# Policy Finetuning: Bridging Sample-Efficient Offline and Online Reinforcement Learning

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## **Abstract**

This paper initiates the theoretical study of policy finetuning towards bridging the gap between (sample-efficient) online RL and offline RL. In this problem, the online RL learner has additional access to a "reference policy"  $\mu$  close to the optimal policy  $\pi_{\star}$  in a certain sense. We first design a sharp offline reduction algorithm—which simply executes  $\mu$  and runs offline policy optimization on the collected dataset—that finds an  $\varepsilon$  near-optimal policy within  $O(H^3SC^*/\varepsilon^2)$ episodes, where  $C^*$  is the single-policy concentrability coefficient between  $\mu$  and  $\pi_{\star}$ . This offline result is the first that matches the sample complexity lower bound in this setting, and resolves a recent open question in offline RL. We then establish an  $\Omega(H^3S\min\{C^*,A\}/\varepsilon^2)$  sample complexity lower bound for any policy finetuning algorithm, including those that can adaptively explore the environment. This implies that perhaps surprisingly—the optimal policy finetuning algorithm is either offline reduction or a purely online RL algorithm that does not use  $\mu$ . Finally, we design a new hybrid offline/online algorithm for policy finetuning that achieves better sample complexity than both vanilla offline reduction and purely online RL algorithms, in a relaxed setting where  $\mu$  only satisfies concentrability partially up to a certain time step. Overall, our results offer a quantitative understanding on the benefit of a good reference policy, and make a step towards bridging offline and online RL.

#### 1. Introduction

Sample-efficient RL has been studied in a rich body of theoretical work in two main settings: *online RL*, in which the learner has interactive access to the environment and can execute any policy; and *offline RL*, in which the learner only

has access to an "offline" dataset collected by executing some (one or many) policies within the environment, and is not allowed to further access the environment. These two settings share some common learning goals such as the sample complexity for finding the optimal policy. However, existing algorithms and theories in the online and offline setting seem rather different and disconnected.

Further, on the empirical end, insights and patterns from offline RL often help as well in designing online RL algorithms and improving the sample efficiency in the real world. For example, there are online RL algorithms that alternate between data collection steps using a fixed policy, and policy improvement steps by learning on the collected dataset (Janner et al., 2019). The prevalence of these algorithms also offers practical motivations for us to look for a more unified understanding of online and offline RL in theory. These reasonings motivate us to ask the following question:

Can we bridge sample-efficient offline and online RL from a theoretical perspective?

This paper proposes policy finetuning, a new RL setting that investigates the benefit of a good initial policy in reinforcement learning, and encapsulates challenges of both online and offline RL. In the policy finetuning problem, the learner is given interactive access to the environment and asked to learn a near-optimal policy, but in addition has access to a reference policy  $\mu$  that is good in certain aspects. This setting offers great flexibility for the algorithm design: For example, the algorithm is allowed to either simply collect data from  $\mu$  and run any offline policy optimization algorithm on the collected dataset. It is also allowed to play any other policy interactively, including those that adaptively explores the environment. The policy finetuning problem offers a common playground for both offline and online types of algorithms, and has a unified performance metric (sample complexity for finding the near-optimal policy) for comparing their performance.

We study the policy finetuning problem theoretically in finite-horizon MDPs with H time steps, S states, and A actions. We summarize our contributions as follows.

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• We begin by considering offline reduction algorithms which simply collect data using the reference policy  $\mu$  and run an offline policy optimization algorithm on the collected dataset. This setting equivalent to offline RL with behavior policy  $\mu$ , and thus our result translates to a same result for offline RL as well.

We design an algorithm PEVI-ADV that is able to find an  $\varepsilon$ -optimal policy within  $\widetilde{O}(H^3SC^\star/\varepsilon^2)$  episodes of play, where  $C^\star$  is the *single-policy concentrability* coefficient between  $\mu$  and some optimal policy  $\pi_\star$  (Section 3). This improves over the best existing offline result by an  $H^2$  factor in the same setting and matches the lower bound (up to log factors), thereby resolving the recent open question of (Rashidinejad et al., 2021) on tight offline RL under single-policy concentrability.

- Under the same assumption on  $\mu$ , we establish an  $\Omega(H^3S\min\{C^\star,A\}/\varepsilon^2)$  sample complexity lower bound for any policy finetuning algorithm, including those that adaptively explores the environment (Section 4). This implies that the optimal policy finetuning algorithm is either offline reduction via PEVI-ADV, or a "purely" online RL algorithm from scratch (such as UCBVI), depending on whether  $C^\star \leq A$ . This comes rather surprising, as it rules out possibilities of combining online exploration and knowledge of  $\mu$  to further improve the sample complexity over the aforementioned two baselines.
- Finally, we consider policy finetuning in a more challenging setting where  $\mu$  only satisfies concentrability up to a certain time step. We design a "hybrid offline/online" algorithm HOOVI that combines online exploration and offline data collection, and show that it achieves better sample complexity than both vanilla offline reduction and purely online algorithms in certain cases (Section 5). This gives a positive example on when such hybrid algorithm designs are beneficial.

#### 2. Policy finetuning

We present the basic backgrounds (e.g., Markov Decision Processes, policies, value functions, and visitation distributions) to Appendix B. Specifically, the visitation distribution  $d_h^{\pi}(s,a)$  is defined in (1).

**Policy finetuning** A policy finetuning problem consists of an MDP M and a *reference policy*  $\mu$ . During the learning stage, the learner can perform the following two types of moves:

- (a) Play an episode in the MDP M using any policy (i.e. learner has online interactive access to M).
- (b) Access the values of the reference policy  $\mu_h(a|s)$  for all (h, s, a). For example, the learner can use it to sample

actions  $a \sim \mu_h(\cdot|s)$  for any h, s for arbitrarily many times during learning.

The goal of the learner is to output  $\varepsilon$  near-optimal policy  $\widehat{\pi}$  within as few episodes of play (within the MDP) as possible.

A unique feature about the policy finetuning setting is that it allows both *online interactive plays* via any online RL algorithm (not necessarily using  $\mu$ ), as well as *offline reduction* which simply collects data by executing the reference policy  $\mu$  and do anything with the collected dataset. In particular, this means that any algorithm for offline policy optimization (based on offline datasets) also gives an algorithm for policy finetuning via this offline reduction. Therefore, policy finetuning offers a common playground for both online and offline type algorithms with a unified learning goal.

Assumption on reference policy Throughout most of this paper (except for Section 5), we consider the following assumption on the reference policy  $\mu$ .

**Assumption A** (Single-policy concentrability). *The reference policy*  $\mu$  *satisfies that* 

$$\max_{h \in [H], (s,a) \in \mathcal{S} \times \mathcal{A}} \frac{d_h^{\pi_{\star}}(s,a)}{d_h^{\mu}(s,a)} \le C^{\star}$$

(with the convention 0/0 = 0) for some deterministic optimal policy  $\pi_{\star}$  and constant  $C^{\star} \geq 1$ .

This assumption is considered in the recent work of Rashidinejad et al. (2021) on offline RL and is more relaxed than previously assumed concentrability assumptions which typically requires the supremum concentrability against all possible  $\pi$ 's to be bounded (Chen and Jiang, 2019). We consider this assumption as it both allows efficient offline RL algorithms (Rashidinejad et al., 2021), and is perhaps also a sensible measure of quality for the reference policy in policy finetuning.

# 3. Sharp offline learning via reference-advantage decomposition

We begin by investigating the sharpest sample complexity for policy finetuning via the offline reduction approach. This requires us to design sharp offline RL algorithms that run on the dataset  $\mathcal D$  collected by executing  $\mu$ . We emphasize that this is both an interesting offline RL question on its own right, and also important for our later discussions on lower bounds and other algorithms for policy finetuning, as the sharpest sample complexity via offline reduction provides a solid baseline.

**Sharp offline learning via reference-advantage decomposition** We now design a new sharp algorithm PEVI-ADV (Algorithm 1) which achieves an improved  $\widetilde{O}(H^3SC^\star/\varepsilon^2)$  sample complexity (for small enough  $\varepsilon$ ). This improves over VI-LCB (Algorithm 3) $^1$  by  $\widetilde{O}(H^2)$  and is the first algorithm that matches the sample complexity lower bound.

We instantiate that by carefully using VI-LCB to learn the reference value function  $\hat{V}^{\mathrm{ref}}$ , combined with tight Bernstein bonuses, to shave off another H factor in the sample complexity. The full PEVI-ADV algorithm is provided in Algorithm 1. We now present its guarantee in the following theorem. The proof can be found in Appendix G.

**Theorem 1** (Sharp offline learning via PEVI-ADV). Suppose the reference policy  $\mu$  satisfies the single-policy concentrability (Assumption A). Then w.p. at least  $1-\delta$ , PEVI-ADV (Algorithm 1) outputs a policy  $\widehat{\pi}$  and value estimate  $\widehat{V}$  such that

(a) 
$$\max_{h \in [H]} \sum_{s \in \mathcal{S}} d_h^{\pi_{\star}}(s) (V_h^{\star}(s) - \widehat{V}_h(s)) \leq \varepsilon$$
,

(b) 
$$V_1^{\star}(s_1) - V_1^{\widehat{\pi}}(s_1) \le \varepsilon$$
,

within  $n = \widetilde{O} \left( H^3 S C^{\star} / \varepsilon^2 + H^{5.5} S C^{\star} / \varepsilon \right)$  episodes.

Near-optimal offline RL under single-policy concentrability For small enough  $\varepsilon \leq H^{-2.5}$ , Theorem 1 achieves  $\widetilde{O}(H^3SC^\star/\varepsilon^2)$  sample complexity for finding the  $\varepsilon$  near-optimal policy from the offlien dataset  $\mathcal{D}$ . This is the first cubic horizon dependence for offline RL under single-policy concentrability, which improves over recent works (Jin et al., 2020b; Rashidinejad et al., 2021) in this setting and resolves the open question of (Rashidinejad et al., 2021). For  $C^\star \geq 2$ , our sample complexity further matches the information-theoretical lower bound  $\Omega(H^3SC^\star/\varepsilon^2)$  up to log factors<sup>2</sup>.

# 4. Lower bound for policy finetuning

We now switch gears to considering the policy finetuning problem with any algorithm, not necessarily restricted to the offline reduction approach.

Two baselines: offline reduction & purely online RL A first observation is that naive offline reduction is already a strong baseline for policy finetuning, by our Theorem 1: Our PEVI-ADV algorithm only collects data with  $\mu$  and does not do any online exploration, yet achieves a sharp  $\widetilde{O}(H^3SC^*/\varepsilon^2)$  sample complexity for finding a near-optimal policy.

On the other hand, as the policy finetuning setting allows online interaction, *purely online RL* is another baseline algorithm: Simply run any sample-efficient online RL algorithm

(which typically uses optimism to encourage exploration) from scratch, and disregard the reference policy  $\mu$ . Using any sharp online RL algorithm such as UCBVI (Azar et al., 2017), this approach can find an  $\varepsilon$  near-optimal policy within  $\widetilde{O}(H^3SA/\varepsilon^2)$  episodes of play. Note that whether this is advantageous over the offline reduction boils down to the comparison between  $C^\star$  and A.

Given these two baselines, it is natural to ask whether there exists an algorithm that improves over both — Can we design an algorithm that performs some amount of optimistic exploration, yet also utilizes the knowledge of  $\mu$ , so as to achieve a better rate than both offline reduction and purely online RL?

**Lower bound** We provide an information-theoretic lower bound that (perhaps surprisingly) rules out the possibility of the aforementioned improvement. Define the class of problems

$$\mathcal{M}_{C^\star} := \Big\{ (M, \mu) : \text{ Exists deterministic } \pi_\star \text{ of } M$$
 s.t. 
$$\sup_{h,s,a} \frac{d_h^{\pi_\star}(s,a)}{d_h^{\mu}(s,a)} \leq C^\star \Big\}.$$

We recall that a policy finetuning algorithm for problem  $(M,\mu)$  is defined as any algorithm that can play in the MDP M for n episodes, has full knowledge of the reference policy  $\mu$ , and outputs a policy  $\widehat{\pi}$  after playing in the MDP. With these definitions ready, we now state our lower bound for policy finetuning. The proof of Theorem 2 can be found in Appendix H.

**Theorem 2** (Lower bound for policy finetuning). Suppose  $S, H \geq 3, A \geq 2, C^* \geq 2$ . Then, there exists an absolute constant  $c_0 > 0$  such that for any  $\varepsilon \leq 1/12$  and any online finetuning algorithm that outputs a policy  $\widehat{\pi}$ , if the number of episodes

$$n \le c_0 \cdot H^3 S \min \{C^*, A\} / \varepsilon^2,$$

then there exists a problem instance  $(M, \mu) \in \mathcal{M}_{C^*}$  on which the algorithm suffers from  $\varepsilon$ -suboptimality:

$$\mathbb{E}_M \left[ V_{1,M}^{\star} - V_{1,M}^{\widehat{\pi}} \right] \ge \varepsilon,$$

where the expectation  $\mathbb{E}_M$  is w.r.t. the randomness during the algorithm execution within MDP M.

Either offline reduction or purely online is optimal Theroem 2 shows that any policy finetuning algorithm needs to play at least  $\Omega(H^3S\min\{C^\star,A\}/\varepsilon^2)$  episodes in order to find an  $\varepsilon$  near-optimal policy. Crucially, this implies that either a sharp offline reduction (e.g. our PEVI-ADV algorithm) or purely online RL matches the lower bound (up to log), depending on whether  $C^\star\lesssim A$ . Perhaps surprisingly,

<sup>&</sup>lt;sup>1</sup>Due to the space limit, we defer the designing intuition of PEVI-ADV and its improvements over VI-LCB to Appendix E.

<sup>&</sup>lt;sup>2</sup>This lower bound can be adapted directly from a  $\Omega(SC^*/(1-\gamma)^3\varepsilon^2)$  lower bound of (Rashidinejad et al., 2021, Theorem 7).

this rules out the possibility of designing any algorithm "in between" that combines online exploration and knowledge of  $\mu$  to improve the sample complexity, at least in the worst-case over all problems in  $\mathcal{M}_{C^*}$ . We argue that this "no algorithm in between" phenomenon may be due to the single-policy concentrability assumption being too strong such that offline reduction already achieves a rather competitive sample complexity  $\widetilde{O}(H^3SC^*/\varepsilon^2)$ .

We also remark that Theorem 2 generalizes both the  $\Omega(H^3SA/\varepsilon^2)$  lower bound for online RL (Dann et al., 2017; Yin et al., 2020; Domingues et al., 2021) into the policy finetuning problem, as well as the  $\Omega(H^3SC^\star/\varepsilon^2)$  lower bound for offline RL under single-policy concentrability with  $C^\star \geq 2$  (Rashidinejad et al., 2021)³. Further, Theorem 2 directly implies an  $\Omega(H^3SC^\star/\varepsilon^2)$  lower bound for offline RL with  $2 \leq C^\star \leq O(A)$ , as any algorithm for offline policy optimization is also an algorithm for policy finetuning via the offline reduction.

# 5. Hybrid offline/online algorithm for policy finetuning

Towards circumventing the lower bound in Theorem 2, in this section, we study policy finetuning under more relaxed assumptions on the reference policy  $\mu$ . We consider the following relaxation: We assume  $\mu$  satisfies partial concentrability only up to a certain time-step  $h_{\star} \leq H$ , and may not have any bounded concentrability at steps  $h > h_{\star}$ .

**Assumption B** ( $h_{\star}$ -partial concentrability). The reference policy  $\mu$  satisfies the single-policy concentrability with respect to  $\pi_{\star}$  up to step  $h_{\star}$  only:

$$\max_{h \leq h_{\star}} \max_{s,a \in \mathcal{S} \times \mathcal{A}} \frac{d_{h}^{\pi_{\star}}(s,a)}{d_{h}^{\mu}(s,a)} \leq C^{\text{partial}}$$

(with the convention 0/0 = 0), where  $\pi_{\star}$  is some deterministic optimal policy of the MDP, and constant  $C^{\text{partial}} \geq 1$ .

**Algorithm description** We design a hybrid offline/online algorithm HOOVI (presented in Algorithm 2) for policy finetuning under the partial concentrability assumption. At a high-level, the algorithm consists of two main stages:

- In the first stage, it runs an online algorithm UCBVI-UPLOW which uses optimistic exploration to find a near-optimal policy \( \hat{\pi}^{UCB} \) and an accurate value estimate for steps \( (h\_\* + 1) : H. \)
- In the second stage, we run a TRUNCATED-PEVI-ADV algorithm, which collects data from  $\mu$  and runs

offline policy optimization to find a near-optimal policy  $\widehat{\pi}^{\text{PEVI}}$  for steps  $1:h_{\star}$ , building on the lower value estimate  $\underline{V}_{h_{\star}+1}$  from the first stage.

This strategy makes sense intuitively as the reference policy  $\mu$  does not have guarantees for steps  $h_{\star}+1:H$  and thus the algorithm is required to perform optimistic exploration first to get a good policy. However, additional technical cares are needed in order to make the above algorithm provably sample-efficient. The analysis of the second stage requires the online algorithm in the first stage to not only perform fast exploration (e.g. by using upper confidence bounds), but also output a *lower value estimate* for step  $h_{\star}+1$ , and in addition output a final output policy that achieves at least the value of the lower value estimate at every state  $s \in \mathcal{S}$ . Such lower bounds are not directly available in standard online RL algorithms such as UCBVI (Azar et al., 2017).

We resolve this by designing the UCBVI-UPLOW algorithm (Algorithm 4), which is a modification of the Nash-VI Algorithm of Liu et al. (2020a) into the single-player case. We now state our main theoretical guarantee for the HOOVI algorithm. The proof can be found in Appendix I.

**Theorem 3** (Hybrid online / offline learning for policy fine-tuning). Suppose the reference policy  $\mu$  satisfies the partial concentrability (Assumption B) up to some step  $h_{\star} \leq H$ . Then for small enough  $\varepsilon \leq \min \left\{ h_{\star}^{-2.5}, C^{\mathrm{partial}}/S \right\}$ , HOOVI (Algorithm 2) outputs a policy  $\widehat{\pi}$  such that  $V_1^{\star}(s_1) - V_1^{\widehat{\pi}}(s_1) \leq \varepsilon$  with probability at least  $1 - \delta$ , within

$$n = \widetilde{O}\left(\frac{H^2 h_{\star} S C^{\text{partial}} + (H - h_{\star})^3 S A (C^{\text{partial}})^2}{\varepsilon^2}\right)$$

episodes of play.

Comparison against offline reduction and purely online algorithms The sample complexity in Theorem 3 compares favorably against both naive offline reduction as well as purely online algorithms in certain situations. First, naive offline reduction with  $\mu$  does not have any guarantee since  $\mu$  is not assumed to have a finite single-policy concentrability at  $h \geq h_{\star} + 1$ . We can modify  $\mu$  into  $\mu'$  that plays uniformly within  $\mathcal A$  at steps  $h \geq h_{\star} + 1$ ; the single-policy concentrability coefficient of  $\mu'$  is guaranteed to be finite but scales exponentially as  $O(A^{H-h_{\star}})$  in the worst case, leading to a sample complexity much worse than ours.

On the other hand, a sharp online algorithm can still achieve  $\widetilde{O}(H^3SA/\varepsilon^2)$  in this setting (by optimistic exploration from scratch). Our Theorem 3 is in general incomparable with this, but can be better in cases when both  $C^{\mathrm{partial}}$  and  $H-h_{\star}$  are small, e.g., if  $C^{\mathrm{partial}}=o(A)$  and  $(H-h_{\star})/H=o((C^{\mathrm{partial}})^{-2/3})$ . This makes sense intuitively as our hybrid offline/online algorithm benefits the most if the length requiring exploration  $(H-h_{\star})$  is

 $<sup>^3</sup>$ The lower bound in (Rashidinejad et al., 2021) is  $\Omega(SC^\star/\varepsilon^2(1-\gamma)^3)$  for the infinite-horizon  $\gamma$ -discounted setting, which corresponds to an  $\Omega(H^3SC^\star/\varepsilon^2)$  lower bound for our finite-horizon setting.

small, and the partial concentrability  $C^{\mathrm{partial}}$  is small so that  $\mu$  still has a high-quality for the first  $h_{\star}$  steps. To best of our knowledge, this is first result that characterizes when the sample complexity of such hybrid algorithms can be beneficial over purely online or offline algorithms.

#### 6. Additional materials

We present our main algorithms (PEVI-ADV and HOOVI) in Appendix C, Algorithm 1 and 2. Additional related work is discussed in Appenedix A.

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## A. Related work

Sample-efficient online RL algorithms. A major portion of these works is concerned with the tabular setting with finitely many states and actions (Brafman and Tennenholtz, 2002; Kearns and Singh, 2002; Jaksch et al., 2010; Azar et al., 2017; Dann et al., 2017; Agrawal and Jia, 2017; Jin et al., 2018; Zhang et al., 2020). For episodic MDPs with inhomogeneous transition functions with S states, and S actions, and horizon length S, the optimal sample complexity for finding the S near-optimal policy is S and S achieved by various algorithms such as UCBVI of Azar et al. (2017) and UCB-Advantage of Zhang et al. (2020). Our paper adapts the reference-advantage decomposition technique of Zhang et al. (2020) to designing sharp offline algorithms. Online RL with with large state/action spaces are also studied by using function approximation in conjunction with structural assumptions on the MDP (Jin et al., 2020a; Zanette et al., 2020a; b, Agarwal et al., 2020; Osband and Roy, 2014; Jiang et al., 2017; Sun et al., 2019; Wang et al., 2020; Yang et al., 2020; Du et al., 2021; Jin et al., 2021).

Offline RL Offline/batch RL studies the case where the agent only has access to an offline dataset obtained by executing a *behavior policy* in the environment. Sample-efficient learning results in offline RL typically work by assuming either sup-concentrability assumptions (Munos, 2003; Szepesvári and Munos, 2005; Antos et al., 2008; Munos and Szepesvári, 2008; Farahmand et al., 2010; Tosatto et al., 2017; Chen and Jiang, 2019; Xie and Jiang, 2020)) or lower bounded exploration constants (Yin et al., 2020; 2021) to ensure the sufficient coverage of offline data over all (relevant) states and actions. However, such strong coverage assumptions can often fail to hold in practice (Fujimoto et al., 2019). More recent works address this by using either policy constraint/regularization (Fujimoto et al., 2019; Liu et al., 2020b; Kumar et al., 2019; Wu et al., 2019), or the pessimism principle to optimize conservatively on the offline data (Kumar et al., 2020; Yu et al., 2020; Kidambi et al., 2020; Jin et al., 2020b; Yin et al., 2021; Rashidinejad et al., 2021). The policy-constraint/regularization-based approaches prevent the policy to visit states and actions that has no or low coverage from the offline data. Our proposed offline RL algorithm PEVI-ADV (Algorithm 1) is inspired by the pessimistic value iteration algorithms of (Jin et al., 2020b; Rashidinejad et al., 2021) and achieves an improved sample complexity over these work under the same single-policy concentrability assumption on the behavior policy.

Bridging online and offline RL Kalashnikov et al. (2018) observed empirically that the performance of policies trained purely from offline data can be improved considerably by a small amount of additional online fine-tuning. A recent line of work studied low switching cost RL (Bai et al., 2019; Zhang et al., 2020; Gao et al., 2021; Wang et al., 2021)—which forbits online RL algorithms from switching its policy too often—as an interpolation between the online and offline settings. The same problem is also studied empirically as deployment-efficient RL (Matsushima et al., 2020; Su et al., 2021). While we also attempt to bridge online and offline RL, our work differs from this line in that our policy finetuning setting allows a direct comparison between "fully offline" and "fully online" algorithms, whereas the low switching cost setting prohibits fully online algorithms.

## **B.** Backgrounds

**Markov Decision Processes** In this paper, we consider episodic Markov decision processes (MDPs) with time-inhomogeneous transitions, specified by  $M = (\mathcal{S}, \mathcal{A}, H, \mathbb{P}, r)$ , where  $\mathcal{S}$  is the state space,  $\mathcal{A}$  is the action space, H is the horizon length,  $\mathbb{P} = \{\mathbb{P}_h\}_{h=1}^H$  where  $\mathbb{P}_h(\cdot|s,a) \in \Delta_{\mathcal{S}}$  is the transition probabilities at step h, and  $r = \{r_h : \mathcal{S} \times \mathcal{A} \to [0,1]\}_{h=1}^H$  are the deterministic<sup>4</sup> reward functions at time step  $h \in [H]$ . Without loss of generality, we assume that the initial state  $s_1$  is deterministic<sup>5</sup>.

**Policies, value functions, visitation distributions** A policy  $\pi = \{\pi_h(\cdot|s)\}_{h \in [H], s \in \mathcal{S}}$  consists of distributions  $\pi_h(\cdot|s) \in \Delta_{\mathcal{A}}$ . We use  $\mathbb{E}_{\pi}[\cdot]$  to denote the expectation with respect to the random trajectory induced by  $\pi$  in the MDP M, that is,  $(s_1, a_1, r_1, s_2, a_2, r_2, \ldots, s_H, a_H, r_H)$ , where  $a_h = \pi_h(s_h)$ ,  $r_h = r_h(s_h, a_h)$ ,  $s_{h+1} \sim \mathbb{P}_h(\cdot|s_h, a_h)$ . For each policy  $\pi$ , let  $V_h^{\pi} : \mathcal{S} \to \mathbb{R}$  and  $Q_h^{\pi} : \mathcal{S} \times \mathcal{A} \to \mathbb{R}$  denote its value functions and Q functions at each time step  $h \in [H]$ , that is,

$$V_h^{\pi}(s) \coloneqq \mathbb{E}_{\pi} \left[ \left. \sum_{h'=h}^{H} r_{h'}(s_{h'}, a_{h'}) \right| s_h = s \right], \ Q_h^{\pi}(s, a) \coloneqq \mathbb{E}_{\pi} \left[ \left. \sum_{h'=h}^{H} r_{h'}(s_{h'}, a_{h'}) \right| s_h = s, a_h = a \right].$$

<sup>&</sup>lt;sup>4</sup>While we assume deterministic rewards for simplicity, our results can be straightforwardly generalized to stochastic rewards, as the major difficulty is in learning the transitions rather than learning the rewards.

<sup>&</sup>lt;sup>5</sup>Any MDP with stochastic  $s_1$  is equivalent to an MDP with deterministic by creating a dummy initial state  $s_0$  and increasing the horizon by 1.

The operators  $\mathbb{P}_h$  and  $\mathbb{V}_h$  are defined as  $[\mathbb{P}_h V_{h+1}](s,a) := \mathbb{E}[V_{h+1}(s')|s_h = s, a_h = a]$  and  $[\mathbb{V}_h V_{h+1}](s,a) := \operatorname{Var}[V_{h+1}(s')|s_h = s, a_h = a]$  for any value function  $V_{h+1}$  at time step h+1. We also use  $\widehat{\mathbb{P}}_h$  and  $\widehat{V}_h$  to denote empirical versions of these operators building on estimated models (which will be clear in the context).

We use  $\pi_\star \coloneqq \arg\max_\pi V_1^\pi(s_1)$  to denote any optimal policy, and  $V_h^\star \coloneqq V_h^{\pi_\star}$  and  $Q_h^\star \coloneqq Q_h^{\pi_\star}$  to denote the value function and Q function of  $\pi^\star$  at all  $h \in [H]$ . Throughout this paper, our learning goal is to find an near-optimal policy  $\widehat{\pi}$  such that  $V_1^\star(s_1) - V_1^{\widehat{\pi}}(s_1) \le \varepsilon$ .

Finally, we let  $d_h^{\pi}$  denote the state(-action) visitation distributions of  $\pi$  at time step  $h \in [H]$ :

$$d_h^{\pi}(s) := \mathbb{P}(s_h = s | \pi), \quad \text{and} \quad d_h^{\pi}(s, a) := \mathbb{P}(s_h = s, a_h = a | \pi).$$
 (1)

**Miscellaneous** We use standard  $O(\cdot)$  and  $\Omega(\cdot)$  notation: A = O(B) is defined as  $A \leq CB$  for some absolute constant C > 0 (and similarly for  $\Omega$ ). The tilded notation  $A = \widetilde{O}(B)$  denotes  $A \leq CL \cdot B$  where L is a poly-logarithmic factor of problem parameters.

# C. Main algorithms

This section provides the main algorithms studied in Section 3 (Algorithm 1, PEVI-ADV) and Section 5 (Algorithm 2, HOOVI).

Algorithm 1 Pessimistic Value Iteration with Reference-Advantage Decomposition (PEVI-ADV)

**Require:** Dataset 
$$\mathcal{D} = \left\{ (s_1^{(i)}, a_1^{(i)}, r_1^{(i)}, \dots, s_H^{(i)}, a_H^{(i)}, r_H^{(i)}) \right\}_{i=1}^n$$
 collected by executing  $\mu$  in  $M$ .

1: Split the dataset  $\mathcal{D}$  into  $\mathcal{D}_{ref}$ ,  $\mathcal{D}_0$  and  $\{\mathcal{D}_{h,1}\}_{h=1}^H$  uniformly at random:

$$n_{\text{ref}} \coloneqq |\mathcal{D}_{\text{ref}}| = n/3, \ n_0 \coloneqq |\mathcal{D}_0| = n/3, \ n_{1,h} \coloneqq |\mathcal{D}_{h,1}| \coloneqq n/(3H) \ (n_1 \coloneqq n/3).$$

- 2: Learn a reference value function  $\widehat{V}^{\mathrm{ref}} \leftarrow \mathrm{VI-LCB}(\mathcal{D}_{\mathrm{ref}})$  via VI-LCB (Algorithm 3).
- 3: Let  $N_{h,0}(s,a)$  and  $N_{h,0}(s,a,s')$  denote the visitation count of (s,a) and (s,a,s') at step h within dataset  $\mathcal{D}_0$ . Construct empirical model estimates:

$$\widehat{\mathbb{P}}_{h,0}(s'|s,a) \leftarrow \frac{N_{h,0}(s,a,s')}{N_{h,0}(s,a) \vee 1}, \quad \text{and} \quad \widehat{r}_{h,0}(s,a) \leftarrow r_h(s,a) \mathbb{1} \left\{ N_{h,0}(s,a) \geq 1 \right\}.$$

Similarly define  $N_{h,1}(s,a), N_{h,1}(s,a,s'), (\widehat{r}_{h,1},\widehat{\mathbb{P}}_{h,1})$  for all  $h \in [H]$  based on dataset  $\mathcal{D}_{h,1}$ .

4: Set 
$$b_{h,0}(s,a) \leftarrow c \cdot \left(\sqrt{\frac{[\widehat{\mathbb{V}}_{h,0}\widehat{V}_{h+1}^{\mathrm{ref}}](s,a)\iota}{N_{h,0}(s,a)\vee 1}} + \frac{H\iota}{N_{h,0}(s,a)\vee 1}}\right)$$
 for all  $(h,s,a)$ , where  $\iota := \log(HSA/\delta)$ .

- 5: Set  $\widehat{V}_{H+1}(s) \leftarrow 0$  for all  $s \in \mathcal{S}$ .
- 6: **for** h = H, ..., 1 **do**

7: Set 
$$b_{h,1}(s,a) \leftarrow c \cdot \left(\sqrt{\frac{[\widehat{\mathbb{V}}_{h,1}(\widehat{V}_{h+1} - \widehat{V}_{h+1}^{\mathrm{ref}})](s,a)\iota}{N_{h,1}(s,a)\vee 1}} + \frac{H\iota}{N_{h,1}(s,a)\vee 1}\right)$$
.

8: Perform pessimistic value update for all (s, a):

$$\widehat{Q}_h(s,a) \leftarrow \widehat{r}_{h,0}(s,a) + \left[\widehat{\mathbb{P}}_{h,0}\widehat{V}_{h+1}^{\text{ref}}\right](s,a) - b_{h,0}(s,a) + \left[\widehat{\mathbb{P}}_{h,1}(\widehat{V}_{h+1} - \widehat{V}_{h+1}^{\text{ref}})\right](s,a) - b_{h,1}(s,a);$$

$$\widehat{V}_h(s) \leftarrow \left[\max_{a} \widehat{Q}_h(s,a)\right] \vee 0.$$

- 9: Set  $\widehat{\pi}_h(s) \leftarrow \arg \max_a \widehat{Q}_h(s, a)$  for all  $s \in \mathcal{S}$ .
- 10: **end for**
- 11: **return** Policy  $\widehat{\pi} = {\{\widehat{\pi}_h\}_{h \in [H]}}$

#### Algorithm 2 Hybrid Offline/Online Value Iteration (HOOVI)

**Require:** MDP M, reference policy  $\mu$ .

- 1: # Stage 1: Learn step  $h_{\star} + 1$ : H via optimistic online exploration
- 2: for Episode  $k = 1, \ldots, n_{\text{UCB}} = n/2$  do
- 3: Receive initial state  $s_1$  and play with policy  $\mu$  up to step  $h_{\star}$ . Arrive at state  $s_{h_{\star}+1}$ .
- 4: Play step  $h_{\star} + 1$  to H using the UCBVI-UPLOW algorithm (Algorithm 4).
- 5: end for
- 6: Denote the final output of UCBVI-UPLOW as

$$(\overline{V}_{h_{\star}+1}, \underline{V}_{h_{\star}+1}, \widehat{\pi}_{(h_{\star}+1):H}^{\text{UCB}}) \leftarrow \text{UCBVI-UPLow}(n_{\text{UCB}}).$$

- 7: # Stage 2: Learn step 1 :  $h_{\star}$  via executing  $\mu$  + pessimistic offline policy optimization
- 8: Collect  $\mathcal{D} \leftarrow \{n n_{\text{UCB}} \text{ episodes of data using policy } \mu \text{ up to step } h_{\star}\}.$
- 9: Learn policy  $\widehat{\pi}_{1:h_{\star}}^{\text{PEVI}}$  via the Truncated-PEVI-ADV(Algorithm 5):

$$\widehat{\pi}_{1:h_{\star}}^{\text{PEVI}} \leftarrow \text{Truncated-PEVI-ADV}(\mathcal{D}, h_{\star}, \underline{V}_{h_{\star}+1}).$$

10: **return** Policy  $\widehat{\pi} = (\widehat{\pi}_{1:h_{\star}}^{\text{PEVI}}, \widehat{\pi}_{(h_{\star}+1):H}^{\text{UCB}}).$ 

#### D. Technical tools

**Lemma D.1** (Binomial concentration). Suppose  $N \sim \text{Bin}(n,p)$  where  $n \geq 1$  and  $p \in [0,1]$ . Then with probability at least  $1 - \delta$ , we have

$$\frac{p}{N \vee 1} \le \frac{8\log(1/\delta)}{n}.$$

*Proof.* If  $p \le 8 \log(1/\delta)/n$ , the result clearly holds regardless of the value of N. Suppose  $p > 8 \log(1/\delta)/n$ , then by the multiplicative Chernoff bound, we have

$$\mathbb{P}\left(N < \frac{1}{2}np\right) \le \exp\left(-\frac{(1/2)^2np}{2}\right) = \exp(-np/8) \le \delta.$$

Therefore, with probability at least  $1 - \delta$ , we have  $N \ge np/2$  and thus

$$\frac{p}{N \vee 1} \le \frac{p}{N} \le \frac{2}{n} \le \frac{8\log(1/\delta)}{n}.$$

This shows the desired result.

#### E. VI-LCB and PEVI-ADV

We provide detailed discussion between VI-LCB and PEVI-ADV in this section.

We show that a finite-horizon variant of the VI-LCB (Value Iteration with Lower Confidence Bounds) algorithm of Rashidine-jad et al. (2021) achieves sample complexity  $\widetilde{O}(H^5SC^*/\varepsilon^2)$  for finding an  $\varepsilon$  near-optimal policy. This result is similar to the  $\widetilde{O}(SC^*/(1-\gamma)^5\varepsilon^2)$  guarantee<sup>6</sup> for the original VI-LCB in infinite-horizon discounted MDPs (Rashidinejad et al., 2021, Theorem 6). The main ingredients of our VI-LCB algorithm is a pessimistic value iteration procedure in which we perform value iteration on the empirical model estimated from the dataset  $\mathcal{D}$ , along with a negative Hoeffding bonus term to impose pessimism. Due to space constraints, the algorithm description (Algorithm 3) and the proof of Theorem E.1 are deferred to Appendix F.

<sup>&</sup>lt;sup>6</sup>(Rashidinejad et al., 2021) can achieve a faster rate in case  $C^* \leq 1 + \widetilde{O}(1/N)$ . However, we focus on the case  $C^* = 1 + \Theta(1)$  where the guarantee of Rashidinejad et al. (2021) is  $\widetilde{O}(SC^*/(1-\gamma)^5\varepsilon^2)$ .

**Theorem E.1** (VI-LCB for finite-horizon MDPs). Suppose the reference policy  $\mu$  satisfies the single-policy concentrability (Assumption A). Then with probability at least  $1 - \delta$ , VI-LCB (Algorithm 3) outputs a policy  $\widehat{\pi}$  and value estimate  $\widehat{V}$  such that

(a) 
$$\max_{h \in [H]} \sum_{s \in \mathcal{S}} d_h^{\pi_{\star}}(s) (V_h^{\star}(s) - \widehat{V}_h(s)) \leq \varepsilon$$
,

(b) 
$$V_1^{\star}(s_1) - V_1^{\widehat{\pi}}(s_1) \le \varepsilon$$
,

within  $n = \widetilde{O}(H^5SC^*/\varepsilon^2)$  episodes.

Theorem E.1 serves two main purposes. First, the  $\widetilde{O}(H^5SC^*/\varepsilon^2)$  sample complexity asserted in Theorem E.1(b) provides a first result for offline RL (and offline reduction for policy finetuning) under single-policy concentrability in finite-horizon MDPs. Second, the value estimation bound in Theorem E.1(a) shows that the estimated value function  $\widehat{V}_h(s)$  provided by VI-LCB is close to the optimal value  $V_h^*(s)$  at every step  $h \in [H]$ , in terms of the weighted average with  $d_h^{\pi_*}(s)$ . Our next algorithm PEVI-ADV builds on this property so that VI-LCB can be used as a "warm-up" learning procedure that provides a high-quality value estimate.

PEVI-ADV adds two new ingredients over VI-LCB in order to achieve the  $\widetilde{O}(H^2)$  improvement:

- 1. We replace the Hoeffding-style bonus in VI-LCB with a Bernstein-style bonus. This shaves off one *H* factor via the total variance property (Lemma G.4).
- 2. Both VI-LCB and our PEVI-ADV use data splitting to make sure that the estimated value  $\widehat{V}_{h+1}$  and empirical transitions  $\widehat{\mathbb{P}}_h$  are estimated using different subsets of  $\mathcal{D}$ , this yields conditional independence that is required in bounding concentration terms of the form  $(\widehat{\mathbb{P}}_h \mathbb{P}_h)\widehat{V}_{h+1}$ . However, applied naively, this data splitting induces one undesired H factor in the sample complexity as we need to split  $\mathcal{D}$  into H folds and thus each  $\mathbb{P}_h$  is estimated using only n/H episodes of data.

As a technical crux of this algorithm, we overcome this issue by adapting the *reference-advantage decomposition* technique of Zhang et al. (2020). This technique proposes to learn an initial reference value function  $\hat{V}^{\text{ref}}$  of good quality in a certain sense, and then performing the following type of approximate value iteration (using the right-hand side as the algorithm update):

$$\mathbb{P}_h \widehat{V}_{h+1} \approx \widehat{\mathbb{P}}_{h,0} \widehat{V}_{h+1}^{\mathrm{ref}} + \widehat{\mathbb{P}}_{h,1} (\widehat{V}_{h+1} - \widehat{V}_{h+1}^{\mathrm{ref}}).$$

Above,  $\widehat{V}_{h+1}$ ,  $\widehat{\mathbb{P}}_{h,0}$ , and  $\widehat{P}_{h,1}$  are estimated on three disjoint subsets of the data. The advantage of this approach is that, due to this new independence structure,  $\widehat{\mathbb{P}}_{h,0}$  for different  $h \in [H]$  can be estimated on the same set of trajectories without H-fold splitting, which shaves off the H factor within this part. On the other hand, estimating  $\widehat{\mathbb{P}}_{h,1}$  still requires H-fold splitting, yet this would not hurt the sample complexity if the magnitude of  $(\widehat{V}_{h+1} - \widehat{V}_{h+1}^{\mathrm{ref}})$  is much smaller than its naive upper bound O(H)—we show this can be achieved by using VI-LCB to learn  $\widehat{V}^{\mathrm{ref}}$ .

# F. Proof of Theorem E.1

Throughout the proofs we let C > 0 denote an absolute constant that can vary from line to line. This C is not to be confused with the single-policy concentrability coefficient  $C^*$  in Assumption A.

# F.1. Algorithm

We first present the VI-LCB algorithm in Algorithm 3. This algorithm is an analogue of the original VI-LCB algorithm of (Rashidinejad et al., 2021) for finite-horizon MDPs (instead of infinite-horizon discounted MDPs). Within the algorithm, the constant c in Line 5 is chosen to be the same c > 0 as in Lemma F.1.

## Algorithm 3 Value Iteration with Lower Confidence Bounds (VI-LCB) for episodic MDPs

**Require:** Offline dataset 
$$\mathcal{D} = \left\{ (s_1^{(i)}, a_1^{(i)}, r_1^{(i)}, \dots, s_H^{(i)}, a_H^{(i)}, r_H^{(i)}) \right\}_{i=1}^n$$
.

- 1: Randomly split the dataset  $\mathcal{D}$  into  $\{\mathcal{D}_h\}_{h=1}^H$  with  $|\mathcal{D}_h| = n/H$ .
- 2: Let  $N_h(s, a)$  and  $N_h(s, a, s')$  denote the visitation count of (s, a) and (s, a, s') at step h within dataset  $\mathcal{D}_h$ . Construct empirical model estimates:

$$\widehat{r}_h(s, a) \leftarrow r_h(s, a) \mathbb{1} \left\{ N_h(s, a) \ge 1 \right\},$$

$$\widehat{\mathbb{P}}_h(s'|s, a) \leftarrow \frac{N_h(s, a, s')}{N_h(s, a) \vee 1}.$$

- 3: Set  $\widehat{V}_{H+1}(s) \leftarrow 0$  for all  $s \in \mathcal{S}$ .
- 4: **for** h = H, ..., 1 **do**
- 5: Set  $b_h(s,a) \leftarrow c \cdot \sqrt{\frac{H^2 \iota}{N_h(s,a)\vee 1}}$  (where  $\iota := \log(HSA/\delta)$ ).
- 6: Perform value update for all (s, a):

$$\widehat{Q}_h(s,a) \leftarrow \widehat{r}_h(s,a) + \left[\widehat{\mathbb{P}}_h \widehat{V}_{h+1}\right](s,a) - b_h(s,a);$$

$$\widehat{V}_h(s) \leftarrow \left[\max_a \widehat{Q}_h(s,a)\right] \vee 0.$$

- 7: Set  $\widehat{\pi}_h(s) \leftarrow \arg\max_a \widehat{Q}_h(s, a)$  for all  $s \in \mathcal{S}$ .
- 8: end for
- 9: **return** Value estimate  $\widehat{V} = \left\{\widehat{V}_h\right\}_{h \in [H]}$ , policy  $\widehat{\pi} = \left\{\widehat{\pi}_h\right\}_{h \in [H]}$ .

#### F.2. Some lemmas

**Lemma F.1** (Concentration). Under the setting of Theorem E.1, there exists an absolute constant c > 0 such that the concentration event  $\mathcal{E}$  holds with probability at least  $1 - \delta$ , where

$$\mathcal{E} := \left\{ \left| \left[ \widehat{r}_h - r_h \right](s, a) + \left[ (\widehat{\mathbb{P}}_h - \mathbb{P}_h) \widehat{V}_{h+1} \right](s, a) \right| \le c \cdot \sqrt{\frac{H^2 \iota}{N_h(s, a) \vee 1}} = b_h(s, a), \quad and \right.$$

$$\frac{1}{N_h(s, a) \vee 1} \le c \cdot \frac{H \iota}{n d_h^{\mu}(s, a)} \quad for \ all \ (h, s, a) \in [H] \times \mathcal{S} \times \mathcal{A} \right\},$$

and  $\iota := \log(HSA/\delta)$ .

Proof of Lemma F.1. Fix any (h, s, a). The first claim holds trivially if  $N_h(s, a) = 0$ , as  $\widehat{r}_h(s, a) = \widehat{\mathbb{P}}_h(\cdot | s, a) = 0$  by definition, and thus the left-hand side is upper bounded by  $H + 1 \le 2H \le 2\sqrt{H^2 \iota}$ . If  $N_h(s, a) \ge 1$ , conditioned on  $N_h(s, a)$ , we have

$$\begin{split} \widehat{r}_h(s,a) &= r_h(s,a), \\ \left| \left[ (\widehat{\mathbb{P}}_h - \mathbb{P}_h) \widehat{V}_{h+1} \right] (s,a) \right| &\leq c \cdot \sqrt{\frac{H^2 \log(HSA/\delta)}{N_h(s,a)}}, \end{split}$$

where the last inequality is obtained by the Azuma-Hoeffding inequality with probability at least  $1 - \delta/(2HSA)$ , using the fact that the data used in obtaining  $\widehat{V}_{h+1}$  (due to the data splitting in Algorithm 3). Therefore

$$\left| \left[ \widehat{r}_h - r_h \right](s, a) + \left[ (\widehat{\mathbb{P}}_h - \mathbb{P}_h) \widehat{V}_{h+1} \right](s, a) \right| \le c \cdot \sqrt{\frac{H^2 \iota}{N_h(s, a) \vee 1}}.$$

Further taking the union bound yields the first claim over all (h, s, a) with probability at least  $1 - \delta/2$ .

For the second claim, notice that  $N_h(s,a) \sim \text{Bin}(n/H, d_h^{\mu}(s,a))$ . Applying Lemma D.1 yields that

$$\frac{1}{N_h(s,a) \vee 1} \leq \frac{8 \log(2HSA/\delta)}{n/H \cdot d_h^{\mu}(s,a)} \leq c \cdot \frac{H\iota}{nd_h^{\mu}(s,a)}$$

with probability at least  $1 - \delta/(2HSA)$ . Taking the union bound yields the second claim over all (h, s, a) with probability at least  $1 - \delta/2$ .

**Lemma F.2** (Monotonicity for VI-LCB). Let  $\hat{\pi}$  be the output policy of Algorithm 3. Then, on the event  $\mathcal{E}$  defined in Lemma F.1, we have

$$\widehat{V}_h(s) \le V_h^{\widehat{\pi}}(s) \le V_h^{\star}(s)$$

for any  $s \in \mathcal{S}$  and  $h \in [H]$ .

*Proof of Lemma F.2.* We first prove  $\widehat{V}_h(s) \leq V_h^{\widehat{\pi}}(s)$  for any  $s \in \mathcal{S}$  and  $h \in [H]$  by induction. For h = H, and any  $s \in \mathcal{S}, a \in \mathcal{A}$ ,

$$Q_H^{\widehat{\pi}}(s, a) - \widehat{Q}_H(s, a) = r_H(s, a) - \widehat{r}_H(s, a) + b_H(s, a) \ge 0,$$

where the last inequality is by Lemma F.1. Then,

$$\begin{split} &V_H^{\widehat{\pi}}(s) - \widehat{V}_H(s) \\ &= Q_H^{\widehat{\pi}}(s,\widehat{\pi}_H(s)) - \left[\max_a \widehat{Q}_H(s,a)\right] \vee 0 \\ &= Q_H^{\widehat{\pi}}(s,a_{s,H}) - \left[\widehat{Q}_H(s,a_{s,H})\right] \vee 0 \\ &= \left[Q_H^{\widehat{\pi}}(s,a_{s,H}) - \widehat{Q}_H(s,a_{s,H})\right] \wedge Q_H^{\widehat{\pi}}(s,a_{s,H}) \geq 0, \end{split}$$

$$(a_{s,H} \coloneqq \widehat{\pi}_H(s))$$

where the last inequality follows from Lemma F.1, and  $Q_H^{\pi}(s,a) \in [0,1]$  for any  $\pi, s \in \mathcal{S}$ , and  $a \in \mathcal{A}$ .

We now show that, if  $\widehat{V}_{h+1}(s) \leq V_{h+1}^{\widehat{\pi}}(s)$  holds for any s, we also have  $\widehat{V}_h(s) \leq V_h^{\widehat{\pi}}(s)$  for any s. Recall that  $\widehat{V}_h(s) = \max_a \widehat{Q}_h(s,a) \vee 0 = \widehat{Q}_h(s,\widehat{\pi}_h(s)) \vee 0$ . The claim clearly holds in the trivial case of  $\widehat{V}_h(s) = 0$ . Otherwise, we have

$$\begin{split} &V_{h}^{\widehat{\pi}}(s) - \widehat{V}_{h}(s) \\ &= Q_{h}^{\widehat{\pi}}(s, a_{s,h}) - \widehat{Q}_{h}(s, a_{s,h}) \\ &= r_{h}(s, a_{s,h}) + \left[\mathbb{P}_{h}V_{h+1}^{\widehat{\pi}}\right](s, a_{s,h}) - \widehat{r}_{h}(s, a_{s,h}) - \left[\widehat{\mathbb{P}}_{h}\widehat{V}_{h+1}\right](s, a_{s,h}) + b_{h}(s, a_{s,h}) \\ &= r_{h}(s, a_{s,h}) - \widehat{r}_{h}(s, a_{s,h}) + \left[\mathbb{P}_{h}\left(V_{h+1}^{\widehat{\pi}} - \widehat{V}_{h+1}\right)\right](s, a_{s,h}) + \left[\left(\mathbb{P}_{h} - \widehat{\mathbb{P}}_{h}\right)\widehat{V}_{h+1}\right](s, a_{s,h}) + b_{h}(s, a_{s,h}) \\ &\geq r_{h}(s, a_{s,h}) - \widehat{r}_{h}(s, a_{s,h}) + \left[\left(\mathbb{P}_{h} - \widehat{\mathbb{P}}_{h}\right)\widehat{V}_{h+1}\right](s, a_{s,h}) + b_{h}(s, a_{s,h}) \\ &\geq 0, \end{split}$$

where the first inequality follows from  $V_{h+1}^{\widehat{\pi}}(s) \geq \widehat{V}_{h+1}(s)$  for any s, and the last inequality is by Lemma F.1. This completes the proof of  $V_h(s) \leq V_h^{\widehat{\pi}}(s)$ ,  $\forall s \in \mathcal{S}, h \in [H]$ .

The argument  $V_h^{\widehat{\pi}}(s) \leq V_h^{\star}(s)$  holds by definition of  $V_h^{\star}(s) = V_h^{\pi_{\star}}(s) \geq V_h^{\pi}(s)$ , for any  $\pi, s \in \mathcal{S}$ , and  $h \in [H]$ . Thus, we complete the proof.

**Lemma F.3** (Performance decomposition for VI-LCB). On the event E defined in Lemma F.1, we have

$$\sum_{s \in \mathcal{S}} d_h^{\pi_{\star}}(s) (V_h^{\star}(s) - \widehat{V}_h(s)) \le 2 \sum_{h'=h}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_{h'}^{\pi_{\star}}(s,a) b_{h'}(s,a),$$

for any  $h \in [H]$ .

*Proof of Lemma F.3.* Throughout this proof we let  $\widehat{Q}_h(s,\pi_\star) := \widehat{Q}_h(s,\pi_{\star,h}(s))$  for shorthand. We have

$$\begin{split} &\sum_{s \in \mathcal{S}} d_h^{\pi_*}(s) (V_h^*(s) - \widehat{V}_h(s)) \\ &\leq \sum_{s \in \mathcal{S}} d_h^{\pi_*}(s) (V_h^*(s) - \max_a \widehat{Q}_h(s,a)) \\ &\leq \sum_{s \in \mathcal{S}} d_h^{\pi_*}(s) (V_h^*(s) - \max_a \widehat{Q}_h(s,a)) \\ &\leq \sum_{s \in \mathcal{S}} d_h^{\pi_*}(s) (V_h^*(s) - \widehat{Q}_h(s,\pi_*)) \\ &= \sum_{h'=h}^H \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_{h'}^{\pi_*}(s,a) r_{h'}(s,a) - \sum_{s \in \mathcal{S}} d_h^{\pi_*}(s) \widehat{Q}_h(s_1,\pi_*) \\ &= \sum_{h'=h}^H \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_{h'}^{\pi_*}(s,a) r_{h'}(s,a) - \sum_{h'=h}^H \sum_{s,a,s',a'} \left( d_{h'}^{\pi_*}(s,a) \widehat{Q}_{h'}(s,a) - d_{h'+1}^{\pi_*}(s',a') \widehat{Q}_{h'+1}(s',a') \right) \\ &\leq \sum_{h'=h}^H \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_{h'}^{\pi_*}(s,a) r_{h'}(s,a) - \sum_{h'=h}^H \sum_{s,a,s'} \left( d_{h'}^{\pi_*}(s,a) \widehat{Q}_{h'}(s,a) - d_{h'+1}^{\pi_*}(s') \widehat{V}_{h'+1}(s') \right) \quad \text{(by definition of } \widehat{V}_{h'}) \\ &= \sum_{h'=h}^H \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_{h'}^{\pi_*}(s,a) r_h(s,a) - \sum_{h'=h}^H \sum_{s,a,s'} d_{h'}^{\pi_*}(s,a) \left( \widehat{Q}_{h'}(s,a) - d_{h'+1}^{\pi_*}(s') \widehat{V}_{h'+1} \right] (s,a) \right) \\ &= \sum_{h'=h}^H \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_{h'}^{\pi_*}(s,a) \left( r_{h'}(s,a) + \left[ \mathbb{P}_{h'} \widehat{V}_{h'+1} \right] (s,a) - \widehat{Q}_{h'}(s,a) \right) \\ &= \sum_{h'=h}^H \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_{h'}^{\pi_*}(s,a) \left( r_{h'}(s,a) + \left[ \mathbb{P}_{h'} \widehat{V}_{h'+1} \right] (s,a) - \widehat{r}_{h'}(s,a) - \left[ \widehat{\mathbb{P}}_{h'} \widehat{V}_{h'+1} \right] (s,a) + b_{h'}(s,a) \right) \\ &\leq 2 \sum_{h'=h}^H \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_{h'}^{\pi_*}(s,a) b_{h'}(s,a). \quad \text{(by the concentration event } \mathcal{E}) \end{aligned}$$

This completes the proof.

## F.3. Proof of main theorem

We are now ready to prove the Theroem E.1. We first prove part (a). By Lemma F.2, we have

$$\begin{split} & \max_{h \in [H]} \sum_{s \in \mathcal{S}} d_h^{\pi_\star}(s) (V_h^\star(s) - \widehat{V}_h(s)) \\ & \leq 2 \sum_{h=1}^H \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_h^{\pi_\star}(s,a) b_h(s,a) \\ & = c \sum_{h=1}^H \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_h^{\pi_\star}(s,a) \cdot \sqrt{\frac{H^2 \iota}{N_h(s,a) \vee 1}} \\ & = c \sqrt{H^2 \iota} \sum_{h=1}^H \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_h^{\pi_\star}(s,a) \cdot \sqrt{\frac{1}{N_h(s,a) \vee 1}} \\ & \leq c \sqrt{H^2 \iota} \sum_{h=1}^H \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_h^{\pi_\star}(s,a) \cdot \sqrt{\frac{H \iota}{n d_h^\mu(s,a)}} \\ & \leq c \sqrt{H^3 \iota^2} \sum_{h=1}^H \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} \sqrt{d_h^{\pi_\star}(s,a)} \cdot \sqrt{\frac{d_h^{\pi_\star}(s,a)}{n d_h^\mu(s,a)}} \end{split} \tag{by the concentration event $\mathcal{E}$)}$$

Therefore, as long as  $n \ge O(H^5SC^\star \iota^2/\varepsilon^2)$ , we have  $\max_{h \in [H]} \sum_{s \in \mathcal{S}} d_h^{\pi_\star}(s) (V_h^\star(s) - \widehat{V}_h(s)) \le \varepsilon$ . This shows part (a). Further, this bound at h = 1 says

$$V_1^{\star}(s_1) - \widehat{V}_1(s_1) \le \varepsilon$$

(as we assumed deterministic  $s_1$ ). Part (b) follows directly from this and the fact that  $V_1^{\widehat{\pi}}(s_1) \geq \widehat{V}_1(s_1)$  which was shown in Lemma F.2.

#### G. Proof of Theorem 1

#### **G.1. Some Lemmas**

**Lemma G.1** (Concentration). Under the setting of Theorem 1, there exists an absolute constant c > 0 such that the concentration event  $\mathcal{E}$  holds with probability at least  $1 - \delta$ , where

$$\begin{split} \mathcal{E} &:= \left\{ (i) : \left| \left[ \widehat{r}_{h,0} - r_h \right] (s,a) + \left[ (\widehat{\mathbb{P}}_{h,0} - \mathbb{P}_h) \widehat{V}_{h+1}^{\mathrm{ref}} \right] (s,a) \right| \\ &\leq c \cdot \left( \sqrt{\frac{\left[\widehat{\mathbb{V}}_{h,0}(\widehat{V}_{h+1}^{\mathrm{ref}})\right] (s,a)\iota}{N_{h,0}(s,a) \vee 1}} + \frac{H\iota}{N_{h,0}(s,a) \vee 1} \right) = b_{h,0}(s,a), \\ (ii) : \left| \left[ (\widehat{\mathbb{P}}_{h,1} - \mathbb{P}_h)(\widehat{V}_{h+1} - \widehat{V}_{h+1}^{\mathrm{ref}}) \right] (s,a) \right| \\ &\leq c \cdot \left( \sqrt{\frac{\left[\widehat{\mathbb{V}}_{h,1}(\widehat{V}_{h+1} - \widehat{V}_{h+1}^{\mathrm{ref}})\right] (s,a)\iota}{N_{h,1}(s,a) \vee 1}} + \frac{H\iota}{N_{h,1}(s,a) \vee 1} \right) = b_{h,1}(s,a), \\ (iii) : \frac{1}{N_{h,0}(s,a) \vee 1} \leq c \cdot \frac{\iota}{nd_h^{\mu}(s,a)} \quad and \\ (iv) : \frac{1}{N_{h,1}(s,a) \vee 1} \leq c \cdot \frac{H\iota}{nd_h^{\mu}(s,a)} \quad for all \ (h,s,a) \in [H] \times \mathcal{S} \times \mathcal{A} \right\}, \end{split}$$

and  $\iota := \log(HSA/\delta)$ .

Proof of Lemma G.1. Claim (i) holds trivially if  $N_{h,0}(s,a)=0$ , as  $\widehat{r}_{h,0}(s,a)=\widehat{\mathbb{P}}_{h,0}(\cdot|s,a)=0$  by definition, and thus the left-hand side is upper bounded by  $H+1\leq 2H\leq H\iota$ . If  $N_{h,0}(s,a)\geq 1$ , conditioned on  $N_{h,0}(s,a)$ , we have

$$\widehat{r}_{h,0}(s,a) = r_h(s,a),$$

$$\left| \left[ (\widehat{\mathbb{P}}_{h,0} - \mathbb{P}_h) \widehat{V}_{h+1}^{\text{ref}} \right](s,a) \right| \le c \cdot \left( \sqrt{\frac{\left[\widehat{\mathbb{V}}_{h,0}(\widehat{V}_{h+1}^{\text{ref}})\right](s,a) \log(HSA/\delta)}{N_{h,0}(s,a) \vee 1}} + \frac{H \log(HSA/\delta)}{N_{h,0}(s,a) \vee 1} \right)$$

where the last inequality is obtained by the empirical Bernstein inequality (Maurer and Pontil, 2009, Theorem 4) with probability at least  $1 - \delta/(2HSA)$ . Therefore

$$\left| \left[ \widehat{r}_{h,0} - r_h \right](s,a) + \left[ (\widehat{\mathbb{P}}_{h,0} - \mathbb{P}_h) \widehat{V}_{h+1}^{\text{ref}} \right](s,a) \right| \le c \cdot \left( \sqrt{\frac{\left[ \widehat{\mathbb{V}}_{h,0} (\widehat{V}_{h+1}^{\text{ref}}) \right](s,a)\iota}{N_{h,0}(s,a) \vee 1}} + \frac{H\iota}{N_{h,0}(s,a) \vee 1} \right).$$

Further taking the union bound yields the first claim over all (h,s,a) with probability at least  $1-\delta/4$ . The claim (ii) also follows from the similar argument. Claims (iii) and (iv) can be obtained directly from Lemma D.1 and a union bound, in a similar fashion as in the proof of Lemma F.1. (Note that  $N_{h,0}(s,a) \sim \text{Bin}(n_0,d_h^{\mu}(s,a))$  and  $N_{h,1} \sim \text{Bin}(n_{1,h},d_h^{\mu}(s,a))$  where  $n_0=n/3$  and  $n_{1,h}=n/(3H)$  due to our data splitting schedule.) This completes the proof.

**Lemma G.2** (Monotonicity for PEVI-ADV). Let  $\widehat{\pi}$  be the output policy of Algorithm 1. Then, on the event  $\mathcal{E}$  defined in Lemma G.1, we have

$$\widehat{V}_h(s) \le V_h^{\widehat{\pi}}(s) \le V_h^{\star}(s)$$

for any  $s \in \mathcal{S}$  and  $h \in [H]$ .

*Proof of Lemma G.2.* We provide the proof by induction. For h = H, and any s, a,

$$Q_H^{\hat{\pi}}(s,a) - \hat{Q}_H(s,a) = r_H(s,a) - \hat{r}_{H,0}(s,a) + b_{H,0}(s,a).$$
(2)

Eq.(2) is non-negative the concentration event  $\mathcal{E}(i)$  by Lemma G.1. Thus, we have  $Q_H^{\widehat{\pi}}(s,a) - \widehat{Q}_H(s,a) \geq 0$  for any s,a, and then

$$\begin{split} &V_H^{\widehat{\pi}}(s) - \widehat{V}_H(s) \\ &= Q_H^{\widehat{\pi}}(s, \widehat{\pi}_H(s)) - \left[ \max_a \widehat{Q}_H(s, a) \right] \vee 0 \\ &= Q_H^{\widehat{\pi}}(s, a_{s,H}) - \left[ \widehat{Q}_H(s, a_{s,H}) \right] \vee 0 \\ &= \left[ Q_H^{\widehat{\pi}}(s, a_{s,H}) - \widehat{Q}_H(s, a_{s,H}) \right] \wedge Q_H^{\widehat{\pi}}(s, a_{s,H}) \\ &\geq 0, \end{split}$$

$$(a_{s,H} \coloneqq \widehat{\pi}_H(s))$$

$$\geq 0,$$

where the last inequality follows from the result of Eq.(2) is positive, and  $Q_H^{\pi}(s,a) \in [0,1]$  for any  $\pi,s \in \mathcal{S}, a \in \mathcal{A}$ .

We now show that, if  $\widehat{V}_{h+1}(s) \leq V_{h+1}^{\widehat{\pi}}(s)$  holds for any s, we also have  $\widehat{V}_h(s) \leq V_h^{\widehat{\pi}}(s)$  for any s. Recall that  $\widehat{V}_h(s) = \max_a \widehat{Q}_h(s,a) \vee 0 = \widehat{Q}_h(s,\widehat{\pi}_h(s)) \vee 0$ . The claim clearly holds in the trivial case of  $\widehat{V}_h(s) = 0$ . Otherwise, we have

$$\begin{split} &V_{h}^{\widehat{\pi}}(s) - \widehat{V}_{h}(s) \\ &= Q_{h}^{\widehat{\pi}}(s, a_{s,h}) - \widehat{Q}_{h}(s, a_{s,h}) \\ &= r_{h}(s, a_{s,h}) + \left[\mathbb{P}_{h}V_{h+1}^{\widehat{\pi}}\right](s, a_{s,h}) - \widehat{r}_{h,0}(s, a_{s,h}) - \left[\widehat{\mathbb{P}}_{h,0}\widehat{V}_{h+1}^{\text{ref}}\right](s, a_{s,h}) \\ &- \left[\widehat{\mathbb{P}}_{h}(\widehat{V}_{h+1} - \widehat{V}_{h+1}^{\text{ref}})\right](s, a_{s,h}) + b_{h,0}(s, a_{s,h}) + b_{h,1}(s, a_{s,h}) \\ &= r_{h}(s, a_{s,h}) - \widehat{r}_{h,0}(s, a_{s,h}) + \left[\mathbb{P}_{h}\left(V_{h+1}^{\widehat{\pi}} - \widehat{V}_{h+1}\right)\right](s, a_{s,h}) + \left[\left(\mathbb{P}_{h} - \widehat{\mathbb{P}}_{h,0}\right)\widehat{V}_{h+1}^{\text{ref}}\right](s, a_{s,h}) \\ &+ \left[\left(\mathbb{P}_{h} - \widehat{\mathbb{P}}_{h}\right)\left(\widehat{V}_{h+1} - \widehat{V}_{h+1}^{\text{ref}}\right)\right](s, a_{s,h}) + b_{h,0}(s, a_{s,h}) + b_{h,1}(s, a_{s,h}) \\ &\geq r_{h}(s, a_{s,h}) - \widehat{r}_{h,0}(s, a_{s,h}) + \left[\left(\mathbb{P}_{h} - \widehat{\mathbb{P}}_{h,0}\right)\widehat{V}_{h+1}^{\text{ref}}\right](s, a_{s,h}) \end{split}$$

$$+ \left[ \left( \mathbb{P}_h - \widehat{\mathbb{P}}_h \right) \left( \widehat{V}_{h+1} - \widehat{V}_{h+1}^{\text{ref}} \right) \right] (s, a_{s,h}) + b_{h,0}(s, a_{s,h}) + b_{h,1}(s, a_{s,h})$$

where the last inequality follows from  $V_{h+1}^{\widehat{\pi}}(s) \geq \widehat{V}_{h+1}(s)$  for any s. Note that Eq.(3) is also non-negative under  $\mathcal{E}(\mathbf{i} \& \mathbf{ii})$  by Lemma G.1. This completes the proof of  $V_h(s) \leq V_h^{\widehat{\pi}}(s), \ \forall s \in \mathcal{S}, h \in [H]$ .

**Lemma G.3** (Performance decomposition for PEVI-ADV). On the event E defined in Lemma G.1, we have

$$\sum_{s \in \mathcal{S}} d_h^{\pi_{\star}}(s) (V_h^{\star}(s) - \widehat{V}_h(s)) \le 2 \sum_{h'=h}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_{h'}^{\pi_{\star}}(s,a) (b_{h',0}(s,a) + b_{h',1}(s,a)),$$

for any  $h \in [H]$ .

*Proof of Lemma G.3.* Throughout this proof we let  $\widehat{Q}_h(s,\pi_\star) := \widehat{Q}_h(s,\pi_{\star,h}(s))$  for shorthand. On the event  $\mathcal{E}$ , we have

$$\begin{split} &\sum_{s \in \mathcal{S}} d_{h}^{\pi_{*}}(s) (V_{h}^{*}(s) - \hat{V}_{h}(s)) \\ &\leq \sum_{s \in \mathcal{S}} d_{h}^{\pi_{*}}(s) (V_{h}^{*}(s) - \max_{a} \hat{Q}_{h}(s, a)) \\ &\leq \sum_{s \in \mathcal{S}} d_{h}^{\pi_{*}}(s) (V_{h}^{*}(s) - \max_{a} \hat{Q}_{h}(s, a)) \\ &\leq \sum_{s \in \mathcal{S}} d_{h}^{\pi_{*}}(s) (V_{h}^{*}(s) - \hat{Q}_{h}(s, \pi_{*})) \\ &= \sum_{h' = h}^{H} \sum_{(s, a) \in \mathcal{S} \times \mathcal{A}} d_{h'}^{\pi_{*}}(s, a) r_{h'}(s, a) - \sum_{s \in \mathcal{S}} d_{h}^{\pi_{*}}(s) \hat{Q}_{h}(s_{1}, \pi_{*}) \\ &= \sum_{h' = h}^{H} \sum_{(s, a) \in \mathcal{S} \times \mathcal{A}} d_{h'}^{\pi_{*}}(s, a) r_{h'}(s, a) - \sum_{h' = h}^{H} \sum_{s, a, s', a'} \left( d_{h'}^{\pi_{*}}(s, a) \hat{Q}_{h'}(s, a) - d_{h' + 1}^{\pi_{*}}(s', a') \hat{Q}_{h' + 1}(s', a') \right) \\ &\leq \sum_{h' = h}^{H} \sum_{(s, a) \in \mathcal{S} \times \mathcal{A}} d_{h'}^{\pi_{*}}(s, a) r_{h'}(s, a) - \sum_{h' = h}^{H} \sum_{(s, a) \in \mathcal{S}} \left( d_{h'}^{\pi_{*}}(s, a) \hat{Q}_{h'}(s, a) - d_{h' + 1}^{\pi_{*}}(s') \hat{V}_{h' + 1}(s') \right) \quad \text{(by definition of } \hat{V}_{h'}) \\ &= \sum_{h' = h}^{H} \sum_{(s, a) \in \mathcal{S} \times \mathcal{A}} d_{h'}^{\pi_{*}}(s, a) r_{h}(s, a) - \sum_{h' = h}^{H} \sum_{(s, a) \in \mathcal{S} \times \mathcal{A}} d_{h'}^{\pi_{*}}(s, a) \left( \hat{Q}_{h'}(s, a) - \left[ \mathbb{P}_{h'} \hat{V}_{h' + 1} \right] (s, a) \right) \\ &= \sum_{h' = h}^{H} \sum_{(s, a) \in \mathcal{S} \times \mathcal{A}} d_{h'}^{\pi_{*}}(s, a) \left( r_{h'}(s, a) - \hat{r}_{h', 0}(s, a) + \left[ \mathbb{P}_{h'} \hat{V}_{h' + 1} \right] (s, a) - \left[ \mathbb{P}_{h', 0} \hat{V}_{h' + 1}^{\text{ref}} \right] (s, a) \\ &= \sum_{h' = h}^{H} \sum_{(s, a) \in \mathcal{S} \times \mathcal{A}} d_{h'}^{\pi_{*}}(s, a) \left( r_{h'}(s, a) - \hat{r}_{h', 0}(s, a) + b_{h', 1}(s, a) \right) \\ &\leq 2 \sum_{h' = h}^{H} \sum_{(s, a) \in \mathcal{S} \times \mathcal{A}} d_{h'}^{\pi_{*}}(s, a) (b_{h', 0}(s, a) + b_{h', 1}(s, a)). \quad \text{(by Lemma G.1)} \end{aligned}$$

This completes the proof.

**Lemma G.4** (Total variance lemma). On the event  $\mathcal{E}$  defined in Lemma G.1, the reference value function  $\widehat{V}^{\mathrm{ref}}$  obtained in Algorithm 1 satisfies

$$\sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_h^{\pi_{\star}}(s,a) \left[ \mathbb{V}_h \widehat{V}_{h+1}^{\text{ref}} \right](s,a) \le H^2 + c \sqrt{\frac{H^9 S C^{\star} \iota^2}{n_{\text{ref}}}},$$

where c is an absolute constant.

*Proof of Lemma G.4.* We first decompose our target as follows,

$$\begin{split} &\sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_h^{\pi_\star}(s,a) [\mathbb{V}_h(\widehat{V}_{h+1}^{\mathrm{ref}})](s,a) \\ &= \underbrace{\sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_h^{\pi_\star}(s,a) [\mathbb{V}_h V_{h+1}^\star](s,a)}_{(\mathrm{II})} + \underbrace{\sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_h^{\pi_\star}(s,a) [\mathbb{V}_h \widehat{V}_{h+1}^{\mathrm{ref}} - \mathbb{V}_h V_{h+1}^\star](s,a)}_{(\mathrm{II})}. \end{split}$$

We now bound term (I) and term (II) separately.

Let  $\mathcal{F}_{h+1}$  denote the  $\sigma$ -algebra that contains all information about the trajectory up to  $s_{h+1}$  but not  $a_{h+1}$ . We have

$$\begin{split} &(\mathbf{I}) = \sum_{h=1}^{H} \mathbb{E}_{d^{\pi_{\star}}} \left[ \operatorname{Var} \left[ V_{h+1}^{\star}(s_{h+1}) \middle| s_{h}, a_{h} \right] \right] \\ &= \sum_{h=1}^{H} \mathbb{E}_{d^{\pi_{\star}}} \left[ \mathbb{E} \left[ \left( V_{h+1}^{\star}(s_{h+1}) + r_{h}(s_{h}, a_{h}) - V_{h}^{\star}(s_{h}) \right)^{2} \middle| s_{h}, a_{h} \right] \right] \\ &= \sum_{h=1}^{H} \mathbb{E}_{d^{\pi_{\star}}} \left[ \left( V_{h+1}^{\star}(s_{h+1}) + r_{h}(s_{h}, a_{h}) - V_{h}^{\star}(s_{h}) \right)^{2} \right] \\ &= \sum_{h=1}^{H} \mathbb{E}_{d^{\pi_{\star}}} \left[ \left( V_{h+1}^{\star}(s_{h+1}) + r_{h}(s_{h}, a_{h}) - V_{h}^{\star}(s_{h}) \right)^{2} \right] \\ &+ 2 \sum_{1 \leq h < h' \leq H} \mathbb{E}_{d^{\pi_{\star}}} \left[ \left( V_{h+1}^{\star}(s_{h+1}) + r_{h}(s_{h}, a_{h}) - V_{h}^{\star}(s_{h}) \right)^{2} \right] \\ &= 0, \text{ because } \left( V_{h+1}^{\star}(s_{h+1}) + r_{h}(s_{h}, a_{h}) - V_{h}^{\star}(s_{h}) \right) \mathbb{E}_{d^{\pi_{\star}}} \left[ V_{h'+1}^{\star}(s_{h'+1}) + r_{h'}(s_{h'}, a_{h'}) | \mathcal{F}_{h+1}| = 0 \text{ for any } h < h' \right] \\ &= \mathbb{E}_{d^{\pi_{\star}}} \left[ \left( \sum_{h=1}^{H} \left( V_{h+1}^{\star}(s_{h+1}) + r_{h}(s_{h}, a_{h}) - V_{h}^{\star}(s_{h}) \right) \right)^{2} \right] \\ &= \mathbb{E}_{d^{\pi_{\star}}} \left[ \left( \sum_{h=1}^{H} r_{h}(s_{h}, a_{h}) + \sum_{h=1}^{H} \left( V_{h+1}^{\star}(s_{h+1}) - V_{h}^{\star}(s_{h}) \right) \right)^{2} \right] \\ &= \mathbb{E}_{d^{\pi_{\star}}} \left[ \left( \sum_{h=1}^{H} r_{h}(s_{h}, a_{h}) - V_{1}^{\star}(s_{1}) \right)^{2} \right] \\ &= \mathbb{E}_{d^{\pi_{\star}}} \left[ \left( \sum_{h=1}^{H} r_{h}(s_{h}, a_{h}) - V_{1}^{\star}(s_{1}) \right)^{2} \right] \\ &= \mathbb{E}_{d^{\pi_{\star}}} \left[ \left( \sum_{h=1}^{H} r_{h}(s_{h}, a_{h}) - V_{1}^{\star}(s_{1}) \right)^{2} \right] \\ &= \mathbb{E}_{d^{\pi_{\star}}} \left[ \left( \sum_{h=1}^{H} r_{h}(s_{h}, a_{h}) - V_{1}^{\star}(s_{1}) \right)^{2} \right] \\ &= \mathbb{E}_{d^{\pi_{\star}}} \left[ \left( \sum_{h=1}^{H} r_{h}(s_{h}, a_{h}) - V_{1}^{\star}(s_{1}) \right)^{2} \right] \\ &= \mathbb{E}_{d^{\pi_{\star}}} \left[ \left( \sum_{h=1}^{H} r_{h}(s_{h}, a_{h}) - V_{1}^{\star}(s_{1}) \right)^{2} \right] \\ &= \mathbb{E}_{d^{\pi_{\star}}} \left[ \left( \sum_{h=1}^{H} r_{h}(s_{h}, a_{h}) - V_{1}^{\star}(s_{1}) \right)^{2} \right] \\ &= \mathbb{E}_{d^{\pi_{\star}}} \left[ \left( \sum_{h=1}^{H} r_{h}(s_{h}, a_{h}) - V_{1}^{\star}(s_{1}) \right)^{2} \right] \\ &= \mathbb{E}_{d^{\pi_{\star}}} \left[ \left( \sum_{h=1}^{H} r_{h}(s_{h}, a_{h}) - V_{1}^{\star}(s_{1}) \right)^{2} \right] \\ &= \mathbb{E}_{d^{\pi_{\star}}} \left[ \left( \sum_{h=1}^{H} r_{h}(s_{h}, a_{h}) - V_{1}^{\star}(s_{1}) \right] \\ &= \mathbb{E}_{d^{\pi_{\star}}} \left[ \left( \sum_{h=1}^{H} r_{h}(s_{h}, a_{h}) - V_{1}^{\star}(s_{1}) \right)^{2} \right] \\ &= \mathbb{E}_{d^{\pi_{\star}}} \left[ \left( \sum_{h=1}^{H} r_{h}$$

For (II),

$$\begin{aligned} &(\mathrm{II}) = \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_h^{\pi_{\star}}(s,a) [\mathbb{V}_h \widehat{V}_{h+1}^{\mathrm{ref}} - \mathbb{V}_h V_{h+1}^{\star}](s,a) \\ &= \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_h^{\pi_{\star}}(s,a) \left[ \mathbb{P}_h \left( \widehat{V}_{h+1}^{\mathrm{ref}} \right)^2 - \left( \mathbb{P}_h \widehat{V}_{h+1}^{\mathrm{ref}} \right)^2 - \mathbb{P}_h \left( V_{h+1}^{\star} \right)^2 + \left( \mathbb{P}_h V_{h+1}^{\star} \right)^2 \right] (s,a) \\ &\leq \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_h^{\pi_{\star}}(s,a) \left[ \left| \mathbb{P}_h (\widehat{V}_{h+1}^{\mathrm{ref}} + V_{h+1}^{\star}) (\widehat{V}_{h+1}^{\mathrm{ref}} - V_{h+1}^{\star}) \right| \end{aligned}$$

$$\begin{split} &+ \left| \mathbb{P}_{h}(\widehat{V}_{h+1}^{\mathrm{ref}} + V_{h+1}^{\star}) \mathbb{P}_{h}(\widehat{V}_{h+1}^{\mathrm{ref}} - V_{h+1}^{\star}) \right| \right](s, a) \\ &\leq 4H \sum_{h=1}^{H} \sum_{(s, a) \in \mathcal{S} \times \mathcal{A}} d_{h}^{\pi_{\star}}(s, a) \left[ \left| \mathbb{P}_{h}(\widehat{V}_{h+1}^{\mathrm{ref}} - V_{h+1}^{\star}) \right| \right](s, a) \\ &\leq 4H \sum_{h=1}^{H} \sum_{(s, a) \in \mathcal{S} \times \mathcal{A}} d_{h+1}^{\pi_{\star}}(s') \left[ V_{h+1}^{\star} - \widehat{V}_{h+1}^{\mathrm{ref}} \right](s') \\ &\leq 4H^{2} \max_{h \in [H]} \sum_{(s, a) \in \mathcal{S} \times \mathcal{A}} d_{h}^{\pi_{\star}}(s) \left( V_{h}^{\star} - \widehat{V}_{h}^{\mathrm{ref}} \right)(s) \\ &\leq c \sqrt{\frac{H^{9} S C^{\star} \iota^{2}}{n_{\mathrm{ref}}}}, \end{split} \tag{As } \widehat{V}_{h+1}^{\mathrm{ref}} = 0$$

where the last inequality follows from Lemma G.5. Combining (I) and (II), we complete the proof.

**Lemma G.5** (Guarantees for  $\hat{V}^{ref}$ ). On the event  $\mathcal{E}$  defined in Lemma G.1, the reference value function  $\hat{V}^{ref}$  obtained in Algorithm 1 satisfies

$$\max_{h \in [H]} \sum_{s \in S} d_h^{\pi_{\star}}(s) \Big( V_h^{\star}(s) - \widehat{V}_h^{\text{ref}}(s) \Big) \le c \sqrt{\frac{H^5 S C^{\star} \iota^2}{n_{\text{ref}}}},$$

where c > 0 is an absolute constant.

*Proof of Lemma G.5.* This is a direct corollary of Theorem E.1 (cf. the end of its proof in Section F.3).  $\Box$ 

#### G.2. Proof of the Main Theorem

We now provide the proof of Theorem 1. We assume we are on the good event  $\mathcal{E}$  defined in Lemma G.1, which happens with probability at least  $1 - \delta$ . By Lemma G.3, we know

$$\sum_{s \in \mathcal{S}} d_h^{\pi_{\star}}(s) (V_h^{\star}(s) - \widehat{V}_h(s))$$

$$\leq 2 \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_h^{\pi_{\star}}(s,a) b_{h,0}(s,a) + 2 \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_h^{\pi_{\star}}(s,a) b_{h,1}(s,a),$$

$$\underbrace{\sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_h^{\pi_{\star}}(s,a) b_{h,0}(s,a)}_{(D)} + 2 \underbrace{\sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_h^{\pi_{\star}}(s,a) b_{h,1}(s,a)}_{(D)},$$

for any  $h \in [H]$ .

We first study the term (I) of Eq.(4). Observe that for any (s, a),

$$\begin{split} & [\widehat{\mathbb{V}}_{h,0}\widehat{V}_{h+1}^{\mathrm{ref}}](s,a) - [\mathbb{V}_{h}\widehat{V}_{h+1}^{\mathrm{ref}}](s,a) \\ & = \widehat{\mathbb{P}}_{h,0}(\widehat{V}_{h+1}^{\mathrm{ref}})^2 - (\widehat{\mathbb{P}}_{h,0}\widehat{V}_{h+1}^{\mathrm{ref}})^2 - (\mathbb{P}_{h}(\widehat{V}_{h+1}^{\mathrm{ref}})^2 - (\mathbb{P}_{h}\widehat{V}_{h+1}^{\mathrm{ref}})^2) \\ & \leq |(\widehat{\mathbb{P}}_{h,0} - \mathbb{P}_{h})(\widehat{V}_{h+1}^{\mathrm{ref}})^2| + |(\widehat{\mathbb{P}}_{h,0} + \mathbb{P}_{h})\widehat{V}_{h+1}^{\mathrm{ref}} \cdot (\widehat{\mathbb{P}}_{h,0} - \mathbb{P}_{h})\widehat{V}_{h+1}^{\mathrm{ref}}| \\ & \leq |(\widehat{\mathbb{P}}_{h,0} - \mathbb{P}_{h})(\widehat{V}_{h+1}^{\mathrm{ref}})^2| + 2H|(\widehat{\mathbb{P}}_{h,0} - \mathbb{P}_{h})\widehat{V}_{h+1}^{\mathrm{ref}}| \\ & \leq c\sqrt{\frac{H^4\iota}{N_0(s,a)\vee 1}}. \end{split} \tag{$(|\widehat{V}^{\mathrm{ref}}| \leq H)$}$$

where the last inequality follows from the Azuma-Hoeffding inequality and the fact that  $\widehat{V}_{h+1}^{\mathrm{ref}}(s)$  is obtained from data independent of  $\widehat{P}_{h,0}$ .

Thus, we obtain the following bound for term (I)

(I) = 
$$\sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_h^{\pi_{\star}}(s,a) b_{h,0}(s,a)$$

$$= c \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_{h}^{\pi_{*}}(s,a) \left( \sqrt{\frac{[\widehat{\mathbb{V}}_{h,0}(\widehat{V}_{h+1}^{\mathrm{ref}})](s,a)\iota}{N_{h,0}(s,a) \vee 1}} + \frac{H\iota}{N_{h,0}(s,a) \vee 1} \right)$$

$$\leq c \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_{h}^{\pi_{*}}(s,a) \left( \sqrt{\frac{[\mathbb{V}_{h}(\widehat{V}_{h+1}^{\mathrm{ref}})](s,a)\iota + \sqrt{\frac{H^{4}\iota}{N_{0}(s,a) \vee 1}}}{N_{h,0}(s,a) \vee 1}} + \frac{H\iota}{N_{h,0}(s,a) \vee 1} \right)$$

$$\leq c \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_{h}^{\pi_{*}}(s,a) \left( \sqrt{\frac{[\mathbb{V}_{h}(\widehat{V}_{h+1}^{\mathrm{ref}})](s,a)\iota}{N_{h,0}(s,a) \vee 1}} + \frac{H\iota^{1/4}}{(N_{h,0}(s,a) \vee 1)^{3/4}} + \frac{H\iota}{N_{h,0}(s,a) \vee 1} \right)$$

$$\leq c \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_{h}^{\pi_{*}}(s,a) \left( \sqrt{\frac{[\mathbb{V}_{h}(\widehat{V}_{h+1}^{\mathrm{ref}})](s,a)\iota}{N_{h,0}(s,a) \vee 1}} + \sqrt{\frac{1}{N_{h,0}(s,a) \vee 1}} + \frac{H^{2}\iota^{1/2} + H\iota}{N_{h,0}(s,a) \vee 1} \right)$$

$$= c \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_{h}^{\pi_{*}}(s,a) \sqrt{\frac{[\mathbb{V}_{h}(\widehat{V}_{h+1}^{\mathrm{ref}})](s,a)\iota}{N_{h,0}(s,a) \vee 1}}} + c \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_{h}^{\pi_{*}}(s,a) \sqrt{\frac{1}{N_{h,0}(s,a) \vee 1}}}$$

$$+ c \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_{h}^{\pi_{*}}(s,a) \frac{H^{2}\iota^{1/2} + H\iota}{N_{h,0}(s,a) \vee 1}}$$

$$= c \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_{h}^{\pi_{*}}(s,a) \frac{H^{2}\iota^{1/2} + H\iota}{N_{h,0}(s,a) \vee 1}}$$

$$= c \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_{h}^{\pi_{*}}(s,a) \frac{H^{2}\iota^{1/2} + H\iota}{N_{h,0}(s,a) \vee 1}}$$

$$= c \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_{h}^{\pi_{*}}(s,a) \frac{H^{2}\iota^{1/2} + H\iota}{N_{h,0}(s,a) \vee 1}}$$

$$= c \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_{h}^{\pi_{*}}(s,a) \frac{H^{2}\iota^{1/2} + H\iota}{N_{h,0}(s,a) \vee 1}}$$

$$= c \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_{h}^{\pi_{*}}(s,a) \frac{H^{2}\iota^{1/2} + H\iota}{N_{h,0}(s,a) \vee 1}$$

$$= c \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_{h}^{\pi_{*}}(s,a) \frac{H^{2}\iota^{1/2} + H\iota}{N_{h,0}(s,a) \vee 1}$$

where the last inequality follows from Cauchy-Schwarz inequality.

We now discuss the three terms in Eq.(6) separately:

$$\begin{split} &(\text{I.a}) = \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_{h}^{\pi_{\star}}(s,a) \sqrt{\frac{[\mathbb{V}_{h}(\widehat{V}_{h+1}^{\text{ref}})](s,a)\iota}{N_{h,0}(s,a) \vee 1}} \\ &\leq \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_{h}^{\pi_{\star}}(s,a) \cdot \sqrt{\frac{[\mathbb{V}_{h}(\widehat{V}_{h+1}^{\text{ref}})](s,a)\iota^{2}}{n_{0}d_{h}^{\mu}(s,a)}} \qquad \text{(by the concentration event } \mathcal{E}(\text{iii})) \\ &\leq \sqrt{\frac{C^{\star}\iota^{2}}{n_{0}}} \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} \sqrt{d_{h}^{\pi_{\star}}(s,a)[\mathbb{V}_{h}(\widehat{V}_{h+1}^{\text{ref}})](s,a)} \\ &= \sqrt{\frac{C^{\star}\iota^{2}}{n_{0}}} \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} \sqrt{\mathbb{1}\{a = \pi_{\star}(s)\}d_{h}^{\pi_{\star}}(s,a)[\mathbb{V}_{h}(\widehat{V}_{h+1}^{\text{ref}})](s,a)} \\ &\leq \sqrt{\frac{C^{\star}\iota^{2}}{n_{0}}} \sqrt{\sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} \mathbb{1}\{a = \pi_{\star}(s)\}} \cdot \sqrt{\sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_{h}^{\pi_{\star}}(s,a)[\mathbb{V}_{h}(\widehat{V}_{h+1}^{\text{ref}})](s,a)} \\ &\leq \sqrt{\frac{HSC^{\star}\iota^{2}}{n_{0}}} \sqrt{\sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_{h}^{\pi_{\star}}(s,a)[\mathbb{V}_{h}(\widehat{V}_{h+1}^{\text{ref}})](s,a)}} \end{aligned} \tag{by Cauchy-Schwarz inequality)} \\ &\leq \sqrt{\frac{HSC^{\star}\iota^{2}}{n_{0}}} \sqrt{H^{2} + c\sqrt{\frac{H^{9}SC^{\star}\iota^{2}}{n_{\text{ref}}}}} \end{aligned} \tag{8}$$

(follows from the total variance lemma (Lemma G.4))

$$\leq \sqrt{\frac{H^3SC^{\star}\iota^2}{n_0}} + c\sqrt{\frac{HSC^{\star}\iota^2}{n_0}} \sqrt[4]{\frac{H^9SC^{\star}\iota^2}{n_{\text{ref}}}}$$

$$\leq \sqrt{\frac{H^3SC^*\iota^2}{n_0}} + c\left(\sqrt{\frac{H^3SC^*\iota^2}{n_0}} + \frac{H^4SC^*\iota^2}{\sqrt{n_0n_{\text{ref}}}}\right)$$

$$\leq c\left(\sqrt{\frac{H^3SC^*\iota^2}{n_0}} + \frac{H^4SC^*\iota^2}{\sqrt{n_0n_{\text{ref}}}}\right).$$
(by  $\sqrt{ab} \leq (a+b)/2$ )

Term (I.b) is a smaller-order term compared with (I.a):

$$\begin{split} \text{(I.b)} &= \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_h^{\pi_\star}(s,a) \sqrt{\frac{1}{N_{h,0}(s,a) \vee 1}} \\ &\leq \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_h^{\pi_\star}(s,a) \cdot \sqrt{\frac{\iota}{n_0 d_h^{\mu}(s,a)}} \qquad \text{(by the concentration event } \mathcal{E}(\text{iii})) \\ &\leq \sqrt{\frac{C^{\star}\iota}{n_0}} \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} \sqrt{d_h^{\pi_\star}(s,a)} \\ &= \sqrt{\frac{C^{\star}\iota}{n_0}} \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} \sqrt{1\{a = \pi_\star(s)\} d_h^{\pi_\star}(s,a)} \\ &\leq \sqrt{\frac{C^{\star}\iota}{n_0}} \sqrt{\sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} 1\{a = \pi_\star(s)\}} \cdot \sqrt{\sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_h^{\pi_\star}(s,a)} \\ &\leq \sqrt{\frac{H^2C^{\star}\iota}{n_0}}. \qquad \text{(by Cauchy–Schwarz inequality)} \\ &\leq \sqrt{\frac{H^2C^{\star}\iota}{n_0}}. \qquad \qquad (9) \end{split}$$

Finally, term (I.c)

$$\begin{aligned} \text{(I.c)} &= \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_h^{\pi_{\star}}(s,a) \frac{H^2 \iota^{1/2} + H \iota}{N_{h,0}(s,a) \vee 1} \\ &\leq \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_h^{\pi_{\star}}(s,a) \cdot \frac{H^2 \iota^{3/2} + H \iota^2}{n_0 d_h^{\mu}(s,a)} \\ &\leq \frac{H^3 S C^{\star} \iota^{3/2} + H^2 S C^{\star} \iota^2}{n_0}. \end{aligned} \tag{by the concentration event $\mathcal{E}$(iii))}$$

Substituting Eq.(8), Eq.(9), and Eq.(10) into Eq.(6), we obtain

$$(I) = \sum_{h=1}^{H} \sum_{(s,a)\in\mathcal{S}\times\mathcal{A}} d_h^{\pi_{\star}}(s,a) b_{h,0}(s,a)$$

$$\leq c \cdot \left( \sqrt{\frac{H^3 S C^{\star} \iota^2}{n_0}} + \frac{H^4 S C^{\star} \iota^2}{\sqrt{n_0 n_{\text{ref}}}} + \frac{H^3 S C^{\star} \iota^{3/2} + H^2 S C^{\star} \iota^2}{n_0} \right).$$
(11)

We now study the term (II) of Eq.(4). Let  $g_{h+1} \coloneqq \widehat{V}_{h+1} - \widehat{V}_{h+1}^{\mathrm{ref}}$  (which by our data splitting only depends on the datasets  $\mathcal{D}_{\mathrm{ref}}, \mathcal{D}_0$  and is independent of  $\mathcal{D}_{1,h}$ ). By a similar argument as Eq.(5), we have

$$[\widehat{\mathbb{V}}_{h,1}g](s,a) - [\mathbb{V}_h g](s,a) \le c\sqrt{\frac{H^4\iota}{N_1(s,a) \vee 1}}.$$

for any (s, a). Thus,

$$(II) = \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_{h}^{\pi_{\star}}(s,a) b_{h,1}(s,a)$$

$$= c \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_{h}^{\pi_{\star}}(s,a) \left( \sqrt{\frac{\left[\widehat{\mathbb{V}}_{h}(\widehat{V}_{h+1} - \widehat{V}_{h+1}^{ref})\right](s,a)\iota}{N_{h,1}(s,a) \vee 1}} + \frac{H\iota}{N_{h,0}(s,a) \vee 1} \right)$$

$$\leq c \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_{h}^{\pi_{\star}}(s,a) \left( \sqrt{\frac{\left[\mathbb{V}_{h}(\widehat{V}_{h+1} - \widehat{V}_{h+1}^{ref})\right](s,a)\iota}{N_{h,1}(s,a) \vee 1}} + \frac{H\iota}{N_{h,0}(s,a) \vee 1} \right)$$

$$\leq c \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_{h}^{\pi_{\star}}(s,a) \left( \sqrt{\frac{\left[\mathbb{V}_{h}(\widehat{V}_{h+1} - \widehat{V}_{h+1}^{ref})\right](s,a)\iota}{N_{h,1}(s,a) \vee 1}} + \sqrt{\frac{1}{N_{h,1}(s,a) \vee 1}} + \frac{H^{2}\iota^{1/2} + H\iota}{N_{h,1}(s,a) \vee 1} \right)$$

$$= c \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_{h}^{\pi_{\star}}(s,a) \sqrt{\frac{\left[\mathbb{V}_{h}(\widehat{V}_{h+1} - \widehat{V}_{h+1}^{ref})\right](s,a)\iota}{N_{h,1}(s,a) \vee 1}}}$$

$$= c \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_{h}^{\pi_{\star}}(s,a) \sqrt{\frac{\left[\mathbb{V}_{h}(\widehat{V}_{h+1} - \widehat{V}_{h+1}^{ref})\right](s,a)\iota}{N_{h,1}(s,a) \vee 1}}}$$

$$+ c \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_{h}^{\pi_{\star}}(s,a) \sqrt{\frac{1}{N_{h,1}(s,a) \vee 1}}} + c \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_{h}^{\pi_{\star}}(s,a) \frac{H^{2}\iota^{1/2} + H\iota}{N_{h,1}(s,a) \vee 1}}.$$
(12)

Now, we also bound (II.a), (II.b) and (II.c) separately:

$$\begin{split} &(\text{II.a}) = \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_h^{\pi_\star}(s,a) \sqrt{\frac{\left[\mathbb{V}_h(\hat{V}_{h+1} - \hat{V}_{h+1}^{\text{ref}})\right](s,a)\iota}{N_{h,1}(s,a) \vee 1}} \\ &\leq \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_h^{\pi_\star}(s,a) \cdot \sqrt{\frac{H\left[\mathbb{V}_h(\hat{V}_{h+1} - \hat{V}_{h+1}^{\text{ref}})\right](s,a)\iota^2}{n_1 d_h^{\mu}(s,a)}} & \text{(by the concentration event } \mathcal{E}(\text{iv})) \\ &\leq \sqrt{\frac{HC^\star \iota^2}{n_1}} \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} \sqrt{d_h^{\pi_\star}(s,a) \left[\mathbb{V}_h(\hat{V}_{h+1} - \hat{V}_{h+1}^{\text{ref}})\right](s,a)} \\ &= \sqrt{\frac{HC^\star \iota^2}{n_1}} \sum_{h=1}^{H} \sum_{s} \sqrt{d_h^{\pi_\star}(s) \left[\mathbb{V}_h(\hat{V}_{h+1} - \hat{V}_{h+1}^{\text{ref}})\right](s,\pi_{\star,h}(s))} \\ &\leq \sqrt{\frac{H^2SC^\star \iota^2}{n_1}} \sum_{h=1}^{H} \sum_{s} d_h^{\pi_\star}(s) \left[\mathbb{V}_h(\hat{V}_{h+1} - \hat{V}_{h+1}^{\text{ref}})\right](s,\pi_{\star,h}(s))} \\ &\leq \sqrt{\frac{H^2SC^\star \iota^2}{n_1}} \sum_{h=1}^{H} \sum_{s} d_h^{\pi_\star}(s) \left[\mathbb{P}_h(\hat{V}_{h+1} - \hat{V}_{h+1}^{\text{ref}})^2\right](s,\pi_{\star,h}(s))} \\ &\leq \sqrt{\frac{H^4SC^\star \iota^2}{n_1}} \sum_{h\in\{1,2,\ldots,H\}} \int_{h\in\{1,2,\ldots,H\}} d_h^{\pi_\star}(s) \left[\mathbb{P}_h(\hat{V}_{h+1} - \hat{V}_{h+1}^{\text{ref}})^2\right](s,\pi_{\star,h}(s))} \\ &\leq \sqrt{\frac{H^4SC^\star \iota^2}{n_1}} \sum_{h\in\{1,2,\ldots,H\}} \int_{h\in\{1,2,\ldots,H\}} d_h^{\pi_\star}(s) \left[\mathbb{P}_h(\hat{V}_{h+1} - \hat{V}_{h+1}^{\text{ref}})^2\right](s,\pi_{\star,h}(s))} \end{aligned}$$

$$\leq \sqrt{\frac{H^{4}SC^{\star}\iota^{2}}{n_{1}}} \max_{h \in \{1,2,\dots,H\}} \sum_{s} d_{h}^{\pi_{\star}}(s) \Big[ \mathbb{P}_{h}(V_{h+1}^{\star} - \widehat{V}_{h+1}^{\mathrm{ref}})^{2} \Big] (s, \pi_{\star,h}(s)) \quad \text{(by } \widehat{V}_{h+1} \leq V_{h+1}^{\star} \text{ from Lemma G.2)}$$

$$= \sqrt{\frac{H^{4}SC^{\star}\iota^{2}}{n_{1}}} \max_{h \in \{1,2,\dots,H\}} \sum_{s'} d_{h+1}^{\pi_{\star}}(s') \left( V_{h+1}^{\star}(s') - \widehat{V}_{h+1}^{\mathrm{ref}}(s') \right)^{2}$$

$$\leq \sqrt{\frac{H^{4}SC^{\star}\iota^{2}}{n_{1}}} \max_{h \in \{1,2,\dots,H\}} \sum_{s} d_{h}^{\pi_{\star}}(s) \left( V_{h}^{\star}(s) - \widehat{V}_{h}^{\mathrm{ref}}(s) \right) \cdot H$$

$$\leq c \frac{H^{5.5}SC^{\star}\iota^{2}}{\sqrt{n_{1}n_{\mathrm{ref}}}}, \tag{13}$$

where the last inequality follows from the guarantee for  $\widehat{V}^{\mathrm{ref}}$  in Lemma G.5:

$$\max_{h \in \{1,2,\dots,H\}} \sum_s d_h^{\pi_\star}(s) (V_h^\star(s) - \widehat{V}_h^{\mathrm{ref}}(s)) \leq c \sqrt{\frac{H^5 S C^\star \iota^2}{n_{\mathrm{ref}}}}.$$

By similar arguments as Eq.(9) and Eq.(10), we also have the bounds on (II.b) and (II.c) as follows:

$$\begin{split} &(\text{II.b}) = \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_h^{\pi_{\star}}(s,a) \sqrt{\frac{1}{N_{h,1}(s,a) \vee 1}} \\ &\leq \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_h^{\pi_{\star}}(s,a) \cdot \sqrt{\frac{H\iota}{n_1 d_h^{\mu}(s,a)}} \qquad \text{(by the concentration event } \mathcal{E}(\text{iv})) \\ &\leq \sqrt{\frac{HC^{\star}\iota}{n_1}} \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} \sqrt{d_h^{\pi_{\star}}(s,a)} \\ &= \sqrt{\frac{HC^{\star}\iota}{n_1}} \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} \sqrt{\mathbbm{1}\{a = \pi_{\star}(s)\}} d_h^{\pi_{\star}}(s,a) \\ &\leq \sqrt{\frac{HC^{\star}\iota}{n_1}} \sqrt{\sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} \mathbbm{1}\{a = \pi_{\star}(s)\}} \cdot \sqrt{\sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_h^{\star}(s,a)} \\ &\leq \sqrt{\frac{H^3SC^{\star}\iota}{n_1}}. \end{aligned} \tag{by Cauchy–Schwarz inequality)}$$

$$(\text{II.c}) = \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_h^{\pi_{\star}}(s,a) \frac{H^2 \iota^{1/2} + H \iota}{N_{h,1}(s,a) \vee 1}$$

$$\leq \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{S} \times \mathcal{A}} d_h^{\pi_{\star}}(s,a) \cdot \frac{H^3 \iota^{3/2} + H^2 \iota^2}{n_1 d_h^{\mu}(s,a)} \qquad \text{(by the concentration event } \mathcal{E}(\text{iv}))$$

$$\leq \frac{H^4 S C^{\star} \iota^{3/2} + H^3 S C^{\star} \iota^2}{n_1}. \qquad (15)$$

Substituting Eq.(13), Eq.(14), and Eq.(15) into Eq.(12), we obtain

(II) = 
$$\sum_{h=1}^{H} \sum_{(s,a) \in S \times A} d_h^{\pi_{\star}}(s,a) b_{h,1}(s,a)$$

$$\leq c \cdot \left( \frac{H^{5.5}SC^{\star}\iota^{2}}{\sqrt{n_{1}n_{\text{ref}}}} + \sqrt{\frac{H^{3}SC^{\star}\iota}{n_{1}}} + \frac{H^{4}SC^{\star}\iota^{3/2} + H^{3}SC^{\star}\iota^{2}}{n_{1}} \right).$$
(16)

By definition, we know  $n_{\text{ref}} = n_0 = n_1 = n/3$ . Therefore, combining Eq.(16) and Eq.(11), we obtain

$$V_1^{\star}(s_1) - \widehat{V}_1(s_1) \le 2 \cdot (\mathbf{I}) + 2 \cdot (\mathbf{II})$$

$$\le c \cdot \left( \sqrt{\frac{H^3 S C^{\star} \iota^2}{n}} + \frac{H^{5.5} S C^{\star} \iota^2}{n} \right).$$

The right-hand-side is upper bounded by  $\varepsilon$  as long as

$$n \ge \widetilde{O}\left(H^3SC^*\iota^2/\varepsilon^2 + \frac{H^{5.5}SC^*\iota^2}{\varepsilon}\right)$$

Finally, by the monotonicity property in Lemma G.2, the above also implies the guarantee on  $\hat{\pi}$ :

$$V_1^{\star}(s_1) - V_1^{\widehat{\pi}}(s_1) \le c \cdot \left(\sqrt{\frac{H^3 S C^{\star} \iota^2}{n}} + \frac{H^{5.5} S C^{\star} \iota^2}{n}\right) \le \varepsilon.$$

This completes the proof.

#### H. Proof of Theorem 2

To avoid notational clash, in this proof we use upper-case letters  $S_h$ ,  $A_h$ ,  $R_h$  to denote the actual states and actions seen during the algorithm execution (which are random variables), and reserve the lower-case letters  $s_i$ ,  $s_g$ ,  $s_b$ , a for indexing the (fixed) states and actions of the MDP.

Define an integer

$$K := \min \{ \lfloor C^* \rfloor, A \}.$$

By our assumption that  $C^{\star} \geq 2$ , we have  $2 \leq K \leq A$  and  $K \in [2/3,1] \cdot \min\{C^{\star},A\}$ . Therefore, it suffices to prove the desired performance lower bound for  $n \leq c_0 \cdot H^3 SK/\varepsilon^2$ .

Construction of hard instances We now construct a family of MDPs with S+2 states, 2H+1 steps, and A actions for any  $S \ge 1$  and  $H \ge 1$ . (This rescaling only affects S, H by at most a multiplicative constant and thus does not affect our result.)

Each MDP  $M_{a^*}$  is indexed by a vector  $a^* = (a_{h,i}^*) \in [A]^{HS}$  and is specified as follows:

- State space: There are S "bandit states"  $\{s_i\}_{i\in[S]}$ , one "good state"  $s_g$ , and one "bad state"  $s_b$ .
- The action space is A := [A].
- Transitions:
  - At each  $h \in \{1, \dots, H\}$ , the bandit state  $s_i$  can only transition to  $s_i$  itself,  $s_q$ , or  $s_b$ . The transition probabilities are

$$\begin{cases} \mathbb{P}_h(s_i|s_i,a) = 1 - \frac{1}{H} \quad \text{for all } a \in [A], \\ \mathbb{P}_h(s_g|s_i,a) = \mathbb{P}_h(s_b|s_i,a) = \frac{1}{2H} \quad \text{for all } a \neq a_{h,i}^\star, \\ \mathbb{P}_h(s_g|s_i,a_{h,i}^\star) = \frac{1}{H} \bigg(\frac{1}{2} + \tau \bigg), \quad \mathbb{P}_h(s_b|s_i,a_{h,i}^\star) = \frac{1}{H} \bigg(\frac{1}{2} - \tau \bigg), \end{cases}$$

where  $\tau \leq 1/3$  is a parameter to be determined.

- At  $h \ge H + 1$ , all bandit states transit to one of  $s_g$  and  $s_b$  with probability 1/2 each.
- $s_q$  and  $s_b$  are absorbing states:  $\mathbb{P}_h(s_q|s_q,a) = \mathbb{P}_h(s_b|s_b,a)$  for all  $h \in [2H+1]$  and all  $a \in [A]$ .
- Initial state distribution is uniform on all bandit states:  $S_1 \sim \mathrm{Unif}\{s_i\}_{i \in [S]}$
- Reward: The bandit states do not receive any reward. The good state and bad state also do not receive any reward at  $h \le H + 1$ . Finally, for  $h \ge H + 2$ , the good state receives reward 1 and the bad state receives reward 0 regardless of the action taken:

$$r_h(s_a, a) = 1$$
 and  $r_h(s_b, a) = 0$  for  $H + 2 \le h \le 2H + 1$ .

We also let  $M_0$  denote the "null" MDP which has the same construction as the above except that there is no "special" actions  $a_{h,i}^{\star}$ , that is,

$$\mathbb{P}_h(s_g|s_i, a) = \mathbb{P}_h(s_b|s_i, a) = \frac{1}{2H}$$
 for all  $a \in [A]$ .

**Policies**  $\pi_{\star}$  and  $\mu$  In MDP  $M_{a^{\star}}$ , at any bandit state  $s_i$  and time step  $h \leq H$ , the optimal action to take is  $a_{h,i}^{\star}$  since it induces a slightly higher probability of transiting to the "good state"  $s_g$  than all other actions. At all other states or time steps, the action does not affect anything (the transition and reward do not depend on the action), so for example we could take a=1. To summarize, the following deterministic policy  $\pi_{\star}$  is an optimal policy for  $M_{a^{\star}}$ :

- $\pi_{\star,h}(s_i) = a_{h,i}^{\star}$  for all  $i \in [S]$  and  $h \in [H]$ .
- $\pi_{\star,h}(s_i) = 1 \text{ for all } h \ge H + 1;$
- $\pi_{\star,h}(s_q) = \pi_{\star,h}(s_b) = 1$  for all  $h \in [2H+1]$ .

We define our reference policy  $\mu$  as follows

- $\mu_h(a|s_i) = \frac{1}{K} \mathbb{1} \{1 \le a \le K\}$  for all  $i \in [S]$ , and  $h \in [H]$ .
- $\mu_h(1|s) = 1$  whenever  $h \ge H + 1$  or  $s \in \{s_a, s_b\}$ .

The following lemma shows that  $\mu$  satisfies  $C^*$ -concentrability with respect to  $\pi_*$  as long as all optimal actions  $a_{h,i}^* \in \{1,\ldots,K\}$ . The proof of this lemma is deferred to Section H.1.

**Lemma H.1** ( $\mu$  satisfies single-policy concentrability). For any  $\mathbf{a}^{\star} \in \{1, \dots, K\}^{HS}$ , in the MDP  $M_{\mathbf{a}^{\star}}$ , we have

$$\sup_{h,s,a} \frac{d_h^{\pi_\star}(s,a)}{d_h^{\mu}(s,a)} \leq K \leq C^\star,$$

where  $\pi_{\star}$  (the optimal policy for  $M_{a^{\star}}$ ) and  $\mu$  are defined as above.

Lemma H.1 shows that the following family of problems is indeed a subset of the class  $\mathcal{M}_{C^*}$ :

$$\left\{ \left(M_{\boldsymbol{a}^{\star}},\mu\right):\boldsymbol{a}^{\star}\in\left[K\right]^{HS}\right\} \subset\mathcal{M}_{C^{\star}}.$$

We further let  $\nu$  denote the uniform (prior) distribution on  $[K]^{HS}$ , that is,  $\nu(a^* = a_0) = 1/K^{HS}$  for all  $a_0 \in [K]^{HS}$ .

 $\mu$  is uninformative Note that in the above family of problems, the reference policy  $\mu$  is the same for all MDPs. Therefore  $\mu$  is uninformative in the sense that the set of all online finetuning algorithms that utilize  $\mu$  in its execution is equivalent to the set of all usual online RL algorithms for this particular class of MDPs (which by definition may utilize the additional knowledge that this class of MDPs has a policy  $\mu$  with good concentrability). In the following, we assume  $\hat{\pi}$  is any online RL algorithm for this class of MDPs.

Without loss of generality, we further restrict attention to algorithms that output a deterministic policy (i.e.  $\widehat{\pi}_h(s) \in [A])^7$ . For any deterministic policy  $\widehat{\pi}$  and any index  $a_{\star}$ , define the *bandit best-arm identification* loss for any  $(h, i) \in [H] \times [S]$  as

$$\ell_{h,i}(\widehat{\pi}, \boldsymbol{a}_{\star}) := \mathbb{P}_{\boldsymbol{a}_{\star}}(\widehat{\pi}_{h}(s_{i}) \neq a_{h,i}^{\star}),$$

and the total bandit loss as

$$L(\widehat{\pi}, \boldsymbol{a}_{\star}) := \sum_{(h, i) \in [H] \times [S]} \ell_{h, i}(\widehat{\pi}, \boldsymbol{a}_{\star}) = \mathbb{E}_{\boldsymbol{a}_{\star}} \big[ \# \big\{ (h, i) : \widehat{\pi}_{h}(s_{i}) \neq a_{h, i}^{\star} \big\} \big].$$

The loss L measures the expected number of (h,i) pairs on which the algorithm failed to identify the best arm  $a_{h,i}^{\star}$ . A large loss will translate to a high suboptimality bound, as we make precise in the following lemma. The proof can be found in Section H.2.

**Lemma H.2.** For any  $a^* \in [A]^{HS}$  and any algorithm outputing a deterministic policy  $\widehat{\pi}$ , we have

$$\mathbb{E}_{\boldsymbol{a}^{\star}} \left[ V_{1,M_{\boldsymbol{a}^{\star}}}^{\star} - V_{1,M_{\boldsymbol{a}^{\star}}}^{\widehat{\pi}} \right] = \sum_{h=1}^{H} \sum_{i=1}^{S} \frac{1}{S} \left( 1 - \frac{1}{H} \right)^{h-1} \tau \cdot \ell_{h,i}(\widehat{\pi}, \boldsymbol{a}^{\star}) \geq \frac{\tau}{3S} L(\widehat{\pi}, \boldsymbol{a}^{\star}).$$

With Lemma H.2 at hand, establishing lower bound on the expected suboptimality reduces to establishing a lower bound on the total bandit loss  $L(\widehat{\pi}, \mathbf{a}^*)$ .

**Lower bounding the total bandit loss** Fix any (h,i), and consider the individual bandit loss  $\mathbb{E}_{\boldsymbol{a}^* \sim \nu}[\ell_{h,i}(\widehat{\pi}, \boldsymbol{a}^*)]$  averaged over the prior  $\boldsymbol{a}^* \sim \nu$ . For any algorithm  $\widehat{\pi}$ , we decompose the algorithm into (1) the data collection algorithm  $\mathcal{A}$  from which we collect the observed data  $X \sim (\mathbb{P}_{\boldsymbol{a}^*}, \mathcal{A})$ , and (2) the estimator  $\widehat{\pi}_h(s_i) = f(X)$  for some measurable function  $f: \mathcal{X} \to [A]$ . We have

$$\mathbb{E}_{\boldsymbol{a}^{\star} \sim \nu}[\ell_{h,i}(\widehat{\boldsymbol{\pi}}, \boldsymbol{a}^{\star})] \geq \inf_{f} \mathbb{E}_{\boldsymbol{a}^{\star} \sim \nu} \mathbb{E}_{X \sim (\mathbb{P}_{\boldsymbol{a}^{\star}}, \mathcal{A})} \big[ a_{h,i}^{\star} \neq f(X) \big].$$

Fixing A, the  $\inf_f$  is taken at the Bayes estimator of  $a_{h,i}^{\star}$ , which is a function of the posterior  $a_{h,i}^{\star}|X$  (see, e.g. (Lehmann and Casella, 2006, Theorem 1.1 of Section 4)).

By construction of our MDP  $M_{a^*}$ , the prior distribution of  $a_{h,i}^*$  is uniform in [K], and the only data that reveal information about  $a_{h,i}^*$  (i.e. data whose likelihood is affected by  $a_{h,i}^*$ ) is the observed transitions from state  $s_i$  at step h (i.e.  $\{(A_h, S'_{h+1}) : S_h = s_i\}$ ). Therefore, the posterior distribution  $a_{h,i}^*|X$  depends only on  $\{(A_h, S'_{h+1}) : S_h = s_i\}$  as well. Further, a set of sufficient statistics for this posterior is the visitation counts  $\{N_h(s_i, a, s') : a \in [A], s' \in \mathcal{S}\}$ , where  $N_h(s_i, a, s')$  denote the visitation count of  $(s_i, a, s')$  at step h within the data X. Therefore, we can restrict the  $\inf_f$  to the inf over functions of the vistation counts only (denoted as g), and obtain that

$$\mathbb{E}_{\boldsymbol{a}^{\star} \sim \nu}[\ell_{h,i}(\widehat{\boldsymbol{\pi}}, \boldsymbol{a}^{\star})] \geq \inf_{g} \mathbb{E}_{\boldsymbol{a}^{\star} \sim \nu} \mathbb{P}_{X \sim (\mathbb{P}_{\boldsymbol{a}^{\star}}, \mathcal{A})} \left[ a_{h,i}^{\star} \neq g(\{N_{h}(s_{i}, a, s') : a \in [A], s' \in \mathcal{S}\}) \right]$$

$$\geq \inf_{g} \mathbb{E}_{\boldsymbol{a}^{\star} \sim \nu} \mathbb{P}_{X \sim (\mathbb{P}_{\boldsymbol{0}}, \mathcal{A})} \left[ a_{h,i}^{\star} \neq g(\{N_{h}(s_{i}, a, s') : a \in [A], s' \in \mathcal{S}\}) \right]$$

$$- \mathbb{E}_{\boldsymbol{a}^{\star} \sim \nu} \text{TV}(\{N_{h}(s_{i}, a, s')\}|_{\mathbb{P}_{\boldsymbol{0}}, \mathcal{A}}, \{N_{h}(s_{i}, a, s')\}|_{\mathbb{P}_{\boldsymbol{a}^{\star}}, \mathcal{A}})$$

$$\stackrel{(i)}{\geq} \inf_{g} \mathbb{E}_{\boldsymbol{a}^{\star}_{-(h,i)} \sim \nu_{-(h,i)}} \frac{1}{K} \sum_{a_{h,i}^{\star} = 1}^{K} \mathbb{P}_{X \sim (\mathbb{P}_{\boldsymbol{0}}, \mathcal{A})} \left[ a_{h,i}^{\star} \neq g(\{N_{h}(s_{i}, a, s') : a \in [A], s' \in \mathcal{S}\}) \right]$$

$$- \mathbb{E}_{\boldsymbol{a}^{\star} \sim \nu} \sqrt{\frac{1}{2} \text{KL}(\{N_{h}(s_{i}, a, s')\}|_{\mathbb{P}_{\boldsymbol{0}}, \mathcal{A}} |\{N_{h}(s_{i}, a, s')\}|_{\mathbb{P}_{\boldsymbol{a}^{\star}}, \mathcal{A}})}$$

$$\stackrel{(ii)}{\geq} \frac{K - 1}{K} - \mathbb{E}_{\boldsymbol{a}^{\star} \sim \nu} \sqrt{\frac{1}{2} \sum_{a = 1}^{A} \mathbb{E}_{\mathbb{P}_{\boldsymbol{0}}, \mathcal{A}} [N_{h}(s_{i}, a)] \cdot \text{KL}(\mathbb{P}_{\boldsymbol{0}, h}(\cdot | s_{i}, a) || \mathbb{P}_{\boldsymbol{a}^{\star}, h}(\cdot | s_{i}, a))}$$

<sup>&</sup>lt;sup>7</sup>This is because we can replace  $\mathbb{P}_{a_{\star}}(\widehat{\pi}_h(s) \neq a_{h,i}^{\star})$  in our proof for deterministic policies with  $\mathbb{E}_{a_{\star}}[1 - \widehat{\pi}_h(a_{h,i}^{\star}|s)]$  for stochastic policies, and the proof will follow analogously.

$$\stackrel{(iii)}{\geq} \frac{1}{2} - \mathbb{E}_{\boldsymbol{a}^{\star} \sim \nu} \sqrt{\frac{1}{2}} \mathbb{E}_{\mathbb{P}_{\mathbf{0}}, \mathcal{A}} \Big[ N_{h}(s_{i}, a_{h,i}^{\star}) \Big] \cdot \text{KL} \Big( \mathbb{P}_{0,h}(\cdot | s_{i}, a_{h,i}^{\star}) \| \mathbb{P}_{\boldsymbol{a}^{\star}, h}(\cdot | s_{i}, a_{h,i}^{\star}) \Big) \\
\stackrel{(iv)}{\geq} \frac{1}{2} - \mathbb{E}_{\boldsymbol{a}^{\star} \sim \nu} \sqrt{\mathbb{E}_{\mathbb{P}_{\mathbf{0}}, \mathcal{A}} \Big[ N_{h}(s_{i}, a_{h,i}^{\star}) \Big] \cdot 2\tau^{2} / H} \\
\stackrel{(v)}{\geq} \frac{1}{2} - \sqrt{\frac{1}{K}} \sum_{a=1}^{K} \mathbb{E}_{\mathbb{P}_{\mathbf{0}}, \mathcal{A}} [N_{h}(s_{i}, a)] \cdot 2\tau^{2} / H} \\
\geq \frac{1}{2} - \sqrt{\mathbb{E}_{\mathbb{P}_{\mathbf{0}}, \mathcal{A}} [N_{h}(s_{i})] \cdot 2\tau^{2} / H K}.$$

Above, (i) used Pinsker's inequality; (ii) used the KL divergence decomposition (Lattimore and Szepesvári, 2020, Lemma 15.1), and the fact that  $\frac{1}{K} \sum_{a_{h,i}^{\star}=1}^{K} \mathbb{P}_{X \sim (\mathbb{P}_{\mathbf{0}}, \mathcal{A})} \left[ a_{h,i}^{\star} \neq g(\{N_h(s_i, a, s') : a \in [A], s' \in \mathcal{S}\}) \right]$  is at least (K-1)/K for any g (it equals either (K-1)/K or 1 depending on whether  $g \in [K]$ ); (iii) used our construction that  $\mathbb{P}_{\mathbf{0}}$  and  $\mathbb{P}_{\boldsymbol{a}^{\star}}$  at step h and state  $s_i$  only differ in the arm  $a_{h,i}^{\star}$ ; (iv) used the bound that

$$\mathrm{KL}\bigg(\bigg(1 - \frac{1}{H}, \frac{1}{2H}, \frac{1}{2H}\bigg)\bigg\|\bigg(1 - \frac{1}{H}, \frac{1}{H}\bigg(\frac{1}{2} + \tau\bigg), \frac{1}{H}\bigg(\frac{1}{2} - \tau\bigg)\bigg)\bigg) = \frac{1}{2H}\log\frac{1}{1 - 4\tau^2} \le 4\tau^2/H$$

for  $\tau \in [0, 0.4]$ ; and finally (v) used Jensen's inequality and the fact that  $a_{h,i}^{\star} \sim \mathrm{Unif}([K])$  under  $\nu$ .

Summing the preceding bound over all (h, i), we get that for any algorithm  $\widehat{\pi}$ ,

$$\mathbb{E}_{\boldsymbol{a}^{\star} \sim \nu}[L(\widehat{\boldsymbol{\pi}}, \boldsymbol{a}^{\star})] = \sum_{h=1}^{H} \sum_{i=1}^{S} \mathbb{E}_{\boldsymbol{a}^{\star} \sim \nu}[\ell_{h,i}(\widehat{\boldsymbol{\pi}}, \boldsymbol{a}^{\star})]$$

$$\geq \frac{HS}{2} - \sum_{h=1}^{H} \sum_{i=1}^{S} \sqrt{\mathbb{E}_{\mathbb{P}_{0}, \mathcal{A}}[N_{h}(s_{i})] \cdot 2\tau^{2}/HK}$$

$$\geq HS \left\{ \frac{1}{2} - \sqrt{\frac{1}{HS}} \sum_{h=1}^{H} \sum_{i=1}^{S} \mathbb{E}_{\mathbb{P}_{0}, \mathcal{A}}[N_{h}(s_{i})] \cdot 2\tau^{2}/HK} \right\} = HS \left( \frac{1}{2} - \sqrt{2\tau^{2}n/HSK} \right).$$

Therefore, as long as  $\sqrt{2\tau^2 n/HSK} \le 1/4$ , i.e.  $n \le HSK/(32\tau^2)$ , we have

$$\mathbb{E}_{\boldsymbol{a}^{\star} \sim \nu}[L(\widehat{\pi}, \boldsymbol{a}^{\star})] \geq HS/4.$$

**Bandit loss to MDP suboptimality loss** By the above lower bound on the average risk, for any algorithm  $\widehat{\pi}$ , there must exist some instance  $a^* \in [K]^{HS}$  for which  $L(\widehat{\pi}, a^*) \ge HS/4$ . On this  $a^*$ , by Lemma H.2, we get

$$\mathbb{E}_{\boldsymbol{a}^{\star}}\Big[V_{1,M_{\boldsymbol{a}^{\star}}}^{\star}-V_{1,M_{\boldsymbol{a}^{\star}}}^{\widehat{\pi}}\Big] \geq \frac{\tau}{3S} \cdot L(\widehat{\pi},\boldsymbol{a}^{\star}) \geq \tau H/12.$$

Finally, for any  $\varepsilon \le 1/12$ , take  $\tau = 12\varepsilon/H \le 1/3$ , we have the following: as long as

$$n \le \frac{HSK}{32\tau^2} = \frac{H^3SK}{32 \cdot 12^2 \varepsilon^2},$$

(which is satisfied if  $n \leq c_0 \cdot H^3 S \min \{C^\star, A\} / \varepsilon^2$  for some absolute  $c_0 > 0$ ), we have  $\mathbb{E}_{\boldsymbol{a}^\star} \big[ V_{1, M_{\boldsymbol{a}^\star}}^\star - V_{1, M_{\boldsymbol{a}^\star}}^{\widehat{\pi}} \big] \geq \varepsilon$ . This is the desired result.

#### H.1. Proof of Lemma H.1

Fix any  $a^*$ , we show that  $d_h^{\pi_\star}(s,a)/d_h^{\mu}(s,a) \leq K$  for all (s,a). Note that it suffices to consider actions taken by  $\pi_\star$  only.

**Bandit states** For any bandit state  $s \in \{s_i\}_{i \in [S]}$  and any  $h \leq H$ , by construction of our MDP, we have  $d_h^{\pi_{\star}}(s_i) = d_h^{\mu}(s_i) = (1 - \frac{1}{H})^{h-1}$ ,  $\pi_{\star,h}(a_{h,i}^{\star}|s_i) = 1$ , and  $\mu_h(a_{h,i}^{\star}|s_i) = 1/K$ , therefore

$$\frac{d_h^{\pi_{\star}}(s_i, a_{h,i}^{\star})}{d_h^{\mu}(s_i, a_{h,i}^{\star})} = \frac{d_h^{\pi_{\star}}(s_i) \cdot \pi_{\star,h}(a_{h,i}^{\star}|s_i)}{d_h^{\mu}(s_i) \cdot \mu_h(a_{h,i}^{\star}|s_i)} = K.$$

At h=H+1, we have  $d_h^{\pi_\star}(s_i)=d_h^\mu(s_i)=(1-1/H)^H$ , and both  $\pi_\star$  and  $\mu$  takes action 1 deterministically, and thus  $d_h^{\pi_\star}(s_i,1)/d_h^\mu(s_i,1)=1$ . At  $h\geq H+2$ , we have  $d_h^{\pi_\star}(s_i)=d_h^\mu(s_i)=0$ . This verifies the K-concentrability for all  $s_i$ .

Good state and bad state For the good state  $s_g$  and bad state  $s_b$ , since both  $\pi_\star$  and  $\mu$  takes deterministic action 1 at all h, it suffices to bound distribution ratio  $d_h^{\pi_\star}(s_{\{g,b\}})/d_h^{\mu}(s_{\{g,b\}})$  over the states only (instead of joint state-actions).

Recall that  $\pi_{\star}$  always takes the optimal action  $a_{h,i}^{\star}$  which leads to  $1/H \cdot (1/2 + \tau)$  transition probability to the "good state"  $s_g$ . Thus at any  $h \leq H + 1$ , we have

$$d_h^{\pi_{\star}}(s_g) = \sum_{h'=1}^{h-1} \sum_{i=1}^{S} \frac{1}{S} \left( 1 - \frac{1}{H} \right)^{h'-1} \cdot \frac{1}{H} \left( \frac{1}{2} + \tau \right) = \left( \sum_{h'=1}^{h-1} \left( 1 - \frac{1}{H} \right)^{h'-1} \cdot \frac{1}{H} \right) \cdot \left( \frac{1}{2} + \tau \right).$$

In contrast,  $\mu$  only takes the optimal action  $a_{h,i}^{\star}$  with probability 1/K, and thus we have

$$d_{h}^{\mu}(s_{g}) = \left(\sum_{h'=1}^{h-1} \left(1 - \frac{1}{H}\right)^{h'-1} \cdot \frac{1}{H}\right) \cdot \left(\frac{1}{2} + \frac{\tau}{K}\right).$$

Therefore

$$\frac{d_h^{\pi_*}(s_g)}{d_h^{\mu}(s_g)} = \frac{1/2 + \tau}{1/2 + \tau/K} \le \frac{1/2 + \tau}{1/2} \le 2 \le K.$$

Similarly, for the "bad state"  $s_b$  we have

$$\frac{d_h^{\pi_*}(s_b)}{d_h^{\mu}(s_b)} = \frac{1/2 - \tau}{1/2 - \tau/K} \le 1 \le K.$$

For  $h \ge H + 2$ , we have

$$\frac{d_h^{\pi_{\star}}(s_g)}{d_h^{\mu}(s_g)} = \frac{d_{H+1}^{\pi_{\star}}(s_g) + \frac{1}{2} \cdot (1 - 1/H)^H}{d_{H+1}^{\mu}(s_g) + \frac{1}{2} \cdot (1 - 1/H)^H} \le 2 \le K,$$

and similarly

$$\frac{d_h^{\pi_{\star}}(s_b)}{d_h^{\mu}(s_b)} = \frac{d_{H+1}^{\pi_{\star}}(s_b) + \frac{1}{2} \cdot (1 - 1/H)^H}{d_{H+1}^{\mu}(s_b) + \frac{1}{2} \cdot (1 - 1/H)^H} \le 1 \le K,$$

This verifies the K-concentrability for  $(s_q, s_b)$  as well.

#### H.2. Proof of Lemma H.2

Fix any  $a^\star \in [A]^{HS}$ , by construction of our MDP  $M_{a^\star}$ , only the good state  $s_g$  receives a +1 reward starting at  $h \in \{H+2,\ldots,2H+1\}$ . Along each trajectory, there will be exactly one transition from the bandit states  $\{s_i\}$  to one of  $(s_g,s_b)$ . This transition can happen at step  $h \leq H$  and state  $s_i$  with probability  $1/H \cdot (1/2+\tau)$  if the optimal action  $a^\star_{h,i}$  is taken, or probability 1/(2H) if any other action is taken. The transition can also happen at step h=H+1 but with the same transition probability regardless of the policy. Further, note that the state distribution  $d^\pi_h(s_i) = 1/S \cdot (1-1/H)^{h-1} =: d_h(s_i)$  (for  $h \leq H$ ) does not depend on the policy  $\pi$ . Therefore, we have

$$V_{1,M_{\boldsymbol{a}^{\star}}}^{\star} - V_{1,M_{\boldsymbol{a}^{\star}}}^{\widehat{\pi}}$$

$$= \sum_{h=1}^{H} \sum_{i=1}^{S} d_h(s_i) \cdot \left[ \frac{1}{H} \left( \frac{1}{2} + \tau \right) - \frac{1}{2H} \right] \cdot \mathbb{1} \left\{ \widehat{\pi}_h(s_i) \neq a_{h,i}^{\star} \right\} \cdot H$$

$$= \sum_{h=1}^{H} \sum_{i=1}^{S} \frac{1}{S} \left( 1 - \frac{1}{H} \right)^{h-1} \tau \cdot \mathbb{1} \left\{ \widehat{\pi}_h(s_i) \neq a_{h,i}^{\star} \right\}.$$

Taking expectation with respect to the algorithm execution within the MDP  $M_{a^*}$ , we get

$$\begin{split} & \mathbb{E}_{\boldsymbol{a}^{\star}} \left[ V_{1,M_{\boldsymbol{a}^{\star}}}^{\star} - V_{1,M_{\boldsymbol{a}^{\star}}}^{\widehat{\boldsymbol{\pi}}} \right] = \sum_{h=1}^{H} \sum_{i=1}^{S} \frac{1}{S} \left( 1 - \frac{1}{H} \right)^{h-1} \boldsymbol{\tau} \cdot \underbrace{\mathbb{P}_{\boldsymbol{a}^{\star}} \left( \widehat{\boldsymbol{\pi}}_{h}(s_{i}) \neq a_{h,i}^{\star} \right)}_{\ell_{h,i}(\widehat{\boldsymbol{\pi}}, \boldsymbol{a}^{\star})} \\ & = \sum_{h=1}^{H} \sum_{i=1}^{S} \frac{1}{S} \underbrace{\left( 1 - \frac{1}{H} \right)^{h-1}}_{\geq (1-1/H)^{H-1} \geq e^{-1} \geq 1/3} \boldsymbol{\tau} \cdot \ell_{h,i}(\widehat{\boldsymbol{\pi}}, \boldsymbol{a}^{\star}) \\ & \geq \frac{\tau}{3S} \cdot \sum_{h=1}^{H} \sum_{i=1}^{S} \ell_{h,i}(\widehat{\boldsymbol{\pi}}, \boldsymbol{a}^{\star}) = \frac{\tau}{3S} \cdot L(\widehat{\boldsymbol{\pi}}, \boldsymbol{a}^{\star}). \end{split}$$

This proves the lemma.

#### I. Proofs for Section 5

#### I.1. Algorithm UCBVI-UPLOW

We present the UCBVI-UPLOW algorithm in Algorithm 4. This algorithm is a specialization of the NASH-VI algorithm of (Liu et al., 2020a) (originally developed for two-player Markov games) into the case with a single player, and with additional modifications on the output value functions and policy that are similar to the certified policy technique of (Bai et al., 2020). Above, the BONUS function on Line 7 is taken as the Bernstein bonus:

BONUS
$$(t, \widehat{\sigma}^2) := c \Big( \sqrt{\widehat{\sigma}^2 \iota / t} + (H - h_\star)^2 S \iota / t \Big),$$

where  $\iota := \log(HSAn/\delta)$  is a log factor and c > 0 is some absolute constant.

We now present the main guarantee for UCBVI-UPLOW, which is going to be used in proving the main theorem.

**Lemma I.1** (Theoretical guarantee for UCBVI-UPLOW). Suppose Algorithm 4 is run for  $n_{\text{UCB}}$  episodes. Then, the output lower value estimate  $\underline{V}_{h_{\star}+1}^{\text{out}}$  and the policy  $\pi_{h_{\star}+1:H}^{\text{out}}$  satisfies the following with probability at least  $1-\delta$ :

(a) Small error in lower value estimates:  $0 \le \underline{V}_{h_{\star}+1}^{\mathrm{out}}(s) \le V_{h_{\star}+1}^{\star}(s)$  for all  $s \in \mathcal{S}$ , and

$$\sum_{s \in \mathcal{S}} d_{h_{\star}+1}(s) \left( V_{h_{\star}+1}^{\star}(s) - \underline{V}_{h_{\star}+1}^{\text{out}}(s) \right) \le O\left( \sqrt{\frac{(H - h_{\star})^3 S A \iota^3}{n_{\text{UCB}}}} + \frac{(H - h_{\star})^3 S^2 A \iota^3}{n_{\text{UCB}}} \right),$$

where  $d_{h_{\star}+1}(\cdot)$  is the distribution of the initial state  $s_{h_{\star}+1}$ .

(b)  $\pi^{\text{out}}$  achieves at least  $\underline{V}^{\text{out}}$  value: we have  $V_{h_{\star}+1}^{\pi^{\text{out}}}(s) \geq \underline{V}_{h_{\star}+1}^{\text{out}}(s)$  for all  $s \in \mathcal{S}$ .

*Proof.* First notice that Algorithm 4 is a special case of the NASH-VI algorithm for two-player Markov games (Liu et al., 2020a, Algorithm 1), where the number of actions for the min-player is one so that the Markov game reduces to a single-player MDP, and the game starts at step  $h_{\star}+1$  (so that the horizon length is  $H-h_{\star}$  instead of H).

Therefore, by (Liu et al., 2020a, Theorem 4), with probability at least  $1 - \delta/2$  the following happens

$$\sum_{k=1}^{n_{\text{UCB}}} \overline{V}_{h_{\star}+1}^{k}(s_{h_{\star}+1}^{k}) - \underline{V}_{h_{\star}+1}^{k}(s_{h_{\star}+1}^{k}) \le \sqrt{(H-h_{\star})^{3} SAn_{\text{UCB}}\iota} + (H-h_{\star})^{3} S^{2} A \iota^{2},$$

where  $\iota := \log(HSA/\delta)$ . Further, (Liu et al., 2020a, Lemma 22) implies that for any (s,k),

$$\overline{V}_{h_{\star}+1}^{k}(s) \ge V_{h_{\star}+1}^{\star}(s) \ge V_{h_{\star}+1}^{\pi^{k}}(s) \ge \underline{V}_{h_{\star}+1}^{k}(s)$$

on the same good event. Using the relation betwen  $\overline{V}_{h_\star+1}^k$  and  $V_{h_\star+1}^\star$  yields

$$\sum_{s \in \mathcal{S}} N_{h_{\star}+1}(s) \left( V_{h_{\star}+1}^{\star}(s) - \underline{V}_{h_{\star}+1}^{\text{out}}(s) \right)$$

$$\stackrel{(i)}{=} \sum_{k=1}^{n_{\text{UCB}}} V_{h_{\star}+1}^{\star}(s_{h_{\star}+1}^{k}) - \underline{V}_{h_{\star}+1}^{k}(s_{h_{\star}+1}^{k}) \le \sqrt{(H - h_{\star})^{3} SA n_{\text{UCB}} \iota} + (H - h_{\star})^{3} S^{2} A \iota^{2},$$

where (i) used the definition of our  $\underline{V}^{\text{out}}$  in Line 28. Now, since  $N_{h_{\star}+1}(s) \sim \text{Bin}(n_{\text{UCB}}, d_{h_{\star}+1}(s))$ , by Lemma D.1 and a union bound over  $s \in \mathcal{S}$ , we have with probability at least  $1 - \delta/2$  that

$$N_{h_{\star}+1}(s) \lor 1 \ge \frac{1}{C_L} \cdot n_{\text{UCB}} d_{h_{\star}+1}(s)$$

simultaneously for all  $s \in \mathcal{S}$ .

Plugging this into the preceding bound further yields

$$\begin{split} &\sum_{s \in \mathcal{S}} d_{h_{\star}+1}(s) \left( V_{h_{\star}+1}^{\star}(s) - \underline{V}_{h_{\star}+1}^{\text{out}}(s) \right) \\ &\leq \frac{C\iota}{n_{\text{UCB}}} \sum_{s \in \mathcal{S}} \left( N_{h_{\star}+1}(s) \vee 1 \right) \cdot \left( V_{h_{\star}+1}^{\star}(s) - \underline{V}_{h_{\star}+1}^{\text{out}}(s) \right) \\ &\leq \frac{C\iota}{n_{\text{UCB}}} \sum_{s \in \mathcal{S}} N_{h_{\star}+1}(s) \cdot \left( V_{h_{\star}+1}^{\star}(s) - \underline{V}_{h_{\star}+1}^{\text{out}}(s) \right) + \frac{C\iota}{n_{\text{UCB}}} \sum_{s \in \mathcal{S}} \mathbbm{1} \left\{ N_{h_{\star}+1}(s) = 0 \right\} \cdot \underbrace{\left( V_{h_{\star}+1}^{\star}(s) - \underline{V}_{h_{\star}+1}^{\text{out}}(s) \right)}_{\leq H - h_{\star}} \\ &\leq C \sqrt{\frac{(H - h_{\star})^3 S A \iota^3}{n_{\text{UCB}}}} + C \cdot \frac{(H - h_{\star})^3 S^2 A \iota^3 + (H - h_{\star}) S \iota}{n_{\text{UCB}}} \\ &\leq C \left( \sqrt{\frac{(H - h_{\star})^3 S A \iota^3}{n_{\text{UCB}}}} + \frac{(H - h_{\star})^3 S^2 A \iota^3}{n_{\text{UCB}}} \right) \end{split}$$

This shows part (a).

For part (b), by our definition of  $\pi^{\text{out}}$  (Line 31), we have for any  $s \in \mathcal{S}$  that

$$\begin{split} &V_{h_{\star}+1}^{\pi^{\mathrm{out}}}(s) = V_{h_{\star}+1}^{\pi^{(s)}}(s) \\ &= \frac{1}{N_{h_{\star}+1}(s)} \sum_{k: s_{h_{\star}+1}^k = s} V_{h_{\star}+1}^{\pi^k}(s) \\ &\geq \frac{1}{N_{h_{\star}+1}(s)} \sum_{k: s_{h_{\star}+1}^k = s} \underline{V}_{h_{\star}+1}^k(s) = \underline{V}_{h_{\star}+1}^{\mathrm{out}}(s). \end{split}$$

This shows part (b).

#### I.2. Algorithm TRUNCATED-PEVI-ADV

The algorithm TRUNCATED-PEVI-ADV is similar as the PEVI-ADV algorithm (Algorithm 1) except that the algorithm uses a plug-in estimate of  $V_{h_{\star}+1}^{\star}$ , and only performs (pessimistic) value iteration within step 1 to  $h_{\star}$ . For completeness, we describe the algorithm in Algorithm 5.

#### I.3. Proof of Theorem 3

We are now ready to present the proof of Theorem 3. Throughout this proof, C denotes an absolute constant that can vary from line to line, and all "good events" happen with probability at least  $1 - \delta/10$ , which combine to yield the  $1 - \delta$  high probability guarantee for the final bound.

Guarantees for learned values First, Stage 1 in our Algorithm 2 runs the UCBVI-UPLOW algorithm with  $n_{\text{UCB}} = n/2$  episodes with initial state  $s_{h_{\star}+1} \sim d^{\mu}_{h_{\star}+1}$ . Therefore by Lemma I.1, its output lower value estimate  $\underline{V}_{h_{\star}+1}$  satisfies  $\underline{V}_{h_{\star}+1}(s) \leq V^{\star}_{h_{\star}+1}(s)$  for all  $s \in \mathcal{S}$ , and

$$\sum_{s \in \mathcal{S}} d_{h_{\star}+1}^{\mu}(s) \left( V_{h_{\star}+1}^{\star}(s) - \underline{V}_{h_{\star}+1}(s) \right) \le C \left( \sqrt{\frac{(H - h_{\star})^{3} S A \iota^{3}}{n}} + \frac{(H - h_{\star})^{3} S^{2} A \iota^{3}}{n} \right).$$

Since  $\mu$  satisfies  $C^{\text{partial}}$  partial concentration for steps  $1:h_{\star}$  (by Assumption B), it also satisfies the *state-wise* concentrability at step  $h_{\star}+1$ : For any  $s' \in \mathcal{S}$  we have

$$\frac{d_{h_{\star}+1}^{\pi_{\star}}(s')}{d_{h_{\star}+1}^{\mu}(s')} = \frac{\sum_{s,a} d_{h_{\star}}^{\pi_{\star}}(s,a) \mathbb{P}_{h_{\star}}(s'|s,a)}{\sum_{s,a} d_{h_{\star}}^{\mu}(s,a) \mathbb{P}_{h_{\star}}(s'|s,a)} \leq C^{\text{partial}}.$$

Applying this in the preceding bound, we get

$$\sum_{s \in \mathcal{S}} d_{h_{\star}+1}^{\pi_{\star}}(s) \left( V_{h_{\star}+1}^{\star}(s) - \underline{V}_{h_{\star}+1}(s) \right) \leq C \cdot C^{\text{partial}} \left( \sqrt{\frac{(H-h_{\star})^3 S A \iota^3}{n}} + \frac{(H-h_{\star})^3 S^2 A \iota^3}{n} \right) =: \varepsilon_0.$$

Next, in stage 2 we run the TRUNCATED-PEVI-ADV algorithm. In its first (sub)-stage, we learn the reference value function  $\widehat{V}^{\mathrm{ref}}$  via a truncated version of the VI-LCB algorithm (which runs for  $(n-n_{\mathrm{UCB}})/3=n/6$  episodes). Since we set  $\widehat{V}_{h_\star+1}^{\mathrm{ref}} \leftarrow \underline{V}_{h_\star+1}$  and do not update it, we can imitate the proof of Theorem E.1 for steps 1 to  $h_\star$  (which uses the  $C^{\mathrm{partial}}$  partial-concentrability assumed in Assumption B) and obtain  $\widehat{V}_h^{\mathrm{ref}}(s) \leq V_h^\star(s)$  for all  $h \in [h_\star]$ ,  $s \in \mathcal{S}$ , and (by replacing H with  $h_\star$  at appropriate places in the proof in Section F.3)

$$\begin{aligned} & \max_{1 \leq h \leq h_{\star}} \sum_{s \in \mathcal{S}} d_{h}^{\pi_{\star}}(s) \Big( V_{h}^{\star}(s) - \widehat{V}_{h}^{\text{ref}}(s) \Big) \\ & \leq \sum_{h=1}^{h_{\star}} \sum_{s,a} d_{h}^{\pi_{\star}}(s,a) \cdot b_{h}(s,a) + \sum_{s \in \mathcal{S}} d_{h_{\star}+1}^{\pi_{\star}}(s) \Big( V_{h_{\star}+1}^{\star}(s) - \underline{V}_{h_{\star}+1}(s) \Big) \\ & \leq C \sqrt{\frac{H^{2} h_{\star}^{3} S C^{\text{partial}} \iota^{2}}{n}} + \sum_{s \in \mathcal{S}} d_{h_{\star}+1}^{\pi_{\star}}(s) \Big( V_{h_{\star}+1}^{\star}(s) - \underline{V}_{h_{\star}+1}(s) \Big) \\ & \leq C \sqrt{\frac{H^{2} h_{\star}^{3} S C^{\text{partial}} \iota^{2}}{n}} + \varepsilon_{0} =: \varepsilon_{1}. \end{aligned}$$

In its second sub-stage, we learn the final value function  $\widehat{V}$  in a similar fashion as the reference-advantage updates in Algorithm 1 (which runs for  $n_0+n_1$  episodes where  $n_0=n_1=n/6$ ). Notice again we set  $\widehat{V}_{h_\star+1}\leftarrow \underline{V}_{h_\star+1}$  and do not update it. Therefore we can imiate the proof of Theorem 1 (again, this uses the  $C^{\mathrm{partial}}$  partial-concentrability assumed in Assumption B) to obtain  $\widehat{V}_h(s) \leq V_h^\star(s)$  for all  $h \in [h_\star]$ ,  $s \in \mathcal{S}$  and (by replacing H with  $h_\star$  at appropriate places in Section G.2)

$$\begin{aligned} & \max_{1 \leq h \leq h_{\star}} \sum_{s \in \mathcal{S}} d_{h}^{\pi_{\star}}(s) \Big( V_{h}^{\star}(s) - \widehat{V}_{h}(s) \Big) \\ & \leq \sum_{h=1}^{h_{\star}} \sum_{s,a} d_{h}^{\pi_{\star}}(s,a) \cdot \big( b_{h,0}(s,a) + b_{h,1}(s,a) \big) + \sum_{s \in \mathcal{S}} d_{h_{\star}+1}^{\pi_{\star}}(s) \big( V_{h_{\star}+1}^{\star}(s) - \underline{V}_{h_{\star}+1}(s) \big) \\ & \leq C \bigg( \sqrt{\frac{H^{2}h_{\star}SC^{\text{partial}}\iota^{2}}{n}} + \frac{H^{2}h_{\star}SC^{\text{partial}}\iota^{3/2} + Hh_{\star}^{3}SC^{\text{partial}}\iota^{2}}{n} \end{aligned}$$

$$\begin{split} &+\sqrt{\frac{h_{\star}^4SC^{\mathrm{partial}}\iota^2}{n}}\cdot H\cdot\varepsilon_1 + \frac{H^2h_{\star}^2SC^{\mathrm{partial}}\iota^{3/2} + Hh_{\star}^2SC^{\mathrm{partial}}\iota^2}{n} \Big) + \varepsilon_0 \\ &\leq C\bigg(\sqrt{\frac{H^2h_{\star}SC^{\mathrm{partial}}\iota^2}{n}} + \frac{H^2h_{\star}SC^{\mathrm{partial}}\iota^{3/2} + Hh_{\star}^3SC^{\mathrm{partial}}\iota^2}{n} \\ &+\sqrt{\frac{H^2h_{\star}^4SC^{\mathrm{partial}}\iota^2}{n}}\cdot \bigg(\sqrt{\frac{H^2h_{\star}^3SC^{\mathrm{partial}}\iota^2}{n}} + \varepsilon_0\bigg) + \frac{H^2h_{\star}^2SC^{\mathrm{partial}}\iota^{3/2} + Hh_{\star}^2SC^{\mathrm{partial}}\iota^2}{n}\bigg) + \varepsilon_0 \\ =: \varepsilon_2. \end{split}$$

We first let  $\varepsilon_0 \le \varepsilon/2$  which requires

$$n \ge N_0 := C \left[ (H - h_{\star})^3 S A \iota^3 (C^{\text{partial}})^2 + (H - h_{\star})^3 S^2 A \iota^3 / \varepsilon \right].$$

Then to let the rest of the terms above be also bounded by  $\varepsilon/2$ , a sufficient condition is

$$n \ge N_2 := C \left[ \frac{H^2 h_{\star} SC^{\text{partial}} \iota^2}{\varepsilon^2} + \frac{H^2 h_{\star}^{3.5} SC^{\text{partial}} \iota^2}{\varepsilon} + H^2 h_{\star}^4 SC^{\text{partial}} \iota^2 \right].$$

Combined, this shows that  $\max_{1 \leq h \leq h_\star} \sum_{s \in \mathcal{S}} d_h^{\pi_\star}(s) \Big( V_h^\star(s) - \widehat{V}_h(s) \Big) \leq \varepsilon$  if

$$n \geq C \left( \frac{H^2 h_{\star} S C^{\text{partial}} \iota^2 + (H - h_{\star})^3 S A (C^{\text{partial}})^2 \iota^3}{\varepsilon^2} + \frac{H^2 h_{\star}^{3.5} S C^{\text{partial}} \iota^2 + (H - h_{\star})^3 S^2 A C^{\text{partial}} \iota^3}{\varepsilon} + H^2 h_{\star}^4 S C^{\text{partial}} \iota^2 \right)$$

$$\geq \max \{N_0, N_2\}.$$

Further, when  $\varepsilon \leq \min \left\{ h_{\star}^{-2.5}, C^{\mathrm{partial}}/S \right\}$ , the  $\varepsilon^{-2}$  term above dominates and thus a sufficient condition for the above is

$$n \ge \widetilde{O}\left(\frac{H^2 h_{\star} S C^{\text{partial}} + (H - h_{\star})^3 S A (C^{\text{partial}})^2}{\varepsilon^2}\right). \tag{17}$$

Guarantees for output policy We also show that the final output policy  $\widehat{\pi}$  of Algorithm 2 also satisfies  $V_1^\star(s_1) - V_1^{\widehat{\pi}}(s_1) \leq \varepsilon$  building on the above guarantee for  $\widehat{V}$ . First, at step  $h_\star + 1$ , as  $\widehat{\pi}_{(h_\star + 1):H} = \widehat{\pi}_{(h_\star + 1):H}^{\mathrm{UCB}}$ , by Lemma I.1(b) we have for all  $s \in \mathcal{S}$  that

$$V_{h_{\star}+1}^{\widehat{\pi}}(s) \ge \underline{V}_{h_{\star}+1}(s) = \widehat{V}_{h_{\star}+1}(s).$$

Second, using this as a base step for the induction argument in G.2, we get that  $V_h^{\widehat{\pi}}(s) \geq \widehat{V}_h(s)$  for all  $h \in [h_{\star}]$  and s. In particular, at h = 1 we have  $V_1^{\widehat{\pi}}(s_1) \geq \widehat{V}_1(s_1)$ . Therefore

$$V_1^{\star}(s_1) - V_1^{\widehat{\pi}}(s_1) \leq V_1^{\star}(s_1) - \widehat{V}_1(s_1) = \sum_{s \in \mathcal{S}} d^{\pi_{\star}}(s) \Big( V_1^{\star}(s) - \widehat{V}_1(s) \Big) \leq \varepsilon.$$

This shows the desired near-optimality guarantee for  $\widehat{\pi}$  whenever  $\varepsilon \leq \min\left\{h_{\star}^{-2.5}, C^{\mathrm{partial}}/S\right\}$  and the number of episodes n satisfies (17). This proves Theorem 3.

# Algorithm 4 UCB-VI with Upper and Lower Confidence Bounds (UCBVI-UPLOW)

```
Require: Starting time step h_{\star} + 1, end time step H, number of episodes n_{\text{UCB}}.
  1: Initialize: For any (s,a,h,s'): \overline{Q}_h(s,a) \leftarrow H - h_\star, \underline{Q}_h(s,a) \leftarrow 0, N_h(s) = N_h(s,a) = N_h(s,a,s') \leftarrow 0.
  2: for Episode k = 1, \ldots, n_{\text{UCB}} do
            for step h = H, \ldots, h_{\star} + 1 do
  3:
  4:
                for (s, a) \in \mathcal{S} \times \mathcal{A} do
                    t \leftarrow N_h(s, a).
  5:
                    if t > 0 then
  6:
                        \beta \leftarrow \text{Bonus}(t, \widehat{\mathbb{V}}_h[(\overline{V}_{h+1} + \underline{V}_{h+1})/2](s, a))
  7:
                        \gamma \leftarrow c/(H - h_{\star}) \cdot \widehat{\mathbb{P}}_h(\overline{V}_{h+1} - \underline{V}_{h+1})(s, a).
  8:
                        \overline{Q}_h(s,a) \leftarrow \min \Big\{ (r_h + \widehat{\mathbb{P}}_h \overline{V}_{h+1})(s,a) + \gamma + \beta, H - h_{\star} \Big\}.
  9:
                        Q_h(s,a) \leftarrow \max \left\{ (r_h + \widehat{\mathbb{P}}_h \underline{V}_{h+1})(s,a) - \gamma - \beta, 0 \right\}
10:
11:
                end for
12:
13:
                for s \in \mathcal{S} do
                    \pi_h(s) \leftarrow \arg\max_{a \in \mathcal{A}} \overline{Q}_h(s, a).
14:
                    \overline{V}_h(s) \leftarrow \overline{Q}_h(s, \pi_h(s)); \underline{V}_h(s) \leftarrow \underline{Q}_h(s, \pi_h(s)).
15:
                end for
16:
17:
            end for
18:
            Receive an initial state s_{h_{\star}+1} from the MDP.
19:
            for step h = h_{\star} + 1, \dots, H do
                Take action a_h = \pi_h(s_h), observe reward r_h and next state s_{h+1}.
20:
                Add 1 to N_h(s_h), N_h(s_h, a_h), and N_h(s_h, a_h, s_{h+1}).
21:
                \widehat{\mathbb{P}}_h(\cdot|s_h,a_h) \leftarrow N_h(s_h,a_h,\cdot)/N_h(s_h,a_h).
22:
            end for
23:
25: Let (\overline{V}_h^k, \underline{V}_h^k, \pi^k) denote the value estimates and policy at the beginning of episode k.
26: for s \in \mathcal{S} do
27: \overline{V}_{h_{\star}+1}^{\mathrm{out}}(s) \leftarrow \frac{1}{N_{h_{\star}+1}(s)} \sum_{k:s_{h_{\star}+1}^k = s} \overline{V}_{h_{\star}+1}^k(s).
           \underline{V}_{h_{\star}+1}^{\text{out}}(s) \leftarrow \frac{1}{N_{h_{\star}+1}(s)} \sum_{k:s_{h_{\star}+1}^{k}=s} \underline{V}_{h_{\star}+1}^{k}(s).
           Let policy \pi_{h_{\star}+1:H}^{(s)} be the uniform mixture of \pi_{h_{\star}+1:H}^{k} over all \{k: s_{h_{\star}+1}^{k} = s\}.
29:
30: end for
31: return Value estimates (\overline{V}_{h_{\star}+1}^{\text{out}}, \underline{V}_{h_{\star}+1}^{\text{out}}).
                     Mixture policy \pi_{h_{\star}+1:H}^{\text{out}} defined as follows: Play policy \pi_{h_{\star}+1:H}^{(s)} if s_{h_{\star}+1}=s.
```

#### **Algorithm 5** Truncated-PEVI-ADV

1: Split the dataset  $\mathcal{D}$  into  $\mathcal{D}_{ref}$ ,  $\mathcal{D}_0$  and  $\{\mathcal{D}_{h,1}\}_{h=1}^{h_{\star}}$  uniformly at random:

$$n_{\text{ref}} \coloneqq |\mathcal{D}_{\text{ref}}| = n_{\text{offline}}/3, \ n_0 \coloneqq |\mathcal{D}_0| = n_{\text{offline}}/3, \ n_{1,h} \coloneqq |\mathcal{D}_{h,1}| \coloneqq n_{\text{offline}}/(3h_{\star}).$$

- 2: Learn a reference value function  $\hat{V}_{1:h_{\star}}^{\mathrm{ref}} \leftarrow \mathrm{VI-LCB}(\mathcal{D}_{\mathrm{ref}})$  via of a truncated version of VI-LCB(Algorithm 3), with the modification that only the datae from steps  $1:h_{\star}$  are used, and  $\widehat{V}_{h_{\star}+1}^{\mathrm{ref}}\leftarrow V_{h_{\star}+1}^{\mathrm{init}}$  and is not updated. 3: Let  $N_{h,0}(s,a)$  and  $N_{h,0}(s,a,s')$  denote the visitation count of (s,a) and (s,a,s') at step h within dataset  $\mathcal{D}_0$ . Construct
- empirical model estimates:

$$\widehat{r}_{h,0}(s,a) \leftarrow r_h(s,a) \mathbb{1} \left\{ N_{h,0}(s,a) \ge 1 \right\}, \\ \widehat{\mathbb{P}}_{h,0}(s'|s,a) \leftarrow \frac{N_{h,0}(s,a,s')}{N_{h,0}(s,a) \vee 1}.$$

Similarly define 
$$N_{h,1}(s,a), N_{h,1}(s,a,s'), (\widehat{r}_{h,1},\widehat{\mathbb{P}}_{h,1})$$
 for all  $h \in [h_{\star}]$  based on dataset  $\mathcal{D}_{h,1}$ .  
4: For all  $(h,s,a)$ , set  $b_{h,0}(s,a) \leftarrow c \cdot \left(\sqrt{\frac{[\widehat{\mathbb{V}}_{h,0}\widehat{V}_{h+1}^{\mathrm{ref}}](s,a)\iota}{N_{h,0}(s,a)\vee 1}} + \frac{H\iota}{N_{h,0}(s,a)\vee 1}\right)$ , where  $\iota := \log(HSA/\delta)$ .

- 5: Set  $\widehat{V}_{h_{\star}+1}(s) \leftarrow V_{h_{\star}+1}^{\mathrm{init}}(s)$  for all  $s \in \mathcal{S}$ . (Note that  $\widehat{V}_{h_{\star}+1}(s)$  is not updated in the following.) 6: for  $h = h_{\star}, \ldots, 1$  do

7: Set 
$$b_{h,1}(s,a) \leftarrow c \cdot \left( \sqrt{\frac{[\widehat{\mathbb{V}}_{h,1}(\widehat{V}_{h+1} - \widehat{V}_{h+1}^{\mathrm{ref}})](s,a)\iota}{N_{h,1}(s,a)\vee 1}} + \frac{H\iota}{N_{h,1}(s,a)\vee 1} \right).$$

Perform value update for all (s, a)8:

$$\widehat{Q}_h(s,a) \leftarrow \widehat{r}_{h,0}(s,a) + \left[\widehat{\mathbb{P}}_{h,0}\widehat{V}_{h+1}^{\text{ref}}\right](s,a) - b_{h,0}(s,a) + \left[\widehat{\mathbb{P}}_{h,1}(\widehat{V}_{h+1} - \widehat{V}_{h+1}^{\text{ref}})\right](s,a) - b_{h,1}(s,a);$$

$$\widehat{V}_h(s) \leftarrow \left[\max_{a} \widehat{Q}_h(s,a)\right] \vee 0.$$

- Set  $\widehat{\pi}_h(s) \leftarrow \arg \max_a \widehat{Q}_h(s, a)$  for all  $s \in \mathcal{S}$ .
- 10: **end for**
- 11: **return** Policy  $\widehat{\pi} = {\{\widehat{\pi}_h\}_{1 \leq h \leq h_{\star}}}$ .