^i})$$

(defined in Algorithm 1) with some $\mathcal{X} \subset \mathcal{S} \times \mathcal{A}$ satisfying

$$W_h(\mathcal{X}) \leq 2^{-i+1}.$$

Let $\mathcal{X}_i \subset \mathcal{X}, \Pi_i$ be the output. We introduce the following notations. Let K_{ij} denote the total number of episodes taken for j, where the index j changes when the reward r_h^j is reset. Let m_i denote the number of j. Thus, we have

$$\sum_{j=1}^{m_i} K_{ij} = K_i.$$

Let $V_0^{*,ij}$ denote the optimal value function on the reward function r_h^j, $V_0^{k,ij}$ denote the value function for the policy π_k on the reward function r_h^j. Then,

$$V_0^{k,ij} \leq V_0^{*,ij} \leq \sup_\pi \mathbb{E}_\pi[\mathbb{I}\{(s_h, a_h) \in \mathcal{X}\}] = W_h(\mathcal{X}) \leq 2^{-(i-1)}.$$

Now we define some events.

$$\mathcal{C}_{1,\delta} = \Big\{\sum_{j=1}^{m_i}\Big(\sum_{k=1}^{K_{ij}} V_0^{*,ij} - \sum_{k=1}^{K_{ij}} V_0^{k,ij}\Big) \leq 2c_{\text{se}}\sqrt{S^2A^2H^2V_0^{*,i1}K_i\log(HK_i)\log(\frac{MHK_i}{\delta})}$$
$$+ 2c_{\text{se}}S^3A^2H^6\log(HK_i)\log(\frac{MHK_i}{\delta})\Big\},$$
$$\mathcal{C}_{2,\delta} = \Big\{\Big|\sum_{j=1}^{m_i}\sum_{k=1}^{K_{ij}}\sum_{h=1}^{H} R_h^j(s_h^{j,k}, a_h^{j,k}) - \sum_{j=1}^{m_i}\sum_{k=1}^{K_{ij}} V_0^{k,ij}\Big| \leq \sqrt{4K_i 2^{-i}\log\frac{2}{\delta}} + 2\log\frac{2}{\delta}\Big\},$$
$$\mathcal{D}_{1,\delta} = \Big\{\forall(s,a) \in \mathcal{X}, \Big|\sum_{k=1}^{K_i} w_h^{\pi_k}(s,a) - \sum_{k=1}^{K_i}\mathbb{I}_{\{(s_h^k, a_h^k)=(s,a)\}}\Big| \leq \sqrt{2K_iW_h(s)\log\frac{2}{\delta}} + 2\log\frac{2}{\delta}\Big\}$$

for the process during the algorithm,

$$\mathcal{D}_{2,\delta} = \Big\{\forall(s,a) \in \mathcal{X}_i, \Big|\sum_{k=1}^{K_i} w_h^{\pi_k}(s,a) - \sum_{k=1}^{K_i}\mathbb{I}_{\{(s_h^k, a_h^k)=(s,a)\}}\Big| \leq \sqrt{2K_iW_h(s)\log\frac{2}{\delta}} + 2\log\frac{2}{\delta}\Big\}$$

for the process during the replay.

Freedman's inequality is stated below for use in subsequent analysis.

Lemma 11 (Freedman's inequality)**.** *Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a probability space and $\mathcal{F}_0 \subset \mathcal{F}_1 \subset \mathcal{F}_2 \subset \cdots \mathcal{F}$ be a filtration of σ-algebra. Let $\{X_i\}_i$ be random variables such that X_i is $\mathcal{F}_i$-measurable,*

$$|X_i| \leq M,$$
$$\mathbb{E}[X_n|\mathcal{F}_{n-1}] = 0,$$
$$\mathbb{E}[X_n^2|\mathcal{F}_{n-1}] \leq V_n$$

for constants V_n. Then, for any $\delta > 0$, with probability at least $1-\delta$,

$$|\sum_{i=1}^{n} X_i| < 2M\log\frac{2}{\delta} + \sqrt{2\sum_{i=1}^{n} V_n\log\frac{2}{\delta}}.$$

We state properties of the events defined above.

Lemma 12. *If $\delta \in (0,1)$ is the third argument of* `FindExplorableSets`*,*

$$\mathbb{P}(\mathcal{C}_{1,\delta/2}) \geq 1 - \delta/2.$$

Proof. For any fixed K and j,

$$\Big(\sum_{k=1}^{K} V_0^{*,ij} - \sum_{k=1}^{K} V_0^{k,ij}\Big)|\mathcal{F}_{j-1} \leq c_{\text{se}}\sqrt{SAH^2 V_0^{*,i1} K \log(HK)\log(\frac{MHK}{\delta})} + c_{\text{se}} S^2 AH^6 \log(HK)\log(\frac{MHK}{\delta})$$

with probability at least $1-\delta$, where $\mathcal{F}_{j-1}$ is the filtration up to iteration j, and we used $V_0^{*,ij} \leq V_0^{*,i1}$ for all j since the reward function can only decrease as j increases. `FindExplorableSets` stops and restarts StrongEuler if the relevant condition is met, but this is a random stopping condition. Thus, to guarantee that the regret bound holds for any possible value of this stopping time, we union bound over all possible values. Since `FindExplorableSets` runs for at most K_i episodes, we union bound over K_i stopping times. We then have

$$\Big(\sum_{k=1}^{K} V_0^{*,ij} - \sum_{k=1}^{K} V_0^{k,ij}\Big)|\mathcal{F}_{j-1} \leq 2c_{\text{se}}\sqrt{SAH^2 V_0^{*,i1} K \log(HK_i)\log(\frac{2MHK_i}{\delta})} + 2c_{\text{se}} S^2 AH^6 \log(HK_i)\log(\frac{2MHK_i}{\delta})$$

for all $K \in [K_i]$ with probability at least $1 - \frac{\delta}{2SA}$. Since $m_i \leq SA$, union bounding over all j we then have that, with probability at least $1-\delta/2$,

$$\begin{aligned}\sum_{j=1}^{m_i}\Big(\sum_{k=1}^{K_{ij}} V_0^{\star,ij} - \sum_{k=1}^{K_{ij}} V_0^{k,ij}\Big) &\leq \sum_{j=1}^{m_i} 2c_{\text{se}}\sqrt{SAH^2 V_0^{*,i1} K_{ij}\log(HK_i)\log(\frac{2MHK_i}{\delta})} \\ &\quad + 2c_{\text{se}} S^3 A^2 H^6 \log(HK_i)\log(\frac{2MHK_i}{\delta}) \\ &\leq 2c_{\text{se}}\sqrt{S^2A^2H^2 V_0^{*,i1} K_i \log(HK_i)\log(\frac{2MHK_i}{\delta})} \\ &\quad + 2c_{\text{se}} S^3 A^2 H^6 \log(HK_i)\log(\frac{2MHK_i}{\delta}),\end{aligned}$$

where the last inequality follows from Jensen's inequality. □

Lemma 13. *For any* $\delta \in (0,1)$,

$$\mathbb{P}(\mathcal{C}_{2,\delta}) \geq 1-\delta.$$

Proof. For each $k \in [K_i]$, we have that $X_k := \sum_{h=1}^{H} R_h(s_h^k, a_h^k) \sim \text{Bernoulli}(V_0^{\pi_k})$. Then $|X_k - V_0^{\pi_k}| \leq 1$, $\mathbb{E}[(X_k - V_0^{\pi_k})^2|\mathcal{F}_{k-1}] = V_0^{\pi_k}(1-V_0^{\pi_k}) \leq V_0^{\pi_k} \leq W_h(\mathcal{X}) \leq 2^{-i+1}$. Thus, if we apply Lemma 11, we obtain the statement. □

Lemma 14. *For any* $\delta \in (0,1)$,

$$\mathbb{P}(\mathcal{D}_{1,\delta}) \geq 1 - |\mathcal{X}|\delta \geq 1 - SA\delta.$$

Proof. Since $X_k := \mathbb{I}_{\{(s_h^k, a_h^k)=(s,a)\}} \sim \text{Bernoulli}(w_h^{\pi_k}(s,a))$,

$$\mathbb{E}[(X_k - w_h^{\pi_k}(s,a))^2|\mathcal{F}_{k-1}] = w_h^{\pi_k}(s,a)(1-w_h^{\pi_k}(s,a)) \leq w_h^{\pi_k}(s,a) \leq W_h(s).$$

By Lemma 11, we have that

$$\left|\sum_{k=1}^{K_i} w_h^{\pi_k}(s,a) - \sum_{k=1}^{K_i} \mathbb{I}_{\{(s_h^k,a_h^k)=(s,a)\}}\right| \leq \sqrt{2K_i W_h(s)\log\frac{2}{\delta}} + 2\log\frac{2}{\delta}$$

with probability at least $1-\delta$. Union bounding over $\mathcal{X}$ leads to the statement. □

Lemma 15. *For any* $\delta \in (0,1)$,

$$\mathbb{P}(\mathcal{D}_{2,\delta}) \geq 1 - |\mathcal{X}_i|\delta \geq 1 - SA\delta.$$

Proof. Since $X_k := \mathbb{I}_{\{(s_h^k, a_h^k)=(s,a)\}} \sim \text{Bernoulli}(w_h^{\pi_k}(s,a))$,

$$\mathbb{E}[(X_k - w_h^{\pi_k}(s,a))^2 | \mathcal{F}_{k-1}] = w_h^{\pi_k}(s,a)(1 - w_h^{\pi_k}(s,a)) \le w_h^{\pi_k}(s,a) \le W_h(s).$$

By Lemma 11 and union bound over $\mathcal{X}_i$, the statement follows. □

Lemma 16. *If $\delta \in (0,1)$ is the third argument of `FindExplorableSets`, the event $\mathcal{C}_{1,\delta/2} \cap \mathcal{C}_{2,\delta/2}$ implies*

$$W_h(\mathcal{X} \setminus \mathcal{X}_i) \le 2^{-i}.$$

Proof. Putting Lemma 12, 13 and union bounding over these events, we have that with probability at least $1-\delta$,

$$\sum_{j=1}^{m_i}\sum_{k=1}^{K_{ij}}\sum_{h=1}^{H} R_h^j(s_h^{j,k}, a_h^{j,k}) \ge \sum_{j=1}^{m_i}\sum_{k=1}^{K_{ij}} V_0^{\star,ij} - \sqrt{4K_i 2^{-i}\log\frac{4}{\delta}} - 2c_{\text{se}}\sqrt{S^2A^2H^2V_0^{*,i1}K_i\log(HK_i)\log(\frac{2MHK_i}{\delta})} - C_{\mathcal{R}}$$

where we denote

$$C_{\mathcal{R}} := 2c_{\text{se}}S^3A^2H^6\log(HK_i)\log(\frac{2MHK_i}{\delta}) + 2\log\frac{4}{\delta}.$$

Assume that $V_0^{*,im_i} > 2^{-i}$. Using that the reward decreases monotonically so $V_0^{*,im_i} \le V_0^{*,ij}$ for any $j \le m_i$, we can lower bound the above as

$$\begin{aligned}
&\ge 2^{-i}K_i - \sqrt{4K_i 2^{-i}\log\frac{4}{\delta}} - 2c_{\text{se}}\sqrt{S^2A^2H^2V_0^{*,i1}K_i\log(HK_i)\log(\frac{2MHK_i}{\delta})} - C_{\mathcal{R}} \\
&\ge 2^{-i}K_i - 3c_{\text{se}}\sqrt{S^2A^2H^2 2^{-i}K_i\log(HK_i)\log(\frac{2MHK_i}{\delta})} - C_{\mathcal{R}}
\end{aligned}$$

where the second inequality follows since $V_0^{*,i1} \le 2^{-i+1}$ and $\sqrt{4K_i 2^{-i}\log\frac{4}{\delta}}$ will then be dominated by the regret term. Lemma 10 gives

$$K_i \ge 2^i \max\left\{4C_{\mathcal{R}}, 144c_{\text{se}}^2S^2A^2H^2\log(HK_i)\log(\frac{2MHK_i}{\delta})\right\}$$

which implies

$$\frac{1}{4}2^{-i}K_i - C_{\mathcal{R}} \ge 0$$

and

$$\begin{aligned}
&\frac{1}{4}2^{-i}K_i - 3c_{\text{se}}\sqrt{S^2A^2H^2 2^{-i}K_i\log(HK_i)\log(\frac{2MHK_i}{\delta})} \\
&\quad\ge \frac{2^i \cdot 144c_{\text{se}}^2S^2A^2H^2\log(HK_i)\log(\frac{2MHK_i}{\delta})}{4\cdot 2^i} \\
&\quad\quad - 3c_{\text{se}}\sqrt{S^2A^2H^2 2^{-i}\log(HK_i)\log(\frac{2MHK_i}{\delta})\cdot 2^i 144c_{\text{se}}^2S^2A^2H^2\log(HK_i)\log(\frac{2MHK_i}{\delta})} \\
&\quad= 0.
\end{aligned}$$

Thus, we can lower bound the above as

$$2^{-i}K_i - 3c_{\text{se}}\sqrt{S^2A^2H^2 2^{-i}K_i\log(HK_i)\log(\frac{2MHK_i}{\delta})} - C_{\mathcal{R}} \ge \frac{1}{2}2^{-i}K_i.$$

Note that we can collect a total reward of at most $|\mathcal{X}|N_i$. However, by our choice of

$$N_i = K_i/(4|\mathcal{X}|\cdot 2^i),$$

we have that

$$|\mathcal{X}|N_i = \frac{1}{4\cdot 2^i}K_i < \frac{1}{2\cdot 2^i}K_i.$$

This is a contradiction. Thus, we must have that $W_h(\mathcal{X}\setminus\mathcal{X}_i) \le V_0^{*,im_i} \le 2^{-i}$. □

Lemma 17. *The event $\mathcal{C}_{\delta/2}$ with $\delta \geq \frac{\delta_{\mathrm{samp}}}{SAH}$ implies*

$$W_h(\mathcal{X}) \geq \frac{|\mathcal{X}_i|}{2^{i+3}|\mathcal{X}|}.$$

Proof.

$$\begin{aligned}
N_i|\mathcal{X}_i| \leq \sum_{j=1}^{m_i}\sum_{k=1}^{K_{ij}} R_h^j(s_h^{j,k}, a_h^{j,k}) &\leq \sum_{j=1}^{m_i}\sum_{k=1}^{K_{ij}} V_0^{k,ij} + \sqrt{4K_i 2^{-i}\log\frac{4}{\delta}} + 2\log\frac{4}{\delta} \\
&\leq K_i W_h(\mathcal{X}) + \sqrt{4K_i 2^{-i}\log\frac{4}{\delta}} + 2\log\frac{4}{\delta} \\
&\leq K_i W_h(\mathcal{X}) + \frac{K_i}{2^{i+4}SA} + \frac{K_i}{2^{i+10}SA} \\
&\leq K_i W_h(\mathcal{X}) + \frac{K_i}{2^{i+3}SA},
\end{aligned}$$

where the forth inequality follows from $K_i \geq 2^{i+11}S^2A^2\log\frac{4SAH}{\delta_{\mathrm{samp}}}$. Then,

$$W_h(\mathcal{X}) \geq \frac{N_i|\mathcal{X}_i|}{K_i} - \frac{1}{2^{i+3}SA} = \frac{|\mathcal{X}_i|}{2^{i+2}|\mathcal{X}|} - \frac{1}{2^{i+3}SA} \geq \frac{|\mathcal{X}_i|}{2^{i+3}|\mathcal{X}|}.$$

□

Lemma 18. *The event $\mathcal{D}_{1,\delta} \cap \mathcal{D}_{2,\delta}$ with $\delta \geq \frac{\delta_{\mathrm{samp}}}{2SAH}$ implies that after rerunning each policy in Π_i once, the number of samples collected for each $(s,a) \in \mathcal{X}_i$ is at least $\frac{1}{4}N_i$.*

Proof. Let $\mathbb{I}^1, \mathbb{I}^2$ denote the indicator of an event during `FindExplorableSets`, and an event during rerunning policies respectively. For a pair $(s,a) \in \mathcal{X}_i$, we have

$$\begin{aligned}
\sum_{k=1}^{K_i}\mathbb{I}^1_{\{(s_h^k,a_h^k)=(s,a)\}} - \sum_{k=1}^{K_i} w_h^{\pi_k}(s,a) &\leq \sqrt{2K_i W_h(s)\log\frac{2}{\delta}} + 2\log\frac{2}{\delta} \\
\sum_{k=1}^{K_i} w_h^{\pi_k}(s,a) - \sum_{k=1}^{K_i}\mathbb{I}^2_{\{(s_h^k,a_h^k)=(s,a)\}} &\leq \sqrt{2K_i W_h(s)\log\frac{2}{\delta}} + 2\log\frac{2}{\delta}
\end{aligned}$$

Then the number of samples of (s,a) collected during the rerunning satisfies

$$\begin{aligned}
\sum_{k=1}^{K_i}\mathbb{I}^2_{\{(s_h^k,a_h^k)=(s,a)\}} &\geq \sum_{k=1}^{K_i}\mathbb{I}^1_{\{(s_h^k,a_h^k)=(s,a)\}} - 2\sqrt{2K_i W_h(s)\log\frac{2}{\delta}} - 4\log\frac{2}{\delta} \\
&\geq N_i - 2\sqrt{2K_i W_h(s)\log\frac{2}{\delta}} - 4\log\frac{2}{\delta} \\
&\geq N_i - 2\sqrt{2^{-i+2}K_i\log\frac{2}{\delta}} - 4\log\frac{2}{\delta} \\
&\geq N_i - \frac{K_i}{2^{i+3.5}SA} - \frac{K_i}{2^{i+9}S^2A^2} \\
&\geq N_i - \frac{K_i}{2^{i+2.5}SA} \\
&\geq N_i - \frac{K_i}{2^{i+2.5}|\mathcal{X}|} = N_i(1-\frac{1}{\sqrt{2}}) \geq \frac{1}{4}N_i,
\end{aligned}$$

where the forth inequality follows from $\delta \geq \frac{\delta_{\mathrm{samp}}}{4SAH}$ and $\log\frac{2SAH}{\delta_{\mathrm{samp}}} \leq \frac{K_i}{2^{i+11}S^2A^2}$. □

Lemma 19. *The event $\mathcal{D}_{1,\delta}$ with $\delta \geq \frac{\delta_{\mathrm{samp}}}{2SAH}$ implies*

$$W_h(s) > \frac{1}{2^{i+3}|\mathcal{X}|} \text{ for each } (s,a) \in \mathcal{X}_i, \quad W_h(\mathcal{X}_i) > \frac{|\mathcal{X}_i|}{2^{i+3}|\mathcal{X}|}.$$

Proof. In the proof of the previous lemma, we showed that

$$\sqrt{2^{-i+2}K_i \log \frac{2}{\delta}} + 2\log\frac{2}{\delta} \leq \frac{N_i}{2\sqrt{2}} < \frac{N_i}{2}$$

when $\delta \geq \frac{\delta_{\mathrm{samp}}}{2SAH}$. Using this, we have

$$N_i \leq \sum_{k=1}^{K_i} \mathbb{I}^1_{\{(s_h^k, a_h^k)=(s,a)\}} \leq \sum_{k=1}^{K_i} w_h^{\pi_k}(s,a) + \sqrt{2^{-i+2}K_i \log \frac{2}{\delta}} + 2\log\frac{2}{\delta} < K_i W_h(s) + \frac{N_i}{2}$$

for each $(s,a) \in \mathcal{X}_i$. Thus,

$$W_h(s) > \frac{N_i}{2K_i} = \frac{1}{2^{i+3}|\mathcal{X}|}.$$

On the other hand,

$$|\mathcal{X}_i|N_i \leq \sum_{(s,a)\in\mathcal{X}_i} \sum_{k=1}^{K_i} \mathbb{I}^1_{\{(s_h^k, a_h^k)=(s,a)\}} \leq \sum_{k=1}^{K_i} w_h^{\pi_k}(\mathcal{X}_i) + |\mathcal{X}_i| \left(\sqrt{2^{-i+2}K_i \log \frac{2}{\delta}} + 2\log\frac{2}{\delta} \right) < K_i W_h(\mathcal{X}_i) + \frac{|\mathcal{X}_i|N_i}{2}.$$

Thus,

$$W_h(\mathcal{X}_i) > \frac{|\mathcal{X}_i|N_i}{2K_i} = \frac{|\mathcal{X}_i|}{2^{i+3}|\mathcal{X}|}.$$

□

We finally give a guarantee of `FindExplorableSets`.

Theorem C.1. *If we run*

$$\texttt{FindExplorableSets}(\mathcal{X}, h, \delta, K_i = K_i(\delta, \delta_{\mathrm{samp}} = SAH\delta), N_i = \frac{K_i}{4|\mathcal{X}|2^i})$$

for a subset $\mathcal{X} \subset \mathcal{S} \times \mathcal{A}$ with $W_h(\mathcal{X}) \leq 2^{-i+1}$ and returns subset $\mathcal{X}_i \subset \mathcal{X}$, policy set Π_i, then

1. *$W_h(\mathcal{X} \setminus \mathcal{X}_i) \leq 2^{-i}$ with probability at least $1-\delta$.*
2. *With probability at least $1 - SA\delta$,*
   - *(1) If we rerun each policy in Π_i once, the number of samples collected for each $(s,a) \in \mathcal{X}_i$ is at least $\frac{1}{4}N_i$.*
   - *(2) $W_h(s) > \frac{1}{2^{i+3}|\mathcal{X}|}$ for each $(s,a) \in \mathcal{X}_i$ and $W_h(\mathcal{X}_i) > \frac{|\mathcal{X}_i|}{2^{i+3}|\mathcal{X}|}$.*

Proof. By Lemma 12, 13, 14, 15, 16, 18, and 19, the theorem follows. □

C.2 Proof of Theorem 3.1

Before proving Theorem 3.1, we introduce a useful lemma related to the Lambert W-function. The Lambert function $W(s) : [0,\infty) \to [0,\infty)$ is defined by

$$x = W(x)\exp(W(x)), \quad \text{for } x \geq 0.$$

Then the following holds.

Lemma 20. *(Orabona and Pal, 2016, Lemma 17)*

$$0.6321 \log(1+x) \leq W(x) \leq \log(1+x) \text{ for } x \geq 0.$$

We define

$$c(B) = 4JC_K(\frac{1}{8SAH}, \frac{1}{8}, J) = \mathrm{poly}(S, A, H, \log(B)),$$
$$C_{\mathrm{L2E}}(B) = SH^2 c(B). \tag{5}$$

Recall that C_K was defined in equation 4. We now give a proof of Theorem 3.1

Theorem C.2 (Theorem 3.1)**.** *Consider running Algorithm 1 with $B \geq c(B)$. Then, the following statements hold.*

1. *The total budget used is at most B.*
2. *For any $\varepsilon \geq 2SH^2\varepsilon_B$, with probability at least $1 - \exp\left(-\tilde{\Theta}\left(\frac{\varepsilon B}{C_{\mathrm{L2E}}(B)}\right)\right)$,*

   (1) The reachability of each set $\mathcal{X}_i$ satisfies

   $$\frac{|\mathcal{X}_i|}{|\mathcal{X}|} \cdot 2^{-i-3} \leq W_h(\mathcal{X}_i) \leq 2^{-i+1} \quad \textit{for all } i \leq i_\varepsilon := \left\lceil \log_2\left(\frac{2SH^2}{\varepsilon}\right)\right\rceil,$$

   (2) The remaining elements, $\bar{\mathcal{X}} := \mathcal{X} \setminus \cup_{i=1}^{i_\varepsilon}\mathcal{X}_i$ satisfy

   $$\sup_\pi \sum_{(s,a)\in\bar{\mathcal{X}}} w_h^\pi(s,a) \leq \frac{\varepsilon}{2SH^2}.$$

   (3) Moreover, for any $i \leq i_\varepsilon$, if each policy in Π_i is executed A times, then every state-action pair $(s,a) \in \mathcal{X}_i$ is visited at least $\frac{1}{8}AN_i$ times.

   Here, the probability accounts for both the randomness in the execution of the algorithm and the resampling process.

Proof. We first prove that the total budget used is at most B. Let $\delta = \frac{1}{8SAH}$. By the definition of δ_i,

$$\begin{aligned}
\log\frac{1}{\delta_i} &= 0.6321 L_i \log\frac{1}{\delta} \cdot \log\log\frac{1}{\delta} \\
&\leq 1 + 0.6321 L_i \log\frac{1}{\delta} \cdot \log\log\frac{1}{\delta} \\
&\leq (1 + L_i \log\frac{1}{\delta} \cdot \log\log\frac{1}{\delta})^{0.6321} \\
&\leq \exp(W(L_i \log\frac{1}{\delta} \cdot \log\log\frac{1}{\delta})).
\end{aligned}$$

Thus,

$$\log\frac{1}{\delta_i} \cdot \log\log\frac{1}{\delta_i} \leq W(L_i \log\frac{1}{\delta} \cdot \log\log\frac{1}{\delta}) \exp(W(L_i \log\frac{1}{\delta} \cdot \log\log\frac{1}{\delta})) = L_i \log\frac{1}{\delta} \cdot \log\log\frac{1}{\delta}. \tag{6}$$

The total budget used is

$$\begin{aligned}
\sum_{j=1}^{J} K_j(\delta_j, SAH\delta_j) &\leq \sum_{j=1}^{J} 2^{j+1} C_K(\delta_j, SAH\delta_j, J) \\
&\leq \sum_{j=1}^{J} 2^{J+1} C_K(\frac{1}{8SAH}, \frac{1}{8}, J) \\
&\leq 2J(1 + \frac{\log(2)B}{c(B)})^{0.6321} C_K(\frac{1}{8SAH}, \frac{1}{8}, J) \\
&\leq 2J(1 + \frac{B}{c(B)}) C_K(\frac{1}{8SAH}, \frac{1}{8}, J),
\end{aligned}$$

where the second inequality follows from equation 6 and that C_K has $\log(\frac{1}{\delta})\log\log(\frac{1}{\delta})$ dependence. If $B \geq c(B)$, then the above is bounded by

$$\frac{4JB}{c(B)} C_K(\frac{1}{8SAH}, \frac{1}{8}, J) = B.$$

We now prove the second part. By union bounding Theorem C.1 over $i = 1, 2, \dots i_\varepsilon$, (1) hold with probability at least

$$1 - \sum_{i=1}^{i_\varepsilon} \delta_i \geq 1 - i_\varepsilon \delta_{i_\varepsilon}.$$

Here, $\delta_{i_\varepsilon} = \exp(-\tilde{\Theta}(L_{i_\varepsilon}))$ by the definition and

$$L_{i_\varepsilon} = 2^{J-i_\varepsilon} \geq \frac{\varepsilon}{4SH^2}(1+\frac{\log(2)B}{c(B)})^{0.6321} \geq \frac{\varepsilon}{4SH^2}(1+0.6321\frac{\log(2)B}{c(B)}) \geq \frac{\varepsilon}{4SH^2}\cdot 0.6321\frac{\log(2)B}{c(B)}.$$

Thus, (1) holds with probability at least $1 - \exp\left(-\tilde{\Theta}\left(\frac{\varepsilon B}{C_{\mathrm{L2E}}(B)}\right)\right)$. Similarly, (2) holds with probability at least

$$1 - SA\sum_{i=1}^{i_\varepsilon} \delta_i.$$

Since SA becomes $\log(SA)$ when moving into the exponential, (2) also holds with probability at least $1 - \exp\left(-\tilde{\Theta}\left(\frac{\varepsilon B}{C_{\mathrm{L2E}}(B)}\right)\right)$. We next compute the probability that (3) holds. For simplicity, let's consider the level $i = i_\varepsilon$, in which the failure probability $SA\delta_{i_\varepsilon}$ is dominant. For the collection of samples via rerunning policies to be successful, we need both $\mathcal{D}_{1,\delta_{i_\varepsilon}}$ and $\mathcal{D}_{2,\delta_{i_\varepsilon}}$ to hold. $\mathcal{D}_{1,\delta_{i_\varepsilon}}$ holds with probability at least $1 - \frac{SA\delta_{i_\varepsilon}}{2}$. On the event $\mathcal{D}_{1,\delta_{i_\varepsilon}}$, consider rerunning each policy in Π_{i_ε} for A times. By Lemma 21, with probability $1 - \exp(-\frac{1}{2}A\log(\frac{1}{eSA\delta_{i_\varepsilon}}))$, at least for $\frac{A}{2}$ trials of repetition, we collect $\frac{N_{i_\varepsilon}}{4}$ samples of each $(s,a) \in \mathcal{X}_{i_\varepsilon}$, which means we collect at least $\frac{AN_{i_\varepsilon}}{8}$ samples of each $(s,a) \in \mathcal{X}_{i_\varepsilon}$. Thus, the probability that there exists some $(s,a) \in \mathcal{X}_{i_\varepsilon}$, the sample number of which is less than $\frac{AN_{i_\varepsilon}}{8}$ is

$$\exp\left(-\frac{1}{2}A\log(\frac{1}{eSA\delta_{i_\varepsilon}})\right) = \exp\left(-\tilde{\Theta}\left(\frac{\varepsilon AB}{C_{\mathrm{L2E}}(B)}\right)\right).$$

However, the failure probability of $\mathcal{D}_{1,\delta_{i_\varepsilon}}$ is already $\exp\left(-\tilde{\Theta}\left(\frac{\varepsilon B}{C_{\mathrm{L2E}}(B)}\right)\right)$, which is more dominant. Thus, (3) also holds with probability $1 - \exp\left(-\tilde{\Theta}\left(\frac{\varepsilon B}{C_{\mathrm{L2E}}(B)}\right)\right)$. The theorem is proven. □

C.3 BOOSTING TECHNIQUE

In this subsection, we develop an alternative algorithm of FB-L2E. The core mechanism of this alternative is the boosting technique, which repeatedly executes independent trials. The number of repetitions and the failure probability is in the exponential relationship as we can see in the following lemma.

Lemma 21. *Let $\mathcal{E}$ be an event from a random trial such that $\mathbb{P}(\mathcal{E}) \leq \delta$ Let $\alpha \in (\delta, 1)$. Let N be the number of trials where $\mathcal{E}$ is true out of L trials. Assume $\alpha > \delta$. Then,*

$$\mathbb{P}(\frac{N}{L} \geq \alpha) \leq \exp\left(-\alpha L \ln\left(\frac{\alpha}{e\delta}\right)\right)$$

Proof. Recall the KL divergence based concentration inequality where $\hat{\mu}_n$ is the sample mean of n Bernoulli i.i.d. random variables with head probability μ:

$$\mathbb{P}(\hat{\mu}_n - \mu \geq \varepsilon) \leq \exp(-n\mathsf{kl}(\mu+\varepsilon, \mu)) .$$

Note that N/L can be viewed as the sample mean of Bernoulli trials with $\mu := \mathbb{P}(\mathcal{E})$. Then,

$$\begin{aligned}\mathbb{P}(N \geq \alpha L) &= \mathbb{P}(\frac{N}{L} \geq \alpha) \\ &= \mathbb{P}(\frac{N}{L} - \mu \geq \alpha - \mu)\end{aligned}$$

Algorithm 4 **F**ixed **B**udget **L**earn to **E**xplore with **B**oosting for **S**ingleton (FB-L2E-BS)

function FB-L2E-BS($\mathcal{X} = \{(s,a)\} \subseteq \mathcal{S} \times \mathcal{A}$, step h, budget B)
  if $|\mathcal{X}| = 0$ **then**
    return $\{(\emptyset, \emptyset, 0,)\}$
  end if
  $J \leftarrow \lceil 0.6321 \log_2(1 + \frac{\log(2)B}{c(B)}) \rceil$
  for $j = 1, \ldots, J$ **do**
    $K_j \leftarrow K_j(\frac{1}{8SAH}, \frac{1}{8}), \quad N_j \leftarrow K_j/(4|\mathcal{X}| \cdot 2^j), \quad L_j \leftarrow 2^{J-j}$
    for $m = 1, \ldots, L_j$ **do**
      $\mathcal{Y}_{j,m}, \Pi_{j,m} = \texttt{FindExplorableSets}(\mathcal{X}, h, \frac{1}{8SAH}, K_j, N_j)$
    end for
    Calculate the votes: $\forall (s,a) \in \mathcal{X}, v_{s,a} \leftarrow \sum_{m=1}^{L_j} \mathbb{1}\{(s,a) \in \mathcal{Y}_{j,m}\}$.
    Filter out only if chosen at least half the time: $\mathcal{X}_j \leftarrow \{(s,a) \mid v_{s,a} \geq L_j/2\}$
    $\Pi_j = \cup_{m=1}^{L_j} \Pi_{j,m}$
    $\mathcal{X} \leftarrow \mathcal{X} \backslash \mathcal{X}_j$
  end for
  return $\{(\mathcal{X}_j, \Pi_j, N_j)\}_{j=1}^{J}$
end function

$$
\begin{aligned}
&\leq \exp(-L\mathsf{kl}(\alpha, \mu)) \\
&= \exp\left(-L\left(\alpha \ln(\alpha/\mu) + (1-\alpha)\ln\frac{1-\alpha}{1-\mu}\right)\right) \\
&\overset{(a)}{\leq} \exp\left(-L\left(\alpha\ln(\alpha/\mu) - \alpha\right)\right) \\
&\leq \exp\left(-L\left(\alpha\ln(\alpha/\delta) - \alpha\right)\right)
\end{aligned}
$$

where (a) is by the following derivation:

$$
\begin{aligned}
(1-\alpha)\ln\frac{1-\alpha}{1-\mu} &= -(1-\alpha)\ln\frac{1-\mu}{1-\alpha} \\
&= -(1-\alpha)\ln\left(1 + \frac{\alpha-\mu}{1-\alpha}\right) \\
&\geq -(\alpha - \mu) \\
&\geq -\alpha
\end{aligned}
$$

□

The alternative algorithm, FB-L2E-BS is described in Algorithm 0. Although it only applies to singleton subsets (subset of size 1), one can flexibly change the regret minimization algorithm in FINDEXPLORABLESETS. It was crucial for our result that the regret bound of STRONGEULER has $\log(\frac{1}{\delta})$ dependence. However, for FB-L2E-BS, we can use algorithms such as EULER, which has $\log^3(\frac{1}{\delta})$ dependence in the lower order term.

We briefly argue that the statements of Theorem 3.1 also hold for FB-L2E-BS used for singleton subset. The total budget used is

$$
\begin{aligned}
\sum_{j=1}^{J} 2^{J-j} K_j &= J 2^{J+1} C_K(\frac{1}{8SAH}, \frac{1}{8}, J) \\
&\leq 2J(1 + \frac{\log(2)B}{c(B)})^{0.6321} C_K(\frac{1}{8SAH}, \frac{1}{8}, J) \\
&\leq 2J(1 + \frac{\log(2)B}{c(B)}) C_K(\frac{1}{8SAH}, \frac{1}{8}, J).
\end{aligned}
$$

If $B \geq c(B)$, then the above is bounded by

$$\frac{4JB}{c(B)} C_K(\frac{1}{8SAH}, \frac{1}{8}, J) = B.$$

Let $\delta = \frac{1}{8SAH}, \delta_{\text{samp}} = \frac{1}{8}$. The crucial part for other statements in Theorem 3.1, was to make the failure probability of the j-th iteration in the form of

$$(c_1\delta)^{c_2 L_j} \tag{7}$$

for some constant c_1, c_2, which was done by defining δ_i as this form in FB-L2E. Once we get equation 7, the dominant term becomes $(c_1\delta)^{c_2 L_{i_\varepsilon}} = \exp\left(-\tilde{\Theta}\left(\frac{\varepsilon B}{C_{\text{L2E}}(B)}\right)\right)$. We show that equation 7 can also be obtained for FB-L2E-BS.

Assume $W_h(s) \in (2^{-i}, 2^{-i+1}]$ for $i \leq J$. Let's call i as the *reachable index* of s at h. Let $\mathcal{N}_j$ be the event that (s, a) is not filtered in j-th boosted FES. By Lemma 16,

$$\mathbb{P}\left((s,a) \text{ is not filtered in } i\text{-th step by a single FES}| \cap_{j=1}^{i-1} \mathcal{N}_j\right) \leq \delta.$$

If we apply Lemma 21, we obtain the form of equation 7 as

$$\mathbb{P}\left(\cap_{j=1}^{i} \mathcal{N}_j\right) \leq \mathbb{P}\left(\mathcal{N}_i| \cap_{j=1}^{i-1} \mathcal{N}_j\right) \leq \exp\left(-\frac{1}{2} L_i \log \frac{1}{2e\delta}\right).$$

We say that (s, a) is *upper well-filtered* at h if (s, a) is filtered in the index j for some $j \leq i$.

Now we consider the j-th boosted FES for some $j \leq i - 4$. By Lemma 14, 19,

$$\mathbb{P}\left((s,a) \text{ is filtered in } j\text{-th step by a single FES}| \cap_{k=1}^{j-1} \mathcal{N}_k\right) \leq \frac{\delta_{\text{samp}}}{2SAH}.$$

Thus, by Lemma 21, we obtain the form of equation 7 as

$$\mathbb{P}\left(\cap_{k=1}^{j-1} \mathcal{N}_k, \quad \mathcal{N}_j^{\mathsf{c}}\right) \leq \mathbb{P}\left(\mathcal{N}_j^{\mathsf{c}}| \cap_{k=1}^{j-1} \mathcal{N}_k\right) \leq \exp\left(-\frac{1}{2} L_j \log \frac{SAH}{e\delta_{\text{samp}}}\right).$$

We say that (s, a) is *lower well-filtered* at h if (s, a) is not filtered in the indices j with $j \leq i - 4$. We also say that (s, a) is *well-filtered* at h if (s, a) is both upper and lower well-filtered at h. We have

$$\mathbb{P}\left((s,a) \text{ is not lower well-filtered at } h\right) \leq \sum_{j=1}^{i-4} \exp\left(-\frac{1}{2} L_j \log \frac{SAH}{e\delta_{\text{samp}}}\right) \leq i \exp\left(-\frac{1}{2} L_i \log \frac{SAH}{e\delta_{\text{samp}}}\right).$$

Thus, we have

$$\mathbb{P}\left((s,a) \text{ is well-filtered at } h\right) \geq 1 - \exp\left(-\frac{1}{2} L_i \log \frac{1}{2e\delta}\right) - i \exp\left(-\frac{1}{2} L_i \log \frac{SAH}{e\delta_{\text{samp}}}\right).$$

Recall that $\varepsilon \geq 2SH^2\varepsilon_B$ and $i_\varepsilon := \lceil \log_2(\frac{2SH^2}{\varepsilon}) \rceil$. We define the set

$$\mathcal{S}_\varepsilon = \{(s,h) : \text{the reachable index of } s \text{ at } h \leq i_\varepsilon\}$$

and the event

$$\mathcal{M}_\varepsilon = \{(s,a) \text{ is well-filtered at } h \text{ for all } (s,h) \in S_\varepsilon\}.$$

By using the monotonicity of L_i and union bound, we have the following.

Lemma 22.

$$\begin{aligned}\mathbb{P}(\mathcal{M}_\varepsilon) &\geq 1 - SH \exp\left(-\frac{1}{2} L_{i^*} \log \frac{1}{2e\delta}\right) - SHi_\varepsilon \exp\left(-\frac{1}{2} L_{i^*} \log \frac{SAH}{e\delta_{\text{samp}}}\right) \\ &= 1 - \exp\left(-\tilde{\Theta}\left(\frac{\varepsilon B}{C_{\text{L2E}}(B)}\right)\right).\end{aligned}$$

Let $W_h(S) \in (2^{-i}, 2^{-i+1}]$ and assume that $\mathcal{D}_{1,\delta}$ happened for at least $\frac{L_j}{2}$, where j is the index that (s,a) is filtered. We denote the number of (s,a) samples at horizon h when running each policy in a policy set Π A times as $N^A_\Pi(s,a,h)$. Let $I \subset [L_j]$ be the set of indices that $\mathcal{D}_{1,\delta}$ happened, which means $|I| \geq L_j/2$. Assume $m \in I$. If we rerun each policy in $\Pi_{j,m}$ once,

$$\mathbb{P}(\#\text{ of } (s,a) \text{ samples at horizon } h < \frac{1}{4}N_j) \leq \frac{\delta_{\text{samp}}}{H}$$

by Lemma 18. Now consider rerunning each policy in $\Pi_{j,m}$ A times. Since running policies are independent, we can think of the process as A repetition of running each policy in $\Pi_{j,m}$ once. Thus, we get

$$\mathbb{P}(N^A_{\Pi_{j,m}}(s,a,h) < \frac{1}{8}AN_j) \leq \mathbb{P}(\sum_{i=1}^{A} \mathbb{I}^i_{\{N^1_{\Pi_{j,m}}(s,a,h) < \frac{1}{4}N_j\}} \geq \frac{A}{2}) \leq \exp(-\frac{A}{2}\ln(H/2e\delta_{\text{samp}})),$$

where $\mathbb{I}^i$ is the indicator function for i-th repetition of running each policy in $\Pi_{j,m}$ and the second inequality follows from Lemma 21. If we rerun each policy in Π_j A times,

$$\begin{aligned}\mathbb{P}(N^A_{\Pi_j} < \frac{1}{32}AN_jL_j) \leq \mathbb{P}(\sum_{m\in I} \mathbb{I}_{\{N^A_{\Pi_{j,m}}(s,a,h) < \frac{1}{8}AN_j\}} \geq \frac{|I|}{2}) &\leq \exp(-\frac{Y}{2}\ln(1/2e\exp(-\frac{A}{2}\ln(H/2e\delta_{\text{samp}})))) \\ &\leq \exp(-\frac{L_j}{4}\ln(1/2e\exp(-\frac{A}{2}\ln(H/2e\delta_{\text{samp}})))) \\ &\leq \exp\left(-\tilde{\Theta}\left(AL_j\right)\right)\end{aligned}$$

by Lemma 21. If this happens, let's say that (s,a) is *well-collected* at horizon h for A repetition. However, the failure probability

$$\mathbb{P}(\mathcal{D}_{1,\delta} \text{ happened less than } \frac{L_j}{2}) \leq \exp\left(-\tilde{\Theta}\left(L_j\right)\right),$$

which is more dominant. Thus, the following holds.

Lemma 23. *Consider s whose reachable index at h is $i \leq i_\varepsilon$. If we replay policies saved for (s,a) A times, the number T_{hs} of (s,a) samples we get satisfies*

$$\mathbb{P}\left(T_{hs} < \frac{AN_iL_i}{16}\right) \leq \exp\left(-\tilde{\Theta}\left(\frac{\varepsilon B}{C_{\text{L2E}}(B)}\right)\right).$$

D Analysis of SAR

Fix $\varepsilon \geq 0$. We say that an arm i of a bandit m is ε-*good* if $\mu_{m,1} - \mu_{m,i} \leq \varepsilon$. An arm is ε-*bad* if it is not ε-good. Let $g_m(\varepsilon)$ denote the number of ε-good arms in bandit m. We write $k^* := \max\left\{k : \bar{\Delta}_{(KM+1-k)} > \varepsilon\right\}$ and define the following two key events:

$$\begin{aligned}\mathcal{E}_1 &= \left\{\forall k \in [k^*], \quad \tfrac{\varepsilon}{2}\text{-good pairs are not rejected at the end of phase } k\right\} \\ \mathcal{E}_2 &= \{\forall k \in [(k^*+1), \ldots, K], \quad \text{for every active bandit } m \text{ containing an } \varepsilon\text{-bad arm} \\ &\qquad\qquad \text{at the beginning of phase } k, \text{ an } \tfrac{\varepsilon}{2}\text{-good arm in bandit } m \text{ is not rejected}\Big\}\end{aligned}$$

We first show that the intersection of these two events leads to a successful good arm identification for every bandit.

Lemma 24. *Suppose $\mathcal{E}_1 \cap \mathcal{E}_2$ holds. Then for every $m \in [M]$, the accepted arm is ε-good.*

Proof. Suppose the conclusion is not true; i.e., there exists a bandit m for which an ε-bad arm (m,b) has been accepted. Then, there exists a phase $k \in [KM-1]$ where the best arm $(m,1)$ is rejected from bandit m. Due to $\mathcal{E}_1$ and the fact that arm $(m,1)$ is an $\frac{\varepsilon}{2}$-good arm, we know $k \geq k^*+1$. Now, at the beginning of phase k, the bandit m must contain both (m,b) and $(m,1)$. However, due to $\mathcal{E}_2$, the arm $(m,1)$ cannot be rejected, which contradicts our supposition. □

Furthermore, consider the following event

$$\mathcal{E}_0 = \left\{ \forall m \in [M], \forall i \in [K], \forall k \in [MK-1],\ \left|\hat{\mu}_{m,i}(n_k) - \mu_{m,i}\right| < \frac{1}{8}(\bar{\Delta}_{(MK+1-k)} \vee \bar{\Delta}_{(g(\varepsilon)+1)}) \right\}$$

Lemma 25. $\mathcal{E}_0 \implies \mathcal{E}_1 \cap \mathcal{E}_2$

Proof. Assume $\mathcal{E}_0$. To show $\mathcal{E}_1$, it suffices to show that, for every $k \in [k^*]$, if no $\frac{\varepsilon}{2}$-good arm was rejected before phase k then no $\frac{\varepsilon}{2}$-good arm will be rejected in phase k (i.e., either accepts an arm or rejects a non-$\frac{\varepsilon}{2}$-good arm).

So, let $k \in [k^*]$, which implies that $\bar{\Delta}_{(MK+1-k)} > \varepsilon$ by definition, and assume that no $\frac{\varepsilon}{2}$-good arm was rejected before phase k. Furthermore, $\mathcal{E}_1$ is trivially true if the phase k accepts an arm. Thus, it suffices to assume that the phase k does not accept an arm.

We claim that, at the beginning of phase k, there exists an arm $(\bar{m}, \bar{i}) \in S$ such that

$$\mu_{\bar{m},1} - \mu_{\bar{m},\bar{i}} \geq \bar{\Delta}_{(MK+1-k)} \,.$$

Hereafter, we omit (n_k) from $\hat{\mu}_{\cdot,\cdot}(n_k)$. To prove this claim, first note that there exists $(m', i') \in S$ such that

$$\bar{\Delta}_{m',i'} \geq \bar{\Delta}_{(MK+1-k)} \,.$$

(To see this, first, confirm that this is true with equality if the arm $(MK+1-k)$ is rejected or accepted at each phase k; now, notice that if an arm other than $(MK+1-k)$ was rejected or accepted, then it only makes the equality into $\geq$.) Then, we have the following two cases:

- If $i' \neq 1$, then $\bar{\Delta}_{m',i'} = \mu_{m',1} - \mu_{m',i'}$ by definition, so we can take $\bar{m} = m'$ and $\bar{i} = i'$ to prove the claim.
- If $i' = 1$, then, since phase k does not accept an arm, there must exist another surviving arm $i'' \neq 1$ in bandit m'. Since $\bar{\Delta}_{m',i''} = \mu_{m',1} - \mu_{m',i''}$ and

  $$\bar{\Delta}_{m',i''} \geq \bar{\Delta}_{m',2} = \bar{\Delta}_{m',1} = \bar{\Delta}_{m',i'} \geq \bar{\Delta}_{(MK+1-k)} \,,$$

  we can choose $\bar{m} = m'$ and $\bar{i} = i''$ to prove the claim.

Assume that $\mathcal{E}_1$ is false; i.e., an $\frac{\varepsilon}{2}$-good arm in bandit m is rejected. This implies that there exists an active bandit m such that

$$\exists g \in [g_m(\tfrac{\varepsilon}{2})] : \hat{\mu}_{m,\hat{1}_m} - \hat{\mu}_{m,g} \geq \hat{\mu}_{\bar{m},\hat{1}_{\bar{m}}} - \hat{\mu}_{\bar{m},\bar{i}} \,.$$

Note that, using $\mathcal{E}_0$ and $\mu_{m,\hat{1}_m} - \mu_{m,g} \leq \mu_{m,1} - \mu_{m,g} \leq \frac{\varepsilon}{2} < \frac{1}{2}\bar{\Delta}_{(MK+1-k)}$,

$$\begin{aligned}
(\text{LHS}) &= \hat{\mu}_{m,\hat{1}_m} - \mu_{m,\hat{1}_m} + \mu_{m,\hat{1}_m} - \mu_{m,g} + \mu_{m,g} - \hat{\mu}_{m,g} \\
&< \frac{\bar{\Delta}_{(MK+1-k)}}{8} + \frac{\bar{\Delta}_{(MK+1-k)}}{2} + \frac{\bar{\Delta}_{(MK+1-k)}}{8} \\
&= \frac{3}{4}\bar{\Delta}_{(MK+1-k)} \,.
\end{aligned}$$

On the other hand,

$$\begin{aligned}
(\text{RHS}) &\geq \hat{\mu}_{\bar{m},1} - \hat{\mu}_{\bar{m},\bar{i}} \qquad ((m,1) \in S \text{ since no } \tfrac{\varepsilon}{2}\text{-good arm rejected before phase } k) \\
&= \hat{\mu}_{\bar{m},1} - \mu_{\bar{m},1} + \mu_{\bar{m},1} - \mu_{\bar{m},\bar{i}} + \mu_{\bar{m},\bar{i}} - \hat{\mu}_{\bar{m},\bar{i}} \\
&> -\frac{1}{8}\bar{\Delta}_{(MK+1-k)} + \bar{\Delta}_{(MK+1-k)} - \frac{1}{8}\bar{\Delta}_{(MK+1-k)} \\
&\geq \frac{3}{4}\bar{\Delta}_{(MK+1-k)} \,.
\end{aligned}$$

This is a contradiction.

We now prove $\mathcal{E}_2$. Suppose not; there exists a phase $k \geq k^* + 1$ and a bandit m active at the beginning of phase k where an $\frac{\varepsilon}{2}$-good arm (g, m) is rejected even if there was a surviving bad arm (b, m). This means that

$$\hat{\mu}_{m,g} \leq \hat{\mu}_{m,b}$$

On the other hand, note that $k \geq k^* + 1$ implies $\bar{\Delta}_{(MK+1-k)} \leq \bar{\Delta}_{(g(\varepsilon)+1)}$, so $\bar{\Delta}_{(MK+1-k)} \vee \bar{\Delta}_{(g(\varepsilon)+1)} = \bar{\Delta}_{(g(\varepsilon)+1)}$. Thus,

$$\begin{aligned}
\hat{\mu}_{m,g} - \hat{\mu}_{m,b} &= \hat{\mu}_{m,g} - \mu_{m,g} + \mu_{m,g} - \mu_{m,b} + \mu_{m,b} - \hat{\mu}_{m,b} \\
&> -\frac{1}{8}\bar{\Delta}_{(g(\varepsilon)+1)} + \mu_{m,g} - \mu_{m,b} - \frac{1}{8}\bar{\Delta}_{(g(\varepsilon)+1)} && (\mathcal{E}_0) \\
&\geq -\frac{1}{8}\bar{\Delta}_{(g(\varepsilon)+1)} + \frac{1}{2}\bar{\Delta}_{(g(\varepsilon)+1)} - \frac{1}{8}\bar{\Delta}_{(g(\varepsilon)+1)} && \text{(definition of } g \text{ and } b) \\
&> 0
\end{aligned}$$

This is a contradiction. □

Let

$$H_1(\varepsilon) := \sum_{i=1}^{MK} \frac{1}{(\bar{\Delta}_{(i)} \vee \varepsilon)^2}, \quad H_2(\varepsilon) := \max_{i \geq g(\varepsilon)+1} \frac{i}{\bar{\Delta}^2_{(i)}}.$$

We present a relation between these two gap-dependent quantities.

Lemma 26. $H_2(\varepsilon) \leq H_1(\varepsilon) \leq \frac{g(\varepsilon)}{\varepsilon^2} + \log(\frac{MK}{g(\varepsilon)})H_2(\varepsilon)$.

Proof. Let $i^* = \arg\max_{i \geq g(\varepsilon)+1} i\bar{\Delta}_i^{-2}$. Note that

$$\begin{aligned}
H_1(\varepsilon) = \sum_{i \geq 1} (\bar{\Delta}_i \vee \varepsilon)^{-2} &\geq \sum_{i=1}^{g(\varepsilon)} \bar{\Delta}^{-2}_{g(\varepsilon)+1} + \sum_{i \geq g(\varepsilon)+1} \Delta_i^{-2} \\
&\geq \sum_{i=1}^{g(\varepsilon)} \bar{\Delta}^{-2}_{g(\varepsilon)+1} + \sum_{i=g(\varepsilon)+1}^{i^*} \bar{\Delta}^{-2}_{i^*} \\
&= \sum_{i=1}^{g(\varepsilon)} \bar{\Delta}^{-2}_{g(\varepsilon)+1} + (i^* - g(\varepsilon))\bar{\Delta}^{-2}_{i^*} \\
&= \sum_{i=1}^{g(\varepsilon)} \bar{\Delta}^{-2}_{g(\varepsilon)+1} + H_2(\varepsilon) - g(\varepsilon)\bar{\Delta}^{-2}_{i^*} \\
&\geq \sum_{i=1}^{g(\varepsilon)} \bar{\Delta}^{-2}_{g(\varepsilon)+1} + H_2(\varepsilon) - g(\varepsilon)\bar{\Delta}^{-2}_{g(\varepsilon)+1} \\
&\geq H_2(\varepsilon).
\end{aligned}$$

For the right inequality,

$$\begin{aligned}
H_1(\varepsilon) = \sum_{i \geq 1} \frac{1}{i} i(\bar{\Delta}_i \vee \varepsilon)^{-2} &= \\
&\leq \sum_{i=1}^{g(\varepsilon)} \frac{1}{i} i\varepsilon^{-2} + \sum_{i=g(\varepsilon)+1}^{MK} \frac{1}{i} H_2(\varepsilon) \\
&\leq \frac{g(\varepsilon)}{\varepsilon^2} + \log(\frac{MK}{g(\varepsilon)})H_2(\varepsilon).
\end{aligned}$$

□

We are now ready to prove Theorem 3.2.

Theorem D.1 (Refinement of Theorem 3.2)**.** If we run Algorithm 2 with $B \geq MK$, then the total number of budget used is at most B and

$$\mathbb{P}(\exists m \in [M] : \mu_{m,1} - \mu_{m,J_B(m)} > \varepsilon) \leq 2M^2K^2 \exp\left(-\frac{B - MK}{128\sigma^2 \overline{\log}(MK) \cdot \max_{i \geq g(\varepsilon)+1} i\bar{\Delta}_{(i)}^{-2}}\right)$$
$$\leq 2M^2K^2 \exp\left(-\frac{B - MK}{128\sigma^2 \overline{\log}(MK) \cdot \sum_{i \in [MK]} (\bar{\Delta}_{(i)} \vee \varepsilon)^{-2}}\right).$$

Proof. For the first part, the total budget used is bounded as

$$\sum_{k=1}^{MK-1} n_k(B, M, K) + n_{MK-1}(B, M, K) \leq MK + \frac{B - MK}{\overline{\log}(MK)} \left(\frac{1}{2} + \sum_{k=1}^{MK-1} \frac{1}{MK + 1 - k}\right) = B,$$

where we used $\lceil x \rceil \leq 1 + x$ For the second part, it suffices to bound $\mathbb{P}(\overline{\mathcal{E}}_0)$ by Lemma 24 and Lemma 25. Fix a bandit m and an arm i. Then,

$$\mathbb{P}\left(\exists k \in [KM-1] : \left|\hat{\mu}_{m,i}(n_k) - \mu_{m,i}\right| \geq \frac{1}{8}(\bar{\Delta}_{(MK+1-k)} \vee \bar{\Delta}_{(g(\varepsilon)+1)})\right)$$
$$\leq \sum_{k=1}^{KM-1} 2\exp\left(-\frac{n_k}{2\sigma^2} \cdot \frac{(\bar{\Delta}_{(MK+1-k)} \vee \bar{\Delta}_{(g(\varepsilon)+1)})^2}{64}\right)$$
$$\leq \sum_{k=1}^{KM-1} 2\exp\left(-\frac{B - MK}{\overline{\log}(MK) \cdot (MK + 1 - k)} \frac{(\bar{\Delta}_{(MK+1-k)} \vee \bar{\Delta}_{(g(\varepsilon)+1)})^2}{128\sigma^2}\right)$$
$$\leq 2MK \exp\left(-\frac{B - MK}{128\sigma^2 \overline{\log}(MK) \cdot \max_{i \in [2..MK]} i(\bar{\Delta}_{(i)} \vee \bar{\Delta}_{(g(\varepsilon)+1)})^{-2}}\right)$$
$$\leq 2MK \exp\left(-\frac{B - MK}{128\sigma^2 \overline{\log}(MK) \cdot \max_{i \geq g(\varepsilon)+1} i\bar{\Delta}_{(i)}^{-2}}\right).$$

Taking a union bound over $m \in [M]$ and $i \in [K]$ and Lemma 26 completes the proof. □

Note that when $\varepsilon = 0$, this theorem recovers the best arm identification result of Bubeck et al. (2013).

Remark 27. *If we set $M = 1$, SAR becomes a single bandit algorithm. Consider running this single bandit SAR to each bandit $m \in [M]$ with budget B/M. Then, we have*

$$\mathbb{P}(\mu_{m,1} - \mu_{m,J(m)} > \varepsilon) \leq \exp\left(-\tilde{\Theta}\left(\frac{B/M}{\sum_i (\bar{\Delta}_{m,i} \vee \varepsilon)^{-2})}\right)\right)$$

for each bandit $m \in [M]$. This yields

$$\mathbb{P}(\exists m \in [M] : mu_{m,1} - \mu_{m,J(m)} > \varepsilon) \leq \exp\left(-\tilde{\Theta}\left(\frac{B/M}{\max_m \sum_i (\bar{\Delta}_{m,i} \vee \varepsilon)^{-2})}\right)\right),$$

which is worse than the result of Theorem 3.2 since

$$\sum_m \sum_i (\bar{\Delta}_{m,i} \vee \varepsilon)^{-2}) \leq M \max_m \sum_i (\bar{\Delta}_{m,i} \vee \varepsilon)^{-2}).$$

Due to this difference, if we use single bandit algorithm in BREA, we get the term

$$\exp\left(-\tilde{\Theta}\left(\frac{B}{H^5 \max_{h \in [H]} C_h^2 S \max_{s \in \mathcal{S}} W_h(s)^{-1} \sum_{a \in \mathcal{A}} (\bar{\Delta}_h(s,a) \vee \frac{\varepsilon}{W_h(s)})^{-2}}\right)\right),$$

which is worse than the actual term

$$\exp\left(-\tilde{\Theta}\left(\frac{B}{H^5 \max_{h \in [H]} C_h^2 \sum_{s \in \mathcal{S}} W_h(s)^{-1} \sum_{a \in \mathcal{A}} (\bar{\Delta}_h(s,a) \vee \frac{\varepsilon}{W_h(s)})^{-2}}\right)\right)$$

of Theorem 3.3.

E Proof of Theorem 3.3 and Corollary 3

In this section, we provide an analysis of BREA. Recall that $\varepsilon \geq 2SH^2\varepsilon_B$ and $i_\varepsilon = \lceil \log_2(\frac{2SH^2}{\varepsilon}) \rceil$ We define the events

$$
\begin{aligned}
\mathcal{M}_{h,\varepsilon} =& \Big\{ \text{For any } s \in \mathcal{S}, \\
& \quad \text{FB-L2E}(\{(s,1)\}, h, B') \text{ outputs } \mathcal{X}_i = \{(s,1)\} \text{ for some } i \leq i_\varepsilon \implies 2^{-i-3} \leq W_h(s) \leq 2^{-i+1}, \\
& \quad \text{FB-L2E}(\{(s,1)\}, h, B') \text{ outputs } \mathcal{X}_i = \emptyset \text{ for all } i \in [i_\varepsilon] \implies W_h(s) \leq \frac{\varepsilon}{2SH^2} \Big\}, \\
\mathcal{M}_\varepsilon =& \cup_{h=1}^H \mathcal{M}_{h,\varepsilon}, \\
\mathcal{L}_{h,\varepsilon} =& \Big\{ \text{For any } i \leq i_\varepsilon \text{ and any phase } k \in [|\mathcal{Z}_{hi}|A - 1], \\
& \quad \text{each } (s,a) \in A_k \text{ is collected at least } \lfloor \frac{n_k}{N_i^{sh}} \rfloor \frac{N_i^{sh}}{8} \text{ times} \Big\}, \\
\mathcal{L}_\varepsilon =& \cup_{h=1}^H \mathcal{L}_{h,\varepsilon} \\
\mathcal{E}_h =& \Big\{ \Delta_h^{\hat{\pi}}(s, \hat{\pi}_h(s)) \leq \frac{\varepsilon}{2C_h H W_h(s)} \text{ for all } s \in \cup_{i=1}^{i_\varepsilon} \mathcal{Z}_{hi} \Big\}.
\end{aligned}
\tag{8}
$$

Before proving Theorem 3.3, we provide lemmas that will give us a relation between the suboptimality gap and its empirical estimate.

Lemma 28. *Let $0 < a \leq b$ and assume $f_1, f_2 \geq 0$ satisfy $|f_1 - f_2| \leq b$. Then*

$$(f_1 \vee a)^{-2} \leq (\frac{a}{2b} f_2 \vee a)^{-2}.$$

Proof. If $f_1 \leq a$, then $(f_1 \vee a)^{-2} = a^{-2}$. On the other hand, $f_2 \leq f_1 + b \leq a + b \leq 2b$. Thus,

$$(f_1 \vee a)^{-2} = a^{-2} = (\frac{a}{2b} f_2 \vee a)^{-2}.$$

If $f_1 > a$, then $(f_1 \vee a)^{-2} = f_1^{-2} < a^{-2}$. Also, $f_2 \leq f_1 + b < f_1 + \frac{f_1}{a} b = f_1(1 + \frac{b}{a}) \leq \frac{2b}{a} f_1$. Thus,

$$(f_1 \vee a)^{-2} = f_1^{-2} < (\frac{a}{2b} f_2 \vee a)^{-2}.$$

□

Lemma 29. *On $\cap_{h'=H}^{h+1} \mathcal{E}_{h'} \cap \mathcal{M}_\varepsilon \cap \mathcal{L}_\varepsilon$, we have*

$$(\Delta_h^{\hat{\pi}}(s,a) \vee \frac{\varepsilon}{2C_h H W_h(s)})^{-2} \leq 16 C_h^2 H^2 (\Delta_h(s,a) \vee \frac{2\varepsilon}{W_h(s)})^{-2}.$$

Proof. By Lemma 7, for any policy π'

$$
\begin{aligned}
\sum_s w_{h+1}^{\pi'}(s)(V_{h+1}^*(s) - V_{h+1}^{\hat{\pi}}(s)) &\leq \sum_{h'=h+1}^H \sup_\pi \sum_s w_{h'}^\pi(s) \varepsilon_h(s) \\
&\leq \sum_{h'=h+1}^H \sup_\pi \sum_{i \leq i_\varepsilon} \sum_{s \in \mathcal{Z}_{hi}} w_{h'}^\pi(s) \frac{\varepsilon}{2C_h H W_h(s)} + H \sum_{h'=h+1}^H \sum_{s \notin \cup_{i \leq i_\varepsilon} \mathcal{Z}_{hi}} \sup_\pi w_{h'}^\pi(s) \\
&\leq \sum_{h'=h+1}^H \frac{\varepsilon}{2H} + \sum_{h'=h+1}^H SH \frac{\varepsilon}{2SH^2} \\
&\leq \varepsilon.
\end{aligned}
$$

By Lemma 8,

$$|\Delta_h(s,a) - \Delta_h^{\hat{\pi}}(s,a)| \leq \frac{\varepsilon}{W_h(s)}.$$

By applying Lemma 28 with $f_1 = \Delta_h^{\hat{\pi}}(s,a), f_2 = \Delta_h(s,a), a = \frac{\varepsilon}{2C_h H W_h(s)}, b = \frac{\varepsilon}{W_h(s)}$, the proof is done. □

Theorem E.1 (Theorem 3.3)**.** *If we run Algorithm 3 with*

$$B \geq \max\{2SHc(\frac{B}{2SH}), 2SA\varepsilon_{\frac{B}{2SH}} \log_2 \frac{1}{\varepsilon_{\frac{B}{2SH}}}\},$$

then the total number of budget used is at most B. Moreover, for any $\varepsilon \geq 2SH^2\varepsilon_{\frac{B}{2SH}}$,

$$\mathbb{P}\left(V_0^* - V_0^{\hat{\pi}} > \varepsilon\right) \leq \exp\left(-\tilde{\Theta}\left(\frac{\varepsilon B}{C_{\mathrm{L2E}}(\frac{B}{2SH})}\right)\right) + \exp\left(-\tilde{\Theta}\left(\frac{B}{H^5 \max_{h\in[H]} C_h^2 \sum_{s\in\mathcal{S}} W_h(s)^{-1} \sum_{a\in\mathcal{A}} (\bar{\Delta}_h(s,a) \vee \frac{\varepsilon}{W_h(s)})^{-2}}\right)\right).$$

Proof. The budget used from the first part is

$$SH\lfloor \frac{B}{2SH} \rfloor \leq \frac{B}{2}$$

by Theorem 3.1. For the second part, we use

$$\begin{aligned}
&\sum_{i=1}^{|\mathcal{Z}_{hi}|A-1} T_i(s,a) + T_{|\mathcal{Z}_{hi}|A-1}(s,a) \\
\leq &\frac{1}{N_i}\left(\sum_{i=1}^{|\mathcal{Z}_{hi}|A-1} n_i + n_{|\mathcal{Z}_{hi}|A-1}\right) \\
\leq &\frac{\lfloor B''2^{-i-2}\rfloor}{2^{i+2}} \leq B'' = \frac{B}{2HJ} \qquad \text{(Theorem 3.2)}
\end{aligned}$$

for each multiple bandit $\mathcal{Z}_{hi}$. Thus, the budget used in the second part is at most $\frac{B}{2}$, the total budget used is at most B.

We now prove the probability bound. By Theorem 3.1 and that $B \geq 2SHc(\frac{B}{2SH})$, we have

$$\begin{aligned}
\mathbb{P}(\mathcal{M}_\varepsilon^{\mathsf{c}}) &\leq SH \exp\left(-\tilde{\Theta}\left(\frac{\varepsilon B}{C_{\mathrm{L2E}}(\frac{B}{2SH})}\right)\right) = \exp\left(-\tilde{\Theta}\left(\frac{\varepsilon B}{C_{\mathrm{L2E}}(\frac{B}{2SH})}\right)\right), \\
\mathbb{P}(\mathcal{L}_\varepsilon^{\mathsf{c}}) &\leq S^2A^2H \exp\left(-\tilde{\Theta}\left(\frac{\varepsilon B}{C_{\mathrm{L2E}}(\frac{B}{2SH})}\right)\right) = \exp\left(-\tilde{\Theta}\left(\frac{\varepsilon B}{C_{\mathrm{L2E}}(\frac{B}{2SH})}\right)\right). \qquad (9)
\end{aligned}$$

We can decompose the probability as

$$\begin{aligned}
\mathbb{P}(V_0^* - V_0^{\hat{\pi}} > \varepsilon) &\leq \mathbb{P}(V_0^* - V_0^{\hat{\pi}} > \varepsilon, \mathcal{M}_\varepsilon, \mathcal{L}_\varepsilon) + \mathbb{P}(\mathcal{M}_\varepsilon^{\mathsf{c}}) + \mathbb{P}(\mathcal{L}_\varepsilon^{\mathsf{c}}) \\
&\leq \mathbb{P}(V_0^* - V_0^{\hat{\pi}} > \varepsilon, \mathcal{M}_\varepsilon, \mathcal{L}_\varepsilon) + \exp\left(-\tilde{\Theta}\left(\frac{\varepsilon B}{C_{\mathrm{L2E}}(\frac{B}{2SH})}\right)\right). \qquad (10)
\end{aligned}$$

Assume that $\mathcal{M}_\varepsilon, \mathcal{L}_\varepsilon, \{\mathcal{E}_h\}_{h=1}^H$ holds. Then, by Lemma 7,

$$\begin{aligned}
V_0^* - V_0^{\hat{\pi}} &\leq \sum_{h=1}^H \sup_\pi \sum_s w_h^\pi(s)\varepsilon_h(s) \\
&\leq \sum_{h=1}^H \sup_\pi \sum_{i\leq i_\varepsilon} \sum_{s\in\mathcal{Z}_{hi}} w_h^\pi(s) \frac{\varepsilon}{2C_h H W_h(s)} + H\sum_{h=1}^H \sum_{s\notin\cup_{i\leq i_\varepsilon}\mathcal{Z}_{hi}} \sup_\pi w_h^\pi(s) \\
&\leq \sum_{h=1}^H \frac{\varepsilon}{2H} + SH^2\frac{\varepsilon}{2SH^2} \\
&\leq \frac{\varepsilon}{2} + \frac{\varepsilon}{2} = \varepsilon,
\end{aligned}$$

where the second inequality follows from the definition of C_h. Thus, we have

$$\mathbb{P}(V_0^* - V_0^{\hat{\pi}} > \varepsilon, \mathcal{M}_\varepsilon, \mathcal{L}_\varepsilon) \leq \sum_{h=1}^{H} \mathbb{P}(\mathcal{E}_h^{\mathsf{c}}, \mathcal{M}_\varepsilon, \mathcal{L}_\varepsilon, \cap_{h'=H}^{h+1} \mathcal{E}_{h'}). \tag{11}$$

We try to bound $\mathbb{P}(\mathcal{E}_h^{\mathsf{c}}, \mathcal{M}_\varepsilon, \mathcal{L}_\varepsilon, \cap_{h'=H}^{h+1} \mathcal{E}_{h'})$.

On the event $\mathcal{L}_\varepsilon$, every multiple bandit instance $\mathcal{Z}_{hi}$ effectively collects samples so that SAR with budget $\Theta(\frac{B}{2HJ} 2^{-i-2})$ is run. On the event $\mathcal{M}_\varepsilon$, this is $\Theta(\frac{BW_h(s)}{HJ}) = \Theta(\frac{BW_h(s)}{H})$. To be precise, the minimum budget of SAR is $\min_{s \in \mathcal{Z}_h} \frac{BW_h(s)}{2HJ} \geq \frac{B\varepsilon \frac{B}{2SH}}{2HJ}$ and this is more or equal to SA by the hypothesis of Theorem 3.3. Thus, by Theorem 3.2, we have

$$\begin{aligned}
&\mathbb{P}\left(\Delta_h^{\hat{\pi}}(s, \hat{\pi}_h(s)) > \frac{\varepsilon}{2C_h H W_h(s)} \text{ for some } s \in \mathcal{Z}_{hi}, \mathcal{M}_\varepsilon, \mathcal{L}_\varepsilon, \cap_{h'=H}^{h+1} \mathcal{E}_{h'} | \mathcal{F}_{h+1}\right) \\
&\leq \exp\left(-\tilde{\Theta}\left(\frac{B}{H^3 \sum_{(s,a) \in \mathcal{Z}_{hi} \times \mathcal{A}} W_h(s)^{-1} (\bar{\Delta}_h^{\hat{\pi}}(s,a) \vee \frac{\varepsilon}{2C_h H W_h(s)})^{-2}}\right)\right) \\
&= \exp\left(-\tilde{\Theta}\left(\frac{B}{H^3 \sum_{s \in \mathcal{Z}_{hi}} W_h(s)^{-1} \sum_{a \geq 2} (\Delta_h^{\hat{\pi}}(s,a) \vee \frac{\varepsilon}{2C_h H W_h(s)})^{-2}}\right)\right) \\
&\leq \exp\left(-\tilde{\Theta}\left(\frac{B}{C_h^2 H^5 \sum_{s \in \mathcal{Z}_{hi}} W_h(s)^{-1} \sum_{a \geq 2} (\Delta_h(s,a) \vee \frac{\varepsilon}{W_h(s)})^{-2}}\right)\right) \\
&\leq \exp\left(-\tilde{\Theta}\left(\frac{B}{C_h^2 H^5 \sum_{(s,a) \in \mathcal{Z}_{hi} \times \mathcal{A}} W_h(s)^{-1} (\bar{\Delta}_h(s,a) \vee \frac{\varepsilon}{W_h(s)})^{-2}}\right)\right),
\end{aligned} \tag{12}$$

where the second inequality follows from Lemma 29, $\mathcal{F}_{h+1}$ is a filtration up to learning in step $h+1$. Thus, we have

$$\begin{aligned}
\mathbb{P}(\mathcal{E}_h^{\mathsf{c}}, \mathcal{M}_\varepsilon, \mathcal{L}_\varepsilon, \cap_{h'=H}^{h+1} \mathcal{E}_{h'}) &\leq i_\varepsilon \exp\left(-\tilde{\Theta}\left(\frac{B}{C_h^2 H^5 \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} W_h(s)^{-1} (\Delta_h(s,a) \vee \frac{\varepsilon}{W_h(s)})^{-2}}\right)\right) \\
&= \exp\left(-\tilde{\Theta}\left(\frac{B}{C_h^2 H^5 \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} W_h(s)^{-1} (\Delta_h(s,a) \vee \frac{\varepsilon}{W_h(s)})^{-2}}\right)\right).
\end{aligned}$$

If we plug this into equation 11 and equation 10, we get the probability bound of the theorem. □

Corollary 30 (Exact statement of Corollary 3)**.** *If*

$$2SH^2 \varepsilon_{\frac{B}{2SH}} < \varepsilon^* := \min\{\min_{s,h}^{+} W_h(s), 2H \min_{s,a,h}^{+} C_h W_h(s) \bar{\Delta}_h(s,a)\},$$

we obtain a guarantee of the best policy identification, given by

$$\begin{aligned}
\mathbb{P}\left(V_0^* - V_0^{\hat{\pi}} > 0\right) &\leq \exp\left(-\tilde{\Theta}\left(\frac{\varepsilon^* B}{C_{\mathrm{L2E}}(\frac{B}{2SH})}\right)\right) \\
&\quad + \exp\left(-\tilde{\Theta}\left(\frac{B}{H^5 \max_{h \in [H]} C_h^2 \sum_{s \in \mathcal{S}} W_h(s)^{-1} \sum_{a \in \mathcal{A}} (\bar{\Delta}_h(s,a) \vee \frac{\varepsilon^*}{W_h(s)})^{-2}}\right)\right).
\end{aligned}$$

Furthermore, if the optimal action in each state s at each step h is unique, then

$$\begin{aligned}
\mathbb{P}\left(V_0^* - V_0^{\hat{\pi}} > 0\right) &\leq \exp\left(-\tilde{\Theta}\left(\frac{\varepsilon^* B}{C_{\mathrm{L2E}}(\frac{B}{2SH})}\right)\right) \\
&\quad + \exp\left(-\tilde{\Theta}\left(\frac{B}{H^3 \max_{h \in [H]} \sum_{s \in \mathcal{S}} W_h(s)^{-1} \sum_{a \in \mathcal{A}} \bar{\Delta}_h(s,a)^{-2}}\right)\right).
\end{aligned}$$

Proof. Let's take any $\varepsilon_{\frac{B}{2SH}} \leq \varepsilon < \varepsilon^*$ and assume that the events $\mathcal{M}_\varepsilon, \mathcal{L}_\varepsilon, \cap_{h=1}^H \mathcal{E}_h$ hold. By the definition of $\mathcal{M}_\varepsilon$ in equation 8, $\varepsilon < 2SH^2 \min^+_{s,h} W_h(s)$ implies that any state s with $W_h(s) > 0$ lies in $\mathcal{Z}_h$ for any $h \in [H]$. Since $\Delta_H^{\hat{\pi}}(s,a) = \Delta_H(s,a)$, the event $\mathcal{E}_H$ and that $\varepsilon < 2H \min^+_{s,a,h} C_h W_h(s) \Delta_h(s,a)$ implies that $\hat{\pi}_H(s)$ is an optimal action for all $s \in \mathcal{Z}_H$. Then this implies that $\Delta_{H-1}^{\hat{\pi}}(s,a) = \Delta_{H-1}(s,a)$ holds for all s, a. Again, the event $\mathcal{E}_{H-1}$ and that $\varepsilon < 2H \min^+_{s,a,h} C_h W_h(s) \Delta_h(s,a)$ implies that $\hat{\pi}_{H-1}(s)$ is an optimal action for all $s \in \mathcal{Z}_{H-1}$. Repeating this procedure, we can conclude that $\hat{\pi}$ is optimal. The first probability bound follows by limiting the result of Theorem 3.3 as $\varepsilon \to \varepsilon^*-$.

Next, we further assume the uniqueness of the optimal actions. In equation 12 of the proof of Theorem 3.3, we may apply tha fact that $\Delta_h^{\hat{\pi}}(s,a) = \Delta_h(s,a)$ and $\varepsilon < 2H \min^+_{s,a,h} C_h W_h(s) \Delta_h(s,a)$ instead of Lemma 29 so that we obtain

$$
\begin{aligned}
&\mathbb{P}\left(\Delta_h^{\hat{\pi}}(s, \hat{\pi}_h(s)) > \frac{\varepsilon}{2C_h H W_h(s)} \text{ for some } s \in \mathcal{Z}_{hi}, \mathcal{M}_\varepsilon, \mathcal{L}_\varepsilon, \cap_{h'=H}^{h+1} \mathcal{E}_{h'} | \mathcal{F}_{h+1}\right) \\
&\leq \exp\left(-\tilde{\Theta}\left(\frac{B}{H^3 \sum_{(s,a)\in\mathcal{Z}_{hi}\times\mathcal{A}} W_h(s)^{-1} (\bar{\Delta}_h^{\hat{\pi}}(s,a) \vee \frac{\varepsilon}{2C_h H W_h(s)})^{-2}}\right)\right) \\
&= \exp\left(-\tilde{\Theta}\left(\frac{B}{H^3 \sum_{s\in\mathcal{Z}_{hi}} W_h(s)^{-1} \sum_{a\geq 2} (\Delta_h^{\hat{\pi}}(s,a) \vee \frac{\varepsilon}{2C_h H W_h(s)})^{-2}}\right)\right) \\
&= \exp\left(-\tilde{\Theta}\left(\frac{B}{H^3 \sum_{s\in\mathcal{Z}_{hi}} W_h(s)^{-1} \sum_{a\geq 2} (\Delta_h(s,a) \vee \frac{\varepsilon}{2C_h H W_h(s)})^{-2}}\right)\right) \\
&= \exp\left(-\tilde{\Theta}\left(\frac{B}{H^3 \sum_{s\in\mathcal{Z}_{hi}} W_h(s)^{-1} \sum_{a\geq 2} \Delta_h(s,a)^{-2}}\right)\right) \\
&\leq \exp\left(-\tilde{\Theta}\left(\frac{B}{H^3 \sum_{s\in\mathcal{S}} W_h(s)^{-1} \sum_{a\in\mathcal{A}} \bar{\Delta}_h(s,a)^{-2}}\right)\right).
\end{aligned}
$$

Union bound over h, combining with the exploration term and taking the limit as $\varepsilon \to \varepsilon^*-$ give the second probability bound. □

F Proof of Theorem 3.4

We present a modified algorithm, BREAP in Algorithm 5

BREAP additionally refine the policy. Intuitively, BREAP gathers good arms from the second part, additionally collects samples of them, and picks the empirically best actions.

Consider the situation where we run SAR with the set $\mathcal{Z}_{hi} \times \mathcal{A}$. Let

$$\hat{\Delta}_h^{\hat{\pi}}(s,a) := \max_{a'} \hat{Q}_h^{\hat{\pi}}(s,a') - \hat{Q}_h^{\hat{\pi}}(s,a)$$

and

$$\hat{g}_{hi}^{\hat{\pi}}(\varepsilon) := |\{(s,a) \in \mathcal{Z}_{hi} \times \mathcal{A} : \hat{\Delta}_h^{\hat{\pi}}(s,a) \leq \varepsilon\}|.$$

We define the set $\widehat{\mathrm{OPT}}_h(\varepsilon)$ as the last $\hat{g}_{hi}^{\hat{\pi}}(\frac{\varepsilon}{\hat{W}_h(s)})$ surviving pairs.

Let k^* be

$$\max\{k : \bar{\Delta}_{(|\mathcal{Z}_{hi}|A+1-k)} < \varepsilon\},$$

where $\bar{\Delta}_{(1)} \geq \bar{\Delta}_{(2)} \geq \ldots \geq \bar{\Delta}_{(|\mathcal{Z}_{hi}|A)}$ and define the events

$$\mathcal{G}_{0,\varepsilon}(\mathcal{Z}_{hi}) = \{\forall k, \forall (s,a) \in \mathcal{Z}_{hi} \times \mathcal{A}, \quad |\hat{Q}_h^{\hat{\pi}}(s,a,n_k) - Q_h^{\hat{\pi}}(s,a)| < \frac{1}{8}(\bar{\Delta}_{(|\mathcal{Z}_{hi}|A+1-k)} \vee \frac{\varepsilon}{W_h(s)})\}$$

$$\mathcal{G}_{1,\varepsilon}(\mathcal{Z}_{hi}) = \{\forall k \in [k^*], \quad \frac{\varepsilon}{2W_h(s)} - \text{good pairs are not rejected at phase } k\}$$

$\mathcal{G}_{2,\varepsilon}(\mathcal{Z}_{hi}) = \{\forall k > k^*, \quad \frac{\varepsilon}{2W_h(s)} -$ good pairs are not rejected at phase k if there exists a bad pair in the same state$\}$

as in Appendix D. We omit $\mathcal{Z}_{hi}$ when there is no confusion. We also redefine the events

$$\mathcal{E}_h = \{\sup_{\pi} \sum_{s \in \mathcal{Z}_{h1:i_\varepsilon}} w_h^\pi(s) \Delta_h^{\hat{\pi}}(s, \hat{\pi}(s)) \leq \frac{\varepsilon}{2H}\},$$

where $\mathcal{Z}_{h1:i_\varepsilon} = \cup_{i=1}^{i_\varepsilon} \mathcal{Z}_{hi}$.

We state some lemmas describing the properties of SAR process.

Lemma 31. *Under the events $\mathcal{M}_\varepsilon, \mathcal{L}_\varepsilon$, the event $\mathcal{G}_{0,\varepsilon}$ implies $\mathcal{G}_{1,\varepsilon}$ and $\mathcal{G}_{2,\varepsilon}$.*

Proof. This is just a restatement of Lemma 25. □

Lemma 32. *Under the events $\mathcal{M}_\varepsilon, \mathcal{L}_\varepsilon$,*

$$\mathbb{P}(\mathcal{G}_{0,\varepsilon}^{\mathsf{c}}) \leq \exp\left(-\tilde{\Theta}\left(\frac{W_h(s)B}{H^3 \max_i i(\Delta_{(i)} \bar{\vee} \frac{\varepsilon}{W_h(s)})^{-2}}\right)\right).$$

Proof. This is just a restatement of Theorem 3.2. □

Lemma 33. *Under the events $\mathcal{M}_\varepsilon, \mathcal{L}_\varepsilon, \mathcal{G}_{0,\varepsilon}$, if a pair (s,a) is rejected in a phase $k \in [k^*]$, then*

$$\Delta_h^{\hat{\pi}}(s,a) > \frac{1}{2}\bar{\Delta}_{(|\mathcal{Z}_{hi}|A+1-k)}.$$

Proof. There exists a pair (s', a') in the remaining set at the beginning of phase k such that

$$\Delta_h^{\hat{\pi}}(s', a') \geq \bar{\Delta}_{(|\mathcal{Z}_{hi}|A+1-k)}.$$

Since (s,a) is eliminated in phase $k \leq k^*$,

$$\hat{\Delta}_h(s,a)_k \geq \hat{\Delta}_h(s',a')_k,$$

where the subscript k is for the empirical gap until phase k. Let $a_s^* \in \arg\max_a \hat{Q}_h^{\hat{\pi}}(s,a)_k$. Then we have

$$\begin{aligned}
\hat{\Delta}_h(s,a)_k &= \hat{Q}_h^{\hat{\pi}}(s,\hat{a}_s)_k - \hat{Q}_h^{\hat{\pi}}(s,a)_k \\
&= \hat{Q}_h^{\hat{\pi}}(s,\hat{a}_s)_k - Q_h^{\hat{\pi}}(s,\hat{a}_s) + Q_h^{\hat{\pi}}(s,\hat{a}_s) - Q_h^{\hat{\pi}}(s,a) + Q_h^{\hat{\pi}}(s,a) - \hat{Q}_h^{\hat{\pi}}(s,a)_k \\
&< \frac{\bar{\Delta}_{(|\mathcal{Z}_{hi}|A+1-k)}}{8} + Q_h^{\hat{\pi}}(s,a_s^*) - Q_h^{\hat{\pi}}(s,a) + \frac{\bar{\Delta}_{(|\mathcal{Z}_{hi}|A+1-k)}}{8} \\
&= \Delta_h^{\hat{\pi}}(s,a) + \frac{\bar{\Delta}_{(|\mathcal{Z}_{hi}|A+1-k)}}{4}
\end{aligned}$$

under $\mathcal{G}_0$. On the other hand,

$$\begin{aligned}
\hat{\Delta}_h(s',a')_k &= \hat{Q}_h^{\hat{\pi}}(s',\hat{a}_{s'})_k - \hat{Q}_h^{\hat{\pi}}(s',a')_k \\
&\geq \hat{Q}_h^{\hat{\pi}}(s',a_{s'}^*)_k - \hat{Q}_h^{\hat{\pi}}(s',a')_k \\
&= \hat{Q}_h^{\hat{\pi}}(s',a_{s'}^*)_k - Q_h^{\hat{\pi}}(s',a_{s'}^*) + Q_h^{\hat{\pi}}(s',a_{s'}^*) - Q_h^{\hat{\pi}}(s',a) + Q_h^{\hat{\pi}}(s',a) - \hat{Q}_h^{\hat{\pi}}(s',a')_k \\
&> -\frac{\bar{\Delta}_{(|\mathcal{Z}_{hi}|A+1-k)}}{8} + \Delta_h^{\hat{\pi}}(s',a') - \frac{\bar{\Delta}_{(|\mathcal{Z}_{hi}|A+1-k)}}{8} \\
&\geq -\frac{\bar{\Delta}_{(|\mathcal{Z}_{hi}|A+1-k)}}{8} + \bar{\Delta}_{(|\mathcal{Z}_{hi}|A+1-k)} - \frac{\bar{\Delta}_{(|\mathcal{Z}_{hi}|A+1-k)}}{8} \\
&= \frac{3\bar{\Delta}_{(|\mathcal{Z}_{hi}|A+1-k)}}{4}
\end{aligned}$$

under $\mathcal{G}_0$. Then

$$\Delta_h^{\hat{\pi}}(s,a) + \frac{\bar{\Delta}_{(|\mathcal{Z}_{hi}|A+1-k)}}{4} > \hat{\Delta}_h(s,a)_k \geq \hat{\Delta}_h(s',a')_k > \frac{3\bar{\Delta}_{(|\mathcal{Z}_{hi}|A+1-k)}}{4},$$

which implies

$$\Delta_h^{\hat{\pi}}(s,a) > \frac{1}{2}\bar{\Delta}_{(|\mathcal{Z}_{hi}|A+1-k)}.$$

□

Lemma 34. *Under the events $\mathcal{M}_\varepsilon, \mathcal{L}_\varepsilon, \mathcal{G}_{0,\varepsilon}$, if a pair (s,a) is accepted in a phase $k \in [k^*]$, then*

$$\Delta_h^{\hat{\pi}}(s,a) = 0.$$

Proof. Since (s,a) is accepted in the phase $k \in [k^*]$, (s,a') for the other actions a' are rejected befor phase k. By Lemma 33, $\Delta_h^{\hat{\pi}}(s,a') > 0$ for the other actions a'. Thus, $\Delta_h^{\hat{\pi}}(s,a) = 0$. □

Lemma 35. *Under the events $\mathcal{M}_\varepsilon$, $\mathcal{L}_\varepsilon$, $\cap_{h'=h+1}^H \mathcal{E}_{h'}$, and $\mathcal{G}_{0,\varepsilon}$,*

$$\hat{\Delta}_h^{\hat{\pi}}(s,a) \le \frac{\varepsilon}{W_h(s)} \implies \Delta_h(s,a) \le \frac{3\varepsilon}{W_h(s)}$$

Proof. Assume that $\hat{\Delta}_h^{\hat{\pi}}(s,a) \le \frac{\varepsilon}{W_h(s)}$. We have

$$\Delta_h(s,a) - \hat{\Delta}_h^{\hat{\pi}}(s,a) \le \underbrace{\Delta_h(s,a) - \Delta_h^{\hat{\pi}}(s,a)}_{\text{(I)}} + \underbrace{\Delta_h^{\hat{\pi}}(s,a) - \hat{\Delta}_h^{\hat{\pi}}(s,a)}_{\text{(II)}}.$$

(I) is less than or equal to $\frac{\varepsilon}{W_h(s)}$ in the good event $\cap_{h'=h+1}^H \mathcal{E}_{h'}$ by Lemma 8. Thus, under $\cap_{h'=h+1}^H \mathcal{E}_{h'}$,

$$\Delta_h(s,a) \le \frac{2\varepsilon}{W_h(s)} + \text{(II)}. \tag{13}$$

Let $a_s^* \in \arg\max Q_h^{\hat{\pi}}(s,a)$. Then we have

$$\begin{aligned}\text{(II)} = \Delta_h^{\hat{\pi}}(s,a) - \hat{\Delta}_h^{\hat{\pi}}(s,a) &= \max_a Q_h^{\hat{\pi}}(s,a) - \max_a \hat{Q}_h^{\hat{\pi}}(s,a) + \hat{Q}_h^{\hat{\pi}}(s,a) - Q_h^{\hat{\pi}}(s,a) \\ &\le \underbrace{Q_h^{\hat{\pi}}(s,a_s^*) - \hat{Q}_h^{\hat{\pi}}(s,a_s^*)}_{\text{(III)}} + \underbrace{\hat{Q}_h^{\hat{\pi}}(s,a) - Q_h^{\hat{\pi}}(s,a)}_{\text{(IV)}}.\end{aligned}$$

(1) If (s,a) is accepted, then

$$\text{(II)} = \Delta_h^{\hat{\pi}}(s,a) - \hat{\Delta}_h^{\hat{\pi}}(s,a) \le \Delta_h^{\hat{\pi}}(s,a) \le \frac{\varepsilon}{W_h(s)}$$

by Theorem 3.2. Thus, $\Delta_h(s,a) \le \frac{3\varepsilon}{W_h(s)}$.

(2) If (s,a) is rejected in some phase $k > k^*$, then

$$\text{(II)} = \Delta_h^{\hat{\pi}}(s,a) - \hat{\Delta}_h^{\hat{\pi}}(s,a) \le \Delta_h^{\hat{\pi}}(s,a) \le \frac{\varepsilon}{W_h(s)}$$

since

$$\mathcal{G}_{0,\varepsilon} \implies \mathcal{G}_{0,2\varepsilon} \implies \mathcal{G}_{1,2\varepsilon}, \quad \mathcal{G}_{2,2\varepsilon}$$

and $\mathcal{G}_{1,2\varepsilon}, \quad \mathcal{G}_{2,2\varepsilon}$ implies that all of the pairs remaining in the end of phase k^* are $\frac{\varepsilon}{W_h(s)}$-good. Thus, $\Delta_h(s,a) \le \frac{3\varepsilon}{W_h(s)}$.

(3) Assume (s,a) is rejected in phase k. By $\mathcal{G}_0$ and Lemma 33,

$$\text{(IV)} < \frac{1}{8}(\bar{\Delta}_{(|\mathcal{Z}_{hi}|A+1-k)} \vee \frac{\varepsilon}{W_h(s)}) \le \frac{1}{8}(2\Delta_h^{\hat{\pi}}(s,a) \vee \frac{\varepsilon}{W_h(s)}).$$

(i) If (s,a_s^*) is accepted, then it is accepted in phase $k' > k$. Thus,

$$\text{(III)} \le \frac{1}{8}(\bar{\Delta}_{(|\mathcal{Z}_{hi}|A+1-k')} \vee \frac{\varepsilon}{W_h(s)}) \le \frac{1}{8}(\bar{\Delta}_{(|\mathcal{Z}_{hi}|A+1-k)} \vee \frac{\varepsilon}{W_h(s)}) \le \frac{1}{8}(2\Delta_h^{\hat{\pi}}(s,a) \vee \frac{\varepsilon}{W_h(s)}).$$

(ii) If (s, a_s^*) is rejected at phase k', then

$$\text{(III)} < \frac{1}{8}(\bar{\Delta}_{(|\mathcal{Z}_{hi}|A+1-k')} \vee \frac{\varepsilon}{W_h(s)}) \leq \frac{1}{8}(2\Delta_h^{\hat{\pi}}(s, a_s^*) \vee \frac{\varepsilon}{W_h(s)}) \leq \frac{1}{8}(2\Delta_h^{\hat{\pi}}(s, a) \vee \frac{\varepsilon}{W_h(s)})$$

also by $\mathcal{G}_0$ and Lemma 33.

Thus,

$$\Delta_h^{\hat{\pi}}(s, a) - \frac{\varepsilon}{W_h(s)} \leq \Delta_h^{\hat{\pi}}(s, a) - \hat{\Delta}_h^{\hat{\pi}}(s, a) = \text{(II)} \leq \text{(III)} + \text{(IV)} < \frac{1}{4}(2\Delta_h^{\hat{\pi}}(s, a) \vee \frac{\varepsilon}{W_h(s)})$$

If $2\Delta_h^{\hat{\pi}}(s, a) > \frac{\varepsilon}{W_h(s)}$, then $\Delta_h^{\hat{\pi}}(s, a) < \frac{2\varepsilon}{W_h(s)}$ which implies $\Delta_h(s, a) \leq \frac{3\varepsilon}{W_h(s)}$ by the event $\cap_{h'=h+1}^{H} \mathcal{E}_{h'}$ and Lemma 8.

If $2\Delta_h^{\hat{\pi}}(s, a) \leq \frac{\varepsilon}{W_h(s)}$, then $\Delta_h^{\hat{\pi}}(s, a) < \frac{5\varepsilon}{4W_h(s)}$ which implies $\Delta_h(s, a) \leq \frac{9\varepsilon}{4W_h(s)}$ by the event $\cap_{h'=h+1}^{H} \mathcal{E}_{h'}$ and Lemma 8.

□

By Lemma 35, we have $|\widehat{\mathrm{OPT}}_h(\varepsilon)| \leq |\,\mathrm{OPT}_h(3\varepsilon)|$. Now we prove Theorem 3.4.

Theorem F.1 (Theorem 3.4)**.** *If we run Algorithm 5 with*

$$B \geq \max\{2SHc(\frac{B}{2SH}), 4Hc(\frac{B}{4H}), 2SA\varepsilon_{\frac{B}{2SH}} \log_2 \frac{1}{\varepsilon_{\frac{B}{2SH}}}\}$$

and an accuracy level $\varepsilon \geq 2SH^2\varepsilon_{\frac{B}{2SH}}$, it uses at most budget B and satisfies the following guarantee:

$$\begin{aligned}\mathbb{P}\left(V_0^* - V_0^{\hat{\pi}} > \varepsilon\right) \leq & \exp\left(-\tilde{\Theta}\left(\frac{\varepsilon B}{\mathrm{poly}(S, A, H, \log B)}\right)\right) \\ & + \exp\left(-\tilde{\Theta}\left(\frac{B}{H^3 \max_{h\in[H]} \sum_{s\in\mathcal{S}} W_h(s)^{-1} \sum_{a\in\mathcal{A}} (\bar{\Delta}_h(s, a) \vee \frac{\varepsilon}{W_h(s)})^{-2}}\right)\right) \\ & + \exp\left(-\tilde{\Theta}\left(\frac{\varepsilon^2 B}{H^5 \max_{h\in[H]} |\,\mathrm{OPT}_h(\varepsilon)|}\right)\right),\end{aligned}$$

where $\mathrm{OPT}_h(\varepsilon) = \{(s, a) \in \mathcal{S} \times \mathcal{A} : \bar{\Delta}_h(s, a) W_h(s) \leq \varepsilon\}$.

Proof. For the budget, the first and the second part each consume at most $\frac{B}{4}$. In the third part total budget of running FB-L2E is at most $\frac{B}{4}$ by Theorem 3.1. We only need to consider the collecting part. Let $K_j = K_j(\delta_j, SAH\delta_j), N_j = \frac{K_j}{2^{j+2}|\widehat{\mathrm{OPT}}_h(\varepsilon) \setminus \cup_{i=1}^{j-1} \mathcal{X}_i|}$. Then, the budget used in collecting is

$$\sum_{j=1}^{J} \frac{K_j}{N_j} n_j = \sum_{j=1}^{J} 2^{i+2} |\widehat{\mathrm{OPT}}_h(\varepsilon) \setminus \cup_{i=1}^{j-1} \mathcal{X}_i| \times \frac{B}{H|\widehat{\mathrm{OPT}}_h(\varepsilon)|} 2^{-2i-4} \leq \frac{B}{4}$$

Next, we prove the probability bound. Let $\mathcal{M}_\varepsilon'$ be the event where all of the FB-L2E in the third part suceed up to ε as in Theorem 3.1. Let $\mathcal{L}_\varepsilon'$ be the event where all of the resampling process up to group reachability level i_ε suceed as in Theorem 3.1. Since $\frac{B}{4H} \leq c(\frac{B}{4H})$,

$$\mathbb{P}(\mathcal{M}_\varepsilon'^{\mathsf{c}}), \mathbb{P}(\mathcal{L}_\varepsilon'^{\mathsf{c}}) \leq \exp\left(-\tilde{\Theta}\left(\frac{\varepsilon B}{\mathrm{poly}(S, A, H, \log B)}\right)\right) \tag{14}$$

by Theorem 3.1. In collecting part, assume the good event

$$\mathcal{H}_{h,\varepsilon} = \{\forall h, \forall s \in \mathcal{Z}_{h,1:i_\varepsilon}, \max_{a'} Q_h^{\hat{\pi}}(s, a') - Q_h^{\hat{\pi}}(s, \hat{\pi}(s)) \leq \varepsilon_h(s) := \frac{\varepsilon}{2HJ2^{-j(s)+1}}\},$$

where $i_\varepsilon = \lceil \log_2(\frac{2SH^2}{\varepsilon}) \rceil$ and $j(s) := \sup\{j : (s,a') \in \mathcal{X}_j \text{ for some } a'\}$. Let $\tilde{\mathcal{X}}_j = \{s : j(s) = j\}$. Then, $\mathcal{H}_{h,\varepsilon} \implies \mathcal{E}_h$ since

$$\sup_\pi \sum_{s \in \mathcal{Z}_{h1:i_\varepsilon}} w_h^\pi(s) \Delta_h^{\hat{\pi}}(s, \hat{\pi}(s)) \le \frac{\varepsilon}{2HJ} \sup_\pi \sum_{j=1}^{i_\varepsilon} \sum_{s \in \tilde{\mathcal{X}}_j} w_h^\pi(s) 2^{-j+1} \le \frac{i_\varepsilon \varepsilon}{2HJ} \le \frac{\varepsilon}{2H}.$$

Let $\mathcal{H}_\varepsilon := \cup_{h=1}^H \mathcal{H}_{h,\varepsilon}$, Then the events $\mathcal{M}_\varepsilon, \mathcal{L}_\varepsilon, \mathcal{M}'_\varepsilon, \mathcal{L}'_\varepsilon, \cap_{h=1}^H \mathcal{E}_h, \mathcal{H}_\varepsilon$ and $\mathcal{G}_{0,\varepsilon}(\mathcal{Z}_{hi})$ for all multiple bandit instances $\mathcal{Z}_{hi}$ with $i \le i_\varepsilon$ implies

$$\begin{aligned}
V_0^* - V_0^{\hat{\pi}} &\le \sum_{h=1}^H \sup_\pi \sum_s w_h^\pi(s) \Delta_h^{\hat{\pi}}(s, \hat{\pi}(s)) \\
&\le \frac{\varepsilon}{2HJ} \sum_{h=1}^H \sup_\pi \sum_{s \in \mathcal{Z}_{h,1:i_\varepsilon}} w_h^\pi(s) 2^{j(s)-1} + H \sum_h \sup_\pi \sum_{s \in \mathcal{Z}^c_{h,1:i_\varepsilon}} w_h^\pi(s) \\
&\le \frac{\varepsilon}{2HJ} \sum_{h=1}^H \sup_\pi \sum_{j=1}^{i_\varepsilon} \sum_{s \in \tilde{\mathcal{X}}_j} w_h^\pi(s) 2^{j-1} + H \sum_h \sum_{s \in \mathcal{Z}^c_{h,1:i^*}} W_h(s) \\
&\le \frac{\varepsilon}{2HJ} \sum_{h=1}^H \sum_{j=1}^{i_\varepsilon} 2^{j-1} \sup_\pi \sum_{(s,a) \in \tilde{\mathcal{X}}_j} w_h^\pi(s,a) + H \sum_h |S 2^{-i_\varepsilon} \\
&\le \frac{\varepsilon}{2HJ} \sum_{h=1}^H \sum_{j=1}^{i_\varepsilon} 2^{j-1} \cdot 2^{-j+1} + \frac{\varepsilon}{2} \\
&\le \frac{\varepsilon}{2} + \frac{\varepsilon}{2} = \varepsilon
\end{aligned}$$

Thus,

$$\begin{aligned}
\mathbb{P}(V_0^* - V_0^{\hat{\pi}} > \varepsilon) \le \mathbb{P}(\mathcal{M}_\varepsilon^{\mathsf{c}} \cup \mathcal{L}_\varepsilon^{\mathsf{c}} \cup \mathcal{M}_\varepsilon'^{\mathsf{c}} \cup \mathcal{L}_\varepsilon'^{\mathsf{c}}) + \sum_{h=1}^H \sum_{i=1}^{i_\varepsilon} \mathbb{P}(\mathcal{M}_\varepsilon, \mathcal{L}_\varepsilon, \mathcal{G}_{0,\varepsilon}(\mathcal{Z}_{hi})^{\mathsf{c}}) \\
+ \sum_{h=1}^H \mathbb{P}(\mathcal{H}_{h,\varepsilon}^{\mathsf{c}}, \mathcal{M}_\varepsilon, \mathcal{L}_\varepsilon, \mathcal{M}'_\varepsilon, \mathcal{L}'_\varepsilon, \bigcup_{h, i \le i_\varepsilon} \mathcal{G}_{0,\varepsilon}(\mathcal{Z}_{hi})).
\end{aligned}$$

The first term is

$$\exp\left(-\tilde{\Theta}\left(\frac{\varepsilon B}{\text{poly}(S, A, H, \log B)}\right)\right)$$

by equation 14 and Theorem 3.1 and the second term is

$$\exp\left(-\tilde{\Theta}\left(\frac{B}{H^3 \max_{h \in [H]} \sum_{s \in \mathcal{S}} W_h(s)^{-1} \sum_{a \in \mathcal{A}} (\bar{\Delta}_h(s,a) \vee \frac{\varepsilon}{W_h(s)})^{-2}}\right)\right)$$

by Lemma 32 and that i_ε is only a logarithmic factor.

It remains to bound the probability of $\mathcal{H}_{h,\varepsilon}^c$ assuming other events

$$\mathcal{M}_\varepsilon, \mathcal{L}_\varepsilon, \mathcal{M}'_\varepsilon, \mathcal{L}'_\varepsilon, \cap_{h'=h+1}^H \mathcal{E}_{h'}, \bigcup_{h, i \le i_\varepsilon} \mathcal{G}_{0,\varepsilon}(\mathcal{Z}_{hi}).$$

Let $a^* \in \arg\max_a Q_h^{\hat{\pi}}(s,a)$ and denote $\varepsilon_h(s) := \frac{\varepsilon}{HJ 2^{-j(s)+1}}$.

$$\begin{aligned}
\varepsilon_h(s) &< \max_a Q_h^{\hat{\pi}}(s,a) - Q^{\hat{\pi}}(s, \hat{\pi}_h(s)) \\
&= Q_h^{\hat{\pi}}(s,a^*) - \hat{Q}_h^{\hat{\pi}}(s,a^*) + \hat{Q}_h^{\hat{\pi}}(s,a^*) - \hat{Q}_h^{\hat{\pi}}(s, \hat{\pi}_h(s)) + \hat{Q}_h^{\hat{\pi}}(s, \hat{\pi}_h(s)) - Q_h^{\hat{\pi}}(s, \hat{\pi}_h(s)) \\
&\le Q_h^{\hat{\pi}}(s,a^*) - \hat{Q}_h^{\hat{\pi}}(s,a^*) + 0 + \hat{Q}_h^{\hat{\pi}}(s, \hat{\pi}_h(s)) - Q_h^{\hat{\pi}}(s, \hat{\pi}_h(s))
\end{aligned}$$

$$\implies \left(\varepsilon_h(s)/2 \le Q_h^{\hat{\pi}}(s,a^*) - \hat{Q}_h^{\hat{\pi}}(s,a^*)\right) \vee \left(\varepsilon_h(s)/2 \le \hat{Q}_h^{\hat{\pi}}(s,\hat{\pi}_h(s)) - Q_h^{\hat{\pi}}(s,\hat{\pi}_h(s))\right)$$

Then, by Hoeffding's inequality, the probability term below can be obtained as

$$\mathbb{P}(\mathcal{H}_{h,\varepsilon}^c | \mathcal{M}_\varepsilon, \mathcal{L}_\varepsilon, \mathcal{M}'_\varepsilon, \mathcal{L}'_\varepsilon, \cap_{h'=h+1}^H \mathcal{E}_{h'}, \bigcup_{h,i\le i_\varepsilon} \mathcal{G}_{0,\varepsilon}(\mathcal{Z}_{hi})) \le$$

$$\mathbb{P}(\exists (s,a) \in \widehat{\mathrm{OPT}}_h(\varepsilon), |\max_{a'} Q_h^{\hat{\pi}}(s,a') - \hat{Q}_h^{\hat{\pi}}(s,a)| \ge \varepsilon_h(s) | \mathcal{M}_\varepsilon, \mathcal{L}_\varepsilon, \mathcal{M}'_\varepsilon, \mathcal{L}'_\varepsilon, \cap_{h'=h+1}^H \mathcal{E}_{h'}, \bigcup_{\mathcal{Z}_{hi}} \mathcal{G}_{0,\varepsilon}(\mathcal{Z}_{hi}))$$

$$\le \exp\left(-\tilde{\Theta}\left(\frac{1}{2^{2j(s)}} n_0 \cdot \frac{1}{H^2} \cdot \frac{\varepsilon^2}{H^2(2^{-2j(s)})}\right)\right)$$

$$= \exp\left(-\tilde{\Theta}\left(\frac{B}{|\widehat{\mathrm{OPT}}_h(\varepsilon)|} \cdot \frac{\varepsilon^2}{H^5}\right)\right)$$

$$\le \exp\left(-\tilde{\Theta}\left(\frac{B}{|\mathrm{OPT}_h(3\varepsilon)|} \cdot \frac{\varepsilon^2}{H^5}\right)\right).$$

This proves the theorem. □

Algorithm 5 **B**ackward **R**eachability **E**stimation, **A**ction elimination and **P**olicy refinement (BREAP)

input: Budget B, error level ε
$B' \leftarrow \lfloor \frac{B}{4SH} \rfloor, \quad J \leftarrow \lceil 0.6321 \log_2(1 + \frac{\log(2)B'}{c(B')}) \rceil$
$B'' \leftarrow \frac{B}{4HJ}$
for $h = H, H-1, \ldots, 1$ **do**
  $\mathcal{Z}_h \leftarrow \emptyset$
  for $s \in \mathcal{S}$ **do** $\{(\mathcal{X}_j^{sh}, \Pi_j^{sh}, N_j^{sh})\}_{j=1}^{J} \leftarrow$ FB-L2E($\{(s,1)\}, h, B'$) (1 is an arbitrary action)
    if $\mathcal{X}_h^{sh} = \{(s,1)\}$ for some $j \in [J]$ **then**
      $\widehat{W}_h(s) \leftarrow 2^{-j+1}, \quad \mathcal{Z}_h \leftarrow \mathcal{Z}_h \cup \{s\}$
    end if
  end for
  $\widehat{\mathrm{OPT}}_h(\varepsilon) \leftarrow \emptyset$
  for $i = 1$ to J **do**
    $\mathcal{Z}_{hi} \leftarrow \{s \in \mathcal{Z}_h : \widehat{W}_h(s) = 2^{-i+1}\}, \quad A_1 \leftarrow \mathcal{Z}_{hi} \times \mathcal{A},$
    $\forall (s,a) \in A_1, \quad N(s,a) \leftarrow 0, \quad T(s,a) \leftarrow 0, \quad T_0(s,a) \leftarrow 0, \quad Q(s,a) \leftarrow 0$
    for $k = 1$ to $|\mathcal{Z}_{hi}|A - 1$ **do**
      $n_k \leftarrow n_k(\lfloor B'' 2^{-i-2} \rfloor, |\mathcal{Z}_{hi}|, A)$ (as defined in equation 1)
      for $(s,a) \in A_k$ **do**
        $T_k(s,a) \leftarrow \lfloor \frac{n_k}{N_i^s h} \rfloor$
        Rerun each policy in Π_i^{sh} for $T_k - T_{k-1}$ times
        for each time $t = T(s,a) + 1$ to $T_k(s,a)$ **do**
          if (s,a) is visited at step h **then**
            Take action a and extend a trajectory using $\{\hat{\pi}_{h'}\}_{h'=h+1}^{H}$
            $N(s,a) \leftarrow N(s,a) + 1$
            $Q(s,a) \leftarrow Q(s,a) + \sum_{h'=h}^{H} R_{h'}^t(s_{h'}^t, a_{h'}^t)$
          end if
        end for
        $\hat{Q}_h^{\hat{\pi}}(s,a) \leftarrow Q(s,a)/N(s,a)$ **if** $N(s,a) > 0$ **else** 0
        $T(s,a) \leftarrow T_k(s,a)$
      end for
      if $\exists$ state s with unique surviving pair (s,a) in A_k **then**
        $\hat{\pi}_h(s) \leftarrow a, \quad A_{k+1} \leftarrow A_k \setminus \{(s,a)\}$
      else
        $\forall (s,a) \in A_k, \quad \widehat{\Delta}_h^{\hat{\pi}}(s,a) \leftarrow \max_{a:(s,a)\in A_k} \hat{Q}_h^{\hat{\pi}}(s,a) - \hat{Q}_h^{\hat{\pi}}(s,a)$
        $(s', a') \leftarrow \arg\max_{(s,a)\in A_k} \widehat{\Delta}_h^{\hat{\pi}}(s,a)$ (Break ties arbitrarily)
        $A_{k+1} \leftarrow A_k \setminus \{(s', a')\}$
      end if
    end for
    $\forall (s,a) \in \mathcal{Z}_{hi} \times \mathcal{A}, \hat{Q}_h^{\hat{\pi}}(s,a) \leftarrow Q(s,a)/N(s,a)$ **if** $N(s,a) > 0$ **else** 0
    $\forall (s,a) \in \mathcal{Z}_{hi} \times \mathcal{A}, \hat{\Delta}_h^{\hat{\pi}}(s,a) \leftarrow \max_{a'} \hat{Q}_h^{\hat{\pi}}(s,a') - \hat{Q}_h^{\hat{\pi}}(s,a)$
    $\hat{g}_{hi}^{\hat{\pi}}(\varepsilon) \leftarrow |\{(s,a) \in \mathcal{Z}_{hi} \times \mathcal{A} : \hat{\Delta}_h^{\hat{\pi}}(s,a)\widehat{W}_h(s) \leq \varepsilon\}|$
    $\widehat{\mathrm{OPT}}_h(\varepsilon) \leftarrow \widehat{\mathrm{OPT}}_h(\varepsilon) \cup \{\text{survived pairs in the end of phase } |\mathcal{Z}_{hi}|A - \hat{g}_{hi}^{\hat{\pi}}(\varepsilon) + 1\}$
    $\hat{\pi}_h(s) \leftarrow a$ for (s,a) accepted up to phase $|\mathcal{Z}_{hi}|A - \hat{g}_{hi}^{\hat{\pi}}(\varepsilon) + 1$
  end for
  For each $s \in \mathcal{S} \setminus \mathcal{Z}_h$, set $\hat{\pi}_h(s)$ as any action
  $\{(\mathcal{X}_j, \Pi_j, N_j)\}_{j=1}^{J} \leftarrow$ FB-L2E($\widehat{\mathrm{OPT}}_h(\varepsilon), h, \frac{B}{4H}$)
  $\forall j \in [J], n_j \leftarrow \frac{B}{H|\widehat{\mathrm{OPT}}_h(\varepsilon)|} 2^{-2j-4}$
  for $j = 1$ to J **do**
    rerun each policy in Π_j, $\lceil \frac{n_j}{N_j} \rceil$ times
  end for
  Compute the empirical $\hat{Q}_h^{\hat{\pi}}(s,a)$
  $\hat{\pi}(s) \leftarrow \arg\max_a \hat{Q}_h^{\hat{\pi}}(s,a)$ for all active state s in $\widehat{\mathrm{OPT}}_h(\varepsilon)$
end for
return $\hat{\pi}$