Efficient Reinforcement Learning in Factored MDPs with Application to Constrained RL

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Abstract

Reinforcement learning (RL) in episodic factored Markov decision processes (FMDPs) is studied. We propose an algorithm called FMDP-BF, which leverages the factorization structure of the FMDP. The algorithm’s regret is shown to be exponentially smaller than optimal algorithms in non-factored MDPs, and improves on the best previous result for FMDPs (Osband and Van Roy, 2014) by a factored of $\sqrt{H|S_i|}$, where $|S_i|$ is the cardinality of the factored state subspace and $H$ is the planning horizon. To show the optimality of our bounds, we also provide a lower bound for FMDP, which indicates that our algorithm is near-optimal w.r.t timestep $T$, horizon $H$ and factored state-action subspace cardinality. Finally, as an application, we study a new formulation of constrained RL, known as RL with knapsack constraints (RLwK), and provides the first sample-efficient algorithm based on FMDP-BF.

1. Introduction

Reinforcement learning (RL) is concerned with sequential decision making problems where an agent interacts with a stochastic environment and aims to maximize its cumulative rewards. The environment is usually modeled as a Markov Decision Process (MDP) whose transition kernel and reward function are unknown to the agent. A main challenge of the agent is efficiently explore in the MDP, so as to minimize its regret, or the related sample complexity of exploration.

Extensive study has been done on the tabular case, in which almost no prior knowledge is assumed on the MDP dynamics. The regret or sample complexity bounds typically depend polynomially on the cardinality of state and action spaces (e.g., Strehl et al., 2009; Jaksch et al., 2010; Azar et al., 2017; Dann et al., 2017; Jin et al., 2018; Zanette and Brunskill, 2019). Moreover, matching lower bounds (e.g., Jaksch et al., 2010) imply that these results cannot be improved without additional assumptions. On the other hand, many RL tasks involve large state and action spaces, for which these regret bounds are still excessively large.
In many practical scenarios, one can often take advantage of specific structures of the MDP to develop more efficient algorithms. For example, in robotics, the state may be high-dimensional, but the subspaces of the state may evolve independently of others, and only depend on a low-dimensional subspace of the previous state. Formally, these problems can be described as factored MDPs (Boutilier et al., 2000; Kearns and Koller, 1999; Guestrin et al., 2003). Most relevant to the present work is Osband and Van Roy (2014), who proposed a posterior sampling algorithm and a UCRL-like algorithm that both satisfy $\sqrt{T}$ regret. Their regret bounds have linear dependence on the time horizon and each factored state subspace. It is unclear whether this bound is tight or not.

In this work, we tackle this problem by proposing algorithms with improved regret bounds, and developing corresponding lower bounds for episodic FMDPs. We propose a sample efficient and computationally efficient algorithm called FMDP-BF based on the principle of optimism in the face of uncertainty, and prove its regret bounds. We also provide a regret lower bound, which implies that our regret bound is near-optimal with respect to the timestep $T$, the planning horizon $H$ and factored state-action subspace cardinality $|\mathcal{X}[Z_i]|$.

As an application, we study a novel formulation of constrained RL, known as RL with knapsack constraints (RLwK), which we believe is natural to capture many scenarios in real-life applications. We apply FMDP-BF to this setting, to obtain a statistically efficient algorithm with a regret bound that is near-optimal in terms of $T$, $S$, $A$, and $H$.

Our contributions are summarized as follows:

1. We propose an algorithm for FMDP, and prove its regret bound that improves on the best previous result of Osband and Van Roy (2014) by a factor of $\sqrt{H|S_i|}$.
2. We prove a regret lower bound for FMDP, which implies the regret bound of FMDP-BF is near-optimal in terms of horizon $H$ and factored state-action subspace cardinality $|\mathcal{X}[Z_i]|$.
3. We apply FMDP-BF in RLwK, a novel constrained RL setting with knapsack constraints, and prove a regret bound that is near-optimal in terms of $S$, $A$ and $H$.

2. Preliminaries

We consider the setting of a tabular episodic Markov decision process (MDP), $(S, A, H, \mathbb{P}, R)$, where $S$ is the set of states, $A$ is the action set, $H$ is the number of steps in each episode. $\mathbb{P}$ is the transition probability matrix so that $\mathbb{P}(-|s,a)$ gives the distribution over states if action $a$ is taken for state $s$, and $R(s,a)$ is the reward distribution of taking action $a$ in state $s$ with support $[0,1]$. We use $R(s,a)$ to denote the expectation $E[R(s,a)]$.

In each episode, the agent starts from an initial state $s_1$ that may be arbitrarily selected. At each step $h \in [H]$, the agent observes the current state $s_h \in S$, takes action $a_h \in A$, receives a reward $r_h$ sampled from $R(s_h,a_h)$, and transits to state $s_{h+1}$ with probability $\mathbb{P}(s_{h+1}|s_h,a_h)$. The episode ends when $s_{H+1}$ is reached.

A policy $\pi$ of an agent is a collection of $H$ policy functions $\{\pi_h : S \rightarrow A\}_{h \in [H]}$. We use $V_h^\pi : S \rightarrow \mathbb{R}$ to denote the value function at step $h$ under policy $\pi$, which gives the expected sum of remaining rewards received under policy $\pi$ starting from $s_h = s$, i.e. $V_h^\pi(s) = E \left[ \sum_{h'=h}^H R(s_{h'}, \pi_{h'}(s_{h'})) \mid s_h = s \right]$. Accordingly, we define $Q_h^\pi(s, a)$ as the expected Q-value function at step $h$: $Q_h^\pi(s, a) = E \left[ R(s_h,a_h) + \sum_{h'=h+1}^H R(s_{h'}, \pi_{h'}(s_{h'})) \mid s_h = s, a_h = a \right]$. We
use $V^*_h$ and $Q^*_h$ to denote the optimal value and Q-functions under optimal policy $\pi^*$ at step $h$.

The agent interacts with the environment for $K$ episodes with a policy $\pi_k = \{\pi_{k,h} : S \to A\}_{h[H]}$ determined before the beginning of the $k$-th episode. The agent’s goal is to maximize its cumulative rewards $\sum_{k=1}^K \sum_{h=1}^H r_{k,h}$ over $T = KH$ steps, or equivalently, to minimize the following expected regret:

$$\text{Reg}(K) \overset{\text{def}}{=} \sum_{k=1}^K \left[ V^*_1(s_{k,1}) - V_{1,\pi_k}^*(s_{k,1}) \right],$$

where $s_{k,1}$ denotes the initial state in episode $k$.

### 2.1 Factored MDPs

A factored MDP is a MDP whose rewards and transitions exhibit certain conditional independence structures. We start with the formal definition of factored MDP (Osband and Van Roy, 2014; Xu and Tewari, 2020; Lu and Van Roy, 2019).

**Definition 1.** (Factored set) Let $X = X_1 \times \cdots \times X_d$ be a factored set. For any subset of indices $Z \subseteq \{1, 2, \ldots, d\}$, we define the scope set $X[Z] := \otimes_{i \in Z} X_i$. Further, for any $x \in X$, define the scope variable $x[Z] \in X[Z]$ to be the value of the variables $x_i \in X_i$ with indices $i \in Z$. If $Z$ is a singleton, we will write $x[i]$ for $x[\{i\}]$.

Let $P(X, Y)$ denote the set of functions that map $x \in X$ to the probability distribution on $Y$.

**Definition 2.** (Factored reward) The reward function class $R \subseteq P(X, \mathbb{R})$ is factored over $S \times A = X = X_1 \times \cdots \times X_d$ with scopes $Z_1, \ldots, Z_m$ if and only if, for all $R \in R$, $x \in X$, there exists functions $\{R_i \in P(X[Z_i], [0, 1])\}_{i=1}^m$ such that

$$\mathbb{E}[r] = \frac{1}{m} \sum_{i=1}^m \mathbb{E}[r_i]$$

where $r \sim R(x)$ is equal to $\frac{1}{m} \sum_{i=1}^m r_i$ with each $r_i \sim R_i(x[Z_i])$ individually observed. We use $R_i$ to denote the expectation $\mathbb{E}[R_i]$.

**Definition 3.** (Factored transition) The transition function class $P \subseteq P(X, S)$ is factored over $S \times A = X = X_1 \times \cdots \times X_d$ and $S = S_1 \times \cdots \times S_n$ with scopes $Z_1, \ldots, Z_n$ if and only if, for all $P \in P$, $x \in X$, $s \in S$, there exists functions $\{P_j \in P(X[Z_j], S_j)\}_{j=1}^n$ such that

$$P(s \mid x) = \prod_{j=1}^n P_j(s[j] \mid x[Z_j])$$

A factored MDP is an MDP with factored rewards and transitions. Let $X = S \times A$. A factored MDP is fully characterized by

$$M = \left( \{X_i\}_{i=1}^d ; \{Z_i^R\}_{i=1}^m ; \{R_i\}_{i=1}^m ; \{S_j\}_{j=1}^n ; \{Z_j^P\}_{j=1}^n ; \{P_j\}_{j=1}^n ; H \right)$$
where \( \{Z^R_i\}_{i=1}^n \) and \( \{Z^P_j\}_{j=1}^n \) are the scopes for the reward and transition functions, which we assume to be known to the agent, \( H \) is the fixed horizon.

For notation simplicity, we use \( X[i:j] \) and \( S[i:j] \) to denote \( X[\cup_{k=i,...,j} Z_k] \) and \( \otimes^j_{k=i} S_k \) respectively. Similarly, We use \( \mathbb{P}[i:j](s'[i:j] \mid s, a) \) to denote \( \prod^j_{k=i} \mathbb{P}(s'[k] \mid (s, a)[Z^P_k]) \). For every \( V: \mathcal{S} \to \mathbb{R} \) and the right-linear operators \( \mathbb{P} \), we define \( \mathbb{P}V(s, a) \stackrel{\text{def}}{=} \sum_{s' \in \mathcal{S}} \mathbb{P}(s' \mid s, a)V(s') \). A state-action pair can be represented as \((s, a)\) or \(x\). We also use \((s, a)[Z]\) to denote the corresponding \(x[Z]\) for notation convenience.

We mainly focus on the case where the total time step \( T = KH \) is the dominant factor (compared with \(|S_i|, |X_i| \) and \( H \)). We assume that \( T \geq |X_i| \geq H \) during the analysis.

3. Related Work

**Tabular MDP** Most algorithms in theoretical RL focus on tabular case, where the number of states and actions \( S, A \) are finite, and the regret bound scales polynomially with \( S \) and \( A \). Strong theoretical guarantees (e.g., Dann et al., 2017; Azar et al., 2017; Jin et al., 2018; Zhang and Ji, 2019) have been established in the episodic case and infinite-horizon (average rewards) case with respect to the minimax lower bound (Jaksch et al., 2010).

**Factored MDP** FMDP is a structural assumption that the transition and reward function can be decomposed into independent factors decided by different subsets of state/action set. Episodic FMDP was studied by Osband and Van Roy (2014), in which they proposed both PSRL and UCRL style algorithm with near-optimal Bayesian and frequentist regret bound. In non-episodic setting, Xu and Tewari (2020) recently generalizes the algorithm of Osband and Van Roy (2014) to infinite horizon average reward setting. However, both their results suffer from linear dependence on the horizon and factored state space’s cardinality.

Concurrent with our work is the recent paper by Tian et al. (2020), which also applies UCBVI and EULER to the factored MDP setting. Compared with their results, we propose a more refined variance decomposition theorem for factored Markov chain (Theorem 1), which results in a better regret by a factor of \( \sqrt{n} \); the theorem is also of independent interest with potential use in other problems in factored MDPs. Furthermore, we formulate the RLwK problem, and provide a sample-efficient algorithm based on our algorithm for factored MDPs.

**Constrained MDP and knapsack bandits** Knapsack setting with hard constraints has already been studied in bandits with both sample-efficient and computational-efficient algorithms (Badanidiyuru et al., 2013; Agrawal et al., 2016). This setting may be viewed as a special case of RLwK with \( H = 1 \). In constrained RL, there is a line of works that focus on *soft constraints* where the constraints are satisfied in expectation or with high probability (Brantley et al., 2020; Zheng and Ratliff, 2020), or a violation bound is established (Efroni et al., 2020; Ding et al., 2020). RLwK requires stronger constraints that is almost surely satisfied during the execution of the agents. A more related setting is proposed by Brantley et al. (2020), which studies a sample-efficient algorithm for knapsack episodic setting with hard constraints on all \( K \) episodes. However, we require the constraints to be satisfied *within each episode*, which we believe can better describe the real-world scenarios. The setting of Singh et al. (2020) is closer to ours since they are focusing on “every-time” hard constraints, but they consider the non-episodic case.
4. Main Results

In this section, we introduce our FMDP-BF algorithm, which uses empirical variance to construct a Bernstein-type confidence bonus for value estimation. In Section 4.1, we briefly introduce our estimation error decomposition techniques and the construction of the confidence bonus. In Section 4.2, we give a specific analysis of the variance of factored Markov chain, which helps to give a more precise upper bound on the summation of per-step variance. In Section 4.3, we propose our FMDP-BF algorithm in detail. In Section 4.4, we present the regret bound of Alg. 1. In Section 4.5, we propose the corresponding lower bound for factored MDP. Besides FMDP-BF, we also propose a simpler algorithm called FMDP-CH with a slightly worse regret, which follows the similar idea of UCBVI-CH (Azar et al., 2017). The algorithm and the corresponding analysis is more concise and easy to understand; details are deferred to Section C.

4.1 Estimation Error Decomposition

Our algorithm will follow the principle of “optimism in the face of uncertainty”, which is a standard strategy for efficient exploration (e.g., Strehl et al., 2009; Jaksch et al., 2010; Dann et al., 2017; Azar et al., 2017; Jin et al., 2018; Dong et al., 2019; Zanette and Brunskill, 2019). Like ORLC (Dann et al., 2019) and EULER (Zanette and Brunskill, 2019), our algorithm also maintains both the optimistic and pessimistic estimates of state values to yield an improved regret bound.

We use \( \bar{V}_{k,h} \) and \( \check{V}_{k,h} \) to denote the optimistic value estimation and pessimistic value estimation of \( V^*_h \). To guarantee optimism, we need to add confidence bonus to the estimated value function \( \bar{V}_{k,h} \) in each step, so that \( \bar{V}_{k,h}(s) \geq V^*(s) \) holds for any \( k \in [K] \), \( h \in [H] \) and \( s \in S \). Suppose \( \tilde{R}_{k,i} \) and \( \tilde{P}_{k,j} \) denote the estimation value of each expected factored reward \( R_i \) and factored transition probability \( P_j \) before episode \( k \) respectively. By the definition of the reward \( R \) and the transition \( P \), we use \( \tilde{R}_k \overset{\text{def}}{=} \frac{1}{m} \sum_{i=1}^{m} \tilde{R}_{k,i} \) and \( \tilde{P}_k \overset{\text{def}}{=} \prod_{j=1}^{n} \tilde{P}_{k,j} \) as the estimation of \( \bar{R} \) and \( \bar{P} \). Following the previous framework, this confidence bonus needs to tightly characterize the estimation error of the one-step backup \( \bar{R}(s,a) + \bar{P}V^*_h(s,a) \); in other words, it should compensate for the estimation errors, \( (\tilde{R}_k - \bar{R})(s,a) \) and \( (\tilde{P}_k - \bar{P})V^*_h(s,a) \), respectively.

For the estimation error of rewards \( (\tilde{R}_k - \bar{R})(s_{k,h},a_{k,h}) \), since the reward is defined as the average of \( m \) factored rewards, it is not hard to decompose the estimation error of \( \bar{R}(s,a) \) to the average of the estimation error of each factored rewards. In that case, we separately construct the confidence bonus of each factored reward \( \bar{R}_i \); suppose \( CB_{k,Z}^R(s,a) \) is the confidence bonus that compensates for the estimation error \( \tilde{R}_{k,i} - \bar{R}_i \), then we have \( CB_k^R(s,a) \overset{\text{def}}{=} \frac{1}{m} \sum_{i=1}^{m} CB_{k,Z}^R(s,a) \).

For the estimation error of transition \( (\tilde{P}_k - \bar{P})V^*_{h+1}(s_{k,h},a_{k,h}) \), the main difficulty is that \( \tilde{P}_k \) is the multiplication of \( n \) estimated transition dynamics \( \tilde{P}_{k,j} \). In that case, the estimation error \( (\tilde{P}_k - \bar{P})V^*_{h+1}(s_{k,h},a_{k,h}) \) may be calculated as the multiplication of \( n \) estimation error
for each factored transition $\hat{P}_{k,i}$, which makes the analysis much more difficult. Fortunately, we have the following lemma to address this challenge.

**Lemma 4.1. (Informal)** Let the transition function class $\mathbb{P} \in \mathcal{P}(\mathcal{X},\mathcal{S})$ be factored over $\mathcal{X} = \mathcal{X}_1 \times \cdots \times \mathcal{X}_d$, and $\mathcal{S} = \mathcal{S}_1 \times \cdots \times \mathcal{S}_n$ with scopes $Z^P_1, \cdots, Z^P_n$. For a given function $V: \mathcal{S} \rightarrow \mathbb{R}$, the estimation error of one-step value $|\langle \hat{P}_k - \mathbb{P} \rangle V(s,a)|$ can be decomposed by:

$$ |\langle \hat{P}_k - \mathbb{P} \rangle V(s,a)| \leq \sum_{i=1}^{n} (\hat{P}_{k,i} - \mathbb{P}_i) \left( \prod_{j \neq i,j=1}^{n} \mathbb{P}_j \right) V(s,a) \right) + \beta_{k,h}(s,a)$$

Here, $\beta_{k,h}(s,a)$, formally defined in Lemma D.1, are higher order terms that do no harm to the order of the regret. This lemma allows us to decompose the estimation error $\langle \hat{P}_k - \mathbb{P} \rangle V_{h+1}(s_h,a_k)$ into an additive form, so we can construct the confidence bonus for each factored transition $\mathbb{P}$, separately. Let $CB_{k,Z_j}^P(s,a)$ be the confidence bonus for the estimation error $\langle \hat{P}_{k,i} - \mathbb{P}_i \rangle \left( \prod_{j \neq i,j=1}^{n} \mathbb{P}_j \right) V(s,a)$. Then, $CB_k^P(s,a) \overset{\text{def}}{=} \sum_{j=1}^{n} CB_{k,Z_j}^P(s,a) + \eta_{k,h}(s,a)$, where $\eta_{k,h}(s,a)$ omits higher order factors that will be explicitly given later.

Finally, we define the confidence bonus as the summation of all confidence bonuses for rewards and transition: $CB_k(s,a) = CB_k^R(s,a) + CB_k^F(s,a)$.

### 4.2 Variance of Factored Markov Chain

After the analysis in Section 4.1, the remaining problem is how to define the confidence bonus $CB_k^R(s,a)$ and $CB_k^F(s,a)$. In this subsection, we tackle this problem by deriving the variance decomposition formula for factored MDP. To begin with, we consider a Markov chain with stochastic factored transition and stochastic factored rewards, and deduce the Bellman equation of variance for factored Markov chain. The analysis shows how to define the empirical variance in the confidence bonus for factored MDP and gives an upper bound on the summation of per-step variance (Corollary 1.1).

In the Markov chain setting, the reward is defined to be a mapping from $\mathcal{S}$ to $\mathbb{R}$. Suppose $J_{t_1:t_2}(s)$ denotes the total rewards the agent obtains from step $t_1$ to step $t_2$ (inclusively), given that the agent starts from state $s$ in step $t_1$. $J_{t_1:t_2}$ is a random variable depending on the randomness of the trajectory from step $t_1$ to $t_2$, and stochastic rewards therein. Following this definition of $J_{t_1:t_2}$, we define $J_{1:H}$ to be the total reward obtained during one episode. We use $s_t$ to denote the random state that the agent encounters at step $t$. We define

$$\omega_h^2(s) \overset{\text{def}}{=} \mathbb{E} \left[ (J_{h:H}(s_h) - V_h(s_h))^2 \mid s_h = s \right],$$

to be the variance of the total gain after step $h$, given that $s_h = s$.

We define $\sigma_{R,i}^2(s) \overset{\text{def}}{=} \mathbb{V} [R_i(\xi) \mid \xi = s]$ to be the variance of the $i$-th factored reward, given that the current state is $s$. Given the current state $s$, we define the variance of the next-state value function w.r.t. the $i$-th factored transition in the following way:

$$\sigma_{P,i,h}^2(s) \overset{\text{def}}{=} \mathbb{E}_{s_{h+1}[1:i-1]} \left[ \mathbb{V}_{s_{h+1}[i]} \left[ \mathbb{E}_{s_{h+1}[i+1:n]} [V_{h+1}(s_{h+1})] \right] \right] \mid s_h = s.$$
That is, for each given \( s'[1 : i] \), we firstly take expectation over all possible value of \( s'[i + 1 : n] \) w.r.t. \( \mathbb{P}_{[i+1:n]} \). Then, we calculate the variance of transition \( s'[i] \sim \mathbb{P}_i(\cdot | (s, a)[Z^P_i]) \) given fixed \( s'[1 : i - 1] \). Finally, we take the expectation of this variance w.r.t. \( s'[1 : i - 1] \sim \mathbb{P}_{[1:i-1]} \).

**Theorem 1.** For any horizon \( h \), we have

\[
\omega^2_h(s) = \sum_{s'} \mathbb{P}(s'|s) \omega^2_{h+1}(s') + \sum_{i=1}^n \sigma^2_{P_i,h}(s) + \frac{1}{m^2} \sum_{i=1}^m \sigma^2_{R_i}(s),
\]

Theorem 1 generalizes the analysis of Munos and Moore (1999), which deals with non-factored MDPs and deterministic rewards. From the Bellman equation of variance, we can give an upper bound to the expected summation of per-step variance.

**Corollary 1.1.** Suppose the agent takes policy \( \pi \) during an episode. Let \( w_h(s, a) \) denote the probability of entering state \( s \) and taking action \( a \) in step \( h \). Then we have the following inequality:

\[
\sum_{h=1}^H \sum_{(s,a) \in X} w_h(s, a) \left( \sum_{i=1}^n \sigma^2_{P_i}(V^\pi_{h+1}, s, a) + \frac{1}{m^2} \sum_{i=1}^m \sigma^2_{R_i}(s, a) \right) \leq H^2,
\]

where \( \sigma^2_{R_i}(s, a) \) is the variance of \( i \)-th factored reward given the current state-action pair \( (s, a) \). \( \sigma^2_{P_i}(V^\pi_h, s, a) \) denotes the variance of \( i \)-th factored transition given current state \( s \), i.e. \( \mathbb{E}_{s_{h+1}|[1:i-1]} [V^\pi_{h+1} | \mathbb{E}_{s_{h+1}|[1:i:n]} [V^\pi_{h+1}(s_{h+1})] | s_h = s] \).

This corollary makes it possible to construct confidence bonus with variance for each factored rewards and transition separately. Please refer to Section E.2 for the detailed proof of Theorem 1 and Corollary 1.1.

### 4.3 Algorithm

Our algorithm is formally described in Alg. 1. Denote by \( N_k((s, a)[Z]) \) the number of steps that the agent encounters \( (s, a)[Z] \) during the first \( k \) episodes, and \( N_k((s, a)[Z_j], s_j) \) the number of steps that the agent transits to a state with \( s[j] = s_j \) after encountering \( (s, a)[Z_j] \) during the first \( k \) episodes. In episode \( k \), we estimate the mean value of each factored reward \( R_i \) and each factored transition \( P_i \) with empirical mean value \( \hat{R}_{k,i} \) and \( \hat{P}_{k,i} \) respectively. To be more specific, \( \hat{R}_{k,i}((s, a)[Z^R_i]) = \sum_{t \leq (k-1)H} 1_{\frac{1}{N_{k-1}((s, a)[Z^R_i])}[s[t], a[t], Z^R_i[t]] \cap r_{t,i}} \), where \( r_{t,i} \) denotes the reward \( R_i \) sampled in step \( t \), and \( \hat{P}_{k,i}((s, a)[Z^P_i]) = \frac{N_{k-1}((s, a)[Z^P_i], s[j])}{N_{k-1}((s, a)[Z^P_i], s[j])} \). After that, we construct the optimistic MDP \( \hat{M} \) based on the estimated rewards and transition functions. For a certain \( (s, a) \) pair, the transition function and reward function are denoted as \( \hat{R}_k(s, a) = \frac{1}{m} \sum_{i=1}^m \hat{R}_{k,i}((s, a)[Z^R_i]) \) and \( \hat{P}_k(s' | s, a) = \prod_{j=1}^n \hat{P}_{k,j}(s'[j] | (s, a)[Z^P_j]) \).

Following the analysis in Section 4.1, we separately construct the confidence bonus of each factored reward \( R_i \) with the empirical variance:

\[
CB_{k,Z^R_i}^R(s, a) = \sqrt{\frac{2\sigma^2_{R_{k,i}}(s, a)[L^R_i]}{N_{k-1}((s, a)[Z^R_i])}} + \frac{8L^R_i}{3N_{k-1}((s, a)[Z^R_i])}, \quad i \in \mathbb{Z}.
\]
Algorithm 1 FMDP-BF

Input: \( \delta \)
\( \mathcal{L} = \emptyset \), initialize \( N((s, a)[Z_i]) = 0 \) for any factored set \( Z_i \) and any \((s, a)[Z_i] \in \mathcal{X}[Z_i] \)

for episode \( k = 1, 2, \ldots \) do

Set \( V_{k,H+1}(s) = V_{k,H+1}(s) = 0 \) for all \( s,a \).

Let \( \mathcal{K} = \{(s, a) \in \mathcal{S} \times \mathcal{A} : \cap_{i=1,\ldots,n} N_k((s, a)[Z_i^R]) > 0 \} \)

Estimate \( \hat{R}_{k,i}(s, a) \) as the empirical mean if \( N_{k-1}((s, a)[Z_i^R]) > 0 \), and 1 otherwise
\( \hat{R}(s, a) = \frac{1}{m} \sum_{i=1}^{m} \hat{R}_i((s, a)[Z_i^R]) \)

Estimate \( \hat{P}_k(\cdot \mid s,a) \) with empirical mean value for all \((s, a) \in \mathcal{K} \)

for horizon \( h = H, H - 1, \ldots, 1 \) do

for \( s \in \mathcal{S} \) do

for \( a \in \mathcal{A} \) do

if \((s, a) \in \mathcal{K} \) then

\( Q_{k,h}(s, a) = \min \{ H, \hat{R}_{k}(s, a) + CB_k(s, a) + \hat{P}_k \hat{V}_{k,h+1}(s, a) \} \)

else

\( Q_{k,h}(s, a) = H \)

end if

end for

\( \pi_{k,h}(s) = \arg \max_a Q_{k,h}(s, a) \)
\( \bar{V}_{k,h}(s) = \max_{a \in \mathcal{A}} Q_{k,h}(s, a) \)

\( V_{k,h}(s) = \max \left\{ 0, \hat{R}_k(s, \pi_{k,h}) - CB_k(s, \pi_{k,h}) + \hat{P}_k \bar{V}_{k,h+1}(s, \pi_{k,h}) \right\} \)

end for

end for

for step \( h = 1, \ldots , H \) do

Take action \( a_{k,h} = \arg \max_a Q_{k,h}(s_{k,h}, a) \)

end for

Update history trajectory \( \mathcal{L} = \mathcal{L} \cup \{s_{k,h}, a_{k,h}, r_{k,h}, s_{k,h+1} \}_{h=1,2,\ldots,H} \), and update history counter \( N_{k-1}((s, a)[Z_i]) \).

end for

where \( L_i^R \overset{\text{def}}{=} \log (18mT|\mathcal{X}[Z_i^R]|/\delta) \), and \( \hat{\sigma}_{R,k,i}^2 \) is the empirical variance of the \( i \)-th factored reward \( \hat{R}_i \), i.e.

\[
\hat{\sigma}_{R,k,i}^2(s, a) = \frac{1}{N_{k-1}((s, a)[Z_i^R])} \sum_{t=1}^{(k-1)H} \mathbf{1}[(s_t, a_t)[Z_i^R] = (s, a)[Z_i^R]] \cdot \hat{r}_{t,i}^2 - \left( \hat{R}_{k,i}((s, a)[Z_i^R]) \right)^2.
\]

We define \( L_P = \log (18nTSA/\delta) \) for short. Following the idea of Lemma 4.1, we separately construct the confidence bonus of scope \( Z_i^P \) for transition estimation:

\[
CB_{k,Z_i^P}(s, a) = \sqrt{\frac{4\hat{\sigma}_{P,k,i}^2(V_{k,h+1}, s, a)L_P}{N_{k-1}((s, a)[Z_i^R])}} + \sqrt{\frac{2u_{k,h,i}(s,a)L_P}{N_{k-1}((s, a)[Z_i^R])}} + \eta_{k,h,i}(s, a), \quad i \in [n] \tag{2}
\]

where \( \hat{\sigma}_{P,k,i}(s, a) \) and \( u_{k,h,i}(s,a) \) are defined later. \( \eta_{k,h,i}(s, a) \) omits the additional bonus terms that do not affect the order of the final regret. The precise expression of \( \eta_{k,h,i}(s, a) \) is deferred to Section E.
The definition of \( \hat{\sigma}_{P,k,i}^2(V_{k,h+1}, s, a) \) corresponds to \( \sigma_{P,k,i}^2(V^*_h, s, a) \) in Corollary 1.1, which can be regarded as the empirical variance of transition \( \mathbb{P}_{k,i} \):

\[
\hat{\sigma}_{P,k,i}^2(V_{k,h+1}, s, a) = \mathbb{E}_{s'[1;i-1] \sim \hat{P}_{k,[1,i-1]}(|s,a)} \left[ V(s'[i] \sim \hat{P}_{k,i}(|s,a), \mathbb{P}_{k,i} V_{k,h+1}(s')) \right].
\]

To guarantee optimism, we need to use the empirical variance \( \hat{\sigma}_{P,k,i}^2(V^*, s, a) \) to upper bound the estimation error in the proof. Since we do not know \( V^* \) beforehand, we use \( \hat{\sigma}_{P,k,i}^2(\bar{V}_{k,h+1}, s, a) \) as a surrogate in the confidence bonus. However, we cannot guarantee that \( \hat{\sigma}_{P,k,i}^2(V^*, s, a) \) is upper bounded by \( \hat{\sigma}_{P,k,i}^2(\bar{V}_{k,h+1}, s, a) \). To compensate for the error due to the difference between \( \bar{V}_{h+1}^* \) and \( \bar{V}_{k,h+1} \), we add \( \sqrt{\frac{2u_{k,h,i}(s,a) L^P}{N_{k-1}((s,a)[Z_{i}^P])}} \) to the confidence bonus, where \( u_{k,h,i}(s,a) \) is defined as:

\[
u_{k,h,i}(s,a) = \mathbb{E}_{s'[1;i] \sim \hat{P}_{k,[1,i]}(|s,a)} \left[ \left( \mathbb{E}_{s[i+1:n] \sim \hat{P}_{k,[i+1:n]}(|s,a)} \left( \bar{V}_{k,h+1} - V(s') \right)^2 \right) \right].
\]

### 4.4 Regret

**Theorem 2.** With prob. \( 1 - \delta \), the regret of Alg. 1 with Bernstein-type bonus is upper bounded by

\[
\mathcal{O} \left( \frac{1}{m} \sum_{i=1}^{m} \sqrt{T |\mathcal{X}[Z_i^P]| \log(mT |\mathcal{X}[Z_i^P]| / \delta) + \sqrt{HT \sum_{j=1}^{n} |\mathcal{X}[Z_j^P]| \log(nTSA / \delta)} \right).
\]

Note that the regret bound does not depend on the cardinalities of state and action spaces, but only has square root dependence on the cardinality of each factored subspace \( X[Z_i] \). By leveraging the structure of factored MDP, we achieve regret that scales exponentially smaller compared with that of UCBVI (Azar et al., 2017). The best previous regret bound for episodic factored MDP is achieved by Osband and Van Roy (2014). When transformed to our setting, it is:

\[
\mathcal{O} \left( \frac{1}{m} \sum_{i=1}^{m} \sqrt{|\mathcal{X}[Z_i^P]|T \log(mT |\mathcal{X}[Z_i^P]| / \delta) + \sum_{j=1}^{n} H \sqrt{|\mathcal{X}[Z_j^P]| |S_j| T \log(nTSA / \delta)} \right).
\]

which is worse than our results by a factor of \( \sqrt{H|S_j|} \). Furthermore, we improve the regret by \( \sqrt{n} \), when the cardinality of each factored subspace \( |\mathcal{X}[Z_i^P]| \) are relatively the same.

For clarity, we also present a cleaner single-term regret bound under a symmetric problem setting. Suppose \( \mathcal{M} \) is a set of factored MDP with \( m = n, |S| = S_i, |\mathcal{X}_i| = S_i A_i \) and \( |Z_i^R| = |Z_j^P| = \zeta \) for \( i = 1, \ldots, m \) and \( j = 1, \ldots, n \), we write \( X = (S_i A_i)^\zeta \).

**Corollary 2.1.** Suppose \( M^* \in \mathcal{M} \), with prob. \( 1 - \delta \), the regret of FMDP-BF is upper bounded by \( \mathcal{O} \left( \sqrt{nHXT \log(nTSA / \delta)} \right) \).

The minimax regret bound for non-factored MDP is \( \mathcal{O} \left( \sqrt{HSAT} \right) \). Compared with this result, our algorithm’s regret is exponentially smaller when \( n \) and \( \zeta \) are relatively small.
4.5 Lower Bound

In this subsection, we propose the regret lower bound for factored MDP. The regret bound in Theorem 2 matches the lower bound w.r.t all the parameters except \( n \). If the cardinality of each factored subspace \( |X[Z|^j|T] \) are relatively the same, there is still a gap of \( \sqrt{n} \), which we leave as a possible future work.

**Theorem 3.** For any algorithm \( \text{ALG} \), there exists a factored MDP instance \( M \) such that the expected regret of the algorithm \( \text{ALG} \) over \( T \) steps is lower bounded by
\[
\Omega \left( \frac{1}{m} \sum_{i=1}^{m} \sqrt{|X[Z]^i||T \log(|X[Z]^i||T)} + \frac{1}{n} \sum_{j=1}^{n} \sqrt{H|X[Z]^j||T} \right).
\]

The proof of Theorem 3 is deferred to Section F.

5. RL with Knapsack Constraints

In this section, we study RL with Knapsack constraints, or RLwK, as an application of FMDP-BF.

5.1 Preliminaries

We generalize bandit with knapsack constraints or BwK (Badanidiyuru et al., 2013; Agrawal et al., 2016) to episodic MDPs. We consider the setting of tabular episodic Markov decision process, \((S, A, H, \mathbb{P}, R, C)\), which adds to an episodic MDP with a \( d \)-dimensional stochastic cost vector, \( C(s, a) \). We use \( C_i(s, a) \) to denote the \( i \)-th cost in the cost vector \( C(s, a) \). If the agent takes action \( a \) in state \( s \), it will receive a reward \( r \) sampled from \( R(s, a) \). After that, it suffers a cost \( c \), and transits to state \( s' \) with probability \( \mathbb{P}(s'|s, a) \). In each episode, the agent’s total budget is \( B \). We also use \( B_i \) to denote the total budget of \( i \)-th cost. Without loss of generality, we assume \( B_i \leq B \) for all \( i \). Once the cumulative cost \( \sum_h c_{h,i} \) of any dimension \( i \) in an episode exceeds the total budget \( B_i \), the agent has to terminate the interaction in this episode. If this doesn’t happen, the episode will end in \( H \) steps. The agent’s goal is to maximize its cumulative rewards \( \sum_{k=1}^{K} \sum_{h=1}^{H} r_{k,h} \) in \( K \) episodes.

5.2 Comparison with Other Settings

The RLwK setting appears similar to the episodic constrained RL analyzed in previous work (Efroni et al., 2020; Brantley et al., 2020). However, the two settings are fundamentally different, so their algorithms cannot be used to solve RLwK.

As discussed in Section 3, the episodic constrained RL setting can be roughly divided into two categories. A line of works focus on soft constraints where the constraints are satisfied in expectation, i.e. \( \sum_{h=1}^{H} \mathbb{E}[c_{k,h}] \leq B \). The expectation is taken over the randomness of the trajectories and the random sample of the costs. Another line of work focuses on hard constraints in \( K \) episodes. To be more specific, they assume that the total costs in \( K \) episodes cannot exceed a constant vector \( B \), i.e. \( \sum_{k=1}^{K} \sum_{h=1}^{H} c_{k,h} \leq B \). Once this is violated before episode \( K_1 < K \), the agent will not obtain any rewards in the remaining \( K - K_1 \) episodes. Though both settings are interesting and useful, they do not cover...
many common situations in constrained RL. For example, when playing games, the game is over once the total energy or health reduce to 0. After that, the player may restart the game (starting a new episode) with full initial energy again. In robotics, a robot may episodically interact with the environment and learn a policy to carry out a certain task. The interaction in each episode is over once its energy is used up. In these two examples, we cannot just consider the expected cost or the cumulative cost across all episodes, but counts the cumulative cost in every individual episode. Moreover, in many constrained RL applications, the agent’s optimal action should depend on its remaining budget. For example, in robotics, the robot should do planning and take actions based on its remaining energy. However, previous results do not consider this issue, and use policies that map states to actions. Instead, in RLwK, we need to define the policy as a mapping from states and remaining budget to actions. Section G gives further details, including two examples for illustrating the difference between these settings.

5.3 Algorithm

We make the following assumptions about the cost function for simplicity. Both of them hold if all the stochastic costs are integers.

**Assumption 1.** The budget \( B_i \) as well as the possible value of costs \( C_i(s,a) \) of any state \( s \) and action \( a \) is an integral multiple of the unit cost \( \frac{1}{m} \).

**Assumption 2.** The stochastic cost \( C_i(s,a) \) has finite support. That is, the random variable \( C_i(s,a) \) can only take at most \( n \) possible values.

Assumption 1 is made for computational issue. If it does not hold, we can construct an \( \epsilon \)-net for budget \( B \) with precision \( \epsilon = \frac{1}{m} \), and this construction will not influence the regret. The reason for Assumption 2 is that we need to estimate the distribution of the cost, instead of just estimating its mean value.

From the above discussion, we know that we need to find a policy that is a mapping from state and budget to action. Therefore, it is natural to augment the state with the remaining budget. It follows that the size of augmented state space is \( S \cdot (Bm)^d \). Directly applying UCBVI will lead to a regret of order \( O\left(\sqrt{HSA(1 + dBm)T}\right) \). Our key observation is that the constructed state representation can be represented as a product of subspaces. Each subspace is relatively independent. For example, the transition matrix over the original state space \( S \) is independent of the remaining budget. That is to say, the constructed MDP can be formulated as a factored MDP, and the compact structure of the model can reduce the regret significantly.

By applying Alg. 1 and Theorem 2 to RLwK, we can reduce the regret to the order of \( O\left(\sqrt{HSA(1 + dBm)T}\right) \) roughly, which is exponentially smaller. However, the regret still depends on the total budget \( B \) and the discretization precision \( m \), which may be very large for continuous budget and cost\(^1\). Another observation to tackle the problem is that the cost of taking action \( a \) in state \( s \) only depends on the current state-action pair \((s,a)\), but has no dependence on the remaining budget \( B \). To be more formally,

\[ b_{h+1} = b_h - c_h, \]

\(^1\) For continuous budget and cost, we need to construct \( \epsilon \)-net, in which case \( m \) equals to \( \frac{1}{\epsilon} \).
where $b_h$ is the remaining budget at step $h$, and $c_h$ is the cost suffered in step $h$. As a result, we can further reduce the regret to roughly $O\left(\sqrt{HdSAT}\right)$ by estimating the distribution of cost function. A similar model has been discussed in Brunskill et al. (2009), which is named as noisy offset model.

We denote $V_h^\pi(s, b)$ as the value function in state $s$ at horizon $h$ following policy $\pi$, and the agent’s remaining budget is $b$. For notation simplicity, we use $P_{s}V(s, a, b)$ as a shorthand of $\sum_{s'}P(s'|s, a)V(s', b)$, and $P_{c}V(s, a)$ as a shorthand of $\sum_{c_0}P(C(s, a) = c_0|s, a)V(s', b - c_0)$. We use $P_{C,i}(c_0|s, a)$ to denote the “transition probability” of budget $i$, i.e., $P(C_i(s, a) = c_0|s, a)$. The Bellman Equation of our setting is written as:

$$
V_h^\pi(s, b) = \begin{cases} 
\tilde{R}(s, \pi_h(s, b)) + P_{s}P_{C}V_{h+1}^\pi(s, \pi_h(s, b), b) & b > 0 \\
0 & b \leq 0. 
\end{cases}
$$

Our algorithm follows the same basic idea of Alg. 1. We defer the detailed description to Section G to avoid redundancy and only sketch the difference in this section. Following the definition in the factored MDP setting, we estimate the empirical rewards, transition among states, and “transition” of the remaining budget with empirical mean value. That is:

$$
\hat{R}_k(s, a) = \frac{\sum_{k,h}1[s_{k,h} = s, a_{k,h} = a] \cdot r_{k,h}}{N_{k-1}(s, a)}
$$

$$
\hat{P}_{s,k}(s'|s, a) = \frac{N_{k-1}(s, a, s')}{N_{k-1}(s, a)}
$$

$$
\hat{P}_{C,k,i}(C_i(s, a) = c_0|s, a) = \frac{\sum_{k,h}1[s_{k,h} = s, a_{k,h} = a, c_{k,h,i} = c_0]}{N_{k-1}(s, a)}.
$$

We construct the confidence bonuses for rewards and transition, respectively:

$$
CB_k^R(s, a) = \sqrt{\frac{2\sigma^2_R(s, a) \log(2SAT)}{N_{k-1}(s, a)}} + \frac{8\log(2SAT)}{3N_{k-1}(s, a)}
$$

$$
CB_{k,i}^P(s, a, b) = \sqrt{\frac{4\sigma^2_{p_i}(V_{k,h+1}(s, a, b)L)}{N_{k-1}(s, a)}} + \sqrt{\frac{2u_{k,h,i}(s, a, b)L}{N_{k-1}(s, a)}} + \eta_{k,h}^i(s, a), \quad 0 \leq i \leq d
$$

where $L = \log(2dSAT) + d\log(mB)$ is the logarithmic factors because of union bounds. Note that there is an additive term $d\log(mB)$, which is because that we need to take union bounds over all possible budget $b$. $CB_k^P(s, a)$ is the confidence bonus for state transition estimation $\hat{P}_s$, and $\{CB_{k,i}^P(s, a)\}_{i=1,...,d}$ is the confidence bonus for budget transition estimation $\{\hat{P}_{c,i}\}_{i=1,...,d}$. $\eta_{k,h}^i(s, a)$ omits the higher order terms, which is defined in Section G.

We define the confidence bonus $CB_k(s, a) = CB_k^R(s, a) + \sum_{i=0}^d CB_{k,i}^P(s, a, b)$. With the estimated model and constructed confidence bonus, we are able to calculate the optimistic and the pessimistic value estimation, and then follow the optimistic value in each episode. The regret can be upper bounded by the following theorem:
Theorem 4. With prob. at least $1 - \delta$, the regret of Alg. 3 is upper bounded by

$$O \left( \sqrt{dHSA} \left( \log(SA) + d \log(Bm) \right) \right)$$

Compared with the lower bound for non-factored tabular MDP (Jaksch et al., 2010), this regret bound matches the lower bound w.r.t. $S$, $A$, $H$ and $T$. There may still be a gap in the dependence of the number of constraints $d$, which is often much smaller than other quantities.

It should be noted that, though we achieve a near-optimal regret for RLwK, the computational complexity is high, scaling polynomially with the maximum budget $B$, and exponential on the number of constraints $d$. This is a consequence of the NP-hardness of knapsack problem with multiple constraints (Martello, 1990; Kellerer et al., 2004). However, since the policy is defined on the state and budget space with cardinality $SB^d$, this computational complexity seems unavoidable. How to tackle this problem, such as with approximation algorithms, is interesting future work.

6. Conclusion

We propose a novel RL algorithm for solving FMDPs, which is efficient both statistically and computationally. It improves the best previous regret bound by a factor of $\sqrt{H|S|}$. We also derive a regret lower bound for FMDPs based on the minimax lower bound of multi-armed bandits and episodic tubular MDPs (Jaksch et al., 2010). Further, we formulate the RL with Knapsack constraints (RLwK) setting and establish the connections between our results for FMDP and RLwK by providing a sample efficient algorithms based on FMDP-BF in this new setting. However, we still leave some issues in this work. The regret upper bound and lower bound still has a gap of approximately $\sqrt{n}$, where $n$ is the number of transition factors. For RLwK, there still remains a computational problem in our algorithm, which may be solved by either a more elegant formulation of hard constraint setting or a clever design of new algorithms. We hope to address these issues in the future work.

References

Shipra Agrawal, Nikhil R Devanur, and Lihong Li. An efficient algorithm for contextual bandits with knapsacks, and an extension to concave objectives. In Conference on Learning Theory, pages 4–18, 2016.

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

Ashwinkumar Badanidiyuru, Robert Kleinberg, and Aleksandrs Slivkins. Bandits with knapsacks. In 2013 IEEE 54th Annual Symposium on Foundations of Computer Science, pages 207–216. IEEE, 2013.

Craig Boutilier, Richard Dearden, and Moisés Goldszmit. Stochastic dynamic programming with factored representations. Artificial intelligence, 121(1-2):49–107, 2000.
Kianté Brantley, Miroslav Dudik, Thodoris Lykouris, Sobhan Miryoosefi, Max Simchowitz, Aleksandrs Slivkins, and Wen Sun. Constrained episodic reinforcement learning in concave-convex and knapsack settings. arXiv preprint arXiv:2006.05051, 2020.

Emma Brunskill, Bethany R. Leffler, Lihong Li, Michael L. Littman, and Nicholas Roy. Provably efficient learning with typed parametric models. Journal of Machine Learning Research, 10(68):1955–1988, 2009. URL http://jmlr.org/papers/v10/brunskill09a.html.

Christoph Dann, Tor Lattimore, and Emma Brunskill. Unifying pac and regret: Uniform pac bounds for episodic reinforcement learning. In Advances in Neural Information Processing Systems, pages 5713–5723, 2017.

Christoph Dann, Lihong Li, Wei Wei, and Emma Brunskill. Policy certificates: Towards accountable reinforcement learning. In International Conference on Machine Learning, pages 1507–1516, 2019.

Dongsheng Ding, Xiaohan Wei, Zhuoran Yang, Zhaoran Wang, and Mihailo R Jovanović. Provably efficient safe exploration via primal-dual policy optimization. arXiv preprint arXiv:2003.00534, 2020.

Kefan Dong, Yuanhao Wang, Xiaoyu Chen, and Liwei Wang. Q-learning with ucb exploration is sample efficient for infinite-horizon mdp. arXiv preprint arXiv:1901.09311, 2019.

Yonathan Efroni, Shie Mannor, and Matteo Pirotta. Exploration-exploitation in constrained mdps. arXiv preprint arXiv:2003.02189, 2020.

Carlos Guestrin, Daphne Koller, Ronald Parr, and Shobha Venkataraman. Efficient solution algorithms for factored MDPs. Journal of Artificial Intelligence Research, 19:399–468, 2003.

Thomas Jaksch, Ronald Ortner, and Peter Auer. Near-optimal regret bounds for reinforcement learning. Journal of Machine Learning Research, 11:1563–1600, 2010.

Chi Jin, Zeyuan Allen-Zhu, Sebastien Bubeck, and Michael I Jordan. Is q-learning provably efficient? In Advances in Neural Information Processing Systems, pages 4863–4873, 2018.

Michael Kearns and Daphne Koller. Efficient reinforcement learning in factored mdps. In IJCAI, volume 16, pages 740–747, 1999.

Hans Kellerer, Ulrich Pferschy, and David Pisinger. Multidimensional knapsack problems. In Knapsack problems, pages 235–283. Springer, 2004.

Lihong Li. A unifying framework for computational reinforcement learning theory. PhD thesis, Rutgers University-Graduate School-New Brunswick, 2009.

Xiuuyuan Lu and Benjamin Van Roy. Information-theoretic confidence bounds for reinforcement learning. In Advances in Neural Information Processing Systems, pages 2461–2470, 2019.
Silvano Martello. Knapsack problems: algorithms and computer implementations. *Wiley-Interscience series in discrete mathematics and optimization*, 1990.

Rémi Munos and Andrew Moore. Influence and variance of a markov chain: Application to adaptive discretization in optimal control. In *Proceedings of the 38th IEEE Conference on Decision and Control (Cat. No. 99CH36304)*, volume 2, pages 1464–1469. IEEE, 1999.

Ian Osband and Benjamin Van Roy. Near-optimal reinforcement learning in factored mdps. In *Advances in Neural Information Processing Systems*, pages 604–612, 2014.

Rahul Singh, Abhishek Gupta, and Ness B Shroff. Learning in markov decision processes under constraints. *arXiv preprint arXiv:2002.12435*, 2020.

Alexander L. Strehl, Lihong Li, and Michael L. Littman. Reinforcement learning in finite MDPs: PAC analysis. *Journal of Machine Learning Research*, 10:2413–2444, 2009.

Yi Tian, Jian Qian, and Suvrit Sra. Towards minimax optimal reinforcement learning in factored markov decision processes. *arXiv preprint arXiv:2006.13405*, 2020.

Tsachy Weissman, Erik Ordentlich, Gadiel Seroussi, Sergio Verdu, and Marcelo J Weinberger. Inequalities for the l1 deviation of the empirical distribution. *Hewlett-Packard Labs, Tech. Rep.*, 2003.

Ziping Xu and Ambuj Tewari. Near-optimal reinforcement learning in factored mdps: Oracle-efficient algorithms for the non-episodic setting. *arXiv preprint arXiv:2002.02302*, 2020.

Andrea Zanette and Emma Brunskill. Tighter problem-dependent regret bounds in reinforcement learning without domain knowledge using value function bounds. *arXiv preprint arXiv:1901.00210*, 2019.

Zihan Zhang and Xiangyang Ji. Regret minimization for reinforcement learning by evaluating the optimal bias function. In *Advances in Neural Information Processing Systems*, pages 2827–2836, 2019.

Liyuan Zheng and Lillian J Ratliff. Constrained upper confidence reinforcement learning. *arXiv preprint arXiv:2001.09377*, 2020.
Appendix A. Notations

Before presenting the proof, we define the following notations.

| Symbol | Explanation |
|--------|-------------|
| $s_{k,h}, a_{k,h}$ | The state and action that the agent encounters in episode $k$ and step $h$ |
| $L^P$ | $\log (18nTSA/\delta)$ |
| $L^R$ | $\log (18mT |X[Z^R]| / \delta)$ |
| $X^P$ | $|X[Z^P]|$ |
| $X^R$ | $|X[Z^R]|$ |
| $\mathbb{P}V(s,a)$ | A shorthand of $\sum_{s' \in S} \mathbb{P}(s'|s,a)V(s')$ |
| $\phi_{k,i}(s,a)$ | $\sqrt{\frac{4|S_i|L^P}{N_{k-1}((s,a)[Z^P_j])} + \frac{4|S_i|L^P}{3N_{k-1}((s,a)[Z^P_j])}}$ |
| $\hat{\sigma}_{R,i}^2(s,a)$ | The empirical variance of reward $r_i$ |
| $\sigma_{P,k,i}^2(V,s,a)$ | The next state variance of $\mathbb{P}V$ for the transition $P_i$, i.e. $\mathbb{E}_{s'[1:i-1] \sim P_{[1,i]}(\cdot|s,a)} \left[ V_{s'[i] \sim P_i(\cdot|(s,a)[Z^P])} \left( \mathbb{E}_{s'[i+1:n] \sim P_{[i+1,n]}(\cdot|s,a)} V'(s') \right) \right]$ |
| $\Omega_{k,h}$ | The optimism and pessimism event for $k, h$: $\{ \bar{\mathbb{V}}_{k,h} \geq V_h^* \geq \mathbb{V}_{k,h} \}$ |
| $w_{k,h,Z}(s,a)$ | The probability of entering $(s,a)[Z]$ at step $h$ in episode $k$ |
| $w_{k,Z}(s,a)$ | $\sum_{h=1}^H w_{k,h,Z}(s,a)$ |
| $w_{k,h}(s,a)$ | The probability of entering $(s,a)$ at step $h$ in episode $k$, i.e. $w_{k,h,Z}(s,a)$ with $Z = \{1, 2, \ldots, d\}$ |
| $w_k(s,a)$ | $\sum_{h=1}^H w_{k,h}(s,a)$ |

Appendix B. High Probability Events

In this section, we discuss the high-prob. events, and assume that these events happen during the proof.
Lemma B.1. *(High prob. event)* With prob. at least $1 - 2\delta/3$, the following events hold for any $k, h, s, a$:

$$\left| \hat{R}_{k,i}(s,a) - \bar{R}_i(s,a) \right| \leq \sqrt{\frac{2L_R}{N_{k-1}((s,a)\mid Z_R^i)}} \quad i \in [m] \quad (7)$$

$$\left| \hat{P}_{k,i} \prod_{j \neq i} P_{k,j} V^*_h(s,a) - \prod_{j=1}^n P_j V^*_h(s,a) \right| \leq \sqrt{\frac{2H^2L_P}{N_{k-1}((s,a)\mid Z_P^i)}} \quad i \in [n] \quad (8)$$

$$\left| (\hat{P}_{k,i} - P_{k,i}) (s,a)\mid Z_P^i \right| \leq 2 \sqrt{\frac{|S_i|L_P}{N_{k-1}((s,a)\mid Z_P^i)}} + \frac{4|S_i|L_P}{3N_{k-1}((s,a)\mid Z_P^i)} \quad i \in [n] \quad (9)$$

$$\left| (\hat{P}_{k,i} - P_{k,i}) (s',a)\mid Z_P^i \right| \leq \sqrt{\frac{2P_i(s'[i]((s,a)\mid Z_P^i)L_P}{N_{k-1}((s,a)\mid Z_P^i)}} + \frac{L_P}{3N_{k-1}((s,a)\mid Z_P^i)} \quad i \in [n] \quad (10)$$

$$\sum_{k=1}^K \sum_{h=1}^H \mathbb{P} \left( \hat{V}_{k,h+1} - V_{h+1}^\pi(s_k,h,a_k,h) - \left( \hat{V}_{k,h+1} - V_{h+1}^\pi(s_k,h+1) \right) \right) \leq \sqrt{2HT \log(18SAT)} \quad (11)$$

$$\sum_{k=1}^K \sum_{h=1}^H \mathbb{P} \left( \hat{V}_{k,h+1} - V_{h+1}^\pi(s_k,h,a_k,h) - \left( \hat{V}_{k,h+1} - V_{h+1}^*(s_k,h) \right) \right) \leq \sqrt{2HT \log(18SAT)} \quad (12)$$

We define the above events as $\Lambda_1$, and assume it happens during the proof.

**Proof.** By Hoeffding’s inequality and union bounds over all $i \in [m]$, step $k \in [K]$ and $(s,a) \in \mathcal{X}[Z_R^i]$, we know that Inq. 7 holds with prob. $1 - \frac{\delta}{9}$ for any $i \in [n], k \in [K], (s,a) \in \mathcal{X}[Z_R^i]$. Similarly, by Hoeffding’s inequality and union bounds over all $i \in [n]$, step $t$ and $(s,a) \in \mathcal{X}$, Inq. 8 also holds with prob. $1 - \frac{\delta}{9}$ for any $i, s, a, k$. Inq. 9 is the high probability bound on the $L_1$ norm of the Maximum Likelihood Estimate, which is proved by Weissman et al. (2003). Inq. 10 can be proved with the use of Bernstein inequality and union bound (See Azar et al. (2017) for a similar derivation). Inq. 11 and Inq. 12 can be regarded as the summation of martingale difference sequences, which can be derived with the application of Azuma’s inequality. Finally, we take union bounds over all these inequalities, which indicates that $\Lambda_1$ holds with prob. at least $1 - 2\delta/3$. \qed

For the proof of Thm. 2, we also need to consider the following high-prob. events. We define the following events as $\Lambda_2$. During the proof of Thm. 2, we assume both $\Lambda_1$ and $\Lambda_2$ happen.
Lemma B.2. With prob. at least $1 - \delta/3$, the following events hold for any $k, h, s, a$:

\[
\left| \hat{R}_{k,i}((s,a)|Z_i^R) - \bar{R}_{k,i}((s,a)|Z_i^R) \right| \leq \sqrt{\frac{2\sigma_{\hat{P}_{k,i}^*}}{N_{k-1}((s,a)[Z_i^R])}} \sum_{j=1}^{\infty} \frac{8L_i^R}{3N_{k-1}((s,a)[Z_i^R])}, \quad i \in [m] \tag{13}
\]

\[
\left| \hat{P}_{k,i} - P_i \right| \prod_{j \neq i} \mathbb{P}_j V_{h+1}^*(s,a) \leq \sqrt{\frac{2\sigma_{\hat{P}_{k,i}^*}}{N_{k-1}((s,a)[Z_i^R])}} \sum_{j=1}^{\infty} \frac{2HL^P}{3N_{k-1}((s,a)[Z_i^R])}, \quad i \in [n] \tag{14}
\]

\[
N_k((s,a)[Z_i^P]) \geq \frac{1}{2} \sum_{j < k} w_j Z_i(s,a) - H \log(10nX_i^PH/\delta), \quad i \in [n] \tag{15}
\]

Proof. Inq. 13 can be proved directly by empirical Bernstein inequality. Now we mainly focus on Inq. 14. By Bernstein's inequality and union bounds over all $s, a, k, h$, we know that the following inequality holds with prob. at least $1 - \frac{\delta}{10}$,

\[
\left| \hat{P}_{k,i} - P_i \right| \prod_{j \neq i} \mathbb{P}_j V_{h+1}^*(s,a)
\]

\[
= \sum_{s'[1:i-1] \in \mathcal{X}[1:i-1]} \mathbb{P}(s'[1:i-1]|s,a) \left( \hat{P}_{k,i} - P_i \right) \prod_{j=i+1}^{\infty} \mathbb{P}_j V_{h+1}^*(s,a) \leq \sum_{s'[1:i-1] \in \mathcal{X}[1:i-1]} \mathbb{P}(s'[1:i-1]|s,a) \sqrt{\frac{2 \text{Var}_{s'[i]} \mathbb{P}_i(s,a)[Z_i^P]}{N_{k-1}((s,a)[Z_i^P])}} \left( \mathbb{E}_{s'[i+1:n] \sim \mathbb{P}_{i+1:n}(\cdot|s,a)} V(s') \mid s'[1:i-1] \right) \frac{2HL^P}{3N_{k-1}((s,a)[Z_i^P])} + \frac{2HL^P}{3N_{k-1}((s,a)[Z_i^P])}
\]

The first inequality is due to Jensen’s inequality. That is,

\[
\sum_{s'[1:i-1]} \mathbb{P}(s'[1:i-1]) \sqrt{\frac{C_1}{N_{k-1}((s,a)[Z_i^P])}} \leq \sqrt{\frac{\sum_{s'[1:i-1]} C_1 \mathbb{P}(s'[1:i-1])}{N_{k-1}((s,a)[Z_i^P])}} = \sqrt{2\sigma_{\hat{P}_{k,i}^*}[V_{h+1}^*, s,a] L^P \cdot \frac{1}{N_{k-1}((s,a)[Z_i^P])}}
\]

where $\mathbb{P}(s'[1:i-1])$ is a shorthand of $\mathbb{P}(s'[1:i-1]|s,a)$, and $C_1$ here denotes

\[
2 \text{Var}_{s'[i] \sim \mathbb{P}_i((s,a)[Z_i^P])} \left( \mathbb{E}_{s'[i+1:n] \sim \mathbb{P}_{i+1:n}(\cdot|s,a)} V(s') \mid s'[1:i-1] \right) L^P.
\]
Inq. 15 follows the same proof of the failure event $F^N$ in section B.1 of Dann et al. (2019).

### Appendix C. Omitted details for FMDP-CH

In this section, we introduce our algorithm with Hoeffding-type confidence bonus and present the corresponding regret bound. Our algorithm, which is described in Algorithm 2, is related to UCBVI-CH algorithm (Azar et al., 2017), in the sense that Algorithm 2 reduces to UCBVI-CH if we consider a flat MDP with $m = n = d = 1$.

#### Algorithm 2 FMDP-CH

**Input:** \( \delta \),

- History data \( \mathcal{L} = \emptyset \), initialize \( N((s,a)[Z]) = 0 \) for any factored set \( Z \) and \( (s,a)[Z] \in \mathcal{X}[Z] \)

**for** episode \( k = 1, 2, \ldots \) **do**

- Set \( \hat{V}_{k,H+1}(s) = 0 \) for all \( s \).

5: **Estimate** \( \hat{R}_{k,i}(s,a) \) with empirical mean value if \( N_{k-1}((s,a)[Z^R]) > 0 \), otherwise \( \hat{R}_{k,i}(s,a) = 1 \), then calculate \( \hat{R}(s,a) = \frac{1}{m} \sum_{i=1}^{m} \hat{R}_i((s,a)[Z^R]) \)

- Let \( \mathcal{K}_P = \{(s,a) \in S \times A, \cup_{i \in [d]} N_k((s,a)[Z^P_i]) > 0\} \)

- **Estimate** \( \hat{V}_k \) with empirical mean value for all \( (s,a) \in \mathcal{K}_P \)

**for** horizon \( h = H, H-1, \ldots, 1 \) **do**

**for** all \( (s,a) \in S \times A \) **do**

- **if** \( (s,a) \in \mathcal{K}_P \) **then**

  \( Q_{k,h}(s,a) = \min \{ H, \hat{R}_k(s,a) + CB_k(s,a) + \hat{p}_k \hat{V}_{k,h+1}(s,a) \} \)

**else**

\( Q_{k,h}(s,a) = H \)

**end if**

**end for**

\( \hat{V}_{k,h}(s) = \max_{a \in A} Q_{k,h}(s,a) \)

**end for**

**for** step \( h = 1, \ldots, H \) **do**

- Take action \( a_{k,h} = \arg \max_a Q_{k,h}(s_{k,h}, a) \)

**end for**

**Update** history trajectory \( \mathcal{L} = \mathcal{L} \cup \{(s_{k,h}, a_{k,h}, r_{k,h}, s_{k,h+1})_{h=1,2,\ldots,H}\} \), and update history counter \( N_{k-1}((s,a)[Z]) \).

**end for**

Let \( N_k((s,a)[Z]) \) denote the number of steps that the agent encounters \( (s,a)[Z] \) during the first \( k \) episodes, and \( N_k((s,a)[Z], s_j) \) denotes the number of steps that the agent transits to a state with \( s[j] = s_j \) after encountering \( (s,a)[Z] \) during the first \( k \) episodes. In episode \( k \), we estimate the mean value of each factored reward \( R_i \) and each factored transition \( P_i \) with empirical mean value \( \hat{R}_{k,i} \) and \( \hat{p}_{k,i} \) respectively. To be more specific, \( \hat{R}_{k,i}((s,a)[Z^R_i]) = \frac{\sum_{t \leq (k-1)H+1} (s,a)[Z^R_i] = (s,a)[Z^P_i], r_{t,i}}{N_{k-1}((s,a)[Z^P_i])} \), where \( r_{t,i} \) denotes the reward \( R_i \) sampled in step \( t \), and \( \hat{p}_{k,j}((s,j)[Z^P_j]) = \frac{N_{k-1}((s,a)[Z^P_i], s[j])}{N_{k-1}((s,a)[Z^P_i])} \). After that, we construct the optimistic MDP $\hat{M}$.
Based on the estimated rewards and transition functions. For a certain \((s, a)\) pair, the transition function and reward function are defined as \(\hat{R}_k(s, a) = \frac{1}{m} \sum_{i=1}^m \hat{R}_{k,i}((s, a)[Z_i^R])\) and \(\hat{P}_k(s' | s, a) = \prod_{j=1}^n \hat{P}_{k,j}(s'[j] | (s, a)[Z_i^P])\).

We define \(L^R_i = \log (18mT|\mathcal{X}[Z_i^R]|/\delta), \phi_k(s, a) = \sqrt{\frac{4|S_i|L^P}{N_{k-1}(s,a)|Z_i^P|}} + \frac{4|S_i|L}{3N_{k-1}(s,a)}\) and \(L^P = \log (18nTSA/\delta)\). We separately construct the confidence bonus of each factored reward \(R_i\) and factored transition \(P_i\) in the following way:

\[
CB_{k,Z_i^R}^R(s, a) = \sqrt{\frac{2L_i^R}{N_{k-1}((s,a)[Z_i^R])}}, \quad i \in [m] 
\]

\[
CB_{k,Z_i^P}^P(s, a) = \sqrt{\frac{2H^2L^P}{N_{k-1}((s,a)[Z_i^P])}} + H\phi_k(s, a) \sum_{j=1,j\neq i}^n \phi_k(s,a), \quad i \in [n] 
\]

We define the confidence bonus as the summation of all confidence bonus for rewards and transition, i.e. \(CB_k(s, a) = \frac{1}{m} \sum_{i=1}^m CB_{k,Z_i^R}^R(s, a) + \sum_{j=1}^n CB_{k,Z_j^P}^P(s, a)\).

We propose the following regret upper bound for Alg. 2.

**Theorem 5.** With prob. \(1 - \delta\), the regret of Alg. 2 is upper bounded by

\[
\text{Reg}(K) = \mathcal{O}\left(\frac{1}{m} \sum_{i=1}^m \sqrt{|\mathcal{X}[Z_i^R]|T \log(mT|\mathcal{X}[Z_i^R]|/\delta)} + \sum_{j=1}^n H \sqrt{|\mathcal{X}[Z_j^P]|T \log(nTSA/\delta)} \right) 
\]

Here \(\mathcal{O}\) hides the lower order terms with respect to \(T\).

**Appendix D. Proof of Theorem 5**

**D.1 Estimation Error Decomposition**

**Lemma D.1.** The estimation error can be decomposed in the following way:

\[
|(\hat{P}_k - P)(\cdot|s, a)|_1 \leq \sum_{i=1}^n |(\hat{P}_{k,i} - P_i)(\cdot|(s,a)[Z_i^P])|_1 
\]

\[
|(\hat{P}_k - P)V(s, a)| \leq \sum_{i=1}^n (\hat{P}_{k,i} - P_i) \left( \prod_{j \neq i, j=1}^n P_j \right) V(s, a) 
\]

\[
+ \sum_{i=1}^n \sum_{j \neq i, j=1}^n |V|_\infty \left| (\hat{P}_{k,i} - P_i)(\cdot|(s,a)[Z_i^P]) \right|_1 \left| (\hat{P}_{k,j} - P_j)(\cdot|(s,a)[Z_j^P]) \right|_1, 
\]

here \(V\) denotes any value function mapping from \(S\) to \(\mathbb{R}\), e.g. \(V_{h+1}^*\) or \(\hat{V}_{k,h+1} - V_{h+1}^*\).

**Proof.** Inq. 18 has the same form of Lemma 32 in Li (2009) and Lemma 1 in Osband and Van Roy (2014). We mainly focus on Inq. 19. We can decompose the difference in the
following way:

\[
\left| (\hat{P}_k - P)V(s, a) \right| \\
\leq \left| (\hat{P}_{k,n} - P_n) \prod_{i=1}^{n-1} P_i V(s, a) \right| + \left| P_n \left( \prod_{i=1}^{n-1} \hat{P}_{k,i} - \prod_{i=1}^{n-1} P_i \right) V(s, a) \right| + \left| (\hat{P}_{k,n} - P_n) \left( \prod_{i=1}^{n-1} \hat{P}_{k,i} - \prod_{i=1}^{n-1} P_i \right) V^*(s, a) \right|
\]

(20)

For the last term of Inq. 20, we have

\[
\left| (\hat{P}_{k,n} - P_n) \left( \prod_{i=1}^{n-1} \hat{P}_{k,i} - \prod_{i=1}^{n-1} P_i \right) V(s, a) \right|
\leq \left| (\hat{P}_{k,n} - P_n) \left( \cdot |(s, a)[Z_n^P] \right)_1 \prod_{i=1}^{n-1} \hat{P}_{k,i} (\cdot |(s, a)[Z_i^P]) - \prod_{i=1}^{n-1} P_i (\cdot |(s, a)[Z_i^P]) \right|_1 |V|_\infty
\]

\[
\leq \left| (\hat{P}_{k,n} - P_n) \left( \cdot |(s, a)[Z_n^P] \right)_1 \sum_{i=1}^{n-1} \left| \left( \hat{P}_{k,i} - P_i \right) (\cdot |(s, a)[Z_i^P]) \right|_1 \right|_1 |V|_\infty,
\]

Where the last inequality is due to Inq. 18.

For the second part of Inq. 20, we can further decompose the term as:

\[
\left| P_{n} \left( \hat{P}_{k,n-1} - P_{n-1} \right) \prod_{i=1}^{n-2} P_i V(s, a) \right|
\leq \left| P_{n} \left( \hat{P}_{k,n-1} - P_{n-1} \right) \prod_{i=1}^{n-2} P_i V(s, a) \right| + \left| P_{n} P_{n-1} \left( \prod_{i=1}^{n-2} \hat{P}_{k,i} - \prod_{i=1}^{n-2} P_i \right) V(s, a) \right|
\]

\[
\leq \left| P_{n} \left( \hat{P}_{k,n-1} - P_{n-1} \right) \left( \prod_{i=1}^{n-2} \hat{P}_{k,i} - \prod_{i=1}^{n-2} P_i \right) V(s, a) \right|
\]

(21)

Following the same decomposition technique, we can prove Inq. 19 by recursively decomposing the second term over all possible \( n \):

\[
|(\hat{P}_k - P)V^*(s, a)| \leq \sum_{i=1}^{n} \left| (\hat{P}_{k,i} - P_i) \left( \prod_{j \neq i, j=1}^{n} P_j \right) V(s, a) \right|
\]

\[
+ \sum_{i=1}^{n} \sum_{j \neq i, j=1}^{n} \left| (\hat{P}_{k,i} - P_i) (\cdot |(s, a)[Z_i^P]) \right|_1 \cdot \left| (\hat{P}_{k,j} - P_j) (\cdot |(s, a)[Z_j^P]) \right|_1 \cdot |V|_\infty
\]

\[\square\]
Lemma D.2. Under event $\Lambda_1$, then the following Inequality holds:

$$|\hat{R}_k(s, a) - \bar{R}(s, a)| \leq \frac{1}{m} \sum_{i=1}^{m} \sqrt{\frac{2L^R_i}{N_k-1((s, a)[Z^P_i])}}$$ \hspace{1cm} (22)

$$|\hat{P}_k - \mathbb{P}||\mathbb{P} - \hat{P}_k||\mathbb{P} - \hat{P}_k||\mathbb{P} - \hat{P}_k|| \leq \sum_{i=1}^{n} \left( \sqrt{\frac{4L^P}{N_k-1((s, a)[Z^P_i])}} + \frac{4L^P}{3N_k-1((s, a)[Z^P_i])} \right)$$ \hspace{1cm} (23)

$$|\hat{P}_k - \mathbb{P}|V^*(s, a) | \leq \sum_{i=1}^{n} \sum_{j \neq i, j=1}^{n} H \left( \sqrt{\frac{4|S_i|L^P}{N_k-1((s, a)[Z^P_i])}} + \frac{4|S_j|L^P}{3N_k-1((s, a)[Z^P_j])} \right) \left( \sqrt{\frac{4|S_j|L^P}{N_k-1((s, a)[Z^P_j])}} + \frac{4|S_j|L^P}{3N_k-1((s, a)[Z^P_j])} \right)$$ \hspace{1cm} (24)

Proof. Inq. 22 can be proved by Lemma B.1:

$$|\hat{R}_k(s, a) - \bar{R}(s, a)| \leq \frac{1}{m} \sum_{i=1}^{m} |\hat{R}_k(s, a) - \bar{R}(s, a)| \leq \sum_{i=1}^{m} \sqrt{\frac{2L^R_i}{N_k-1((s, a)[Z^P_i])}}$$

Inq. 23 follows directly by applying Lemma B.1 to Lemma D.1.

$$|\hat{P}_k - \mathbb{P}||\mathbb{P} - \hat{P}_k||\mathbb{P} - \hat{P}_k|| \leq \sum_{i=1}^{n} \left( \sqrt{\frac{4L^P}{N_k-1((s, a)[Z^P_i])}} + \frac{4L^P}{3N_k-1((s, a)[Z^P_i])} \right)$$

Similarly, Inq 24 can be proved by:

$$|\hat{P}_k - \mathbb{P}|V^*(s, a) | \leq \sum_{i=1}^{n} \left( \prod_{j \neq i, j=1}^{n} \hat{P}_{k,i} - \mathbb{P}_i \right) V^*(s, a) + \sum_{i=1}^{n} \sum_{j \neq i, j=1}^{n} H \left( \hat{P}_{k,i} - \mathbb{P}_i \right) \left( s, a \right) \cdot \left( \hat{P}_{k,j} - \mathbb{P}_j \right) \left( s, a \right)$$

$$\leq \sum_{i=1}^{n} \sqrt{\frac{2L^2}{N_k-1((s, a)[Z^P_i])}} + \sum_{i=1}^{n} \sum_{j \neq i, j=1}^{n} H \left( \sqrt{\frac{4|S_i|L^P}{N_k-1((s, a)[Z^P_i])}} + \frac{4|S_j|L^P}{3N_k-1((s, a)[Z^P_j])} \right) \left( \sqrt{\frac{4|S_j|L^P}{N_k-1((s, a)[Z^P_j])}} + \frac{4|S_j|L^P}{3N_k-1((s, a)[Z^P_j])} \right)$$

D.2 Optimism

Lemma D.3. (Optimism) Under event $\Lambda_1$, $V_{k,h}(s) \geq V^*_h(s)$ for any $k, h, s$. 

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Proof. We prove the Lemma by induction. Firstly, for \( h = H + 1 \), the inequality holds trivially since \( \hat{V}_{k,H+1}(s) = V^*_{H+1}(s) = 0 \).

\[
\hat{V}_{k,h}(s) - V^*_h(s) \\
\geq \hat{R}_k(s, \pi^*_h(s)) + CB_k(s, \pi^*_h(s)) + \hat{P}_k \hat{V}_{k,h+1}(s, \pi^*_h(s)) - \hat{R}(s, \pi^*_h(s)) - \hat{P}V^*_h(s, \pi^*_h(s)) \\
= \hat{R}_k(s, \pi^*_h(s)) - \hat{R}(s, \pi^*_h(s)) + CB_k(s, \pi^*_h(s)) + \hat{P}_k(\hat{V}_{k,h+1} - V^*_h(s, \pi^*_h(s))) + (\hat{P}_k - \hat{P})V^*_h(s, \pi^*(s)) \\
\geq \hat{R}_k(s, \pi^*_h(s)) - \hat{R}(s, \pi^*_h(s)) + CB_k(s, \pi^*_h(s)) + (\hat{P}_k - \hat{P})V^*_h(s, \pi^*(s)) \\
\geq 0
\]

The first inequality is due to \( \hat{V}_{k,h}(s) \geq \hat{Q}_{k,h}(s, \pi^*_h(s)) \). The second inequality follows by induction condition that \( \hat{V}_{k,h+1}(s) \geq V^*_h(s) \) for all \( s \). The last inequality is due to Inq. 22 and Inq. 24 in Lemma D.2.

D.3 Proof of Theorem 5

Now we are ready to prove Thm. 5.

Proof. (Proof of Thm. 5)

\[
V^*_h(s,k,h) - V^*_{\pi_k}(s,k,h) \\
\leq \hat{V}_{k,h}(s,k,h) - V^*_{\pi_k}(s,k,h) \\
= \hat{R}_k(s,k,h, \pi_k(h,k,s)) + \hat{P}_k \hat{V}_{k,h+1}(s,k,h, \pi_k(h,k,s)) + CB_k(s,k,h, \pi_k(h,k,s)) \\
- \hat{R}(s,k,h, \pi_k(h,k,s)) - \hat{P}V^*_{\pi_k}(s,k,h, \pi_k(h,k,s)) \\
= \hat{V}_{k,h+1}(s,k,h+1) - V^*_{\pi_k}(s,k,h+1) + \hat{R}_k(s,k,h, \pi_k(h,k,s)) - \hat{R}(s,k,h, \pi_k(h,k,s)) + CB_k(s,k,h, \pi_k(h,k,s)) \\
+ \hat{P}(\hat{V}_{k,h+1} - V^*_{\pi_k})(s,k,h, \pi_k(h,k,s)) - (\hat{V}_{k,h+1} - V^*_{\pi_k})(s,k,h+1) \\
+ (\hat{P}_k - \hat{P})V^*_{\pi_k}(s,k,h, \pi_k(h,k,s)) \\
+ (\hat{P}_k - \hat{P})(\hat{V}_{k,h+1} - V^*_{\pi_k})(s,k,h, \pi_k(h,k,s))
\]

The first inequality is due to optimism \( \hat{V}_{k,h}(s,k,h) \geq V^*_{\pi_k}(s,k,h) \). The first equality is due to Bellman equation for \( V^*_{\pi_k} \) and \( \hat{V}_{k,h} \).

For notation simplicity, we define

\[
\delta^1_{k,h} = \hat{R}_k(s, \pi_{k,h}(s,k,h)) - \hat{R}(s, \pi_{k,h}(s,k,h)) \\
\delta^2_{k,h} = \hat{P}(\hat{V}_{k,h+1} - V^*_{\pi_k})(s,k,h, \pi_k(h,k,s)) - (\hat{V}_{k,h+1} - V^*_{\pi_k})(s,k,h+1) \\
\delta^3_{k,h} = (\hat{P}_k - \hat{P})V^*_{\pi_k}(s,k,h, \pi_k(h,k,s))
\]

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Firstly we focus on the upper bound of \((\hat{\mathbb{P}}_{k,h} - \mathbb{P})(\hat{V}_{k,h+1} - V^*_h)(s_{k,h}, a_{k,h})\). We bound this term following the idea of Azar et al. (2017).

\[
\left( \hat{\mathbb{P}}_k - \mathbb{P} \right) \left( \hat{V}_{k,h+1} - V^*_h \right) (s_{k,h}, a_{k,h}) \\
\leq \sum_{i=1}^{n} \left( \hat{\mathbb{P}}_i - \mathbb{P}_i \right) \prod_{j=1, j \neq i}^n \mathbb{P}_j \left( \hat{V}_{k,h+1} - V^*_h \right) (s_{k,h}, a_{k,h}) \\
+ \sum_{i=1}^{n} \sum_{j=1}^{n} H \left( \left| \mathbb{P}_i - \mathbb{P}_j \right| (\cdot \mid (s_{k,h}, a_{k,h})[Z^P_i]) \right) \left( \left| \hat{\mathbb{P}}_j - \mathbb{P}_j \right| (\cdot \mid (s_{k,h}, a_{k,h})[Z^P_j]) \right)
\]

\[
\leq \sum_{i=1}^{n} \left( \sum_{s'[i] \in S[i]} \sqrt{2 \mathbb{P}_i(s'[i] | \mathcal{X}[Z^P_i]) L^P \over N_{k-1}((s, a)[Z^P_i])} \prod_{j=1, j \neq i}^n \mathbb{P}_j \left( \hat{V}_{k,h+1} - V^*_h \right) (s_{k,h}, a_{k,h}) \right) + \sum_{i=1}^{n} \sum_{j=1}^{n} H \left( \sqrt{4 |S_i| L^P \over N_{k-1}((s, a)[Z^P_i])} + \sqrt{4 |S_j| L^P \over N_{k-1}((s, a)[Z^P_j])} \right)
\]

The first inequality is due to Lemma D.1 The second inequality is because of Lemma B.1, and the last inequality is due to the fact that \(\left| \hat{V}_{k,h+1} - V^*_h \right|_\infty \leq H\).

For each \(i \in [n]\), we consider those \(s'[i]\) satisfying \(N_{k-1}((s, a)[Z^P_i]) \mathbb{P}_i(s'[i] | (s_{k,h}, a_{k,h})[Z^P_i]) \geq 2n^2 H^2 L^P\) and \(N_{k-1}((s, a)[Z^P_j]) \mathbb{P}_i(s'[i] | (s_{k,h}, a_{k,h})[Z^P_i]) \leq 2n^2 H^2 L^P\) separately.

For those \(s'[i]\) satisfying \(N_{k-1}((s, a)[Z^P_i]) \mathbb{P}_i(s'[i] | (s_{k,h}, a_{k,h})[Z^P_i]) \geq 2n^2 H^2 L^P\), the first term can be bounded by

\[
\sum_{i=1}^{n} \sum_{s'[i] \in S[i]} \sqrt{2 \mathbb{P}_i(s'[i] | \mathcal{X}[Z^P_i]) L^P \over N_{k-1}((s, a)[Z^P_i])} \prod_{j=1, j \neq i}^n \mathbb{P}_j \left( \hat{V}_{k,h+1} - V^*_h \right) (s_{k,h}, a_{k,h})
\]

\[
= \sum_{i=1}^{n} \sum_{s'[i] \in S[i]} \mathbb{P}_i(s'[i] | \mathcal{X}[Z^P_i]) \sqrt{2 L^P \over \mathbb{P}_i(s'[i] | \mathcal{X}[Z^P_i]) N_{k-1}((s, a)[Z^P_i])} \prod_{j=1, j \neq i}^n \mathbb{P}_j \left( \hat{V}_{k,h+1} - V^*_h \right) (s_{k,h}, a_{k,h})
\]

\[
\leq \frac{1}{H} \mathbb{P} \left( \hat{V}_{k,h+1} - V^*_h \right) (s_{k,h}, a_{k,h})
\]

\[
= \frac{1}{H} \left( \hat{V}_{k,h+1} - V^*_h \right) (s_{k,h+1}, a_{k,h+1})
\]

\[
+ \frac{1}{H} \left( \mathbb{P} \left( \hat{V}_{k,h+1} - V^*_h \right) (s_{k,h}, a_{k,h}) - \left( \hat{V}_{k,h+1} - V^*_h \right) (s_{k,h+1}, a_{k,h+1}) \right)
\]

where the second term can be regarded as a martingale difference sequence, and we denote it as \(\delta_{k,h}^4\).
For those $s'[i]$ satisfying $N_{k-1}((s,a)[Z_i^P])P_i(s'[i]|s_{k,h},a_{k,h}) \leq 2n^2H^2L^P$, the summation can be bounded by
\[
\sum_{i=1}^{n} \frac{nH^2|S_i|L^P}{N_{k-1}((s,a)[Z_i^P])}
\]

For notation simplicity, we define $\delta_{k,h}^5$ as:
\[
\delta_{k,h}^5 = \sum_{i=1}^{n} \sum_{j \neq i, j=1}^{n} H \left( \sqrt{\frac{4|S_i|L^P}{N_{k-1}((s,a)[Z_i^P])}} + \frac{4|S_i|L^P}{3N_{k-1}((s,a)[Z_i^P])} \right) \left( \sqrt{\frac{4|S_j|L^P}{N_{k-1}((s,a)[Z_j^P])}} + \frac{4|S_j|L^P}{3N_{k-1}((s,a)[Z_j^P])} \right)
\]

\[
+ \sum_{i=1}^{n} \frac{2nH^2|S_i|L^P}{N_{k-1}((s,a)[Z_i^P])}
\]

To sum up, by the above analysis, we prove that:
\[
(\hat{\Delta}_{k,h} - \bar{\Delta}) (\hat{V}_{k,h+1} - V_{k,h}^*) (s_{k,h}, \pi_{k,h}(s_{k,h})) \leq \frac{1}{H} (\hat{V}_{k,h+1} - V_{k+1}^*) (s_{k,h+1}, a_{k,h+1}) + \delta_{k,h}^4 + \delta_{k,h}^5
\]

Now we are ready to summarize all the terms in the regret. Firstly, we recursively calculate the regret for all $h \in [H]$. 

\[
V_1(s_{k,1}, a_{k,1}) - V_1^\pi_k(s_{k,1}, a_{k,1}) \leq \hat{V}_{k,1}(s_{k,1}, a_{k,1}) - V^\pi_k(s_{k,1}, a_{k,1})
\]

\[
\leq CB(s_{k,1}, a_{k,1}) + \delta_{k,1}^1 + \delta_{k,1}^2 + \delta_{k,1}^3 + \delta_{k,1}^4 + \delta_{k,1}^5 + (1 + \frac{1}{H}) (V_{k,2}(s_{k,2}, a_{k,2}) - V^\pi_k(s_{k,2}, a_{k,2}))
\]

\[
\cdots
\]

\[
\leq \sum_{h=1}^{H} \left( 1 + \frac{1}{H} \right)^{h-1} (CB_k(s_h, a_h) + \delta_{k,h}^1 + \delta_{k,h}^2 + \delta_{k,h}^3 + \delta_{k,h}^4 + \delta_{k,h}^5)
\]

\[
\leq \sum_{h=1}^{H} e (CB_k(s_h, a_h) + \delta_{k,h}^1 + \delta_{k,h}^2 + \delta_{k,h}^3 + \delta_{k,h}^4 + \delta_{k,h}^5)
\]

Then we sum up the regret over $k$ episodes,

\[
\text{Reg}(K) \leq \sum_{k=1}^{K} (V_1^*(s_{1,1}) - V_1^\pi_k(s_{1,1}))
\]

\[
\leq \sum_{k=1}^{K} \sum_{h=1}^{H} e (CB_k(s_h, a_h) + \delta_{k,h}^1 + \delta_{k,h}^2 + \delta_{k,h}^3 + \delta_{k,h}^4 + \delta_{k,h}^5)
\]

$\delta_{k,h}^2$ and $\delta_{k,h}^4$ can be regarded as martingale difference sequence, the summation of which can be bounded by $O(H\sqrt{T \log(T)})$ by Lemma B.1, while $\delta_{k,h}^1$ and $\delta_{k,h}^3$ can also be bounded by Lemma B.1. The summation of different terms in $\delta_{k,h}^1, \delta_{k,h}^3, \delta_{k,h}^4$ and $\delta_{k,h}^5$ can be separated into the following categories. In the following proof, we use $C$ to denote the dependence of other parameters except the counters $N_k((s_{k,h}, a_{k,h})|Z_i)$. 

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For those terms of the form \( \frac{C}{\sqrt{N_k((s_k,h,a_k,h))[Z_i]}} \), we have

\[
\sum_{k} \sum_{h} \frac{C}{\sqrt{N_k((s_k,h,a_k,h))[Z_i]}} \leq HC + \sum_{x[Z_i] \in X[Z_i]} \frac{N_k(x[Z_i])}{c} \sum_{c=1}^{N_k(x[Z_i])} \frac{C}{\sqrt{c}}
\]

\[
= HC + \sum_{x[Z_i] \in X[Z_i]} C \sqrt{N_k(x[Z_i])}
\]

\[
\leq HC + C \sqrt{|X[Z_i]| T}
\]

The last inequality is due to Cauchy-Schwarz inequality. This term influence the main factors in the final regret.

For those terms of the form \( \frac{C}{N_k((s_k,h,a_k,h))[Z_i]} \), we have

\[
\sum_{k} \sum_{h} \frac{C}{N_k((s_k,h,a_k,h))[Z_i]} \leq HC + \sum_{x[Z_i] \in X[Z_i]} \frac{N_k(x[Z_i])}{c} \sum_{c=1}^{N_k(x[Z_i])} \frac{C}{c}
\]

\[
\leq HC + \sum_{x[Z_i] \in X[Z_i]} C \ln (N_k(x[Z_i]))
\]

\[
\leq HC + C |X[Z_i]| \ln T,
\]

which has only logarithmic dependence on \( T \).

For those terms of the form \( \frac{C}{\sqrt{N_k((s_k,h,a_k,h))[Z_i] N_k((s_k,h,a_k,h))[Z_j]}} \), we define \( N_k((s,a)[Z_i],(s,a)[Z_j]) \) as the number of times that agent has encountered \((s,a)[Z_i]\) and \((s,a)[Z_j]\) simultaneously for the first \( k \) episodes. It is not hard to find that \( N_k((s,a)[Z_i]) \geq N_k((s,a)[Z_i],(s,a)[Z_j]) \) and \( N_k((s,a)[Z_j]) \geq N_k((s,a)[Z_i],(s,a)[Z_j]) \).

\[
\sum_{k} \sum_{h} \frac{C}{\sqrt{N_k((s_k,h,a_k,h))[Z_i] N_k((s_k,h,a_k,h))[Z_j]}} \leq HC + \sum_{x[Z_i,\cup Z_j] \in X[Z_i \cup Z_j]} C \ln (N_k((s_k,h,a_k,h))[Z_i],(s_k,h,a_k,h)[Z_j])
\]

\[
\leq HC + C |X[Z_i \cup Z_j]| \ln T,
\]

which also has only logarithmic dependence on \( T \).

For other terms with the form \( \frac{C}{N_k((s_k,h,a_k,h))[Z_i] N_k((s_k,h,a_k,h))[Z_j]} \), the summation of these terms has no dependence on \( T \), which is negligible since \( T \) is the dominant factor.

By bounding these different kinds of terms with the above methods, we can finally show that

\[
\text{Reg}(K) = O \left( \frac{1}{m} \sum_{i=1}^{m} \sqrt{|X[Z_i^R]| T \log(10mT|X[Z_i^R]/\delta)} + \sum_{j=1}^{n} H \sqrt{|X[Z_j^*]| T \log(10nTSA/\delta)} \right)
\]

Here \( O \) hides the constant factors. \( \square \)
Appendix E. Proof of Theorem 2

The formal definition of the confidence bonus for Alg. 1 is:

\[
\begin{align*}
CB_{k,Z_i}^R(s,a) &= \sqrt{\frac{2\hat{\sigma}^2_{R,k,i}(s,a)L_i^R}{N_{k-1}((s,a)|Z_i^R)}} + \frac{8L_i^R}{3N_{k-1}((s,a)|Z_i^R)} \\
CB_{k,Z_i}^P(s,a) &= \sqrt{\frac{4\hat{\sigma}^2_{P,k,i}(\hat{V}_{k,h+1},s,a)L_P}{N_{k-1}((s,a)|Z_i^P)}} + \sqrt{\frac{2u_{k,h,i}(s,a)L_P}{N_{k-1}((s,a)|Z_i^P)}} \\
&\quad + \sqrt{\frac{16H^2L_P}{N_{k-1}((s,a)|Z_i^P)}} \sqrt{n} \left( \frac{4|S_j|L_P}{N_{k-1}((s,a)|Z_j^P}) \right)^{\frac{1}{4}} + \frac{4|S_j|L_P}{3N_{k-1}((s,a)|Z_j^P)} \\
&\quad + \sum_{j=1}^{n} H\phi_{k,i}(s,a)\phi_{k,j}(s,a),
\end{align*}
\]

where \(\phi_{k,i}(s,a) = \sqrt{\frac{4|S_i|L_P}{N_{k-1}((s,a)|Z_i^P)}} + \frac{4|S_j|L_P}{3N_{k-1}((s,a)|Z_j^P)}\).

E.1 Estimation Error Decomposition

Lemma E.1. Under event \(\Lambda_1\) and \(\Lambda_2\), we have

\[
\begin{align*}
|\hat{R}_k(s,a) - \bar{R}(s,a)| &\leq \frac{1}{m} \sum_{i=1}^{m} \sqrt{\frac{2\hat{\sigma}^2_{R,i}(s,a)L_i^R}{N_{k-1}((s,a)|Z_i^R)}} + \frac{1}{m} \sum_{i=1}^{m} \frac{8L_i^R}{3N_{k-1}((s,a)|Z_i^R)} \\
|(\hat{\mathbb{P}}_k - \mathbb{P})V^*_{h+1}(s,a)| &\leq \sum_{i=1}^{n} \sqrt{\frac{2\hat{\sigma}^2_{P,i}(\hat{V}_{h+1},s,a)L_P}{N_{k-1}((s,a)|Z_i^P)}} + \frac{2HL_P}{3N_{k-1}((s,a)|Z_i^P)} \\
&\quad + \sum_{i=1}^{n} \sum_{j\neq i,j=1}^{n} H \left( \sqrt{\frac{4|S_i|L_P}{N_{k-1}((s,a)|Z_i^P)}} + \frac{4|S_j|L_P}{3N_{k-1}((s,a)|Z_j^P)} \right) \left( \sqrt{\frac{4|S_j|L_P}{N_{k-1}((s,a)|Z_j^P)}} + \frac{4|S_j|L_P}{3N_{k-1}((s,a)|Z_j^P)} \right).
\end{align*}
\]

Proof. The first inequality follows directly by the definition that \(R(s,a) = \frac{1}{m} \sum_{i=1}^{m} R_i(s,a)\) and Lemma B.2. We now prove the second inequality. By Lemma D.1, we have

\[
|(\hat{\mathbb{P}}_k - \mathbb{P})V^*_{h+1}(s,a)| \leq \sum_{i=1}^{n} \left| (\hat{\mathbb{P}}_{k,i} - \mathbb{P}_i) \left( \prod_{j\neq i,j=1}^{n} \mathbb{P}_j \right) V^*_{h+1}(s,a) \right| \\
+ \sum_{i=1}^{n} \left( \sum_{j\neq i,j=1}^{n} H \left| (\hat{\mathbb{P}}_{k,i} - \mathbb{P}_i) (\cdot|(s,a)|Z_i^P) \right| \right) \left( \left| (\hat{\mathbb{P}}_{k,j} - \mathbb{P}_j) (\cdot|(s,a)|Z_j^P) \right| \right),
\]

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By Inq. 9 in Lemma B.1 and Inq. 14 in Lemma B.2, we have
\[|(\hat{\Phi} - \Phi) V_{h+1}^*(s, a)|\]
\[\leq \sum_{i=1}^{n} \left( \sqrt{2\sigma_i^2 (V_{h+1}^*(s, a)|L^P_{N_{k-1}((s,a)[Z_i^P])}) + \frac{2HL^P}{3N_{k-1}((s,a)[Z_i^P])}} \right) \]
\[+ \sum_{i=1}^{n} \sum_{j \neq i}^{n} H \left( \sqrt{\frac{4|S_i|L^P}{N_{k-1}((s,a)[Z_i^P])}} + \frac{4|S_i|L^P}{3N_{k-1}((s,a)[Z_i^P])} \right) \left( \sqrt{\frac{4|S_j|L^P}{N_{k-1}((s,a)[Z_j^P])}} + \frac{4|S_j|L^P}{3N_{k-1}((s,a)[Z_j^P])} \right) \]
\[\square\]

E.2 Omitted proof in Section 4.2

Proof. (Proof of Theorem 1)

\[\omega_h^2(s)\]
\[= \mathbb{E} [(J_{h:H}(s_h) - V_h(s_h))^2 | s_h = s] \]
\[= \sum_{s'} \mathbb{P}(s'|s) \mathbb{E} [(J_{h+1:H}(s_{h+1}) + r_h - V_h(s_h))^2 | s_h = s, s_{h+1} = s'] \]
\[= \sum_{s'} \mathbb{P}(s'|s) \mathbb{E} [J_{h+1:H}^2(s_{h+1}) + r_h^2 + V_h^2(s_h) | s_h = s, s_{h+1} = s'] \]
\[+ \sum_{s'} \mathbb{P}(s'|s) \mathbb{E} [2r_h(J_{h+1:H}(s_{h+1}) - V_h(s_h)) - 2J_{h+1:H}(s_{h+1})V_h(s_h) | s_h = s, s_{h+1} = s'] \]

Given \(s_h = s, s_{h+1} = s', r_h, V_h(s_h)\) and \(J_{h+1:H}(s_{h+1})\) are conditionally independent, thus we have

\[\mathbb{E}[2r_h(J_{h+1:H}(s_{h+1}) - V_h(s_h)) | s_h = s, s_{h+1} = s'] = \mathbb{E}[2\tilde{R}(s_h)(V_{h+1}(s_{h+1}) - V_h(s_h)) | s_h = s, s_{h+1} = s'] \]
\[\mathbb{E}[2J_{h+1:H}(s_{h+1})V_h(s_h) | s_h = s, s_{h+1} = s'] = \mathbb{E}[2V_{h+1}(s_{h+1})V_h(s_h) | s_h = s, s_{h+1} = s'] \]

Therefore, we have

\[\omega_h^2(s)\]
\[= \sum_{s'} \mathbb{P}(s'|s) \mathbb{E} [J_{h+1:H}^2(s_{h+1}) + r_h^2 + V_h^2(s_h) | s_h = s, s_{h+1} = s'] \]
\[+ \sum_{s'} \mathbb{P}(s'|s) \mathbb{E} [2\tilde{R}(s_h)(V_{h+1}(s_{h+1}) - V_h(s_h)) - 2V_{h+1}(s_{h+1})V_h(s_h) | s_h = s, s_{h+1} = s'] \]
\[= \mathbb{E} [r_h^2 - \tilde{R}^2(s_h) | s_h = s] + \sum_{s'} \mathbb{P}(s'|s) \mathbb{E} [J_{h+1:H}^2(s_{h+1}) - (V_h(s_h) - \tilde{R}(s_h))^2 | s_h = s, s_{h+1} = s'] \]
\[= \mathbb{E} [r_h^2 - \tilde{R}^2(s_h) | s_h = s] + \sum_{s'} \mathbb{P}(s'|s) \mathbb{E} \left[ J_{h+1:H}^2(s_{h+1}) - \left( \sum_{s''} \mathbb{P}(s''|s)V_{h+1}(s'') \right)^2 \right] | s_h = s, s_{h+1} = s' \]
\[= \mathbb{E} [r_h^2 - \tilde{R}^2(s_h) | s_h = s] + \sum_{s'} \mathbb{P}(s'|s)V_{h+1}^2(s') - \left( \sum_{s''} \mathbb{P}(s''|s)V_{h+1}(s'') \right)^2 \]
\[+ \sum_{s'} \mathbb{P}(s'|s) \mathbb{E} [J_{h+1:H}^2(s_{h+1}) - V_{h+1}^2(s_{h+1}) | s_{h+1} = s'] \] (29)
The second equality is due to the fact that $V_h(s) = \bar{R}(s) + \sum_{s'} P(s'|s)V_{h+1}(s')$.

For the factored rewards, since the rewards $r_{h,i}$ are conditionally independent given $s$, we have

$$\mathbb{E} [ r_h^2 - \bar{R}^2(s_h) \mid s_h = s ] = \frac{1}{m^2} \sum_{i=1}^{m} \sigma_{R,i}^2(s)$$

For the factored transition, we decompose the variance in the following way:

$$\sum_{s'} \mathbb{P}(s'|s)V_{h+1}^2(s') - \left( \sum_{s''} \mathbb{P}(s''|s)V_{h+1}(s'') \right)^2 = \sum_{s''[1]} \mathbb{P}(s''[1] \mid s) \left( \sum_{s'[2:n]} \mathbb{P}(s'\pi'|s) \sum_{s''[2:n]} \mathbb{P}(s''\pi'|s)V_{h+1}(s'') \right)^2 - \sum_{s''[2:n]} \mathbb{P}(s''\pi'|s)V_{h+1}(s'') \left( \sum_{s'[2:n]} \mathbb{P}(s'\pi'|s) \sum_{s''[2:n]} \mathbb{P}(s''\pi'|s)V_{h+1}(s'') \right)^2$$

Here $([s'[1], s''[2 : n]])$ denotes the vector $s''$ with $s''[1]$ replaced with $s'[1]$. By subtracting $\sigma_{P,i,h}^2(s)$ for $i = 2, ..., n$ in the above way, we can show that

$$\sum_{s'} \mathbb{P}(s'|s)V_{h+1}^2(s') - \left( \sum_{s''} \mathbb{P}(s''|s)V_{h+1}(s'') \right)^2 - \sum_{i=1}^{n} \sigma_{P,i,h}^2(s) = 0 \quad (30)$$

Plugging Eqn. 30 back to Eqn. 29, we have

$$\omega_h^2(s) = \sum_{s'} \mathbb{P}(s'|s)\omega_{h+1}^2(s') + \sum_{i=1}^{n} \sigma_{P,i,h}^2(s) + \frac{1}{m^2} \sum_{i=1}^{m} \sigma_{R,i}^2(s)$$

\[\square\]

**Proof.** (Proof of Corollary 1.1) We can regard the MDP with given policy $\pi$ as a Markov chain. By Theorem 1, we have

$$\omega_h^2(s) = \sum_{s'} \mathbb{P}(s'|s, \pi(s))\omega_{h+1}^2(s') + \sum_{i=1}^{n} \sigma_{P,i}^2(V_{h}^\pi, s, a) + \frac{1}{m^2} \sum_{i=1}^{m} \sigma_{R,i}^2(s, a)$$

By recursively decomposing the variance until step $H$, we have:

$$\omega_h^2(s_1) = \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{X}} w_h(s, a) \left( \sum_{i=1}^{n} \sigma_{P,i}^2(V_{h}^\pi, s, a) + \frac{1}{m^2} \sum_{i=1}^{m} \sigma_{R,i}^2(s, a) \right)$$

Since $\omega_h^2(s_1) = \mathbb{E} \left[ (J_{h,H}(s_h) - V_h(s))^2 \mid s_h = s \right] \leq H^2$, we can immediately reach the conclusion. \[\square\]
E.3 The ”good” Set Construction

The construction of the ”good” set is similar with that in Dann et al. (2017) and Zanette and Brunskill (2019), though we modify it to handle this more complicated factored setting. The idea is to partition each factored state-action subspace at each episode into two sets, the set of state-action pairs that have been visited sufficiently often (so that we can lower bound these visits by their expectations using standard concentration inequalities) and the set of (s, a) that were not visited often enough to cause high regret. That is:

**Definition 4. (The Good Set)** The set $L_{k,i}$ for factored transition $P_i$ is defined as:

$$L_{k,i} \overset{def}{=} \left\{ (x[Z_i^P]) \in \mathcal{X}[Z_i^P] : \frac{1}{4} \sum_{j < k} w_{j,Z_i^P}(x) \geq H \log(18 n X_i^P H/\delta) + H \right\}$$

The following two Lemmas follow the same idea of Lemma 6 and Lemma 7 in Zanette and Brunskill (2019).

**Lemma E.2.** Under event $\Lambda_1$ and $\Lambda_2$, if $(s,a)[Z_i^P] \in L_{i,k}$, we have

$$N_k((s,a)[Z_i^P]) \geq \frac{1}{4} \sum_{j < k} w_{j,Z_i^P}(s,a).$$

**Proof.** By Lemma B.2, we have

$$N_k((s,a)[Z_i^P]) \geq \frac{1}{2} \sum_{j < k} w_j((s,a)[Z_i^P]) - H \log(18 n X_i^P H/\delta).$$

Since $(s,a)[Z_i^P] \in L_{i,k}$, we have $\frac{1}{4} \sum_{j < k} w_{j,Z_i^P}(x) \geq H \log(18 n X_i^P H/\delta) + H$. That is,

$$N_k((s,a)[Z_i^P]) \geq \frac{1}{2} \sum_{j < k} w_j((s,a)[Z_i^P]) - H \log(18 n X_i^P H/\delta)$$

$$\geq \frac{1}{2} \sum_{j < k} w_j((s,a)[Z_i^P]) - \frac{1}{4} \sum_{j < k} w_j((s,a)[Z_i^P])$$

$$= \frac{1}{4} \sum_{j < k} w_j((s,a)[Z_i^P])$$

**Lemma E.3.** It holds that

$$\sum_{k=1}^K \sum_{h=1}^H \sum_{(s,a)[Z_i^P] \notin L_{k,i}} w_{k,h,Z_i^P}(s,a) \leq 8 H X_i^P \log(10 n X_i^P H/\delta).$$

**Proof.** For those $(s,a)[Z_i^P] \notin L_{k,i}$, we have $\frac{1}{4} \sum_{j < k} w_{j,Z_i^P}(x) \leq H \log(10 n X_i^P H/\delta) + H \leq 2 H \log(10 n X_i^P H/\delta)$. That is,

$$\sum_{k=1}^K \sum_{h=1}^H \sum_{(s,a)[Z_i^P] \notin L_{k,i}} w_{k,h,Z_i^P}(s,a) \leq \sum_{(s,a)[Z_i^P]} 8 H \log(10 n X_i^P H/\delta) \leq 8 H X_i^P \log(10 n X_i^P H/\delta)$$

\[\square\]
Lemma E.2 shows that we can lower bound the visiting count of a certain \((s,a)[Z_i^P]\) if the visiting probability of \((s,a)[Z_i^P]\) is sufficient large. Lemma E.3 shows that those \((s,a)[Z_i^P]\) with little visiting probability cause little contribution to the final regret.

Lemma E.4.

\[
\sum_{k=1}^{K} \sum_{h=1}^{H} \sum_{(s,a)\in L_{k,i}} \frac{w_{k,h,Z_i^P}(s,a)}{N_k((s,a)[Z_i^P])} \leq 4X_i^P.
\]

Proof. For those \((s,a)[Z_i^P] \in L_{k,i}\), we have \(N_k((s,a)[Z_i^P]) \geq \frac{1}{4} \sum_{j<k} w_{j,Z_i^P}(s,a)\). Therefore, we have

\[
\sum_{k=1}^{K} \sum_{h=1}^{H} \sum_{(s,a)\in L_{k,i}} \frac{w_{k,h,Z_i^P}(s,a)}{N_k((s,a)[Z_i^P])} = \sum_{(s,a)[Z_i^P]\in L_{k,i}} \sum_{k=1}^{K} \frac{w_{k,Z_i^P}(s,a)}{N_k((s,a)[Z_i^P])} \leq \sum_{(s,a)[Z_i^P]\in L_{k,i}} 4 \leq 4X_i^P
\]

\[\square\]

Lemma E.5. For factored set \(Z_i^P\) of transition, we have:

\[
\sum_{k=1}^{K} \sum_{h=1}^{H} \sum_{(s,a)\in X} \frac{w_{k,h}(s,a)}{N_{k-1}((s,a)[Z_i^P])} \leq 8X_i^P
\]

(31)

\[
\sum_{k=1}^{K} \sum_{h=1}^{H} \sum_{(s,a)\in X} \frac{w_{k,h}(s,a)}{\sqrt{N_{k-1}((s,a)[Z_i^P])N_{k-1}((s,a)[Z_j^P])}} \leq 8X_i^P
\]

(32)

\[
\sum_{k=1}^{K} \sum_{h=1}^{H} \sum_{(s,a)\in X} \frac{w_{k,h}(s,a)}{\sqrt{N_{k-1}((s,a)[Z_i^P])N_{k-1}((s,a)[Z_j^P])}} \leq 8\sqrt{X_{i,j}^P T^{1/4}}
\]

(33)

where \(X_{i,j}^P = |X[Z_i^P \cup Z_j^P]|\).

For factored set \(Z_i^R\) of rewards, similarly we have:

\[
\sum_{k=1}^{K} \sum_{h=1}^{H} \sum_{(s,a)\in X} \frac{w_{k,h}(s,a)}{N_{k-1}((s,a)[Z_i^R])} \leq 8X_i^R
\]

(34)

\[
\sum_{k=1}^{K} \sum_{h=1}^{H} \sum_{(s,a)\in X} \frac{w_{k,h}(s,a)}{\sqrt{N_{k-1}((s,a)[Z_i^R])N_{k-1}((s,a)[Z_j^R])}} \leq 8X_i^R
\]

(35)

\[
\sum_{k=1}^{K} \sum_{h=1}^{H} \sum_{(s,a)\in X} \frac{w_{k,h}(s,a)}{\sqrt{N_{k-1}((s,a)[Z_i^R])N_{k-1}((s,a)[Z_j^R])}} \leq 8\sqrt{X_{i,j}^R T^{1/4}}
\]

(36)

where \(X_{i,j}^R = |X[Z_i^R \cup Z_j^R]|\).
Proof. We only prove the inequalities for the factored set of transition. The inequalities for the factored set of rewards can be proved in the same manner.

For Inq. 31, we define $\mathcal{X}_i((s, a)[Z^P_i]) = \{x \in \mathcal{X} \mid x[Z^P_i] = (s, a)[Z^P_i]\}$. then we have

\[
\sum_{k=1}^{K} \sum_{h=1}^{H} \sum_{(s, a) \in \mathcal{X}} w_{k,h}(s, a) \frac{1}{N_{k-1}((s, a)[Z^P_i])} \\
= \sum_{k,h} \sum_{(s, a)[Z^P_i] \in \mathcal{X}[Z^P_i]} w_{k,h,Z^P_i}(s, a) \frac{\sum_{(s, a) \in \mathcal{X}_i((s, a)[Z^P_i])} w_{k,h,Z^P_i}(s, a)}{N_{k-1}((s, a)[Z^P_i])} \\
= \sum_{k,h} \sum_{(s, a)[Z^P_i] \in L_{k,i}} w_{k,h,Z^P_i}(s, a) \frac{1}{N_{k-1}((s, a)[Z^P_i])} \\
\leq \sum_{k,h} \sum_{(s, a)[Z^P_i] \notin L_{k,i}} w_{k,h,Z^P_i}(s, a) \frac{1}{N_{k-1}((s, a)[Z^P_i])} + \sum_{k,h} \sum_{(s, a)[Z^P_i] \notin L_{k,i}} w_{k,h,Z^P_i}(s, a) \frac{1}{N_{k-1}((s, a)[Z^P_i])} \\
\leq 4X^P_i + \sqrt{8HX^P_i \log(10nX^P_i H/\delta)} \\
\leq 8X^P_i
\]

In the first equality, we firstly categorize $(s, a)$ based on their value $(s, a)[Z^P_i]$ and sum up over all possible choice of $(s, a)[Z^P_i]$, then we sum up the value in each category in the inner summation. The second equality is due to $\sum_{(s, a) \in \mathcal{X}_i((s, a)[Z^P_i])} w_{k,h,Z^P_i}(s, a) = 1$.

The first inequality is due to Cauchy-Schwarz inequality. The second inequality is due to Lemma E.4 and Lemma E.3. The last inequality is due to the assumption that $X^P_i \geq H \log(10nX^P_i H/\delta)$.

For Inq. 32 and Inq. 33, we define $Z^P_{i,j} = Z^P_i \cup Z^P_j$. For the factored set $Z^P_{i,j}$, similarly we have

\[
\sum_{k=1}^{K} \sum_{h=1}^{H} \sum_{(s, a) \in L_{k,i}} w_{k,h,Z^P_{i,j}}(s, a) \frac{1}{N_k((s, a)[Z^P_{i,j}])} \leq 4X^P_{i,j} \\
\sum_{k=1}^{K} \sum_{h=1}^{H} \sum_{(s, a) \notin L_{k,i}} w_{k,h,Z^P_{i,j}}(s, a) \leq 8HX^P_{i,j} \log(10nX^P_{i,j} H/\delta),
\]

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By the definition of $Z_i^P$, we know that $N_{k-1}((s,a)\mid Z_i^P) \geq N_{k-1}((s,a)\mid Z_{i,j}^P)$ and $N_{k-1}((s,a)\mid Z_j^P) \geq N_{k-1}((s,a)\mid Z_{i,j}^P)$. Therefore, we have

$$\sum_{k=1}^{K} \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{X}} w_{k,h}(s, a) \sqrt{N_{k-1}((s,a)\mid Z_i^P)N_{k-1}((s,a)\mid Z_j^P)} \leq \sum_{k=1}^{K} \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{X}} w_{k,h}(s, a) \sqrt{N_{k-1}((s,a)\mid Z_j^P)}$$

$$\sum_{k=1}^{K} \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{X}} w_{k,h}(s, a) \biggr(\frac{N_{k-1}((s,a)\mid Z_i^P)N_{k-1}((s,a)\mid Z_j^P)}{N_{k-1}((s,a)\mid Z_{i,j}^P)}\biggr)^{\frac{1}{4}} \leq \sum_{k=1}^{K} \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{X}} w_{k,h}(s, a) \biggr(\frac{N_{k-1}((s,a)\mid Z_j^P)}{N_{k-1}((s,a)\mid Z_{i,j}^P)}\biggr)^{\frac{1}{4}}$$

The following proof of Inq. 32 and Inq. 33 shares the same idea of the proof of Inq. 31 \hfill \Box

### E.4 Technical Lemmas about Variance

In this subsection, we prove several technical lemmas about variance. For notation simplicity, we use $E_i$ and $E_{[i,j]}$ as a shorthand of $E_{s'[i] \sim P_{[i]}}((s,a)\mid Z_i^P)$ and $E_{s'[i,j] \sim P_{[i,j]}}((s,a)\mid Z_{i,j}^P)$. Similarly, we use $V_i$ and $V_{[i,j]}$ as a shorthand of $V_{s'[i] \sim P_{[i]}}((s,a)\mid Z_i^P)$ and $V_{s'[i,j] \sim P_{[i,j]}}((s,a)\mid Z_{i,j}^P)$.

For these w.r.t the empirical transition $\hat{P}_k$, we use $\hat{E}_k$ and $\hat{V}_k$ to denote the corresponding expectation and variance. For example, $E_{s'[i] \sim \hat{P}_{k,i}}((s,a)\mid Z_i^P)$ is denoted as $\hat{E}_{k,i}$.

**Lemma E.6.** Under event $\Lambda_1$, $\Lambda_2$, we have:

$$\left| \sigma_{P,k,i}^2(V, s, a) - \sigma_{P,i}^2(V, s, a) \right| \leq 4H^2 \sum_{j=1}^{n} \left( 2 \sqrt{\frac{|S_j| \cdot L^P}{N_{k-1}((s,a)\mid Z_j^P)}} + \frac{4|S_j| \cdot L^P}{3N_{k-1}((s,a)\mid Z_j^P)} \right),$$

where $V$ denotes some given function mapping from $S$ to $\mathbb{R}$.

**Proof.**

$$\left| \sigma_{P,k,i}^2(V, s, a) - \sigma_{P,i}^2(V, s, a) \right| = \left| \hat{E}_{[1:i-1]} \hat{V}_i \hat{E}_{[i+1:n]} V(s') - E_{[1:i-1]} V_i E_{[i+1:n]} V(s') \right| \leq \left| \hat{E}_{[1:i-1]} \hat{V}_i \hat{E}_{[i+1:n]} V(s') - E_{[1:i-1]} V_i E_{[i+1:n]} V(s') \right|$$

$$+ \left| E_{[1:i-1]} V_i \hat{E}_{[i+1:n]} V(s') - E_{[1:i-1]} V_i E_{[i+1:n]} V(s') \right| \leq \left| \hat{E}_{[1:i-1]} \hat{V}_i \hat{E}_{[i+1:n]} V(s') - E_{[1:i-1]} V_i E_{[i+1:n]} V(s') \right|$$

We bound Eq. 38 and 39 separately.

For equ. 38, we have

$$\left| \hat{E}_{[1:i-1]} \hat{V}_i \hat{E}_{[i+1:n]} V(s') - E_{[1:i-1]} V_i E_{[i+1:n]} V(s') \right| = \left| \sum_{s'[1:i-1] \in S[1:i-1]} (\hat{P}_{[1:i-1]} - P_{[1:i-1]}) (s'[1 : i - 1]|s,a) \hat{V}_i \hat{E}_{[i+1:n]} V(s') \right|$$

$$\leq \left| \hat{P}_{[1:i-1]} (\cdot|s,a) - P_{[1:i-1]} (\cdot|s,a) \right|_{1} \cdot \left| \hat{V}_i \hat{E}_{[i+1:n]} V(s') \right|_{\infty}$$

$$\leq H^2 \sum_{j=1}^{i-1} \left| \hat{P}_j (\cdot|s,a) - P_j (\cdot|s,a) \right|_{1}$$

$$\leq H^2 \sum_{j=1}^{i-1} \left( 2 \sqrt{\frac{|S_j| \cdot L^P}{N_{k-1}((s,a)\mid Z_j^P)}} + \frac{4|S_j| \cdot L^P}{3N_{k-1}((s,a)\mid Z_j^P)} \right)$$

(40)
The last inequality is due to Lemma B.1.

For equ. 39, given fixed $s'[1:i-1]$, we have

\[
\left| \hat{V}_i |\hat{E}_{[i+1:n]} V(s') - \nabla_i |\hat{E}_{[i+1:n]} V(s') \right| \leq \left| \hat{E}_i \left( \hat{E}_{[i+1:n]} V(s') \right)^2 - \nabla_i (E_{[i+1:n]} V(s')^2) \right| \\
+ \left| (E_{[i:n]} V(s'))^2 - (\hat{E}_{[i:n]} V(s'))^2 \right| \\
\leq \left| \hat{E}_i \left( \hat{E}_{[i+1:n]} V(s') \right)^2 - \nabla_i (E_{[i+1:n]} V(s')^2) \right| \\
+ \left| E_i \left( \hat{E}_{[i+1:n]} V(s') \right)^2 - E_i (E_{[i+1:n]} V(s')^2) \right| \\
+ \left| (E_{[i:n]} V(s'))^2 - (\hat{E}_{[i:n]} V(s'))^2 \right| \\
\leq \left| \hat{E}_i \left( \hat{E}_{[i+1:n]} V(s') \right)^2 - \nabla_i (E_{[i+1:n]} V(s')^2) \right| \\
+ \left| E_i \left( \hat{E}_{[i+1:n]} V(s') \right)^2 - E_i (E_{[i+1:n]} V(s')^2) \right| \\
+ 2H \left| E_{[i:n]} V(s') - \hat{E}_{[i:n]} V(s') \right| \\
\leq 4H^2 \sum_{j=i}^n \left( 2 \sqrt{\frac{|S_j|L^P}{N_{k-1}((s,a)[Z_j^P])}} + \frac{4|S_j|L^P}{3N_{k-1}((s,a)[Z_j^P])} \right)
\]

This bound doesn’t depend on the given fixed $s'[1:i-1]$. By taking expectation over $s'[1:i-1] \sim P_{[1:i-1]}(\cdot |s,a)$, we have

\[
E_{[1:i-1]} \left| \hat{V}_i |\hat{E}_{[i+1:n]} V(s') - \nabla_i |\hat{E}_{[i+1:n]} V(s') \right| \\
\leq \left| \hat{E}_i \left( \hat{E}_{[i+1:n]} V(s') \right)^2 - \nabla_i (E_{[i+1:n]} V(s')^2) \right| \\
\leq 4H^2 \sum_{j=i}^n \left( 2 \sqrt{\frac{|S_j|L^P}{N_{k-1}((s,a)[Z_j^P])}} + \frac{4|S_j|L^P}{3N_{k-1}((s,a)[Z_j^P])} \right)
\]

Combining with Equ. 40, we have

\[
|\hat{\sigma}_{P,k,i}(V, s, a) - \sigma_{P,i}(V, s, a)| \leq 4H^2 \sum_{j=1}^n \left( 2 \sqrt{\frac{|S_j|L^P}{N_{k-1}((s,a)[Z_j^P])}} + \frac{4|S_j|L^P}{3N_{k-1}((s,a)[Z_j^P])} \right)
\]

\[\square\]
Lemma E.7. Under event $\Lambda_1$, $\Lambda_2$ and $\Omega$, we have

$$\sigma_{P,i}^2(V^*_h, s, a) - 2\hat{\sigma}^2_{P,k,i}(\tilde{V}_{k,h+1}, s, a, \bar{u}) \leq u_{k,h,i}(s, a) + 4H^2 \sum_{j=1}^n \left( \frac{|S_j|L^p}{N_{k-1}((s, a)[Z_j^p])} + \frac{4|S_j|L^p}{3N_{k-1}((s, a)[Z_j^p])} \right),$$

where $u_{k,h,i}(s, a)$ is defined in Eqn. 3.

Proof. We can decompose the difference in the following way:

$$\sigma_{P,i}^2(V^*_h, s, a) - 2\hat{\sigma}^2_{P,k,i}(\tilde{V}_{k,h+1}, s, a, \bar{u}) \leq \hat{\sigma}^2_{P,k,i}(\tilde{V}_{k,h+1}, s, a, \bar{u}) - 2\hat{\sigma}^2_{P,k,i}(\tilde{V}_{k,h+1}, s, a) + \sigma_{P,i}^2(V^*_h, s, a) - \hat{\sigma}^2_{P,k,i}(V^*_h, s, a)$$

By Lemma E.6, we know that

$$|\hat{\sigma}^2_{P,k,i}(V^*_h, s, a) - \sigma_{P,i}^2(V^*_h, s, a)| \leq 4H^2 \sum_{j=1}^n \left( \frac{|S_j|L^p}{N_{k-1}((s, a)[Z_j^p])} + \frac{4|S_j|L^p}{3N_{k-1}((s, a)[Z_j^p])} \right)$$

Now we only need to bound $\hat{\sigma}^2_{P,k,i}(\tilde{V}_{k,h+1}, s, a, \bar{u}) - 2\hat{\sigma}^2_{P,k,i}(\tilde{V}_{k,h+1}, s, a)$. By Lemma 2 of Azar et al. (2017), we know that for two random variables $X \in \mathbb{R}$ and $Y \in \mathbb{R}$, we have

$$\forall(X) \leq 2[\forall(Y) + \forall(X - Y)]$$

That is,

$$\hat{\sigma}^2_{P,k,i}(\tilde{V}_{k,h+1}, s, a, \bar{u}) - 2\hat{\sigma}^2_{P,k,i}(\tilde{V}_{k,h+1}, s, a) = \mathbb{E}_{i_1 \in [0, 1]} \mathbb{E}_{[a+1, n]} V^*_h + 1(s') - 2\mathbb{E}_{i_1 \in [0, 1]} \mathbb{E}_{[a+1, n]} \tilde{V}_{k,h+1}(s') \leq 2\mathbb{E}_{i_1 \in [0, 1]} \mathbb{E}_{[a+1, n]} (V^*_h + 1(s') - \tilde{V}_{k,h+1}(s'))$$

$$= 2\mathbb{E}_{i_1 \in [0, 1]} \mathbb{E}_{i_1 \in [a+1, n]} (V^*_h + 1(s') - \tilde{V}_{k,h+1}(s')) \leq 2\mathbb{E}_{i_1 \in [0, 1]} \left( \mathbb{E}_{i_1 \in [a+1, n]} (V^*_h + 1(s') - \tilde{V}_{k,h+1}(s')) \right)^2$$

$$= u_{k,h,i}(s, a)$$

The first inequality is due to Inq. 44, and the second inequality is due to $\forall X \leq E X^2$ for any random variable $X \in \mathbb{R}$.

To sum up, we have

$$\sigma_{P,i}^2(V^*_h, s, a) - 2\hat{\sigma}^2_{P,k,i}(\tilde{V}_{k,h+1}, s, a, \bar{u}) \leq u_{k,h,i}(s, a) + 8H^2 \sum_{j=1}^n \left( \frac{|S_j|L^p}{N_{k-1}((s, a)[Z_j^p])} + \frac{4|S_j|L^p}{3N_{k-1}((s, a)[Z_j^p])} \right)$$

Lemma E.8. Under event $\Lambda_1$, $\Lambda_2$ and $\Omega$, suppose $\tilde{\text{Reg}}(K) = \sum_{k=1}^K \tilde{V}_{k,1}(s_1) - V^*_{1}(s_1)$, we have:

$$\sum_{k=1}^K \sum_{h=1}^H \sum_{(s,a) \in \mathcal{X}} w_{k,h}(s, a) (\sigma^2_{\tilde{P},i}(V^*_h, s, a, a) - \sigma^2_{P,k,i}(\tilde{V}_{k,h+1}, s, a, \bar{u})) \leq 2H^2 \tilde{\text{Reg}}(K)$$

$$\sum_{k=1}^K \sum_{h=1}^H \sum_{(s,a) \in \mathcal{X}} w_{k,h}(s, a) (\sigma^2_{\tilde{P},i}(\tilde{V}_{k,h+1}, s, a, a) - \sigma^2_{P,k,i}(\tilde{V}_{k,h+1}, s, a, \bar{u})) \leq 2H^2 \tilde{\text{Reg}}(K)$$

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Proof. We only prove the first inequality in detail. By replacing \( V_{h+1}^* \) with \( \tilde{V}_{k,h+1} \), we can prove the second inequality in the same manner.

\[
\sigma^2_{P,i}(V_{h+1}^*, s, a) - \sigma^2_{P,i}(V_{h+1}^{\pi_k}, s, a) = \mathbb{E}_{[1:n]} \left[ \mathbb{V}_i \left( \mathbb{E}_{[i+1:n]} V_{h+1}^* \right) - \mathbb{V}_i \left( \mathbb{E}_{[i+1:n]} V_{h+1}^{\pi_k} \right) \right]
\]

Given fixed \( s'[1 : i - 1] \), we bound the difference of the variances: \( \mathbb{V}_i \left( \mathbb{E}_{[i+1:n]} V_{h+1}^* \right) - \mathbb{V}_i \left( \mathbb{E}_{[i+1:n]} V_{h+1}^{\pi_k} \right) \).

\[
\begin{align*}
\mathbb{V}_i \left( \mathbb{E}_{[i+1:n]} V_{h+1}^* \right) - \mathbb{V}_i \left( \mathbb{E}_{[i+1:n]} V_{h+1}^{\pi_k} \right) &= \mathbb{E}_i \left[ \left( \mathbb{E}_{[i+1:n]} V_{h+1}^* \right)^2 - \left( \mathbb{E}_{[i+1:n]} V_{h+1}^{\pi_k} \right)^2 \right] \\
&\leq \mathbb{E}_i \left[ \left( \mathbb{E}_{[i+1:n]} V_{h+1}^* \right)^2 - \left( \mathbb{E}_{[i+1:n]} V_{h+1}^{\pi_k} \right)^2 \right] \\
&\leq 2H \mathbb{E}_i \left[ \mathbb{E}_{[i+1:n]} V_{h+1}^* - \mathbb{E}_{[i+1:n]} V_{h+1}^{\pi_k} \right] \\
&= 2H \mathbb{E}_{[i:n]} \left[ V_{h+1}^* - V_{h+1}^{\pi_k} \right]
\end{align*}
\]

The first inequality is due to \( V_{h+1}^* \geq V_{h+1}^{\pi_k} \), and the second inequality is due to \( \mathbb{E}_{[i+1:n]} V_{h+1}^* + \mathbb{E}_{[i+1:n]} V_{h+1}^{\pi_k} \leq 2H \).

We then take expectation over all \( s'[1 : i - 1] \), that is

\[
\sigma^2_{P,i}(V_{h+1}^*, s, a) - \sigma^2_{P,i}(V_{h+1}^{\pi_k}, s, a) \leq 2H \mathbb{E}_{[1:n]} \left[ V_{h+1}^* - V_{h+1}^{\pi_k} \right]
\]

Plugging the inequality into the former equation, we have

\[
\begin{align*}
&\sum_{k=1}^K \sum_{H=1}^H \sum_{(s,a)\in \mathcal{X}} w_{k,h}(s,a) \left( \sigma^2_{P,i}(V_{h+1}^*, s, a) - \sigma^2_{P,i}(V_{h+1}^{\pi_k}, s, a) \right) \\
&\leq \sum_{k=1}^K \sum_{H=1}^H \sum_{(s,a)\in \mathcal{X}} w_{k,h}(s,a) 2H \mathbb{E}_{s'\sim \mathbb{P}(\cdot|s,a)} \left[ V_{h+1}^* - V_{h+1}^{\pi_k} \right] \\
&= \sum_{k=1}^K \sum_{H=1}^H \sum_{s\in \mathcal{S}} 2w_{k,h}(s) H \left[ V_{h}^*(s) - V_{h}^{\pi_k}(s) \right] \\
&\leq \sum_{k=1}^K 2H^2 \left[ V_{h}^*(s_1) - V_{h}^{\pi_k}(s_1) \right] \\
&\leq \sum_{k=1}^K 2H^2 \left[ \bar{V}_{k,h}(s_1) - V_{h}^{\pi_k}(s_1) \right] \\
&= 2H^2 \text{Reg}(K)
\end{align*}
\]

For the second inequality, this is because that by lemma E.15 of Dann et al. (2017), we have

\[
\sum_{s} w_{k,h}(s) \left[ V_{h}^*(s) - V_{h}^{\pi_k}(s) \right]
\]

\[
\begin{align*}
&= \sum_{h=1}^H \sum_{s \geq s} w_{k,h}(s) \left( \bar{R}(s, \pi^*(s)) - \bar{R}(s, \pi_k(s)) + \mathbb{P}V_{h+1}^*(s, \pi^*(s)) - \mathbb{P}V_{h+1}^*(s, \pi_k(s)) \right)
\end{align*}
\]

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\[ V_1^*(s_1) - V_1^\pi_k(s_1) = \sum_{h_1=1}^{H} \sum_s w_{k,h_1}(s) \left( \bar{R}(s, \pi^*(s)) - \bar{R}(s, \pi_k(s)) + \mathbb{P}V_{h_1+1}^*(s, \pi^*(s)) - \mathbb{P}V_{h_1+1}^*(s, \pi^k(s)) \right) \]

This means that \( \sum_s w_{k,h}(s) [V_h^*(s) - V_h^\pi_k(s)] \leq V_1^*(s_1) - V_1^\pi_k(s_1) \) for any \( k, h \).

**E.5 Optimism and Pessimism**

The optimism is proved by induction.

**Lemma E.9. (Optimism)** Suppose that \( \Lambda_1, \Lambda_2 \) and \( \Omega_{k,h+1} \) happen, then we have \( \bar{V}_{k,h} \geq V_h^* \).

**Proof.**

\[
\begin{align*}
\bar{V}_{k,h}(s) - V_h^*(s) \\
\geq & \text{CB}_k(s, \pi^*(s)) + \mathbb{P}_k \bar{V}_{k,h+1}(s, \pi^*(s)) - \mathbb{P}V_{h_1}^*(s, \pi^*(s)) + \bar{R}(s, \pi^*(s)) - \bar{R}(s, \pi^k(s)) \\
\geq & \text{CB}_k(s, \pi^*(s)) + (\mathbb{P}_k - \mathbb{P}) V_{h_1}^*(s, \pi^*(s)) + \bar{R}(s, \pi^*(s)) - \bar{R}(s, \pi^k(s)) \\
\geq & \text{CB}_k(s, \pi^*(s)) - \sum_{i=1}^{n} \left( \frac{2\sigma^2_{P,i}(V_{h_1}^*(s, \pi^*(s)))L^F_{i}}{N_{k-1}((s, \pi^*(s))[Z_{i}^F])} - \frac{2HL^P}{3N_{k-1}((s, \pi^*(s))[Z_{i}^F])} \right) \\
& - \sum_{i=1}^{n} \sum_{j \neq i, j=1}^{n} H \phi_{k,i}(s, \pi^*(s)) \phi_{k,j}(s, \pi^*(s)) \\
& - \frac{1}{m} \sum_{i=1}^{m} \sqrt{\frac{2\sigma^2_{R,i}(s, \pi^*(s))L^R_{i}}{N_{k-1}((s, \pi^*(s))[Z_{i}^R])}} - \frac{1}{m} \sum_{i=1}^{m} \frac{8L^R_{i}}{3N_{k-1}((s, \pi^*(s))[Z_{i}^R])}
\end{align*}
\]

where \( \phi_{k,i}(s, a) = \sqrt{\frac{4|S_i|L^P}{N_{k-1}((s,a)[Z_{i}^F])}} + \frac{4|S_i|L^P}{3N_{k-1}((s,a)[Z_{i}^F])} \). The first inequality is due to \( \bar{V}_{k,h}(s) \geq \bar{Q}_{k,h}(s, \pi^*(s)) \). The second inequality is due to induction condition that \( \Omega_{k,h+1} \) happens. The last inequality is due to Lemma E.1.

For the following proof, we use \( a^* \) to denote \( \pi^*(s) \). Plugging the definition of \( \text{CB}_k(s, \pi^*(s)) \) to the above inequality, we have

\[
\begin{align*}
\bar{V}_{k,h}(s) - V_h^*(s) \\
\leq & \sum_{i=1}^{n} \left( \sqrt{\frac{4\hat{\sigma}^2_{P,i}(V_{h_1}^*(s, a^*)L^P_{i}}{N_{k-1}((s, a^*)[Z_{i}^F])}} - \sqrt{\frac{2\sigma^2_{P,i}(V_{h_1}^*(s, a^*)L^F_{i}}{N_{k-1}((s, a^*)[Z_{i}^F])}) \right) \\
& + \sum_{i=1}^{n} \frac{2u_{k,h,i}(s, a)L^P_{i}}{N_{k-1}((s, a^*)[Z_{i}^F])} + \sum_{i=1}^{n} \sqrt{\frac{16H^2L^P}{N_{k-1}((s, a^*)[Z_{i}^F])}} \sum_{j=1}^{n} \left( \frac{4|S_j|L^P}{N_{k-1}((s, a^*)[Z_{j}^F])} \right)^{\frac{1}{2}} + \sqrt{\frac{4|S_j|L^P}{3N_{k-1}((s, a^*)[Z_{j}^F])}}
\end{align*}
\]
We mainly focus on the bound of Equ. 46.
\[
\sqrt{\frac{4\hat{\sigma}_{P,k,i}(V_{h+1}^{*}, s, a^{*})L_{P}}{N_{k-1}((s, a^{*})[Z_{i}^{P}])}} - \sqrt{\frac{2\hat{\sigma}_{P,i}(V_{h+1}^{*}, s, a^{*})L_{P}}{N_{k-1}((s, a^{*})[Z_{i}^{P}])}} 
\geq - \sqrt{\frac{2\sigma_{P,k,i}(V_{h+1}, s, a^{*})L_{P} - 4\hat{\sigma}_{P,k,i}(V_{h+1}, s, a^{*})L_{P}}{N_{k-1}((s, a^{*})[Z_{i}^{P}])} + 2\hat{\sigma}_{P,k,i}(\tilde{V}_{k,h+1}, s, a^{*})} 
\leq \sigma_{P,i}(V_{h+1}^{*}, s, a^{*})
\]
(48)

For those $2\hat{\sigma}_{P,k,i}(\tilde{V}_{k,h+1}, s, a^{*}) \leq \sigma_{P,i}(V_{h+1}^{*}, s, a^{*})$, by Lemma E.7, we have
\[
\sigma_{P,i}(V_{h+1}^{*}, s, a^{*}) - 2\hat{\sigma}_{P,k,i}(\tilde{V}_{k,h+1}, s, a^{*}) 
\leq u_{k,h,i}(s, a^{*}) + 8H^{2}\sum_{j=1}^{n} \left( 2\frac{|S_{j}|L_{P}}{N_{k-1}((s, a^{*})[Z_{j}^{P}])} + \frac{4|S_{j}|L_{P}}{3N_{k-1}((s, a^{*})[Z_{j}^{P}])} \right)
\]
That is,
\[
\sqrt{\frac{2\hat{\sigma}_{P,k,i}(\tilde{V}_{k,h+1}, s, a^{*})L_{P}}{N_{k-1}((s, a^{*})[Z_{i}^{P}])}} - \sqrt{\frac{4\hat{\sigma}_{P,i}(V_{h+1}^{*}, s, a^{*})L_{P}}{N_{k-1}((s, a^{*})[Z_{i}^{P}])}} 
\geq - \sqrt{\frac{2u_{k,h,i}(s, a^{*})L_{P} + 16H^{2}L_{P}\sum_{j=1}^{n} \left( 2\frac{|S_{j}|L_{P}}{N_{k-1}((s, a^{*})[Z_{j}^{P}])} + \frac{4|S_{j}|L_{P}}{3N_{k-1}((s, a^{*})[Z_{j}^{P}])} \right)}{N_{k-1}((s, a^{*})[Z_{i}^{P}])}}
\geq - \sqrt{\frac{2u_{k,h,i}(s, a^{*})L_{P}}{N_{k-1}((s, a^{*})[Z_{i}^{P}])}} - \sqrt{\frac{16H^{2}L_{P}}{N_{k-1}((s, a^{*})[Z_{i}^{P}])}} \sum_{j=1}^{n} \left( \frac{4|S_{j}|L_{P}}{N_{k-1}((s, a^{*})[Z_{j}^{P}])} \right)^{\frac{1}{2}} + \sqrt{\frac{4|S_{j}|L_{P}}{3N_{k-1}((s, a^{*})[Z_{j}^{P}])}}
\]
Combining with Eq. 45, we prove that
\[
\tilde{V}_{k,h} \geq V_{h}^{*}.
\]

\[\Box\]

**Lemma E.10. (Pessimism)** Suppose that $\Lambda_{1}$, $\Lambda_{2}$ and $\Omega_{k,h+1}$ happen, then we have $V_{k,h} \leq V_{h}^{*}$.

**Proof.**
\[
V_{k,h}(s) 
= \hat{R}(s, \pi_{k,h}(s)) - CB_{k}(s, \pi_{k,h}(s)) + \widehat{P}_{k} V_{k,h+1}(s, \pi_{k,h}(s)) 
\leq \hat{R}(s, \pi_{k,h}(s)) - CB_{k}(s, \pi_{k,h}(s)) + \widehat{P}_{k} V_{h+1}^{*}(s, \pi_{k,h}(s)) 
= \bar{R}(s, \pi_{k,h}(s)) + \bar{P} V_{h+1}^{*}(s, \pi_{k,h}(s)) 
\quad + \left( \hat{R}(s, \pi_{k,h}(s)) - \bar{R}(s, \pi_{k,h}(s)) - \frac{1}{m} \sum_{i=1}^{m} CB_{i}^{R}(s, \pi_{k,h}(s)) \right) 
\quad + \left( \widehat{P}_{k} V_{h+1}^{*}(s, \pi_{k,h}(s)) - \bar{P} V_{h+1}^{*}(s, \pi_{k,h}(s)) - \sum_{i=1}^{n} CB_{i}^{P}(s, \pi_{k,h}(s)) \right)
\]

38
The inequality is due to $V_{k,h+1}(s') \leq V^*_h(s')$ since event $\Omega_{k,h+1}$ happens.
Following the proof of Lemma E.9, we know that

$$
\left| \hat{R}(s, \pi_{k,h}(s)) - \bar{R}(s, \pi_k(s)) \right| \leq \frac{1}{m} \sum_{i=1}^{m} CB_i^R(s, \pi_{k,h}(s))
$$

$$
\left| \hat{P}_k V^*_{h+1}(s, \pi_{k,h}(s)) - \bar{P} V^*_{h+1}(s, \pi_{k,h}(s)) \right| \leq \sum_{i=1}^{n} CB_i^P(s, \pi_{k,h}(s))
$$

Therefore, we have

$$
V_{k,h}(s, \pi_{k,h}(s)) \leq \bar{R}(s, \pi_{k,h}(s)) + \bar{P} V^*_{h+1}(s, \pi_{k,h}(s))
$$

$$

\leq \bar{R}(s, \pi_h(s)) + \bar{P} V^*_{h+1}(s, \pi_{h}(s))
$$

$$
\leq V^*_h(s, a)
$$

\[\square\]

**Lemma E.11.** (Optimism and pessimism) Under event $\Lambda_1$ and $\Lambda_2$, we have $\Omega_{k,h}$ holds for all $k$ and $h$.

**Proof.** By Lemma E.9 and Lemma E.10, through induction over all possible $k, h$, we can prove the Lemma. \[\square\]

**E.6 Proof of Theorem 2**

**Proof.** We decompose $\tilde{\text{Reg}}(K) = \sum_{k=1}^{K} (\tilde{V}_k(s_{k,1}, a_{k,1}) - V^*_1(s_{k,1}, a_{k,1}))$ in the classical way (Azar et al., 2017; Zanette and Brunskill, 2019; Dann et al., 2019), that is

$$
\sum_{k=1}^{K} (\tilde{V}_k(s_1, a_1) - V^*_1(s_1, a_1))
$$

$$
\leq \sum_{k,h} \sum_{s_h,a_h} w_{k,h}(s_h, a_h) CB_k(s_h, a_h) + \sum_{k,h} \sum_{s_h,a_h} w_{k,h}(s_h, a_h) \left( \hat{P}_k - \bar{P} \right) V^*_{h+1}(s_h, a_h)
$$

$$
+ \sum_{k,h} \sum_{s_h,a_h} w_{k,h}(s_h, a_h) \left( \hat{P}_k - \bar{P} \right) (\tilde{V}_{k,h+1} - V^*_{h+1}) (s_h, a_h)
$$

$$
+ \sum_{k,h} \sum_{s_h,a_h} w_{k,h}(s_h, a_h) \left( \hat{R}_k(s_h, a_h) - \bar{R}(s_h, a_h) \right)
$$

We bound Equ. 51, 52, 53 and 54 separately by Lemma E.12, Lemma E.13, Lemma E.14 and Lemma E.15. Combining the results of these Lemmas, we have

$$
\tilde{\text{Reg}}(K) \leq C_1 \frac{1}{m} \sum_{i=1}^{m} \sqrt{X_i^R TL_i^R} + C_2 \sum_{i=1}^{n} HTX_i^P L_i^P + C_3 \sqrt{nH^2\tilde{\text{Reg}}(K)} \sum_{i=1}^{n} X_i^P L_i^P
$$

(55)
Here $C_1, C_2, C_3$ denote some constants. Solving the $\text{Reg}(K)$ in Inq 55, we can show that

$$\text{Reg}(K) \leq O \left( \frac{1}{m} \sum_{i=1}^{m} \sqrt{X_i^RT_iL_i^R} + \sqrt{\sum_{i=1}^{n} HTX_i^PL_i^P} \right),$$

where $O$ hides the lower order terms w.r.t $T$.

By the optimism principle (Lemma E.11), we have $V_i^*(s_{k,1}, a_{k,1}) \leq \bar{V}_{k,1}(s_{k,1}, a_{k,1})$. This leads to the final result:

$$\sum_{k=1}^{K} (V_i^*(s_{k,1}, a_{k,1}) - V_i^*(s_{k,1}, a_{k,1})) \leq O \left( \frac{1}{m} \sum_{i=1}^{m} \sqrt{X_i^RT_iL_i^R} + \sqrt{\sum_{i=1}^{n} HTX_i^PL_i^P} \right).$$

\[ \square \]

E.7 Bounding the Main Terms

**Lemma E.12.** Under event $\Lambda_1, \Lambda_2$ and $\Omega_{k,h}$, suppose $\text{Reg}(K) = \sum_{k=1}^{K} \bar{V}_{k,1}(s_1) - V_i^*(s_{k,1})$, we have

$$\sum_{k=1}^{K} \sum_{h=1}^{H} \sum_{s,a} w_{k,h}(s,a) \text{CB}_k(s,a) \leq O \left( \frac{1}{m} \sum_{i=1}^{m} \sqrt{TX_i^RT_iL_i^R} + \sqrt{HT \sum_{i=1}^{n} X_i^PL_i^P} + \sqrt{H^2 n \text{Reg}(K) \sum_{i=1}^{n} X_i^PL_i^P} \right)$$

**Proof.** By the definition of $\text{CB}_k(s,a)$, we have

$$\sum_{k,h,s,a} w_{k,h}(s,a) \text{CB}_k(s,a) \tag{56}$$

$$= \sum_{k,h,s,a} w_{k,h}(s,a) \left( \frac{1}{m} \sum_{i=1}^{m} \text{CB}_R(s,a) + \sum_{i=1}^{n} \text{CB}_P(s,a) \right) \tag{57}$$

$$= \sum_{k,h,s,a} w_{k,h}(s,a) \left( \frac{1}{m} \sum_{i=1}^{m} \frac{2\bar{r}_{k,i}(s,a)L_i^R}{N_{k-1}((s,a)[Z_i^R])} + \sum_{i=1}^{n} \sqrt{\frac{4\bar{r}_{i}^2(s,a)L_i^P}{N_{k-1}((s,a)[Z_i^P])}} \right) \tag{58}$$

$$+ \sum_{k,h,s,a} w_{k,h}(s,a) \frac{1}{m} \sum_{i=1}^{m} \frac{8L_i^R}{3N_{k-1}((s,a)[Z_i^R])} \tag{59}$$

$$+ \sum_{k,h,s,a} w_{k,h}(s,a) \sum_{i=1}^{n} \left( \sqrt{\frac{16H^2L_i^P}{N_{k-1}((s,a)[Z_i^P])}} \sum_{j=1}^{n} \left( \frac{4|S_j|^L}{N_{k-1}((s,a)[Z_j^P])} \right)^{\frac{1}{2}} + \sqrt{\frac{4|S_j|^L}{3N_{k-1}(s,a)[Z_j^P]}} \right) \tag{60}$$

$$+ \sum_{k,h,s,a} w_{k,h}(s,a) \sum_{i=1}^{n} \sum_{j \neq i=1}^{n} \frac{36H|S_i||S_j|(L_i^P)^2}{\sqrt{N_{k-1}((s,a)[Z_i^P])N_{k-1}((s,a)[Z_j^P])}} \tag{61}$$

$$+ \sum_{k,h,s,a} w_{k,h}(s,a) \sum_{i=1}^{n} \frac{2\bar{u}_{k,h,i}(s,a)L_i^P}{N_{k-1}((s,a)[Z_i^P])} \tag{62}$$

40
By Lemma E.5, the upper bound of Eqn. 59, 60 and 61 is $O(T^{1/2})$, which doesn’t contribute to the main factor in the regret. We prove the upper bound of Eqn. 58 and Eqn. 62 in detail.

By Lemma E.6, we have

$$
|\sigma^2_{P,k,i}(\bar{V}_{k,h+1}, s, a) - \sigma^2_{P,i}(\bar{V}_{k,h+1}, s, a)| \leq 4H^2 \sum_{j=1}^{n} \left( 2 \sqrt{\frac{|S_j| |L^P_i|}{N_{k-1}((s, a)[Z^P_j])}} + \frac{4|S_j| |L^P_i|}{3N_{k-1}((s, a)[Z^P_j])} \right),
$$

Then Eqn. 58 can be bounded as

$$
\begin{align*}
&\frac{1}{m} \sum_{i=1}^{m} \sqrt{\frac{2\sigma^2_{R,k,i}(s, a)L^R_i}{N_{k-1}((s, a)[Z^R_i])}} + \sum_{i=1}^{n} \sqrt{\frac{4\sigma^2_{P,k,i}(V_{k,h+1}, s, a)L^P_i}{N_{k-1}((s, a)[Z^P_i])}} \\
&\leq \frac{1}{m} \sum_{i=1}^{m} \sqrt{\frac{2\sigma^2_{R,k,i}(s, a)L^R_i}{N_{k-1}((s, a)[Z^R_i])}} + \sum_{i=1}^{n} \sqrt{\frac{4\sigma^2_{P,i}(V_{k,h+1}, s, a)L^P_i}{N_{k-1}((s, a)[Z^P_i])}} \\
&+ \sum_{i=1}^{n} \sqrt{\frac{4\sigma^2_{P,i}(V_{k,h+1}, s, a) - \sigma^2_{P,k,i}(V_{k,h+1}, s, a)L^P_i}{N_{k-1}((s, a)[Z^P_i])}} \\
&\leq \frac{1}{m} \sum_{i=1}^{m} \sqrt{\frac{2\sigma^2_{R,k,i}(s, a)L^R_i}{N_{k-1}((s, a)[Z^R_i])}} + \sum_{i=1}^{n} \sqrt{\frac{4\sigma^2_{P,i}(V_{k,h+1}, s, a)L^P_i}{N_{k-1}((s, a)[Z^P_i])}} \\
&+ 8H \sum_{i=1}^{n} \sqrt{\frac{L^P_i}{N_{k-1}((s, a)[Z^P_i])}} \sum_{j=1}^{n} \left( \frac{|S_j| |L^P_i|}{N_{k-1}((s, a)[Z^P_j])} \right)^{1/2} + \sqrt{\frac{4|S_j| |L^P_i|}{3N_{k-1}((s, a)[Z^P_j])}}.
\end{align*}
$$

Similar with Eqn. 65, the summation of Eqn. 65 is upper bounded by $O(T^{1/4})$ by Lemma E.5. For Eqn. 63, we have

$$
\begin{align*}
&\sum_{k,h} \sum_{s,a} w_{k,h}(s, a) \frac{1}{m} \sum_{i=1}^{m} \sqrt{\frac{2\sigma^2_{R,k,i}(s, a)L^R_i}{N_{k-1}((s, a)[Z^R_i])}} \\
&\leq \sum_{k,h} \sum_{s,a} w_{k,h}(s, a) \frac{1}{m} \sum_{i=1}^{m} \sqrt{\frac{2L^R_i}{N_{k-1}((s, a)[Z^R_i])}} \\
&\leq \frac{1}{m} \sum_{i=1}^{m} \sqrt{\sum_{k,h} \sum_{s,a} w_{k,h}(s, a) \sqrt{\sum_{k,h} \sum_{s,a} \frac{2w_{k,h}(s, a)L^R_i}{N_{k-1}((s, a)[Z^R_i])}}} \\
&\leq \frac{1}{m} \sum_{i=1}^{m} \sqrt{T} \sum_{k,h} \sum_{s,a} \frac{2w_{k,h}(s, a)L^R_i}{N_{k-1}((s, a)[Z^R_i])}.
\end{align*}
$$

The first inequality is due to $\delta^2_{R,k,i}(s,a) \leq 1$. The second inequality is due to Cauchy-Schwarz inequality. By Lemma E.5, the summation can be bounded by $\frac{1}{m} \sum_{i=1}^{m} X_i^R L_i^{RT}$.

For Eqn. 64, we have

$$
\sum_{k,h} \sum_{s,a} w_{k,h}(s,a) \sum_{i=1}^{n} \sqrt{\frac{4\sigma^2_{P,i}(\bar{V}_{k,h+1}, s,a) L^P}{N_{k-1}((s,a)[Z_i^P]})} 
\leq \sum_{k,h,s,a} w_{k,h}(s,a) L^P \sum_{i=1}^{n} \sigma^2_{P,i}(\bar{V}_{k,h+1}, s,a) \cdot \sum_{k,h,s,a} w_{k,h}(s,a) \sum_{i=1}^{n} \frac{4L^P}{N_{k-1}((s,a)[Z_i^P])}
$$

$$
\leq \sum_{k,h,s,a} w_{k,h}(s,a) L^P \sum_{i=1}^{n} \sigma^2_{P,i}(\bar{V}_{k,h+1}, s,a) \cdot \sum_{i=1}^{n} 4X_i^P L^P
$$

$$
= \sqrt{\sum_{k,h,s,a} w_{k,h}(s,a) L^P \sum_{i=1}^{n} \left( \sigma^2_{P,i}(\bar{V}_{k,h+1}, s,a) - \sigma^2_{P,i}(\bar{V}_{k,h+1}, s,a) \right) \cdot \sum_{i=1}^{n} 4X_i^P L^P}
$$

$$
\leq \sum_{k,h,s,a} w_{k,h}(s,a) \left( \frac{1}{m^2} \sum_{i=1}^{m} \sigma^2_{R,i}(s,a) + \sum_{i=1}^{n} \sigma^2_{P,i}(\bar{V}_{k,h+1}, s,a) \right) \sum_{i=1}^{n} 4X_i^P L^P + 2H^2 n \text{Reg}(K) \sum_{i=1}^{n} X_i^P L^P
$$

$$
\leq \sqrt{HT} \cdot \sqrt{n} 4X_i^P L^P + 2H^2 n \text{Reg}(K) \sum_{i=1}^{n} X_i^P L^P
$$

The first inequality is due to Cauchy-Schwarz inequality. The second inequality is due to Lemma E.5. The third inequality is due to Lemma E.8. The fourth inequality is due to $\sigma^2_{R,k,i}(s,a) \geq 0$, and the last inequality is because of Corollary 1.1.

For Eqn. 62, we have

$$
\sum_{k,h,s,a} w_{k,h}(s,a) \sum_{i=1}^{n} \sqrt{\frac{2u_{k,h,i}(s,a)L^P}{N_{k-1}((s,a)[Z_i^P])}}
\leq \sum_{i=1}^{n} 2L^P \left( \sum_{k,h,s,a} \frac{4w_{k,h}(s,a)}{N_{k-1}((s,a)[Z_i^P])} \right) \left( \sum_{k,h,s,a} w_{k,h}(s,a) u_{k,h,i}(s,a) \right)
\leq \sum_{i=1}^{n} 64X_i^P L^P \left( \sum_{k,h,s,a} w_{k,h}(s,a) u_{k,h,i}(s,a) \right)
$$

(66)
By Lemma E.19, we know that the summation \( \sum_{k,h,s,a} w_{k,h}(s,a) u_{k,h,i}(s,a) \) is of order \( O(T^{\frac{1}{4}}) \). This means that Equ. 66 is of order \( O(T^{\frac{1}{4}}) \), which doesn’t contribute to the main term \( O(\sqrt{T}) \).

\[ \sum_{k=1}^{K} \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{X}} w_{k,h}(s,a) \left( \hat{p}_k - p \right) V^*(s,a) \]

\[ \leq O \left( \sqrt{(HT + nH^2\text{Reg}(K)) \sum_{i=1}^{n} X_i^P L^P} \right) \]

**Proof.** By Lemma E.1, we have

\[ \sum_{k=1}^{k_1} \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{X}} w_{k,h}(s,a) \left( \hat{p}_k - p \right) V^*(s,a) \]

\[ \leq \sum_{k} \sum_{h} \sum_{i=1}^{n} \sum_{(s,a) \in \mathcal{X}} w_{k,h}(s,a) \sqrt{\frac{2\sigma_{P_i}^2(V_{h+1}^*(s,a)L^P)}{N_{k-1}((s,a)|Z_i^P)}} \]

\[ + \sum_{k} \sum_{h} \sum_{i=1}^{n} \sum_{j \neq i, j=1} w_{k,h}(s,a) \sqrt{\frac{36H|S_i||S_j|(L^P)^2}{N_{k-1}((s,a)|Z_i^P)N_{k-1}((s,a)|Z_j^P)}} \]

By Lemma E.5, the second term has only logarithmic dependence on \( T \), which is negligible compared with the main factor. We mainly focus on the first term.

\[ \sum_{k} \sum_{h} \sum_{i=1}^{n} \sum_{(s,a) \in \mathcal{X}} w_{k,h}(s,a) \sqrt{\frac{2\sigma_{P_i}^2(V_{h+1}^*(s,a)L^P)}{N_{k-1}((s,a)|Z_i^P)}} \]

\[ \leq \sum_{k} \sum_{h} \sum_{(s,a) \in \mathcal{X}} 2w_{k,h}(s,a) \sum_{i=1}^{n} \sigma_{P_i}^2(V_{h+1}^*(s,a)) \cdot \sum_{k} \sum_{h} \sum_{(s,a) \in \mathcal{X}} w_{k,h}(s,a) \sigma_{P_i}^2(V_{h+1}^*(s,a)) \cdot \sum_{k} \sum_{h} \sum_{(s,a) \in \mathcal{X}} \frac{w_{k,h}(s,a)L^P}{N_{k-1}((s,\pi(s))|Z_i^P)} \]

\[ \leq \sqrt{(HT + nH^2\text{Reg}(K)) \sum_{i=1}^{n} X_i^P L^P} \]

The first inequality is due to Cauchy-Schwarz inequality. The second inequality is due to \( \sigma_{R,k,i}^2(s,a) \geq 0 \). For the last inequality, the first part is the summation of the variance, which can be bounded by Lemma 1.1 and Lemma E.8, while the second part can be bounded as \( \sum_{i} X_i^P L^P \) by Lemma E.5. ∎

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Lemma E.14. Under event $\Lambda_1$, $\Lambda_2$ and $\Omega$, suppose $\text{Reg}(K) = \sum_{k=1}^{K} \hat{V}_{k,1}(s_1) - V_{1}^*(s_1)$, we have

$$
\sum_{k=1}^{K} \sum_{h=1}^{H} \sum_{s,a \in \mathcal{X}} w_{k,h}(s,a) \left( \hat{P}_k - P \right) \left( \hat{V}_{k,h+1} - V_{h+1}^* \right)(s,a) \leq O \left( H \sqrt{\sum_{i=1}^{n} \sqrt{TX_j |S_j|L^P} \sum_{i=1}^{n} 2 \sqrt{8X_i^P L^P} } \right)
$$

Proof. By Lemma E.5, we can prove that

$$
\left( \hat{P}_k - P \right) \left( \hat{V}_{k,h+1} - V_{h+1}^* \right)(s,a) \leq \sum_{i=1}^{n} \left( \hat{P}_{k,i} - P_i \right) \left[ \sum_{i=1}^{n} \left( \hat{P}_k - P \right)(\cdot|Z_i^P) \right]_1 \left( \hat{P}_{k,j} - P_j \right)(\cdot|Z_j^P) \right]_1
$$

$$
\leq \sum_{i=1}^{n} \left( 2 \sum_{s'|[i] \in S_i} \sqrt{\frac{P_i(s'[i]|\mathcal{X}[Z_i^P])L^P}{N_{k-1}((s,a)[Z_i^P])}} \right) \left( \hat{P}_{i+1:n} \left( \hat{V}_{k,h}(s_k,h,a_k,h) - V_{h}^*(s_k,h,a_k,h) \right) \right)
$$

$$
+ \sum_{i=1}^{n} \sum_{j \neq i,j=1}^{n} 36H \frac{|S| |S_j| (L^P)^2}{N_{k-1}((s,a)[Z_i^P]) N_{k-1}((s,a)[Z_j^P])} + \sum_{i=1}^{n} \frac{|S_i| L^P}{3N_{k-1}((s,a)[Z_i^P])}
$$

The second inequality is due to Lemma B.1

We only focus on the summation of the first term, since the summation of other terms has only logarithmic dependence on $T$ by Lemma E.5.

$$
\sum_{k=1}^{K} \sum_{h=1}^{H} \sum_{s,a \in \mathcal{X}} w_{k,h}(s,a) \sum_{i=1}^{n} \left( 2 \sum_{s'|[i] \in S_i} \sqrt{\frac{P_i(s'[i]|\mathcal{X}[Z_i^P])L^P}{N_{k-1}((s,a)[Z_i^P])}} \right) \left( \hat{P}_{i+1:n} \left( \hat{V}_{k,h}(s_k,h,a_k,h) - V_{h}^*(s_k,h,a_k,h) \right) \right)
$$

$$
= \sum_{i=1}^{n} \left( 2 \sum_{s'|[i] \in S_i} \sqrt{\frac{P_i(s'[i]|\mathcal{X}[Z_i^P])L^P}{N_{k-1}((s,a)[Z_i^P])}} \right) \left( \hat{P}_{i+1:n} \left( \hat{V}_{k,h}(s_k,h,a_k,h) - V_{h}^*(s_k,h,a_k,h) \right) \right)
$$

$$
\leq \sum_{i=1}^{n} \left( 2 \sum_{s'|[i] \in S_i} \sqrt{\frac{P_i(s'[i]|\mathcal{X}[Z_i^P])L^P}{N_{k-1}((s,a)[Z_i^P])}} \right) \left( \hat{P}_{i+1:n} \left( \hat{V}_{k,h}(s_k,h,a_k,h) - V_{h}^*(s_k,h,a_k,h) \right) \right)
$$

$$
\leq \sum_{i=1}^{n} \left( 2 \sqrt{\frac{|S_i| |S_j| L^P \mathbb{E}_{[i+1:n]}(\cdot [Z_i^P])}{N_{k-1}((s,a)[Z_i^P])}} \right) \left( \hat{P}_{i+1:n} \left( \hat{V}_{k,h}(s_k,h,a_k,h) - V_{h}^*(s_k,h,a_k,h) \right) \right)
$$

$$
\leq \sum_{i=1}^{n} \sqrt{\frac{8X_i^P L^P}{H^2 \sum_{i=1}^{n} \sqrt{TX_j |S_j| L^P} } \sum_{i=1}^{n} 2 \sqrt{8X_i^P L^P} } \right)
$$

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The first inequality is due to the fact that $\bar{V}_{k,h} \geq V^*_h \geq V_{k,h}$. The second and the third inequality is due to Cauchy-Schwarz inequality. The last inequality is because of Lemma E.5 and Lemma E.19.

**Lemma E.15.** Under event $\Lambda_1$, $\Lambda_2$ and $\Omega$, we have

$$\sum_{k,h} \sum_{s_h,a_h} w_{k,h}(s_h, a_h) \left( \hat{R}_k(s_h, a_h) - \bar{R}(s_h, a_h) \right) \leq O \left( \frac{1}{m} \sum_{i=1}^{m} \sqrt{TX_i R L_i^R} \right)$$

**Proof.** By Lemma E.1, we have

$$\sum_{k,h} \sum_{s_h,a_h} w_{k,h}(s_h, a_h) \left( \hat{R}_k(s_h, a_h) - \bar{R}(s_h, a_h) \right)$$

$$\leq \frac{1}{m} \sum_{i=1}^{m} \sum_{k,h} \sum_{s_h,a_h} w_{k,h}(s_h, a_h) \left( \sqrt{2\hat{S}_{R,k,i}(s_h, a_h)L_i^R} \right) \left( \frac{2\hat{S}_{R,k,i}(s_h, a_h)L_i^R}{N_{k-1}(s_h, a_h)[Z_i^R]} \right) + \frac{8L_i^R}{3N_{k-1}(s_h, a_h)[Z_i^R]}$$

$$\leq \frac{1}{m} \sum_{i=1}^{m} \sum_{k,h} \sum_{s_h,a_h} w_{k,h}(s_h, a_h) \left( \sqrt{2L_i^R} \right) \left( \frac{2L_i^R}{N_{k-1}(s_h, a_h)[Z_i^R]} \right) + \frac{8L_i^R}{3N_{k-1}(s_h, a_h)[Z_i^R]}$$

$$\leq \frac{1}{m} \sum_{i=1}^{m} \sqrt{\sum_{k,h} \sum_{s_h,a_h} 2w_{k,h}(s_h, a_h)L_i^R} \frac{1}{N_{k-1}(s_h, a_h)[Z_i^R]} + \frac{1}{m} \sum_{i=1}^{m} \sum_{k,h} \sum_{s_h,a_h} w_{k,h}(s_h, a_h) \frac{8L_i^R}{3N_{k-1}(s_h, a_h)[Z_i^R]}$$

The second inequality is due to $\hat{S}_{R,k,i}(s,a) \leq 1$. The last inequality is due to Cauchy-Schwarz inequality. By Lemma E.5, we know that the summation is of order $O \left( \frac{1}{m} \sum_{i=1}^{m} \sqrt{TX_i R L_i^R} \right)$. \hfill Q.E.D

**Lemma E.16.** Under event $\Lambda_1$ and $\Lambda_2$, we have

$$(V_{k,h} - \bar{V}_{k,h})(s) = \mathbb{E}_{\text{trajectories}} \left[ \sum_{i=h}^{H} \left( 2CB_k(s, \pi_{k,i}(s)) + \sum_{j=1}^{n} \frac{2H^2 \log(18nT|X[Z^P]|/\delta)}{N_{k-1}(s, \pi_{k,j}(s))[Z_j^P]} \right) \mid s_h = s, \pi_k \right]$$

The expectation is over all possible trajectories in episode $k$ given $s_h = s$ following policy $\pi_k$.

**Proof.**

$$(V_{k,h} - \bar{V}_{k,h})(s)$$

$$= 2CB_k(s, \pi_{k,h}(s)) + \mathbb{P}_k(V_{k,h+1}(s) - \bar{V}_{k,h+1}(s))$$

$$= 2CB_k(s, \pi_{k,h}(s)) + (\mathbb{P}_k - \mathbb{P})(V_{k,h+1} - \bar{V}_{k,h+1})(s, \pi_{k,h}(s)) + \mathbb{P}(V_{k,h+1} - \bar{V}_{k,h+1})(s, \pi_{k,h}(s))$$

$$\cdots$$

$$= \mathbb{E}_{\text{trajectories}} \left[ \sum_{i=h}^{H} \left( 2CB_k(s, \pi_{k,i}(s_i)) + (\mathbb{P}_k - \mathbb{P})(V_{k,i+1} - \bar{V}_{k,i+1})(s_i, \pi_{k,i}(s_i)) \right) \mid s_h = s, \pi_k \right]$$

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The second term can be bounded as:

\[
(\hat{P}_k - \mathbb{P})(\hat{V}_{k,i+1} - V_{k,i+1})(s_i, \pi_{k,i}(s_i)) \\
\leq |\hat{P}_k - \mathbb{P}|1|\hat{V}_{k,i+1} - V_{k,i+1}|_{\infty}(s_i, \pi_{k,i}(s)) \\
\leq H \sum_{i=1}^{n} |\hat{P}_{k,i} - \mathbb{P}_i|1(|s_i, \pi_{k,i}(s_i)) \\
\leq \sum_{j=1}^{n} \sqrt{\frac{2H^2L^P}{N_{k-1}((s, \pi_{k,j}(s))[Z_j^P]})}
\]

\[\square\]

**Lemma E.17.** Under event \( \Lambda_1 \) and \( \Lambda_2 \), we have

\[
\sum_{k=1}^{K} \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{X}} w_{k,h}(s,a) CB_k^2(s,a) \leq \sum_{i=1}^{m} \frac{2(m+2)H^2L^R_i X_i^R}{m^2} + \sum_{i=1}^{n} 128n(m+n)H^2X_i^P L^P \sum_{j=1}^{n} |S_j|L^P
\]

Which has only logarithmic dependence on \( T \).

Note that this bound is loose w.r.t parameters such as \( H, |S_j|, X_i^P \) and \( X_i^R \). However, it is acceptable since we regard \( T \) as the dominant parameter. This bound doesn’t influence the dominant factor in the final regret.

**Proof.** By the definition of \( CB_k(s,a), CB^R_k(s,a) \) and \( CB^P_k(s,a) \), we have

\[
CB_k^2(s,a) \leq (m+n) \left( \sum_{i=1}^{m} \frac{1}{m^2} (CB_k^R(s,a))^2 + \sum_{i=1}^{n} (CB_k^P(s,a))^2 \right)
\]

\[
\leq 2(m+n) \sum_{i=1}^{m} \frac{1}{m^2} \left( \frac{2H^2L^R_i}{N_{k-1}((s,a)[Z_i^R])} + \frac{64(L_i^R)^2}{9(N_{k-1}((s,a)[Z_i^R])^2)\right)
\]

\[
+ 4n(m+n) \sum_{i=1}^{n} \left( \frac{4H^2L^P}{N_{k-1}((s,a)[Z_i^P])} + \frac{2HL^P}{N_{k-1}((s,a)[Z_i^P])} \right)
\]

The second inequality is due to \( \hat{\sigma}_{R_i}^2(s,a) \leq 1, \hat{\sigma}_{P_i}^2(\hat{V}_{k,h+1}, s, a) \leq H^2 \) and \( u_{k,h,i}(s,a) \leq H \).

Now we are ready to bound \( \sum_{k=1}^{K} \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{X}} w_{k,h}(s,a) CB_k^2(s,a) \):

\[
\sum_{k=1}^{K} \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{X}} w_{k,h}(s,a) CB_k^2(s,a)
\]

\[
\leq \sum_{k=1}^{K} \sum_{h=1}^{H} \sum_{(s,a) \in \mathcal{X}} w_{k,h}(s,a) \left( \sum_{i=1}^{m} \frac{2(m+2)H^2L^R_i}{m^2N_{k-1}((s,a)[Z_i^R])} + \sum_{i=1}^{n} \frac{128n(m+n)H^2L^P \sum_{j=1}^{n} |S_j|L^P}{N_{k-1}((s,a)[Z_i^P])} \right)
\]

\[
\leq \sum_{i=1}^{m} \frac{2(m+2)H^2L^R_i X_i^R}{m^2} + \sum_{i=1}^{n} 128n(m+n)H^2X_i^P L^P \sum_{j=1}^{n} |S_j|L^P
\]

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Lemma E.18. Under event $\Lambda_1$ and $\Lambda_2$, we have

$$\sum_{k=1}^{K} \sum_{h=1}^{H} \sum_{s,a} w_{k,h}(s,a) \mathbb{E}_{s'[1:i] \sim \mathbb{P}_{[1:i]}} (s,a) \left( \mathbb{E}_{s'[i+1:n] \sim \mathbb{P}_{[i+1:n]}} (s,a) \left( \bar{V}_{k,h+1} - V_{k,h+1} \right) \right)^2 \leq O(\log T),$$

where $O$ hides the dependence on other parameters such as $H, X^P, X^R$ except $T$.

Proof. For notation simplicity, we use $\mathbb{E}_{i}$ and $\mathbb{E}_{[i:j]}$ as a shorthand of $\mathbb{E}_{s'[i] \sim \mathbb{P}_{[i]}(s,a|Z^P_{i})}$ and $\mathbb{E}_{s'[i:j] \sim \mathbb{P}_{[i:j]}(s,a|Z^P_{j})}$.

Define $U_k(s,a) = 2CB_k(s,a) + \sum_{j=1}^{n} \sqrt{\frac{2H^2L^P}{N_{i-1}((s,a)|Z^P_{j})}}$. By Lemma E.16, we have

$$\sum_{k=1}^{K} \sum_{h=1}^{H} \sum_{s,a} w_{k,h+1}(s,a) \left( \bar{V}_{k,h+1} - V_{k,h+1} \right)^2 (s,a)$$

$$\leq \sum_{k,h,s,a} w_{k,h+1}(s,a) \left( \sum_{h_1=h+1}^{H} \sum_{s_{h_1},a_{h_1}} \Pr(s_{h_1},a_{h_1}|s_{h+1} = s, a_{h+1} = a) U_k(s_{h_1},a_{h_1}) \right)^2$$

$$\leq \sum_{k,h,s,a} w_{k,h+1}(s,a) H \sum_{h_1=h+1}^{H} \left( \sum_{s_{h_1},a_{h_1}} \Pr(s_{h_1},a_{h_1}|s_{h+1} = s, a_{h+1} = a) U_k(s_{h_1},a_{h_1}) \right)^2$$

$$\leq \sum_{k,h,s,a} w_{k,h+1}(s,a) H \sum_{h_1=h+1}^{H} \sum_{s_{h_1},a_{h_1}} \Pr(s_{h_1},a_{h_1}|s_{h+1} = s, a_{h+1} = a) (U_k(s_{h_1},a_{h_1}))^2$$

$$= \sum_{k,h} H \sum_{h_1=h+1}^{H} \sum_{s_{h_1},a_{h_1}} w_{k,h_1}(s_{h_1},a_{h_1}) (U_k(s_{h_1},a_{h_1}))^2$$

$$\leq \sum_{k,h} H^2 \sum_{s_{h},a_{h}} w_{k,h}(s_{h},a_{h}) (U_k(s_{h},a_{h}))^2$$

(67)
Plugging the definition of $U_k(s,a)$ into Eqn. 67, we have:

$$\sum_{k=1}^{K} \sum_{h=1}^{H} \sum_{s,a} w_{k,h+1}(s,a) (V_{k,h+1} - V_{k,h+1})^2(s,a)$$ (68)

$$\leq \sum_{k,h} 2H^2 \sum_{s_h,a_h} w_{k,h}(s_h,a_h) \left( 2CB_k(s,a) + \sum_{j=1}^{n} \frac{2H^2L^P}{N_{k-1}((s,a)[Z_j^P])} \right)^2$$ (69)

$$\leq \sum_{k,h} 2nH^2 \sum_{s_h,a_h} w_{k,h}(s_h,a_h) \left( CB_k^2(s,a) + \sum_{j=1}^{n} \frac{2H^2L^P}{N_{k-1}((s,a)[Z_j^P])} \right)$$ (70)

$$\leq \sum_{k,h} 2nH^2 \sum_{s_h,a_h} w_{k,h}(s_h,a_h) CB_k^2(s,a) + 16nH^2X^P_k L^P$$ (71)

The last inequality is due to Lemma E.5. We can bound $\sum_{k,h} 2nH^2 \sum_{s_h,a_h} w_{k,h}(s_h,a_h) CB_k^2(s,a)$ by Lemma E.17. Summing up over all terms, we can show that $\sum_{k=1}^{K} \sum_{h=1}^{H} \sum_{s,a} w_{k,h+1}(s,a) (V_{k,h+1} - V_{k,h+1})^2(s,a)$ is of order $O(1)$. □

Lemma E.19. Under event $\Lambda_1$ and $\Lambda_2$, for any $i \in [n]$, we have

$$\sum_{k=1}^{K} \sum_{h=1}^{H} \sum_{(s,a) \in X} w_{k,h}(s,a) u_{k,h,i}(s,a) \leq O(H^2 \sum_{j=1}^{n} \sqrt{TX^P_j |\mathcal{S}_j^P| L^P}),$$

Here $O$ hides the lower order terms w.r.t. $T$.

Proof. For notation simplicity, we use $\mathbb{E}_i$ and $\mathbb{E}_{[i:j]}$ as a shorthand of $\mathbb{E}_{s'[i] \sim P_i((s,a)[Z_i^P])}$ and $\mathbb{E}_{s'[i:j] \sim P_{[i:j]}((s,a)[Z_j^P])}$. For those expectation w.r.t the empirical transition $\hat{P}_k$, we use $\hat{E}_k$ to denote the corresponding expectation. $u_{k,h,i}(s,a)$ is defined as:

$$u_{k,h,i}(s,a) = \hat{E}_{[1:i]} \left[ \left( \hat{E}_{[i+1:n]} (\hat{V}_{k,h+1} - V_{k,h+1}) (s') \right)^2 \right].$$
\[
\sum_{k,h,s,a} w_{k,h}(s, a) \hat{E}[1:i] \left[ (\hat{E}_{[i+1:n]} (\tilde{V}_{k,h+1} - \tilde{V}_{k,h+1}) (s'))^2 \right] 
\]

(72)

\[
= \sum_{k,h,s,a} w_{k,h}(s, a) \hat{E}[1:i] \left[ (\hat{E}_{[i+1:n]} (\tilde{V}_{k,h+1} - \tilde{V}_{k,h+1}) (s'))^2 \right] 
\]

(73)

\[
+ \sum_{k,h,s,a} w_{k,h}(s, a) \hat{E}[1:i] \left[ (\hat{E}_{[i+1:n]} (\tilde{V}_{k,h+1} - \tilde{V}_{k,h+1}) (s'))^2 \right] 
\]

(74)

\[
- \sum_{k,h,s,a} w_{k,h}(s, a) \hat{E}[1:i] \left[ (\hat{E}_{[i+1:n]} (\tilde{V}_{k,h+1} - \tilde{V}_{k,h+1}) (s'))^2 \right] 
\]

\[
+ \sum_{k,h,s,a} w_{k,h}(s, a) \hat{E}[1:i] \left[ (\hat{E}_{[i+1:n]} (\tilde{V}_{k,h+1} - \tilde{V}_{k,h+1}) (s'))^2 \right] 
\]

(75)

That is

We can bound Eqn. 74 and Eqn. 75 by Lemma B.1. For Eqn. 74, we have

\[
\sum_{k,h,s,a} w_{k,h}(s, a) \left| \hat{E}[1:i] (s,a) - P[1:i] (|s,a|) \right|^2 \]

\[
\leq \sum_{k,h,s,a} w_{k,h}(s, a) \sqrt{\sum_{j=1}^{i} \frac{|S_j|L^P}{N_{k-1} ((s,a)[Z^P_j])} H^2} 
\]

\[
\leq 8H^2 \sum_{j=1}^{i} \sqrt{T X^P_j |S_j|L^P} 
\]

The first inequality is due to \( (\hat{E}_{[i+1:n]} (\tilde{V}_{k,h+1} - \tilde{V}_{k,h+1}) (s'))^2 \leq H^2 \) for any given \( s'[1 : i] \).

The second inequality is due to Lemma B.1. The third inequality is due to Lemma E.5.
For Eqn. 75, similarly we have

\[
\sum_{k,h,s,a} w_{k,h}(s,a)\mathbb{E}_{\{i\}} \left[ (\hat{E}_{[i+1:n]} (\hat{V}_{k,h+1} - \hat{V}_{k,h+1}) (s'))^2 \right] \\
- \sum_{k,h,s,a} w_{k,h}(s,a)\mathbb{E}_{\{i\}} \left[ (E_{[i+1:n]} (\hat{V}_{k,h+1} - V_{k,h+1}) (s'))^2 \right] \\
\leq 2H \sum_{k,h,s,a} w_{k,h}(s,a)\mathbb{E}_{\{i\}} \left[ (E_{[i+1:n]} (\hat{V}_{k,h+1} - V_{k,h+1}) (s')) - (E_{[i+1:n]} (\hat{V}_{k,h+1} - V_{k,h+1}) (s')) \right] \\
\leq 2H \sum_{k,h,s,a} w_{k,h}(s,a)\mathbb{E}_{\{i\}} \left[ H \left| \hat{P}_{[i+1:n]}(\cdot|s,a) - \mathbb{P}_{[i+1:n]}(\cdot|s,a) \right| \right] \\
\leq 2H^2 \sum_{k,h,s,a} w_{k,h}(s,a) \sum_{j=i+1}^{n} \sqrt{\frac{|S_j|L_P}{N_{k-1}((s,a)|Z_j^F)}} \\
= 2H^2 \sum_{k,h,s,a} w_{k,h}(s,a) \sum_{j=i+1}^{n} \sqrt{\frac{|S_j|L_P}{N_{k-1}((s,a)|Z_j^F)}} \\
\leq 16H^2 \sum_{j=i+1}^{n} \sqrt{TX_j^P|S_j|L_P}
\]

Eqn. 73 can be bounded by Lemma E.18, which has only logarithmic dependence on T. □

Appendix F. Proof of Theorem 3

Proof. We consider the following two hard instances.

The first instance is an extension of the hard instance in Jaksch et al. (2010). They proposed a hard instance for non-factored weakly-communicating MDP, which indicates that the lower bound in that setting is \( \Omega(\sqrt{DSAT}) \). When transformed to the hard instance for non-factored episodic MDP, it shows a lower bound of order \( \Omega(\sqrt{HSAT}) \) in episodic setting Azar et al. (2017); Jin et al. (2018). Consider a factored MDP instance with \( d = m = n \) and \( X[Z_i^R] = X[Z_i^P] = X_i = S_i \times A_i \), \( i = 1, \ldots, n \). This factored MDP can be decomposed into \( n \) independent non-factored MDPs. By simply setting these \( n \) non-factored MDPs to be the construction used in Jaksch et al. (2010), the regret for each MDP is \( \Omega(\sqrt{H|X[Z_i^P]|T}) \). The total regret is \( \Omega(\sum_{i=1}^{n} \sqrt{H|X[Z_i^P]|T}) \). Note that in our setting, the reward \( R = \frac{1}{m} \sum_{i=1}^{m} R_i \) is \( [0,1] \)-bounded. Therefore, we need to normalize the reward function in the hard instance by a factor of \( \frac{1}{m} \). This leads to a final lower bound of order \( \Omega(\frac{1}{m} \sum_{i=1}^{n} \sqrt{H|X[Z_i^P]|T}) = \Omega(\frac{1}{m} \sum_{i=1}^{n} \sqrt{H|X[Z_i^P]|T}) \). Similar construction has been used to prove the lower bound for factored weakly-communicating MDP Xu and Tewari (2020).

The second hard instance is an extension of the hard instance for stochastic multi-armed bandits. The lower bound of stochastic multi-armed bandits shows that the regret of a MAB problem with \( k_0 \) arms in \( T_0 \) steps is lower bounded by \( \Omega(\sqrt{k_0T_0}) \). Consider a factored MDP instance with \( d = m = n \) and \( X[Z_i^R] = X[Z_i^P] = X_i = S_i \times A_i \), \( i = 1, \ldots, n \). There are \( m \) independent reward functions, each associated with an independent deterministic transition. For reward function \( i \), there are \( \log_2(|S_i|) \) levels of states, which form a binary tree of depth
There are $2^{h-1}$ states in level $h$, and thus $|S_i| - 1$ states in total. Only those states in level $\log_2(|S_i|)$ have non-zero rewards, the number of which is $\frac{|S_i|}{2}$. After taking actions in level $\log_2(|S_i|)$, the agent will transit back to state $s_0$ in level 1. That is to say, the agent can enter "reward states" $\frac{KH}{\log(|S_i|)}$ times in one episode. For each reward function $i$, the instance can be regarded as an MAB problem with $\frac{K|H|}{\log(|S_i|)}$ steps and $|S_i|$ arms, thus the regret for reward $i$ is $\Omega(\sqrt{\frac{X_Z R_i T}{\log(|X_Z R_i|)}})$. In this construction, the total reward function can be regarded as the average of $m$ independent reward functions of $m$ stochastic MDP. This indicates that the lower bound is $\Omega\left(\frac{1}{m} \sum_{i=1}^{m} \sqrt{\frac{X_Z R_i T}{\log(|X_Z R_i|)}} \right)$.

To sum up, the regret is lower bounded by

$$\Omega\left(\max \left\{ \frac{1}{m} \sum_{i=1}^{m} \sqrt{\frac{X_Z R_i T}{\log(|X_Z R_i|)}}, \frac{1}{m} \sum_{j=1}^{n} \sqrt{H X [Z_j^R] T} \right\} \right),$$

which is of the same order as

$$\Omega\left(\frac{1}{m} \sum_{i=1}^{m} \sqrt{\frac{X_Z R_i T}{\log(|X_Z R_i|)}} + \frac{1}{n} \sum_{j=1}^{n} \sqrt{H X [Z_j^R] T} \right).$$

\[\square\]

Appendix G. Omitted Details in Section 5

G.1 Specific instances

We further explain the difference with two specific examples in Fig. G.1. No matter which setting the previous work considers, the main idea of the algorithms in Efroni et al. (2020); Brantley et al. (2020) is to explore the MDP environment, and then find a near-optimal policy satisfying that the expected cumulative cost less than a constant vector $B_0$, i.e. $\mathbb{E}[\sum_{h \in [H]} c_h] \leq B_0$. However, in our setting, the agent has to terminate the interaction once the total costs in this episode exceed budget $B$. Because of this difference, their algorithm will converge to an sub-optimal policy with unbounded regret in our setting. In the first MDP instance (Fig. G.1), the agent starts from state $s_0$. After taking action $a_1$, it will transit to $s_1$ with a deterministic cost $c_1 = 0.5$. After taking action $a_2$, it will transit to
The cost of taking $a_2$ is 0 with prob. 0.5, and 1 with prob 0.5. There are no rewards in state $s_0$. In state $s_1$ and $s_2$, the agent will not suffer any costs. The deterministic rewards are 0.5 and 0.8 respectively. $s_3$ and $s_4$ are termination states. The budget $B_0$ is 0.5. For this MDP instance, the optimal policy is to take action $a_1$ in $s_0$, since the agent can receive total rewards 0.5 by taking $a_1$. If taking action $a_2$, the agent will terminate at state $s_2$ with no rewards with prob. 0.5, which leads to an expected total rewards of 0.4. However, if we run the algorithm in Efroni et al. (2020); Brantley et al. (2020), the algorithm will converge to the policy that always selects action $a_2$ in $s_0$, since the expected cumulative cost of taking $a_2$ is $0.5 \leq B_0$.

We further show that the policies defined in the previous literature are not expressive enough in our setting. In the second instance, the agent starts in state $s_0$ with one action $a_0$. By taking $a_0$, the agent transits to $s_1$ with no rewards. The cost of taking $a_0$ is 0 with prob. 0.5, and 1 with prob 0.5. In $s_1$, the agent needs to decide to take $a_1$ or $a_2$, with deterministic costs of 0 and 0.5 respectively. After taking $a_1$, the agent will transits to $s_2$, in which it can obtain a reward $r_3 = 0.5$. While by taking $a_2$, the agent can transits to $s_3$, and obtain a reward $r_4 = 1$. The budget $B = 0.5$. In this instance, the action taken in $s_1$ depends on the remaining budget of the agent. That is to say, the policy is not expressive enough if it is defined as a mapping from state to action. Instead, we need to define it as a mapping from state and remaining budget to action. However, the previous literature only consider policies on the state space, which cannot deal with this problem.

G.2 Algorithm and Regret

We denote $V_h^\pi(s, b)$ as the value function in state $s$ at horizon $h$ following policy $\pi$, and the agent’s remaining budget is $b$. For notation simplicity, we use $P_s V(s, a, b)$ as a shorthand of $\sum_{s'} P(s'|s, a)V(s', b)$, and $P_C V(s, a)$ as a shorthand of $\sum_{c_0} P(C(s, a) = c_0 | s, a)V(s', b - c_0)$. We use $P_{C,i}(c_0 | s, a)$ to denote the “transition probability” of budget $i$, i.e. $P(C_i(s, a) = c_0 | s, a)$. The Bellman Equation of our setting is written as:

$$
V_h^\pi(s, b) = \begin{cases} 
\hat{R}(s, \pi_h(s, b)) + P_s P_C V_{h+1}^\pi(s, \pi_{h+1}(s, b), b) & b > 0 \\
0 & b \leq 0
\end{cases}
$$

(76)

Suppose $N_k(s, a)$ denotes the number of times $(s, a)$ has been encountered in the first $k$ episodes. We estimate the mean value of $r(s, a)$, the transition matrix $P_s$ and $P_c$ in the following way:

$$
\hat{R}_k(s, a) = \frac{\sum_{k,h} \mathbb{I}[s_{k,h} = s, a_{k,h} = a] \cdot r_{k,h}}{N_{k-1}(s, a)}
$$

$$
\hat{P}_s(s', s, a) = \frac{N_{k-1}(s, a, s')}{N_{k-1}(s, a)}
$$

$$
\hat{P}_{C,i}(C_i(s, a) = c_0 | s, a) = \frac{\sum_{k,h} \mathbb{I}[c_{k,h,i} = c_0, s_{k,h} = s, a_{k,h} = a]}{N_{k-1}(s, a)}
$$

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Following the definition in the factored MDP setting, we define the confidence bonus for rewards and transition respectively:

\[
CB^R_k(s, a) = \sqrt{\frac{2\sigma^2_R(s, a) \log(2SAT)}{N_{k-1}(s, a)}} + \frac{8 \log(2SAT)}{3N_{k-1}(s, a)}
\]

\[
CB^P_{k,i}(s, a, b) = \sqrt{\frac{4\hat{\sigma}_P^2(\hat{V}_{k,h+1}, s, a, b)L}{N_{k-1}(s, a)}} + \sqrt{\frac{2u_{k,h,i}(s, a, b)L}{N_{k-1}(s, a)}}
\]

\[
+ \sqrt{\frac{32H^2L}{N_{k-1}(s, a)}} \sum_{j=1}^n \left( \frac{\sqrt{4|S_i|L^P}}{N_{k-1}(s, a)} + \sqrt{\frac{4|S_j|L^P}{3N_{k-1}(s, a)}} \right)
\]

\[
+ \sum_{j=1}^n H \left( \sqrt{\frac{4|S_i|L^P}{N_{k-1}(s, a)}} + \sqrt{\frac{4|S_j|L^P}{3N_{k-1}(s, a)}} \right)^2, \quad i = 0, \ldots, d,
\]

where \( L = \log(2dSAT) + d \log(mB) \) is the logarithmic factors because of union bounds. The additional \( d \log(mB) \) is because that we need to take union bounds over all possible budget \( b \). This difference compared with factored MDP is mainly due to the noised offset model.

\( CB^R_k(s, a) \) is the confidence bonus for rewards, and \( \hat{\sigma}_R(s, a) \) denotes the empirical variance of reward \( R(s, a) \), which is defined as:

\[
\hat{\sigma}_R(s, a) = \frac{1}{N_{k-1}(s, a)} \sum_{k=1}^{k-1} \sum_{h=1}^H \sum_1 [(s, a)_{k,h} = (s, a)] \cdot (r_{k,h}(s_{k,h}, a_{k,h}))^2 - \left( \bar{R}_k(s, a) \right)^2
\]

\( CB^P_{k,0}(s, a) \) is the confidence bonus for state transition estimation \( \hat{P}_s \), and \( \{CB^P_{k,i}(s, a)\}_{i=1,\ldots,d} \) is the confidence bonus for budget transition estimation \( \{\hat{P}_{c,i}\}_{i=1,\ldots,d} \).

\( \hat{\sigma}^2_P(\hat{V}_{k,h+1}, s, a, b) \) is the empirical variance of corresponding transition:

\[
\hat{\sigma}^2_P(\hat{V}_{k,h+1}, s, a, b) = \text{Var}_{s' \sim \bar{\hat{P}}_{S,k}(|s, a|Z_t^P)} \left( \mathbb{E}_{c \sim \bar{\hat{P}}_{C,k}(|s, a|)} \hat{V}_{k,h+1}(s', b - c) \right)
\]

\[
\hat{\sigma}^2_P(\hat{V}_{k,h+1}, s, a, b) = \mathbb{E}_{s' \sim \bar{\hat{P}}_{S,k}(|s, a|)} \mathbb{E}_{c_{[i-1]} \sim \bar{\hat{P}}_{C,k,[i-1]}(|s, a|)} \left[ \text{Var}_{c_i \sim \bar{\hat{P}}_{C,k,i}(|s, a|)} \left( \mathbb{E}_{c_{[i+1:n]} \sim \bar{\hat{P}}_{C,k,[i+1:d]}(|s, a|)} \hat{V}_{k,h+1}(s', b - c) \right) \right],
\]

where \( \bar{\hat{P}}_{C,k,[d_1:d_2]} = \prod_{i=d_1}^{d_2} \bar{\hat{P}}_{c,k,i} \).

\( \sqrt{\frac{2u_{k,h,i}(s, a, b)}{N_{k-1}(s, a)}} \) is added to compensate the error due to the difference between \( V^*_h \) and \( \hat{V}_{k,h+1} \), where \( u_{k,h,i}(s, a) \) is defined as:

\[
u_{k,h,0}(s, a, b) = \mathbb{E}_{s' \sim \bar{\hat{P}}_{S,k}(|s, a|)} \left[ \left( \mathbb{E}_{c \sim \bar{\hat{P}}_{C,k}(|s, a|)} (\hat{V}_{k,h+1} - \bar{V}_{k,h+1}) (s', b - c) \right)^2 \right]
\]

\[
u_{k,h,i}(s, a, b) = \mathbb{E}_{s' \sim \bar{\hat{P}}_{S,k}(|s, a|)} \mathbb{E}_{c_{[i-1]} \sim \bar{\hat{P}}_{C,k,[i-1]}(|s, a|)} \left[ \left( \mathbb{E}_{c_{[i+1:n]} \sim \bar{\hat{P}}_{C,k,[i+1:d]}(|s, a|)} (\hat{V}_{k,h+1} - \bar{V}_{k,h+1}) (s', b - c) \right)^2 \right].
\]

We calculate the optimistic value function and find the optimal policy \( \pi \) via the following value iteration in our algorithm:
\[
\bar{V}_h(s, b) = \left\{ \begin{array}{ll}
\max_a \left\{ \left[ \hat{R}(s, a) + CB(s, a) + \hat{P}_k \hat{V}_{h+1}(s, a, b) \right] \right\} & b > 0 \\
0 & b \leq 0
\end{array} \right.
\]  

Algorithm 3 UCB Algorithm for RLwK

**Input:** \( \delta \)

Initialize \( N(s, a) = 0 \) for any \( (s, a) \in \mathcal{X} \)

for episode \( k = 1, 2, \ldots \) do

Set \( \bar{V}_{k,H+1}(s, b) = \bar{V}_{k,H+1}(s, b) = 0 \) for all \( s, a, b \).

5: Let \( K = \{(s, a) \in \mathcal{S} \times \mathcal{A} : N_k(s, a) > 0\} \)

for horizon \( h = H, H - 1, \ldots, 1 \) do

for \( s \in \mathcal{S} \) and all possible budget \( b \) from 0 to \( B \) do

for \( a \in \mathcal{A} \) do

if \( (s, a) \in K \) then

10: \( \bar{Q}_{k,h}(s, a, b) = \min \{ H, \hat{R}_k(s, a) + CB_k(s, a) + \hat{P}_{S,k} \hat{P}_{C,k} \bar{V}_{k,h+1}(s, a, b) \} \)

else

\( \bar{Q}_{k,h}(s, a, b) = H \)

end if

end for

end for

15: \( \pi_{k,h}(s, b) = \arg \max_a \bar{Q}_{k,h}(s, a, b) \)

\( \bar{V}_{k,h}(s, b) = \max_{a \in \mathcal{A}} Q_{k,h}(s, a, b) \)

\( \bar{V}_{k,h}(s, b) = \max \left\{ 0, \hat{R}_k(s, \pi_{k,h}) - CB_k(s, \pi_{k,h}, s, b) + \hat{P}_k \bar{V}_{k,h+1}(s, \pi_{k,h}, b) \right\} \)

end for

end for

20: for step \( h = 1, \ldots, H \) do

Take action \( a_{k,h} = \arg \max_a \bar{Q}_{k,h}(s_{k,h}, a) \)

end for

Update history trajectory \( \mathcal{L} = \mathcal{L} \cup \{s_i, a_i, r_i, s_{i+1}\}_{i=1,2,\ldots,t_k} \)

end for

*Proof.* (Proof of Theorem 4) The proof follows almost the same proof framework of Thm. 2. \( \log(SAT) + d \log(Bm) \) is due to union bound over all possible \( T, s, a \) and budget \( b \). This difference is because of the additional union bounds over all budget \( b \). \( \square \)