Provably Efficient Causal Reinforcement Learning with Confounded Observational Data

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Abstract

Empowered by neural networks, deep reinforcement learning (DRL) achieves tremendous empirical success. However, DRL requires a large dataset by interacting with the environment, which is unrealistic in critical scenarios such as autonomous driving and personalized medicine. In this paper, we study how to incorporate the dataset collected in the offline setting to improve the sample efficiency in the online setting. To incorporate the observational data, we face two challenges. (a) The behavior policy that generates the observational data may depend on unobserved random variables (confounders), which affect the received rewards and transition dynamics. (b) Exploration in the online setting requires quantifying the uncertainty given both the observational and interventional data. To tackle such challenges, we propose the deconfounded optimistic value iteration (DOVI) algorithm, which incorporates the confounded observational data in a provably efficient manner. DOVI explicitly adjusts for the confounding bias in the observational data, where the confounders are partially observed or unobserved. In both cases, such adjustments allow us to construct the bonus based on a notion of information gain, which takes into account the amount of information acquired from the offline setting. In particular, we prove that the regret of DOVI is smaller than the optimal regret achievable in the pure online setting when the confounded observational data are informative upon the adjustments.

1 Introduction

Empowered by the breakthrough in neural networks, deep reinforcement learning (DRL) achieves significant empirical successes in various scenarios [19, 23, 36, 37]. Learning an expressive function approximator necessitates collecting a large dataset. Specifically, in the online setting, it requires the agent to interact with the environment for a large number of steps. For example, to learn a human-level policy for playing Atari games, the agent has to interact with a simulator for more than 10^8 steps [13]. However, in most scenarios, we do not have access to a simulator that allows for trial and error without any cost. Meanwhile, in critical scenarios, e.g., autonomous driving and personalized medicine, trial and error in the real world is unsafe and even unethical. As a result, it remains challenging to apply DRL to more scenarios.

To bypass such a barrier, we study how to incorporate the dataset collected offline, namely the observational data, to improve the sample efficiency of RL in the online setting [21]. In contrast to the interventional data collected online in possibly expensive ways, observational data are often abundantly available in various scenarios. For example, in autonomous driving, we have access to trajectories generated by the drivers. As another example, in personalized medicine, we have access to electronic health records from doctors. However, to incorporate the observational data in a provably efficient way, we have to address two challenges.

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- The observational data are possibly confounded. Specifically, there often exist unobserved random variables, namely confounders, that causally affect the agent and the environment at the same time. In particular, the policy used to generate the observational data, namely the behavior policy, possibly depends on the confounders. Meanwhile, the confounders possibly affect the received rewards and the transition dynamics.

  In the example of autonomous driving [9, 22], the drivers may be affected by complicated traffic or poor road design, resulting in traffic accidents even without misconduct. The complicated traffic and poor road design subsequently affect both the action of the drivers and the outcome. Therefore, it is unclear from the observational data whether the accidents are due to the actions adopted by the drivers. Agents trained with such observational data may be unwilling to take any actions under complicated traffic, jeopardizing the safety of passengers.

  In the example of personalized medicine [8, 29], the patients may not be compliant with prescriptions and instructions, which subsequently affects both the treatment and the outcome. As another example, the doctor may prescribe medicine to patients based on patients' socioeconomic status (which could be inferred by the doctor through interacting with the patients). Meanwhile, socioeconomic status affects the patients' health condition and subsequently plays the role of the confounder. In both scenarios, such confounders may be unavailable due to privacy or ethical concerns. Such a confounding issue makes the observational data uninformative and even misleading for identifying and estimating the causal effect, which is crucial for decision-making in the online setting. In all the examples, it is unclear from the observational data whether the outcome is due to the actions adopted.

- Even without the confounding issue, it remains unclear how the observational data may facilitate exploration in the online setting, which is the key to the sample efficiency of RL. At the core of exploration is uncertainty quantification. Specifically, quantifying the uncertainty that remains given the dataset collected up to the current step, including the observational data and the interventional data, allows us to construct a bonus. When incorporated into the reward, such a bonus encourages the agent to explore the less visited state-action pairs with more uncertainty. In particular, constructing such a bonus requires quantifying the amount of information carried over by the observational data from the offline setting, which also plays a key role in characterizing the regret, especially how much the observational data may facilitate reducing the regret.

  Uncertainty quantification becomes even more challenging when the observational data are confounded. Specifically, as the behavior policy depends on the confounders, there is a mismatch between the data generating processes in the offline setting and the online setting. As a result, it remains challenging to quantify how much information carried over from the offline setting is useful for the online setting, as the observational data are uninformative and even misleading due to the confounding issue.

Contribution. To study causal reinforcement learning, we propose a class of Markov decision processes (MDPs), namely confounded MDPs, which captures the data generating processes in both the offline setting and the online setting as well as their mismatch due to the confounding issue. In particular, we study two tractable cases of confounded MDPs in the episodic setting with linear function approximation [7, 16, 42, 43].

- In the first case, the confounders are partially observed in the observational data. Assuming that an observed subset of the confounders satisfies the backdoor criterion [32], we propose the deconfounded optimistic value iteration (DOVI) algorithm, which explicitly corrects for the confounding bias in the observational data using the backdoor adjustment.
- In the second case, the confounders are unobserved in the observational data. Assuming that there exists an observed set of intermediate states that satisfies the frontdoor criterion [32], we propose an extension of DOVI, namely DOVI$^+$, which explicitly corrects for the confounding bias in the observational data using the composition of two backdoor adjustments. We remark that DOVI$^+$ follows the same principle of design as DOVI and defer the discussion of DOVI$^+$ to §A.

In both cases, the adjustments allow DOVI and DOVI$^+$ to incorporate the observational data into the interventional data while bypassing the confounding issue. It further enables estimating the causal effect of a policy on the received rewards and the transition dynamics with enlarged effective sample size. Moreover, such adjustments allow us to construct the bonus based on a notion of information gain, which takes into account the amount of information carried over from the offline setting.

In particular, we prove that DOVI and DOVI$^+$ attain the $\Delta_H \cdot \sqrt{d^3 H^3 T}$-regret up to logarithmic factors, where d is the dimension of features, H is the length of each episode, and $T = HK$ is the number of steps taken in the online setting, where K is the number of episodes. Here the multiplicative factor $\Delta_H > 0$ depends on d, H, and a notion of information gain that quantifies the amount of information obtained from the interventional data additionally when given the properly adjusted observational data. When the observational data are unavailable or uninformative upon the adjustments, Δ_H is a logarithmic factor. Correspondingly, DOVI and DOVI$^+$ attain the optimal $\sqrt{T}$-regret achievable in the pure online setting [7, 16, 42, 43]. When the observational data are sufficiently informative upon the adjustments, Δ_H decreases towards zero as the effective sample size of the observational data increases, which quantifies how much the observational data may facilitate exploration in the online setting.

Related Work. Our work is related to the study of causal bandit [20]. The goal of causal bandit is to obtain the optimal intervention in the online setting where the data generating process is described by a causal diagram. The previous study establishes causal bandit algorithms in the online setting [26, 34], the offline setting [17, 18], and a combination of both settings [11]. In contrast to this line of work, we study causal RL in a combination of the online setting and the offline setting. Causal RL is more challenging than causal bandit, which corresponds to $H = 1$, as it involves the transition dynamics and is more challenging in exploration. See §B for a detailed literature review on causal bandit.

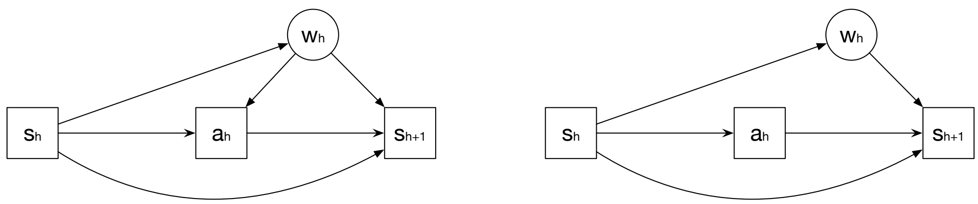
Our work is related to the study of causal RL considered in various settings. [45] propose a model-based RL algorithm that solves dynamic treatment regimes (DTR), which involve a combination of the online setting and the offline setting. Their algorithm hinges on the analysis of sensitivity [3, 27, 38, 44], which constructs a set of feasible models of the transition dynamics based on the confounded observational data. Correspondingly, their algorithm achieves exploration by choosing an optimistic model of the transition dynamics from such a feasible set. In contrast, we propose a model-free RL algorithm, which achieves exploration through the bonus based on a notion of information gain. It is worth mentioning that the assumption of [45] is weaker than ours as theirs does not allow for identifying the causal effect. As a result of partial identification, the regret of their algorithm is the same as the regret in the pure online setting as $T \to +\infty$. In contrast, our work instantiates the following framework in handling confounders for reinforcement learning. (a) First, we propose the estimation equation based on the observations, which identifies the causal effect of actions on the cumulative reward. (b) Second, we conduct point estimation and uncertainty quantification based on observations and the estimation equation. (c) Finally, we conduct exploration based on the uncertainty quantification and achieve the regret reduction in the online setting. Consequently, the regret of our algorithm is smaller than the regret in the pure online setting by a multiplicative factor for all T. [25] propose a model-based RL algorithm in a combination of the online setting and the offline setting. Their algorithm uses a variational autoencoder (VAE) for estimating a structural causal model (SCM) based on the confounded observational data. In particular, their algorithm utilizes the actor-critic algorithm to obtain the optimal policy in such an SCM. However, the regret of their algorithm remains unclear. [6] propose a model-based RL algorithm in the pure online setting that learns the optimal policy in a partially observable Markov decision process (POMDP). The regret of their algorithm also remains unclear. [35] utilize generative adversarial reinforcement learning to reconstruct transition dynamics with confounder, and [40] propose a model-based approach for POMDP based on adjustment with proxy variables. [30] consider off-policy policy evaluation under one-decision confounding and constructs worst-case bounds with theoretical guarantee. [4] utilizes states and actions as proxy variables to tackle off-policy policy evaluation with confounders. In contrast, our work utilizes backdoor and frontdoor adjustments to handle confounded observation.

2 Confounded Reinforcement Learning

Structural Causal Model. We denote a structural causal model (SCM) [32] by a tuple (A, B, F, P). Here A is the set of exogenous (unobserved) variables, B is the set of endogenous (observed) variables, F is the set of structural functions capturing the causal relations, which determines an endogenous variable $v \in B$ based on the other exogenous and endogenous variables, and P is the distribution of all the exogenous variables. We say that a pair of variables Y and Z are confounded by a variable W if they are both caused by W.

An intervention on a set of endogenous variables $X \subseteq B$ assigns a value x to X regardless of the other exogenous and endogenous variables as well as the structural functions. We denote by $\mathrm{do}(X = x)$ the intervention on X and write $\mathrm{do}(x)$ if it is clear from the context. Similarly, a stochastic intervention [10, 28] on a set of endogenous variables $X \subseteq B$ assigns a distribution p to X regardless of the other exogenous and endogenous variables as well as the structural functions. We denote by $\mathrm{do}(X \sim p)$ the stochastic intervention on X.

Confounded Markov Decision Process. To characterize a Markov decision process (MDP) in the offline setting with observational data, which are possibly confounded, we introduce an SCM, where the endogenous variables are the states $\{s_h\}_{h\in[H]}$, actions $\{a_h\}_{h\in[H]}$, and rewards $\{r_h\}_{h\in[H]}$. Let $\{w_h\}_{h\in[H]}$ be the confounders. In §3, we assume that the confounders are partially observed, while in §A, we assume that they are unobserved. The set of structural functions F consists of the transition of states $s_{h+1} \sim \mathcal{P}_h(\cdot \,|\, s_h, a_h, w_h)$, the transition of confounders $w_h \sim \widetilde{\mathcal{P}}_h(\cdot \,|\, s_h)$, the behavior policy $a_h \sim \nu_h(\cdot \,|\, s_h, w_h)$, which depends on the confounder w_h, and the reward function $r_h(s_h, a_h, w_h)$. See Figure 1 for the causal diagram that describes such an SCM.



(a) Offline Setting (b) Online Setting

Figure 1: Causal diagrams of the h-th step of the confounded MDP (a) in the offline setting and (b) in the online setting, respectively.

Here a_h and s_{h+1} are confounded by w_h in addition to s_h. We denote such a confounded MDP by the tuple $(\mathcal{S}, \mathcal{A}, \mathcal{W}, H, \overline{\mathcal{P}}, r)$, where H is the length of an episode, $\mathcal{S}$, $\mathcal{A}$, and $\mathcal{W}$ are the spaces of states, actions, and confounders, respectively, $r = \{r_h\}_{h\in[H]}$ is the set of reward functions, and $\overline{\mathcal{P}} = \{\mathcal{P}_h, \widetilde{\mathcal{P}}_h\}_{h\in H}$ is the set of transition kernels. In the sequel, we assume without loss of generality that r_h takes value in $[0, 1]$ for all $h \in [H]$.

In the online setting that allows for intervention, we assume that the confounders $\{w_h\}_{h\in[H]}$ are unobserved. A policy $\pi = \{\pi_h\}_{h\in[H]}$ induces the stochastic intervention $\mathrm{do}(a_1 \sim \pi_1(\cdot \,|\, s_1), \ldots, a_H \sim \pi_H(\cdot \,|\, s_H))$, which does not depend on the confounders. In particular, an agent interacts with the environment as follows. At the beginning of the k-th episode, the environment arbitrarily selects an initial state s_1^k and the agent selects a policy $\pi^k = \{\pi_h^k\}_{h\in[H]}$. At the h-th step of the k-th episode, the agent observes the state s_h^k and takes the action $a_h^k \sim \pi_h^k(\cdot \,|\, s_h^k)$. The environment randomly selects the confounder $w_h^k \sim \widetilde{\mathcal{P}}_h(\cdot \,|\, s_h^k)$, which is unobserved, and the agent receives the reward $r_h^k = r_h(s_h^k, a_h^k, w_h^k)$. The environment then transits into the next state $s_{h+1}^k \sim \mathcal{P}_h(\cdot \,|\, s_h^k, a_h^k, w_h^k)$.

For a policy $\pi = \{\pi_h\}_{h\in H}$, which does not depend on the confounders $\{w_h\}_{h\in[H]}$, we define the value function $V^\pi = \{V_h^\pi\}_{h\in[H]}$ as follows,

$$V_h^\pi(s) = \mathbb{E}_\pi\biggl[\sum_{j=h}^{H} r_j(s_j, a_j, w_j) \,\bigg|\, s_h = s\biggr], \quad \forall h \in [H], \tag{2.1}$$

where we denote by $\mathbb{E}_\pi$ the expectation with respect to the confounders $\{w_j\}_{j=h}^H$ and the trajectory $\{(s_j, a_j)\}_{j=h}^H$, starting from the state $s_j = s$ and following the policy π. Correspondingly, we define the action-value function $Q^\pi = \{Q_h^\pi\}_{h\in[H]}$ as follows,

$$Q_h^\pi(s, a) = \mathbb{E}_\pi\biggl[\sum_{j=h}^{H} r_j(s_j, a_j, w_j) \,\bigg|\, s_h = s, \mathrm{do}(a_h = a)\biggr], \quad \forall h \in [H]. \tag{2.2}$$

We assess the performance of an algorithm using the regret against the globally optimal policy $\pi^* = \{\pi_h^*\}_{h\in[H]}$ in hindsight after K episodes, which is defined as follows,

$$\mathrm{Regret}(T) = \max_{\pi} \sum_{k=1}^{K} \big(V_1^{\pi}(s_1^k) - V_1^{\pi^k}(s_1^k)\big) = \sum_{k=1}^{K} \big(V_1^{\pi^*}(s_1^k) - V_1^{\pi^k}(s_1^k)\big). \tag{2.3}$$

Here $T = HK$ is the total number of steps.

Our goal is to design an algorithm that minimizes the regret defined in (2.3), where π^* does not depend on the confounders $\{w_h\}_{h\in[H]}$. In the online setting that allows for intervention, it is well understood how to minimize such a regret [2, 14–16]. However, it remains unclear how to efficiently utilize the observational data obtained in the offline setting, which are possibly confounded. In real-world applications, e.g., autonomous driving and personalized medicine, such observational data are often abundant, whereas intervention in the online setting is often restricted. We refer to §C for a comparison between the confounded MDP and other extensions of MDP, including the dynamics treatment regime (DTR), partially observable MDP (POMDP), and contextual MDP (CMDP).

Why is Incorporating Confounded Observational Data Challenging? Straightforwardly incorporating the confounded observational data into an online algorithm possibly leads to an undesirable regret due to the mismatch between the online and offline data generating processes. In particular, due to the existence of the confounders $\{w_h\}_{h\in[H]}$, which are partially observed (§3) or unobserved (§A), the conditional probability $\mathbb{P}(s_{h+1} \,|\, s_h, a_h)$ in the offline setting is different from the causal effect $\mathbb{P}(s_{h+1} \,|\, s_h, \mathrm{do}(a_h))$ in the online setting [33]. More specifically, it holds that

$$\mathbb{P}(s_{h+1} \,|\, s_h, a_h) = \frac{\mathbb{E}_{w_h \sim \widetilde{\mathcal{P}}_h(\cdot \,|\, s_h)}\big[\mathcal{P}_h(s_{h+1} \,|\, s_h, a_h, w_h) \cdot \nu_h(a_h \,|\, s_h, w_h)\big]}{\mathbb{E}_{w_h \sim \widetilde{\mathcal{P}}_h(\cdot \,|\, s_h)}\big[\nu_h(a_h \,|\, s_h, w_h)\big]},$$
$$\mathbb{P}\big(s_{h+1} \,\big|\, s_h, \mathrm{do}(a_h)\big) = \mathbb{E}_{w_h \sim \widetilde{\mathcal{P}}_h(\cdot \,|\, s_h)}\big[\mathcal{P}_h(\cdot \,|\, s_h, a_h, w_h)\big].$$

In other words, without proper covariate adjustments [32], the confounded observational data may be not informative for estimating the transition dynamics and the associated action-value function in the online setting. To this end, we propose an algorithm that incorporates the confounded observational data in a provably efficient manner. Moreover, our analysis quantifies the amount of information carried over by the confounded observational data from the offline setting and to what extent it helps reducing the regret in the online setting.

3 Algorithm and Theory for Partially Observed Confounder

In this section, we propose the Deconfounded Optimistic Value Iteration (DOVI) algorithm. DOVI handles the case where the confounders are unobserved in the online setting but are partially observed in the offline setting. We then characterize the regret of DOVI. We defer the extension of DOVI, namely DOVI+, to §A which handles the case where the confounders are unobserved in both the online setting and the offline setting.

3.1 Algorithm

Backdoor Adjustment. In the online setting that allows for intervention, the causal effect of a_h on s_{h+1} given s_h, that is, $\mathbb{P}(s_{h+1} \,|\, s_h, \mathrm{do}(a_h))$, plays a key role in the estimation of the action-value function. Meanwhile, the confounded observational data may not allow us to identify the causal effect $\mathbb{P}(s_{h+1} \,|\, s_h, \mathrm{do}(a_h))$ if the confounder w_h is unobserved. However, if the confounder w_h is partially observed in the offline setting, the observed subset u_h of w_h allows us to identify the causal effect $\mathbb{P}(s_{h+1} \,|\, s_h, \mathrm{do}(a_h))$, as long as u_h satisfies the following backdoor criterion.

Assumption 3.1 (Backdoor Criterion [32, 33])**.** In the SCM defined in §2 and its induced directed acyclic graph (DAG), for all $h \in [H]$, there exists an observed subset u_h of w_h that satisfies the backdoor criterion, that is,

- the elements of u_h are not the descendants of a_h, and
- conditioning on s_h, the elements of u_h d-separate every path between a_h and s_{h+1}, r_h that has an incoming arrow into a_h.

See Figure 2 for an example that satisfies the backdoor criterion. In particular, we identify the causal effect $\mathbb{P}(s_{h+1} \,|\, s_h, \mathrm{do}(a_h))$ as follows.

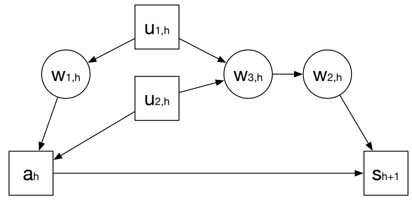


Figure 2: An illustration of the backdoor criterion modified from [32]. The causal diagram corresponds to the h-th step of the confounded MDP conditioning on s_h. Here $w_h = \{w_{1,h}, w_{2,h}, w_{3,h}\}$ is the unobserved confounders and the subset $u_h = \{u_{1,h}, u_{2,h}\}$ satisfies the backdoor criterion.

Proposition 3.2 (Backdoor Adjustment [32])**.** Under Assumption 3.1, it holds for all $h \in [H]$ that

$$\mathbb{P}\big(s_{h+1} \,\big|\, s_h, \mathrm{do}(a_h)\big) = \mathbb{E}_{u_h \sim \mathbb{P}(\cdot \,|\, s_h)}\big[\mathbb{P}(s_{h+1} \,|\, s_h, a_h, u_h)\big],$$

$$\mathbb{E}\big[r_h(s_h, a_h, w_h) \,\big|\, s_h, \mathrm{do}(a_h)\big] = \mathbb{E}_{u_h \sim \mathbb{P}(\cdot \,|\, s_h)}\Big[\mathbb{E}\big[r_h(s_h, a_h, w_h) \,\big|\, s_h, a_h, u_h\big]\Big].$$

Here (s_{h+1}, s_h, a_h, u_h) follows the SCM defined in §2, which generates the confounded observational data.

Proof. See [32] for a detailed proof. $\square$

With a slight abuse of notation, we write $\mathbb{P}(s_{h+1} \mid s_h, a_h, u_h)$ as $\mathcal{P}_h(s_{h+1} \,|\, s_h, a_h, u_h)$ and $\mathbb{P}(u_h \,|\, s_h)$ as $\widetilde{\mathcal{P}}_h(u_h \,|\, s_h)$, since they are induced by the SCM defined in §2. In the sequel, we define $\mathcal{U}$ the space of observed state u_h and write $r_h = r_h(s_h, a_h, w_h)$ for notational simplicity.

Backdoor-Adjusted Bellman Equation. We now formulate the Bellman equation for the confounded MDP. It holds for all $(s_h, a_h) \in \mathcal{S} \times \mathcal{A}$ that

$$Q_h^\pi(s_h, a_h) = \mathbb{E}_\pi\Bigg[\sum_{j=h}^{H} r_j(s_j, a_j, u_j) \,\Bigg|\, s_h, \mathrm{do}(a_h)\Bigg] = \mathbb{E}\big[r_h \,\big|\, s_h, \mathrm{do}(a_h)\big] + \mathbb{E}_{s_{h+1}}\big[V_{h+1}^\pi(s_{h+1})\big],$$

where $\mathbb{E}_{s_{h+1}}$ denotes the expectation with respect to $s_{h+1} \sim \mathbb{P}(\cdot \,|\, s_h, \mathrm{do}(a_h))$. Here $\mathbb{E}[r_h \,|\, s_h, \mathrm{do}(a_h)]$ and $\mathbb{P}(\cdot \,|\, s_h, \mathrm{do}(a_h))$ are characterized in Proposition 3.2. In the sequel, we define the following transition operator and counterfactual reward function,

$$(\mathbb{P}_h V)(s_h, a_h) = \mathbb{E}_{s_{h+1} \sim \mathbb{P}(\cdot \,|\, s_h, \mathrm{do}(a_h))}\big[V(s_{h+1})\big], \quad \forall V : \mathcal{S} \mapsto \mathbb{R},\ (s_h, a_h) \in \mathcal{S} \times \mathcal{A}, \tag{3.1}$$

$$R_h(s_h, a_h) = \mathbb{E}\big[r_h \,\big|\, s_h, \mathrm{do}(a_h)\big], \quad \forall (s_h, a_h) \in \mathcal{S} \times \mathcal{A}. \tag{3.2}$$

We have the following Bellman equation,

$$Q_h^\pi(s_h, a_h) = R_h(s_h, a_h) + (\mathbb{P}_h V_{h+1}^\pi)(s_h, a_h), \quad \forall h \in [H],\ (s_h, a_h) \in \mathcal{S} \times \mathcal{A}. \tag{3.3}$$

Correspondingly, the Bellman optimality equation takes the following form,

$$Q_h^*(s_h, a_h) = R_h(s_h, a_h) + (\mathbb{P}_h V_{h+1}^*)(s_h, a_h), \quad V_h^*(s_h) = \max_{a_h \in \mathcal{A}} Q_h^*(s_h, a_h), \tag{3.4}$$

which holds for all $h \in [H]$ and $(s_h, a_h) \in \mathcal{S} \times \mathcal{A}$. Such a Bellman optimality equation allows us to adapt the least-squares value iteration (LSVI) algorithm [2, 5, 14, 16, 31].

Linear Function Approximation. We focus on the following setting with linear transition kernels and reward functions [7, 16, 42, 43], which corresponds to a linear SCM [33].

Assumption 3.3 (Linear Confounded MDP)**.** We assume that

$$\mathcal{P}_h(s_{h+1} \,|\, s_h, a_h, u_h) = \langle \phi_h(s_h, a_h, u_h), \mu_h(s_{h+1}) \rangle, \quad \forall h \in [H],\ (s_{h+1}, s_h, a_h) \in \mathcal{S} \times \mathcal{S} \times \mathcal{A},$$

where $\phi_h(\cdot, \cdot, \cdot)$ and $\mu_h(\cdot) = (\mu_{1,h}(\cdot), \ldots, \mu_{d,h}(\cdot))^\top$ are $\mathbb{R}^d$-valued functions. We assume that $\sum_{i=1}^d \|\mu_{i,h}\|_1^2 \le d$ and $\|\phi_h(s_h, a_h, u_h)\|_2 \le 1$ for all $h \in [H]$ and $(s_h, a_h, u_h) \in \mathcal{S} \times \mathcal{A} \times \mathcal{U}$. Meanwhile, we assume that

$$\mathbb{E}[r_h \,|\, s_h, a_h, u_h] = \phi_h(s_h, a_h, u_h)^\top \theta_h, \quad \forall h \in [H],\ (s_h, a_h, u_h) \in \mathcal{S} \times \mathcal{A} \times \mathcal{U}, \tag{3.5}$$

where $\theta_h \in \mathbb{R}^d$ and $\|\theta_h\|_2 \le \sqrt{d}$ for all $h \in [H]$.

Such a linear setting generalizes the tabular setting where $\mathcal{S}$, $\mathcal{A}$, and $\mathcal{U}$ are finite.

Proposition 3.4. We define the backdoor-adjusted feature as follows,

$$\psi_h(s_h, a_h) = \mathbb{E}_{u_h \sim \widetilde{\mathcal{P}}_h(\cdot \,|\, s_h)}\big[\phi_h(s_h, a_h, u_h)\big], \quad \forall h \in [H],\ (s_h, a_h) \in \mathcal{S} \times \mathcal{A}. \tag{3.6}$$

Under Assumption 3.1, it holds that

$$\mathbb{P}(s_{h+1} \,|\, s_h, \mathrm{do}(a_h)) = \langle \psi_h(s_h, a_h), \mu_h(s_{h+1}) \rangle, \quad \forall h \in [H],\ (s_{h+1}, s_h, a_h) \in \mathcal{S} \times \mathcal{S} \times \mathcal{A}.$$

Moreover, the action-value functions Q_h^π and Q_h^* are linear in the backdoor-adjusted feature ψ_h for all π.

Proof. See §F.1 for a detailed proof. $\square$

Such an observation allows us to estimate the action-value function based on the backdoor-adjusted features $\{\psi_h\}_{h \in [H]}$ in the online setting. See §D for a detailed discussion. In the sequel, we assume that either the density of $\{\widetilde{\mathcal{P}}_h(\cdot \,|\, s_h)\}_{h \in [H]}$ is known or the backdoor-adjusted feature $\{\psi_h\}_{h \in [H]}$ is known.

In the sequel, we introduce the DOVI algorithm (Algorithm 1). Each iteration of DOVI consists of two components, namely point estimation, where we estimate Q_h^* based on the confounded observational data and the interventional data, and uncertainty quantification, where we construct the upper confidence bound (UCB) of the point estimator.

Algorithm 1 Deconfounded Optimistic Value Iteration (DOVI) for Confounded MDP

Require: Observational data $\{(s_h^i, a_h^i, u_h^i, r_h^i)\}_{i \in [n], h \in [H]}$, tuning parameters $\lambda, \beta > 0$, backdoor-adjusted feature $\{\psi_h\}_{h \in [H]}$, which is defined in (3.6).

1: **Initialization:** Set $\{Q_h^0, V_h^0\}_{h \in [H]}$ as zero functions and V_{H+1}^k as a zero function for $k \in [K]$.
2: **for** $k = 1, \ldots, K$ **do**
3:   **for** $h = H, \ldots, 1$ **do**
4:     Set $\omega_h^k \leftarrow \mathrm{argmin}_{\omega \in \mathbb{R}^d} \sum_{\tau=1}^{k-1} (r_h^\tau + V_{h+1}^\tau(s_{h+1}^\tau) - \omega^\top \psi_h(s_h^\tau, a_h^\tau))^2 + \lambda \|\omega\|_2^2 + L_h^k(\omega)$, where L_h^k is defined in (3.8).
5:     Set $Q_h^k(\cdot, \cdot) \leftarrow \min\{\psi_h(\cdot, \cdot)^\top \omega_h^k + \Gamma_h^k(\cdot, \cdot), H - h\}$, where Γ_h^k is defined in (3.12).
6:     Set $\pi_h^k(\cdot \,|\, s_h) \leftarrow \mathrm{argmax}_{a_h \in \mathcal{A}} Q_h^k(s_h, a_h)$ for all $s_h \in \mathcal{S}$.
7:     Set $V_h^k(\cdot) \leftarrow \langle \pi_h^k(\cdot \,|\, \cdot), Q_h^k(\cdot, \cdot) \rangle_{\mathcal{A}}$.
8:   **end for**
9:   Obtain s_1^k from the environment.
10:   **for** $h = 1, \ldots, H$ **do**
11:     Take $a_h^k \sim \pi_h^k(\cdot \,|\, s_h^k)$. Obtain $r_h^k = r_h(s_h^k, a_h^k, u_h^k)$ and s_{h+1}^k.
12:   **end for**
13: **end for**

Point Estimation. To solve the Bellman optimality equation in (3.4), we minimize the empirical mean-squared Bellman error as follows at each step,

$$\omega_h^k \leftarrow \underset{\omega \in \mathbb{R}^d}{\mathrm{argmin}} \sum_{\tau=1}^{k-1} \big(r_h^\tau + V_{h+1}^\tau(s_{h+1}^\tau) - \omega^\top \psi_h(s_h^\tau, a_h^\tau)\big)^2 + \lambda \|\omega\|_2^2 + L_h^k(\omega), \quad h = H, \ldots, 1, \tag{3.7}$$

where we set $V_{H+1}^k = 0$ for all $k \in [K]$ and V_{h+1}^τ is defined in Line 7 of Algorithm 1 for all $(\tau, h) \in [K] \times [H-1]$. Here k is the index of episode, $\lambda > 0$ is a tuning parameter, and L_h^k is a regularizer, which is constructed based on the confounded observational data. More specifically, we define

$$L_h^k(\omega) = \sum_{i=1}^{n} \big(r_h^i + V_{h+1}^k(s_{h+1}^i) - \omega^\top \phi_h(s_h^i, a_h^i, u_h^i)\big)^2, \quad \forall (k, h) \in [K] \times [H], \tag{3.8}$$

which corresponds to the least-squares loss for regressing $r_h^i + V_{h+1}^k(s_{h+1}^i)$ against $\phi_h(s_h^i, a_h^i, u_h^i)$ for all $i \in [n]$. Here $\{(s_h^i, a_h^i, u_h^i, r_h^i)\}_{(i,h) \in [n] \times [H]}$ are the confounded observational data, where

$u_h^i \sim \widetilde{\mathcal{P}}_h(\cdot \,|\, s_h^i)$, $s_{h+1}^i \sim \mathcal{P}_h(\cdot \,|\, s_h^i, a_h^i, u_h^i)$, and $a_h^i \sim \nu_h(\cdot \,|\, s_h^i, w_h^i)$ with $\nu = \{\nu_h\}_{h\in[H]}$ being the behavior policy. Here recall that, with a slight abuse of notation, we write $\mathbb{P}(s_{h+1} \mid s_h, a_h, u_h)$ as $\mathcal{P}_h(s_{h+1} \,|\, s_h, a_h, u_h)$ and $\mathbb{P}(u_h \,|\, s_h)$ as $\widetilde{\mathcal{P}}_h(u_h \,|\, s_h)$, since they are induced by the SCM defined in §2.

The update in (3.7) takes the following explicit form,

$$\omega_h^k \leftarrow (\Lambda_h^k)^{-1}\biggl(\sum_{\tau=1}^{k-1} \psi_h(s_h^\tau, a_h^\tau) \cdot \bigl(V_{h+1}^k(s_{h+1}^\tau) + r_h^\tau\bigr) \\ + \sum_{i=1}^{n} \phi_h(s_h^i, a_h^i, u_h^i) \cdot \bigl(V_{h+1}^k(s_{h+1}^i) + r_h^i\bigr)\biggr), \tag{3.9}$$

where

$$\Lambda_h^k = \sum_{\tau=1}^{k-1} \psi_h(s_h^\tau, a_h^\tau)\psi_h(s_h^\tau, a_h^\tau)^\top + \sum_{i=1}^{n} \phi_h(s_h^i, a_h^i, u_h^i)\phi_h(s_h^i, a_h^i, u_h^i)^\top + \lambda I. \tag{3.10}$$

Uncertainty Quantification. We now construct the UCB $\Gamma_h^k(\cdot,\cdot)$ of the point estimator $\psi_h(\cdot,\cdot)^\top \omega_h^k$ obtained from (3.9), which encourages the exploration of the less visited state-action pairs. To this end, we employ the following notion of information gain to motivate the UCB,

$$\Gamma_h^k(s_h^k, a_h^k) \propto H(\omega_h^k \,|\, \xi_{k-1}) - H\bigl(\omega_h^k \,|\, \xi_{k-1} \cup \{(s_h^k, a_h^k)\}\bigr), \tag{3.11}$$

where $H(\omega_h^k \,|\, \xi_{k-1})$ is the differential entropy of the random variable ω_h^k given the data ξ_{k-1}. In particular, $\xi_{k-1} = \{(s_h^\tau, a_h^\tau, r_h^\tau)\}_{(\tau,h)\in[k-1]\times[H]} \cup \{(s_h^i, a_h^i, u_h^i, r_h^i)\}_{(i,h)\in[n]\times[H]}$ consists of the confounded observational data and the interventional data up to the $(k-1)$-th episode. However, it is challenging to characterize the distribution of ω_h^k. To this end, we consider a Bayesian counterpart of the confounded MDP, where the prior of ω_h^k is $N(0, I/\lambda)$ and the residual of the regression problem in (3.7) is $N(0,1)$. In such a "parallel" confounded MDP, the posterior of ω_h^k follows $N(\mu_{k,h}, (\Lambda_h^k)^{-1})$, where Λ_h^k is defined in (3.10) and $\mu_{k,h}$ coincides with the right-hand side of (3.9). Moreover, it holds for all $(s_h^k, a_h^k) \in \mathcal{S} \times \mathcal{A}$ that

$$H(\omega_h^k \,|\, \xi_{k-1}) = 1/2 \cdot \log\det\bigl((2\pi e)^d \cdot (\Lambda_h^k)^{-1}\bigr),$$
$$H\bigl(\omega_h^k \,|\, \xi_{k-1} \cup \{(s_h^k, a_h^k)\}\bigr) = 1/2 \cdot \log\det\Bigl((2\pi e)^d \cdot \bigl(\Lambda_h^k + \psi_h(s_h^k, a_h^k)\psi_h(s_h^k, a_h^k)^\top\bigr)^{-1}\Bigr).$$

Correspondingly, we employ the following UCB, which instantiates (3.11), that is,

$$\Gamma_h^k(s_h^k, a_h^k) = \beta \cdot \Bigl(\log\det\bigl(\Lambda_h^k + \psi_h(s_h^k, a_h^k)\psi_h(s_h^k, a_h^k)^\top\bigr) - \log\det(\Lambda_h^k)\Bigr)^{1/2} \tag{3.12}$$

for all $(s_h^k, a_h^k) \in \mathcal{S} \times \mathcal{A}$. Here $\beta > 0$ is a tuning parameter. We highlight that, although the information gain in (3.11) relies on the "parallel" confounded MDP, the UCB in (3.12), which is used in Line 5 of Algorithm 1, does not rely on the Bayesian perspective. Also, our analysis establishes the frequentist regret.

Regularization with Observational Data: A Bayesian Perspective. In the "parallel" confounded MDP, it holds that

$$\omega_h^k \sim N(0, I/\lambda), \quad \omega_h^k \,|\, \xi_0 \sim N\bigl(\mu_{1,h}, (\Lambda_h^1)^{-1}\bigr), \quad \omega_h^k \,|\, \xi_{k-1} \sim N\bigl(\mu_{k,h}, (\Lambda_h^k)^{-1}\bigr),$$

where $\mu_{k,h}$ coincides with the right-hand side of (3.9) and $\mu_{1,h}$ is defined by setting $k = 1$ in $\mu_{k,h}$. Here $\xi_0 = \{(s_h^i, a_h^i, u_h^i, r_h^i)\}_{(i,h)\in[n]\times[H]}$ are the confounded observational data. Hence, the regularizer L_h^k in (3.8) corresponds to using $\omega_h^k \,|\, \xi_0$ as the prior for the Bayesian regression problem given only the interventional data $\xi_{k-1} \setminus \xi_0 = \{(s_h^\tau, a_h^\tau, r_h^\tau)\}_{(\tau,h)\in[k-1]\times[H]}$.

3.2 Theory

The following theorem characterizes the regret of DOVI, which is defined in (2.3).

Theorem 3.5 (Regret of DOVI)**.** Let $\beta = CdH\sqrt{\log(d(T+nH)/\zeta)}$ and $\lambda = 1$, where $C > 0$ and $\zeta \in (0, 1]$ are absolute constants. Under Assumptions 3.1 and 3.3, it holds with probability at least $1 - 5\zeta/2$ that

$$\text{Regret}(T) \leq C' \cdot \Delta_H \cdot \sqrt{d^3 H^3 T} \cdot \sqrt{\log\bigl(d(T+nH)/\zeta\bigr)}, \tag{3.13}$$

where $C' > 0$ is an absolute constant and

$$\Delta_H = \frac{1}{\sqrt{dH^2}} \sum_{h=1}^{H} \bigl(\log\det(\Lambda_h^{K+1}) - \log\det(\Lambda_h^1)\bigr)^{1/2}. \tag{3.14}$$

Proof. See §F.3 for a detailed proof. □

Note that $\Lambda_h^{K+1} \preceq (n+K+\lambda)I$ and $\Lambda_h^1 \succeq \lambda I$ for all $h \in [H]$. Hence, it holds that $\Delta_H = \mathcal{O}(\sqrt{\log(n+K+1)})$ in the worst case. Thus, the regret of DOVI is $\mathcal{O}(\sqrt{d^3H^3T})$ up to logarithmic factors, which is optimal in the total number of steps T if we only consider the online setting. However, Δ_H is possibly much smaller than $\mathcal{O}(\sqrt{\log(n+K+1)})$, depending on the amount of information carried over by the confounded observational data from the offline setting, which is quantified in the following.

Interpretation of Δ_H: An Information-Theoretic Perspective. Let ω_h^* be the parameter of the globally optimal action-value function Q_h^*, which corresponds to π^* in (2.3). Recall that we denote by ξ_0 and ξ_K the confounded observational data $\{(s_h^i, a_h^i, u_h^i, r_h^i)\}_{(i,h)\in[n]\times[H]}$ and the union $\{(s_h^i, a_h^i, u_h^i, r_h^i)\}_{(i,h)\in[n]\times[H]} \cup \{(s_h^k, a_h^k, r_h^k)\}_{(k,h)\in[K]\times[H]}$ of the confounded observational data and the interventional data up to the K-th episode, respectively. We consider the aforementioned Bayesian counterpart of the confounded MDP, where the prior of ω_h^* is also $N(0, I/\lambda)$. In such a "parallel" confounded MDP, we have

$$\omega_h^* \sim N(0, I/\lambda), \quad \omega_h^* \,|\, \xi_0 \sim N\bigl(\mu_{1,h}^*, (\Lambda_h^1)^{-1}\bigr), \quad \omega_h^* \,|\, \xi_K \sim N\bigl(\mu_{K,h}^*, (\Lambda_h^{K+1})^{-1}\bigr), \tag{3.15}$$

where

$$\mu_{1,h}^* = (\Lambda_h^1)^{-1} \sum_{i=1}^{n} \phi_h(s_h^i, a_h^i, u_h^i) \cdot \bigl(V_{h+1}^*(s_{h+1}^i) + r_h^i\bigr),$$

$$\mu_{K,h}^* = (\Lambda_h^{K+1})^{-1} \biggl(\Lambda_h^1 \mu_{1,h}^* + \sum_{\tau=1}^{K} \psi_h(s_h^\tau, a_h^\tau) \cdot \bigl(V_{h+1}^*(s_{h+1}^\tau) + r_h^\tau\bigr)\biggr).$$

It then holds for the right-hand side of (3.14) that

$$1/2 \cdot \log\det(\Lambda_h^{K+1}) - 1/2 \cdot \log\det(\Lambda_h^1) = H(\omega_h^* \,|\, \xi_0) - H(\omega_h^* \,|\, \xi_K). \tag{3.16}$$

The left-hand side of (3.16) characterizes the information gain of intervention in the online setting given the confounded observational data in the offline setting. In other words, if the confounded observational data are sufficiently informative upon the backdoor adjustment, then Δ_H is small, which implies that the regret is small. More specifically, the matrices $(\Lambda_h^1)^{-1}$ and $(\Lambda_h^{K+1})^{-1}$ defined in (3.10) characterize the ellipsoidal confidence sets given ξ_0 and ξ_K, respectively. If the confounded observational data are sufficiently informative upon the backdoor adjustment, Λ_h^{K+1} is close to Λ_h^1. To illustrate, let $\{\psi_h(s_h^\tau, a_h^\tau)\}_{(\tau,h)\in[K]\times[H]}$ and $\{\phi_h(s_h^i, a_h^i, u_h^i)\}_{(i,h)\in[n]\times[H]}$ be sampled uniformly at random from the canonical basis $\{e_\ell\}_{\ell\in[d]}$ of $\mathbb{R}^d$. It then holds that $\Lambda_h^{K+1} \approx (K+n)I/d + \lambda I$ and $\Lambda_h^1 \approx nI/d + \lambda I$. Hence, for $\lambda = 1$ and sufficiently large n and K, we have $\Delta_H = \mathcal{O}(\sqrt{\log(1 + K/(n+d))}) = \mathcal{O}(\sqrt{K/(n+d)})$. For example, for $n = \Omega(K^2)$, it holds that $\Delta_H = \mathcal{O}(n^{-1/2})$, which implies that the regret of DOVI is $\mathcal{O}(n^{-1/2} \cdot \sqrt{d^3H^3T})$. In other words, if the confounded observational data are sufficiently informative upon the backdoor adjustment, the regret of DOVI can be arbitrarily small given a sufficiently large sample size n of the confounded observational data, which is often the case in practice [8, 9, 21, 22, 29].

4 Conclusion

In this paper, we propose the deconfounded optimistic value iteration (DOVI) algorithm and its variant DOVI$^+$, which incorporate the confounded observational data to the online reinforcement learning in a provably efficient manner. DOVI and DOVI$^+$ explicitly adjust for the confounding bias in the observational data via the backdoor and frontdoor adjustments, respectively. In both cases, such adjustments allow us to construct the bonus based on a notion of information gain, which considers the amount of information acquired from the offline dataset. We further conduct regret analysis of DOVI and DOVI$^+$. Our analysis suggests that practitioners can tackle the confounding issue in the offline dataset by estimating the counterfactual reward for value function estimations, given that a proper adjustment such as the backdoor or frontdoor adjustment is available. In the case of backdoor and frontdoor adjustment, we prove that the regret of DOVI is smaller than the optimal regret achievable in the pure online setting when the confounded observational data are informative upon the adjustments, suggesting that one can exploit the confounded observational data in reinforcement learning upon proper adjustments. In our future study, we wish to incorporate proxy variables that are native to MDPs for the adjustments of the offline dataset, such as the variables exploited by [4, 24, 40].

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A Algorithm and Theory for Unobserved Confounder

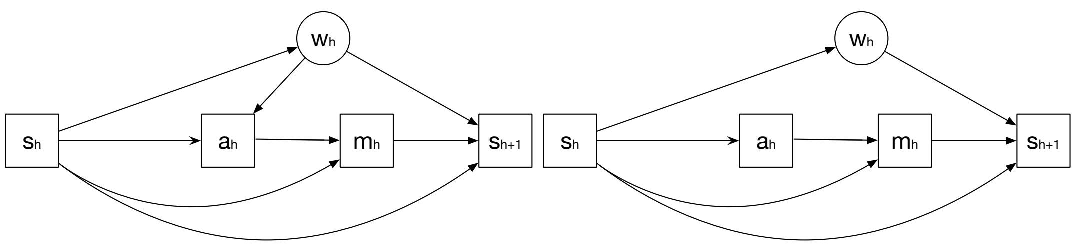
In this section, we extend DOVI to handle the case where the confounders are unobserved in both the online setting and the offline setting. We then characterize the regret of such an extension of DOVI, namely DOVI⁺. In comparison with DOVI, DOVI⁺ additionally incorporates an intermediate state at each step, which extends the length of each episode from H to $2H$.

A.1 Algorithm

Frontdoor Adjustment. Since the confounders $\{w_h\}_{h\in[H]}$ are unobserved in the offline setting, the confounded observational data $\{(s_h^i, a_h^i, r_h^i)\}_{(i,h)\in[n]\times[H]}$ are insufficient for the identification of the causal effect $\mathbb{P}(s_{h+1}\,|\,s_h, \mathrm{do}(a_h))$ [32, 33]. However, such a causal effect is identifiable if we observe the intermediate states $\{m_h\}_{h\in[H]}$ that satisfy the following frontdoor criterion.

Assumption A.1 (Frontdoor Criterion [32, 33])**.** In the SCM defined in §2, for all $h \in [H]$, there additionally exists an observed intermediate state m_h that satisfies the frontdoor criterion, that is,

- m_h intercepts every directed path from a_h to s_{h+1},
- conditioning on s_h, no path between a_h and m_h has an incoming arrow into a_h, and
- conditioning on s_h, a_h d-separates every path between m_h and s_{h+1} that has an incoming arrow into m_h.



(a) Offline Setting (b) Online Setting

Figure 3: Causal diagrams of the h-th step of the confounded MDP with the intermediate state (a) in the offline setting and (b) in the online setting, respectively.

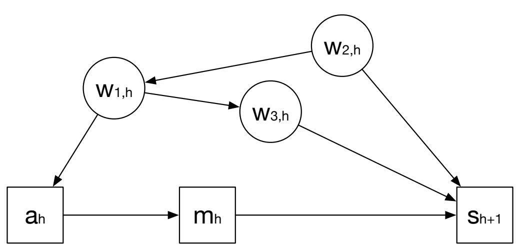


Figure 4: An illustration of the frontdoor criterion. The causal diagram corresponds to the h-th step of the confounded MDP conditioning on s_h. Here $w_h = \{w_{1,h}, w_{2,h}, w_{3,h}\}$ is the confounder and the intermediate state m_h satisfies the frontdoor criterion.

See Figure 3 for the causal diagram that describes such an SCM and Figure 4 for an example that satisfies the frontdoor criterion. Intuitively, Assumption A.1 ensures that, conditioning on s_h, (i) the intermediate state m_h is caused by the action a_h and the causal effect of the action a_h on the next state s_{h+1} is summarized by m_h, while (ii) the action a_h and the intermediate state m_h are not confounded. In the sequel, we denote by $\mathcal{M}$ the space of intermediate states and $\breve{\mathcal{P}}_h(\cdot\,|\,\cdot,\cdot)$ the transition kernel that determines m_h given s_h and a_h. The causal effect $\mathbb{P}(s_{h+1}\,|\,s_h, \mathrm{do}(a_h))$ is identified as follows.

Proposition A.2 (Frontdoor Adjustment [32])**.** Under Assumption A.1, it holds that

$$\mathbb{P}\big(s_{h+1}\,\big|\,s_h, \mathrm{do}(a_h)\big) = \mathbb{E}_{m_h, a_h'}\big[\mathbb{P}(s_{h+1}\,|\,s_h, a_h', m_h)\big],$$

where the expectation $\mathbb{E}_{m_h, a'_h}$ is taken with respect to $m_h \sim \breve{\mathcal{P}}_h(\cdot \,|\, s_h, a_h)$ and $a'_h \sim \mathbb{E}_{w_h \sim \widetilde{\mathcal{P}}_h(\cdot \,|\, s_h)}[\nu_h(\cdot \,|\, s_h, w_h)]$. Here (s_{h+1}, s_h, a_h, m_h) follows the SCM define in §2 with the intermediate states $\{m_h\}_{h \in [H]}$ in the offline setting.

Frontdoor-Adjusted Bellman Equation. In the sequel, we assume without loss of generality that the reward r_h is deterministic and only depends on the state s_h and the action a_h. In parallel to (3.3), we have

$$Q_h^\pi(s_h, a_h) = r_h(s_h, a_h) + \mathbb{E}_{s_{h+1}}\big[V_{h+1}^\pi(s_{h+1})\big], \tag{A.1}$$

where the expectation $\mathbb{E}_{s_{h+1}}$ is taken with respect to $s_{h+1} \sim \mathbb{P}(\cdot \,|\, s_h, \mathrm{do}(a_h))$. We define the the following transition operators,

$$(\mathbb{P}_{h+1/2}V)(s_h, m_h) = \mathbb{E}_{s_{h+1} \sim \mathbb{P}(\cdot \,|\, s_h, \mathrm{do}(m_h))}\big[V(s_{h+1})\big], \quad \forall V : \mathcal{S} \mapsto \mathbb{R},\ (s_h, m_h) \in \mathcal{S} \times \mathcal{M},$$
$$(\mathbb{P}_h \widetilde{V})(s_h, a_h) = \mathbb{E}_{m_h \sim \mathbb{P}(\cdot \,|\, s_h, \mathrm{do}(a_h))}\big[\widetilde{V}(s_h, m_h)\big], \quad \forall \widetilde{V} : \mathcal{S} \times \mathcal{M} \mapsto \mathbb{R},\ (s_h, a_h) \in \mathcal{S} \times \mathcal{A}.$$

We highlight that, under Assumption A.1, the causal effect $\mathbb{P}(m_h \,|\, s_h, \mathrm{do}(a_h))$ coincides with the conditional probability $\mathbb{P}(m_h \,|\, s_h, a_h)$, since a_h and m_h are not confounded given s_h. In the sequel, we define the value function at the intermediate state by $V_{h+1/2}^\pi(s_h, m_h) = (\mathbb{P}_{h+1/2}V_{h+1}^\pi)(s_h, m_h)$. We have the following Bellman equation,

$$\begin{aligned} Q_h^\pi(s_h, a_h) &= r_h(s_h, a_h) + \big(\mathbb{P}_h(\mathbb{P}_{h+1/2}V_{h+1}^\pi)\big)(s_h, a_h) \\ &= r_h(s_h, a_h) + (\mathbb{P}_h V_{h+1/2}^\pi)(s_h, a_h). \end{aligned} \tag{A.2}$$

Correspondingly, the Bellman optimality equation takes the following form,

$$\begin{aligned} &Q_h^*(s_h, a_h) = r_h(s_h, a_h) + (\mathbb{P}_h V_{h+1/2}^*)(s_h, a_h), \\ &V_{h+1/2}^*(s_h, m_h) = (\mathbb{P}_{h+1/2}V_{h+1}^*)(s_h, m_h), \quad V_h^*(s_h) = \max_{a_h \in \mathcal{A}} Q_h^*(s_h, a_h). \end{aligned} \tag{A.3}$$

Linear Function Approximation. In parallel to Assumption 3.3, we focus on the following setting with linear transition kernels and reward functions [7, 16, 42, 43], which corresponds to a linear SCM [33].

Assumption A.3 (Linear Confounded MDP)**.** We assume that

$$\mathcal{P}_h(s_{h+1} \,|\, s_h, m_h, w_h) = \langle \rho_h(s_h, m_h, w_h), \mu_h(s_{h+1}) \rangle, \quad \forall h \in [H],\ (s_h, m_h, w_h) \in \mathcal{S} \times \mathcal{M} \times \mathcal{W},$$
$$\breve{\mathcal{P}}_h(m_h \,|\, s_h, a_h) = \langle \gamma_h(s_h, a_h), \overline{\mu}_h(m_h) \rangle, \quad \forall h \in [H],\ (m_h, s_h, a_h) \in \mathcal{M} \times \mathcal{S} \times \mathcal{A}.$$

where $\rho_h(\cdot,\cdot,\cdot)$, $\gamma_h(\cdot,\cdot)$, $\mu_h(\cdot) = (\mu_{1,h}(\cdot), \ldots, \mu_{d,h}(\cdot))^\top$, and $\overline{\mu}_h(\cdot) = (\overline{\mu}_{1,h}(\cdot), \ldots, \overline{\mu}_{d,h}(\cdot))^\top$ are $\mathbb{R}^d$-valued functions. We assume that $\|\rho_h(s_h, m_h, w_h)\|_2 \le 1$, $\|\gamma_h(s_h, a_h)\|_2 \le 1$, $\sum_{i=1}^d \|\mu_{i,h}\|_1^2 \le d$, and $\sum_{i=1}^d \|\overline{\mu}_{i,h}\|_1^2 \le d$ for all $h \in [H]$ and $(s_h, a_h, m_h, w_h) \in \mathcal{S} \times \mathcal{A} \times \mathcal{M} \times \mathcal{W}$. Meanwhile, we assume that

$$r_h(s_h, a_h) = \gamma_h(s_h, a_h)^\top \theta_h, \quad \forall (h, k) \in [H] \times [K],$$

where $\theta_h \in \mathbb{R}^d$ and $\|\theta_h\|_2 \le \sqrt{d}$ for all $h \in [H]$.

Proposition A.4. We define $\widetilde{\nu}_h(a_h \,|\, s_h) = \mathbb{E}_{w_h \sim \widetilde{\mathcal{P}}_h(\cdot \,|\, s_h)}[\nu_h(a_h \,|\, s_h, w_h)]$, where $\nu = \{\nu_h\}_{h \in [H]}$ is the behavior policy. With a slight abuse of notation, we define the frontdoor-adjusted feature as follows,

$$\phi_h(s_h, a_h, m_h) = \frac{\mathbb{E}_{w_h \sim \widetilde{\mathcal{P}}_h(\cdot \,|\, s_h)}\big[\rho_h(s_h, m_h, w_h) \cdot \nu_h(a_h \,|\, s_h, w_h)\big]}{\widetilde{\nu}_h(a_h \,|\, s_h)}, \quad \forall h \in [H]. \tag{A.4}$$

Under Assumption A.3, it holds that

$$\mathbb{P}(s_{h+1} \,|\, s_h, a_h, m_h) = \langle \phi_h(s_h, a_h, m_h), \mu_h(s_{h+1}) \rangle. \tag{A.5}$$

Proof. See §F.2 for a detailed proof. □

Algorithm 2 DOVI⁺ for Confounded MDP.

Require: Observational data $\{(s_h^i, a_h^i, m_h^i, r_h^i)\}_{i\in[n],h\in[H]}$, tuning parameters $\lambda, \beta > 0$, features $\{\phi_h\}_{h\in[H]}$ and $\{\psi_h\}_{h\in[H]}$, which are defined in (A.4) and (A.6), respectively.

1: **Initialization:** Set $\{Q_h^0, V_{h+1/2}^0, V_h^0\}_{h\in[H]}$ as zero functions and V_{H+1}^k as a zero function for $k \in [K]$.
2: **for** $k = 1, \ldots, K$ **do**
3:   **for** $h = H, \ldots, 1$ **do**
4:     **Update $V_{h+1/2}^k$:**
5:     Set $\omega_{1,h}^k \leftarrow \operatorname{argmin}_{\omega\in\mathbb{R}^d} \sum_{\tau=1}^{k-1} (V_{h+1}^\tau(s_{h+1}^\tau) - \omega^\top \psi_h(s_h^\tau, m_h^\tau))^2 + \lambda\|\omega\|_2^2 + L_{1,h}^k(\omega)$, where $L_{1,h}^k$ is defined in (A.9).
6:     Set $V_{h+1/2}^k(s_h, m_h) \leftarrow \min\{\psi_h(s_h, m_h)^\top \omega_{1,h}^k + \Gamma_{h+1/2}^k(s_h, m_h), H - h\}$ for all $(s_h, m_h) \in \mathcal{S} \times \mathcal{M}$, where $\Gamma_{h+1/2}^k$ is defined in (A.12).
7:     **Update Q_h^k:**
8:     Set $\omega_{2,h}^k \leftarrow \operatorname{argmin}_{\omega\in\mathbb{R}^d} \sum_{\tau=1}^{k-1} (r_h^k + V_{h+1/2}^k(s_h^\tau, m_h^\tau) - \omega^\top \gamma_h(s_h^\tau, a_h^\tau))^2 + \lambda\|\omega\|_2^2 + L_{2,h}^k(\omega)$, where $L_{2,h}^k$ is defined in (A.14).
9:     Set $Q_h^k(s_h, a_h) \leftarrow \min\{\gamma_h(s_h, a_h)^\top \omega_{2,h}^k + \Gamma_h^k(s_h, a_h), H - h\}$ for all $(s_h, a_h) \in \mathcal{S} \times \mathcal{A}$, where Γ_h^k is defined in (A.15).
10:     **Update π_h^k and V_h^k:**
11:     Set $\pi_h^k(\cdot \,|\, s_h) \leftarrow \operatorname{argmax}_{a_h\in\mathcal{A}} Q_h^k(s_h, a_h)$ for all $s_h \in \mathcal{S}$.
12:     Set $V_h^k(\cdot) \leftarrow \langle \pi_h^k(\cdot \,|\, \cdot), Q_h^k(\cdot, \cdot)\rangle_{\mathcal{A}}$.
13:   **end for**
14:   Obtain s_1^k from the environment.
15:   **for** $h = 1, \ldots, H$ **do**
16:     Take $a_h^k \sim \pi_h^k(\cdot \,|\, s_h^k)$. Obtain $r_h^k = r_h(s_h^k, a_h^k)$, m_h^k, and s_{h+1}^k.
17:   **end for**
18: **end for**

DOVI⁺: Update of $V_{h+1/2}^k$. With a slight abuse of notation, we define the following feature,

$$\psi_h(s_h, m_h) = \mathbb{E}_{w_h\sim\widetilde{\mathcal{P}}_h(\cdot \,|\, s_h)}\big[\rho_h(s_h, m_h, w_h)\big]. \tag{A.6}$$

Conditioning on the state s_h, the confounder w_h satisfies the backdoor criterion for identifying the causal effect $\mathbb{P}(s_{h+1} \,|\, s_h, \mathrm{do}(m_h))$, although it is unobserved. In the sequel, we assume that either the density of $\{\widetilde{\mathcal{P}}_h(\cdot \,|\, s_h)\}_{h\in[H]}$ is known to us or the features $\{\phi_h\}_{h\in[H]}$ and $\{\psi_h\}_{h\in[H]}$ are known to us. Following from (A.6), Proposition 3.2, and Assumption A.3, it holds for all $h \in [H]$ and $(s_{h+1}, s_h, m_h) \in \mathcal{S} \times \mathcal{S} \times \mathcal{M}$ that

$$\mathbb{P}\big(s_{h+1} \,\big|\, s_h, \mathrm{do}(m_h)\big) = \langle \psi_h(s_h, m_h), \mu_h(s_{h+1})\rangle. \tag{A.7}$$

Hence, by the Bellman equation and the Bellman optimality equation in (A.2) and (A.3), respectively, the value functions at the intermediate state $V_{h+1/2}^\pi$ and $V_{h+1/2}^*$ are linear in the feature ψ_h for all π. To solve for $V_{h+1/2}^*$ in the Bellman optimality equation in (A.3), we minimize the following empirical mean-squared Bellman error as follows at each step,

$$\omega_{1,h}^k \leftarrow \operatorname*{argmin}_{\omega\in\mathbb{R}^d} \sum_{\tau=1}^{k-1} \big(V_{h+1}^\tau(s_{h+1}^\tau) - \omega^\top \psi_h(s_h^\tau, m_h^\tau)\big)^2 + \lambda\|\omega\|_2^2 + L_{1,h}^k(\omega), \quad h = H, \ldots, 1, \tag{A.8}$$

where we set $V_{H+1}^k = 0$ for all $k \in [K]$ and V_{h+1}^τ is defined in Line 12 of Algorithm 2 for all $(\tau, h) \in [K] \times [H-1]$. Here k is the index of episode, $\lambda > 0$ is a tuning parameter, and $L_{1,h}^k$ is a regularizer, which is constructed based on the confounded observational data. More specifically, we define

$$L_{1,h}^k(\omega) = \sum_{i=1}^n \big(V_{h+1}^\tau(s_{h+1}^i) - \omega^\top \phi_h(s_h^i, a_h^i, m_h^i)\big)^2, \quad \forall (k, h) \in [K] \times [H], \tag{A.9}$$

which corresponds to the least-squares loss for regressing $V_{h+1}^{\tau}(s_{h+1}^i)$ against $\phi_h(s_h^i, a_h^i, m_h^i)$ for all $i \in [n]$. Here $\{(s_h^i, a_h^i, m_h^i, r_h^i)\}_{(i,h)\in[n]\times[H]}$ are the confounded observational data, where $s_{h+1}^i \sim \mathcal{P}_h(\cdot \,|\, s_h^i, a_h^i, w_h^i)$, $m_h^i \sim \breve{\mathcal{P}}_h(\cdot \,|\, s_h^i, a_h^i)$, and $a_h^i \sim \nu_h(\cdot \,|\, s_h^i, w_h^i)$ with $\nu = \{\nu_h\}_{h\in[H]}$ being the behavior policy.

The update in (A.8) takes the following explicit form,

$$\omega_{1,h}^k \leftarrow (\Lambda_{1,h}^k)^{-1}\biggl(\sum_{\tau=1}^{k-1}\psi_h(s_h^\tau, m_h^\tau)\cdot V_{h+1}^k(s_{h+1}^\tau) + \sum_{i=1}^{n}\phi_h(s_h^i, a_h^i, m_h^i)\cdot V_{h+1}^k(s_{h+1}^i)\biggr), \quad \text{(A.10)}$$

where

$$\Lambda_{1,h}^k = \sum_{\tau=1}^{k-1}\psi_h(s_h^\tau, m_h^\tau)\psi_h(s_h^\tau, m_h^\tau)^\top + \sum_{i=1}^{n}\phi_h(s_h^i, a_h^i, m_h^i)\phi_h(s_h^i, a_h^i, m_h^i)^\top + \lambda I. \quad \text{(A.11)}$$

Meanwhile, we employ the following UCB of $\psi_h(s_h^k, m_h^k)^\top\omega_{1,h}^k$ for all $(s_h^k, m_h^k) \in \mathcal{S}\times\mathcal{M}$,

$$\Gamma_{h+1/2}^k(s_h^k, m_h^k) = \beta\cdot\Bigl(\log\det\bigl(\Lambda_{1,h}^k + \psi_h(s_h^k, m_h^k)\psi_h(s_h^k, m_h^k)^\top\bigr) - \log\det(\Lambda_{1,h}^k)\Bigr)^{1/2}. \quad \text{(A.12)}$$

The update of $V_{h+1/2}^k$ is defined in Line 6 of Algorithm 2.

DOVI⁺: Update of Q_h^k. Upon obtaining $V_{h+1/2}^k$, we solve for Q_h^k by minimizing the following empirical mean-squared Bellman error as follows at each step,

$$\begin{aligned}\omega_{2,h}^k \leftarrow \mathop{\mathrm{argmin}}_{\omega\in\mathbb{R}^d}&\sum_{\tau=1}^{k-1}\bigl(r_h^k + V_{h+1/2}^k(s_h^\tau, m_h^\tau) - \omega^\top\gamma_h(s_h^\tau, a_h^\tau)\bigr)^2\\&+\lambda\|\omega\|_2^2 + L_{2,h}^k(\omega),\quad h = H,\ldots,1.\end{aligned} \quad \text{(A.13)}$$

Here $L_{2,h}^k$ is a regularizer, which is defined as follows,

$$L_{2,h}^k(\omega) = \sum_{i=1}^{n}\bigl(r_h^i + V_{h+1/2}^k(s_h^i, m_h^i) - \omega^\top\gamma_h(s_h^i, a_h^i)\bigr)^2, \quad \forall (k,h)\in[K]\times[H]. \quad \text{(A.14)}$$

The update in (A.13) takes the following explicit form,

$$\omega_{2,h}^k \leftarrow (\Lambda_{2,h}^k)^{-1}\biggl(\sum_{\tau=1}^{k-1}\gamma_h(s_h^\tau, a_h^\tau)\cdot\bigl(V_{h+1/2}^k(s_h^\tau, m_h^\tau) + r_h^\tau\bigr) + \sum_{i=1}^{n}\gamma_h(s_h^i, a_h^i)\cdot\bigl(V_{h+1/2}^k(s_h^i, m_h^i) + r_h^i\bigr)\biggr),$$

where

$$\Lambda_{2,h}^k = \sum_{\tau=1}^{k-1}\gamma_h(s_h^\tau, a_h^\tau)\gamma_h(s_h^\tau, a_h^\tau)^\top + \sum_{i=1}^{n}\gamma_h(s_h^i, a_h^i)\gamma_h(s_h^i, a_h^i)^\top + \lambda I.$$

We employ the following UCB of $\gamma_h(s_h^k, a_h^k)^\top\omega_{2,h}^k$ for all $(s_h^k, a_h^k)\in\mathcal{S}\times\mathcal{A}$,

$$\Gamma_h^k(s_h^k, a_h^k) = \beta\cdot\Bigl(\log\det\bigl(\Lambda_{2,h}^k + \gamma_h(s_h^k, a_h^k)\gamma_h(s_h^k, a_h^k)^\top\bigr) - \log\det(\Lambda_{2,h}^k)\Bigr)^{1/2}. \quad \text{(A.15)}$$

The update of Q_h^k is defined in Line 9 of Algorithm 2.

A.2 Theory

In parallel to Theorem 3.5, the following theorem characterizes the regret of DOVI⁺, which is defined in (2.3)

Theorem A.5 (Regret of DOVI⁺)**.** Let $\beta = CdH\sqrt{\log(d(T+nH)/\zeta)}$ and $\lambda = 1$, where $C > 0$ and $\zeta \in (0,1]$ are absolute constants. Under Assumptions A.1 and A.3, it holds with probability at least $1-5\zeta$ that

$$\mathrm{Regret}(T) \le C'\cdot(\Delta_{1,H} + \Delta_{2,H})\cdot\sqrt{d^3H^3T}\cdot\sqrt{\log\bigl(d(T+nH)/\zeta\bigr)},$$

where $C' > 0$ is an absolute constant and

$$\Delta_{1,H} = \frac{1}{\sqrt{dH^2}} \sum_{h=1}^{H} \big(\log \det(\Lambda_{1,h}^{K+1}) - \log \det(\Lambda_{1,h}^{1})\big)^{1/2},$$

$$\Delta_{2,H} = \frac{1}{\sqrt{dH^2}} \sum_{h=1}^{H} \big(\log \det(\Lambda_{2,h}^{K+1}) - \log \det(\Lambda_{2,h}^{1})\big)^{1/2}.$$

Proof. See §F.4 for a detailed proof. □

See the discussion of Theorem 3.5 in §3, where Δ_H corresponds to $\Delta_{1,H}$ and $\Delta_{2,H}$ in Theorem A.5. In particular, $\Delta_{1,H}$ and $\Delta_{2,H}$ admit the same information-theoretic interpretation.

B Literature Review on Causal Bandit

In this section, we present literature review on causal bandit that are closely related to our work. [26] propose the causal upper confidence bound (C-UCB) and causal Thompson Sampling (C-TS) algorithms, which attain the $\sqrt{T}$-regret. [34] propose an algorithm based on importance sampling in policy evaluation. In the pure offline setting, [17, 18] propose algorithms for contextual bandit with confounders in the observational data. Their algorithms are based on the analysis of sensitivity [3, 27, 38, 44], which characterizes the worst-case difference between the causal effect and the conditional density obtained from the confounded observational data. In a combination of the online setting and the offline setting, [11] study multi-armed bandit with both the interventional data and the confounded observational data. In contrast to this line of work, we study causal RL in a combination of the online setting and the offline setting. Causal RL is more challenging than causal bandit, which corresponds to $H = 1$, as it involves the transition dynamics and is more challenging in exploration.

C Connection Between Confounded MDP and Other Extensions of MDP

In what follows, we discuss the connection between confounded MDP and other extensions of MDP and SCM.

- **Dynamic Treatment Regimes (DTR).** In a DTR [45], all the states $\{s_h\}_{h\in[H]}$ are confounded by a global confounder w, whereas in a confounded MDP, each state s_h depends on an individual confounder w_{h-1}, which further depends on the previous state s_{h-1}. If w_{h-1} does not depend on s_{h-1}, the confounded MDP reduces to a DTR by summarizing the confounders into $w = (w_1, \ldots, w_H)$. In addition, we remark that our proposed DOVI and DOVI$^+$ can handle global confounders as long as the backdoor and frontdoor criterion holds, respectively.
- **Contextual MDP (CMDP).** A confounded MDP is similar to a CMDP [12] if we cast the confounders $\{w_h\}_{h\in[H]}$ as the context therein. In a CMDP, which focuses on the online setting, the context is fixed throughout an episode, whereas in a confounded MDP, the confounders $\{w_h\}_{h\in[H]}$ vary across the H steps. Moreover, in a CMDP, the goal is to minimize the regret against the globally optimal policy that depends on the context, which is a stronger benchmark than π^* in (2.3), since π^* does not depend on the confounders $\{w_h\}_{h\in[H]}$.
- **Partially Observable MDP (POMDP).** A confounded MDP is a simplified POMDP [39] if we cast the confounders $\{w_h\}_{h\in[H]}$ as the hidden states therein (assuming that the confounders are unobserved in the offline setting as in §A). A POMDP is more challenging to solve, since marginalizing over the hidden states does not yield an MDP, which is the case in a confounded MDP.

D Mechanism of Utilizing Confounded Observational Data

In this section, we discuss the mechanism of incorporating the confounded observational data.

D.1 Partially Observed Confounder

Corresponding to Line 4 of Algorithm 1, DOVI effectively estimates the causal effect $\mathbb{P}(\cdot \,|\, s_h, \mathrm{do}(a_h))$ using

$$\psi_h(s_h, a_h)^\top (\Lambda_h^k)^{-1} \biggl(\sum_{\tau=1}^{k-1} \psi_h(s_h^\tau, a_h^\tau) \cdot \delta_{s_{h+1}^\tau}(\cdot) + \sum_{i=1}^{n} \phi_h(s_h^i, a_h^i, u_h^i) \cdot \delta_{s_{h+1}^i}(\cdot) \biggr), \tag{D.1}$$

where we denote by $\delta_s(\cdot)$ the Dirac measure at s. To see why it works, let the tuning parameter λ be sufficiently small. By the definition of Λ_h^k in (3.10), we have

$$\begin{aligned} \mathbb{P}\bigl(\cdot \,\big|\, s_h, \mathrm{do}(a_h)\bigr) &= \langle \psi_h(s_h, a_h), \mu_h(\cdot) \rangle \\ &\approx \psi_h(s_h, a_h)^\top (\Lambda_h^k)^{-1} \biggl(\sum_{\tau=1}^{k-1} \psi_h(s_h^\tau, a_h^\tau) \cdot \langle \psi_h(s_h^\tau, a_h^\tau), \mu_h(\cdot) \rangle \\ &\qquad\qquad + \sum_{i=1}^{n} \phi_h(s_h^i, a_h^i, u_h^i) \cdot \langle \phi_h(s_h^i, a_h^i, u_h^i), \mu_h(\cdot) \rangle \biggr). \end{aligned} \tag{D.2}$$

Meanwhile, Assumption 3.3 and Proposition 3.4 imply

$$\begin{aligned} \mathbb{P}\bigl(\cdot \,\big|\, s_h, \mathrm{do}(a_h)\bigr) &= \langle \psi_h(s_h, a_h), \mu_h(\cdot) \rangle, \\ \mathcal{P}_h(\cdot \,|\, s_h, a_h, u_h) &= \langle \phi_h(s_h, a_h, u_h), \mu_h(\cdot) \rangle, \end{aligned}$$

which rely on the backdoor adjustment. Since s_{h+1}^τ and s_{h+1}^i in (D.1) are sampled following $\mathbb{P}(\cdot \,|\, s_h^\tau, \mathrm{do}(a_h^\tau))$ and $\mathcal{P}_h(\cdot \,|\, s_h^i, a_h^i, u_h^i)$, respectively, (D.1) approximates the right-hand side of (D.2) as its empirical version. As $k, n \to +\infty$, (D.1) converges to the right-hand side of (D.2) as well as the causal effect $\mathbb{P}(\cdot \,|\, s_h, \mathrm{do}(a_h))$.

D.2 Unobserved Confounder

If the confounders $\{w_h\}_{h\in[H]}$ are unobserved in the offline setting, the backdoor adjustment in §3 is not applicable. Alternatively, the intermediate states $\{m_h\}_{h\in[H]}$ allow us to estimate the causal effect without observing the confounders. The key is that the frontdoor criterion in Assumption A.1 implies

$$\mathbb{P}\bigl(s_{h+1} \,\big|\, s_h, \mathrm{do}(a_h)\bigr) = \int_{\mathcal{M}} \mathbb{P}\bigl(s_{h+1} \,\big|\, s_h, \mathrm{do}(m_h)\bigr) \cdot \mathbb{P}\bigl(m_h \,\big|\, s_h, \mathrm{do}(a_h)\bigr) \mathrm{d}m_h. \tag{D.3}$$

It remains to estimate $\mathbb{P}(s_{h+1} \,|\, s_h, \mathrm{do}(m_h))$ and $\mathbb{P}(m_h \,|\, s_h, \mathrm{do}(a_h))$ on the right-hand side of (D.3). Since a_h and m_h are not confounded given s_h, the causal effect $\mathbb{P}(m_h \,|\, s_h, \mathrm{do}(a_h))$ coincides with the conditional distribution $\mathbb{P}(m_h \,|\, s_h, a_h)$, which can be estimated based on the observational data. To estimate the causal effect $\mathbb{P}(s_{h+1} \,|\, s_h, \mathrm{do}(m_h))$, we utilize the backdoor adjustment in Proposition 3.2 with u_h replaced by a_h, which is enabled by Assumption A.1. More specifically, it holds that

$$\mathbb{P}\bigl(s_{h+1} \,\big|\, s_h, \mathrm{do}(m_h)\bigr) = \mathbb{E}_{a_h' \sim \mathbb{P}(\cdot \,|\, s_h)} \bigl[\mathcal{P}_h\bigl(s_{h+1} \,\big|\, s_h, a_h', m_h\bigr) \bigr]. \tag{D.4}$$

Correspondingly, we construct the value function at the intermediate state $V_{h+1/2}$ and adapt the value iteration following the Bellman optimality equation in (A.3). To estimate the value functions $\{V_{h+1/2}^k\}_{h\in[H]}$ based on the confounded observational data, we utilize the adjustment in (D.4). Corresponding to Line 5 of Algorithm 2, DOVI⁺ effectively estimates the causal effect $\mathbb{P}(\cdot \,|\, s_h, \mathrm{do}(m_h))$ using

$$\psi_h(s_h, m_h)^\top (\Lambda_{1,h}^k)^{-1} \biggl(\sum_{\tau=1}^{k-1} \psi_h(s_h^\tau, m_h^\tau) \cdot \delta_{s_{h+1}^\tau}(\cdot) + \sum_{i=1}^{n} \phi_h(s_h^i, a_h^i, m_h^i) \cdot \delta_{s_{h+1}^i}(\cdot) \biggr), \tag{D.5}$$

To see why it works, let the tuning parameter λ be sufficiently small. By the definition of $\Lambda_{1,h}^k$ in (A.11), we have

$$\begin{aligned}\mathbb{P}\big(\cdot \,\big|\, s_h, \mathrm{do}(m_h)\big) &= \langle \psi_h(s_h, m_h), \mu_h(\cdot)\rangle \\ &\approx \psi_h(s_h, m_h)^\top (\Lambda_{1,h}^k)^{-1}\Bigg(\sum_{\tau=1}^{k-1} \psi_h(s_h^\tau, m_h^\tau)\cdot \langle \psi_h(s_h^\tau, m_h^\tau), \mu_h(\cdot)\rangle \\ &\qquad + \sum_{i=1}^{n} \phi_h(s_h^i, a_h^i, m_h^i)\cdot \langle \phi_h(s_h^i, a_h^i, m_h^i), \mu_h(\cdot)\rangle\Bigg). \end{aligned} \tag{D.6}$$

Meanwhile, Assumption A.3 and Proposition A.4 imply

$$\begin{aligned}\mathbb{P}\big(\cdot \,\big|\, s_h, \mathrm{do}(m_h)\big) &= \langle \psi_h(s_h, m_h), \mu_h(\cdot)\rangle, \\ \mathbb{P}(\cdot \,|\, s_h, a_h, m_h) &= \langle \phi_h(s_h, a_h, m_h), \mu_h(\cdot)\rangle.\end{aligned}$$

Since s_{h+1}^τ and s_{h+1}^i in (D.6) are sampled following $\mathbb{P}(\cdot \,|\, s_h^\tau, \mathrm{do}(m_h^\tau))$ and $\mathbb{P}(\cdot \,|\, s_h^i, a_h^i, m_h^i)$, respectively, (D.5) approximates the right-hand side of (D.6) as its empirical version. As $k, n \to +\infty$, (D.5) converges to the right-hand side of (D.6) as well as the causal effect $\mathbb{P}(\cdot \,|\, s_h, \mathrm{do}(m_h))$.

E Limitation and Future Study

In this paper, we propose confounded MDP, which captures the data generating processes in both the offline setting and the online setting as well as their mismatch due to the confounding issue. We propose DOVI and DOVI$^+$, which handles the confounding issue if backdoor or frontdoor criteria hold, respectively. Nevertheless, our work requires knowing the linear features in the transition dynamics. Moreover, our work requires taking expectations over the feature embeddings with respect to the variable for adjustment. In reality, such feature and expectation are in general unavailable. It remains unknown if efficient reinforcement learning is possible without knowning the features a priori, which we left as our future study. Moreover, our study is restricted to two types of adjustment, namely, the backdoor and frontdoor adjustment, respectively. The design of DOVI and DOVI$^+$ is tightly related to the estimation equation corresponding to the backdoor and frontdoor adjustments, respectively, which estimates the counterfactual effect of actions on the cumulative rewards. In our future study, we also want to generalize our work for general adjustment with estimation equations given.

F Proof of Main Result

F.1 Proof of Proposition 3.4

Proof. Following from Assumption 3.3 and Proposition 3.2, it holds for all $(s_h, a_h) \in \mathcal{S}\times\mathcal{A}$ that

$$\begin{aligned}\mathbb{P}\big(s_{h+1} \,|\, s_h, \mathrm{do}(a_h)\big) &= \mathbb{E}_{u_h\sim\widetilde{\mathcal{P}}_h(\cdot\,|\,s_h)}\big[\mathcal{P}_h(\cdot \,|\, s_h, a_h, u_h)\big] = \mathbb{E}_{u_h\sim\widetilde{\mathcal{P}}_h(\cdot\,|\,s_h)}\big[\langle \phi_h(s_h, a_h, u_h), \mu_h(s_{h+1})\rangle\big] \\ &= \langle \psi_h(s_h, a_h), \mu_h(s_{h+1})\rangle,\end{aligned}$$

where

$$\psi_h(s_h, a_h) = \mathbb{E}_{u_h\sim\widetilde{\mathcal{P}}_h(\cdot\,|\,s_h)}\big[\phi_h(s_h, a_h, u_h)\big], \quad \forall (s_h, a_H) \in \mathcal{S}\times\mathcal{A}.$$

Similarly, following from Assumption 3.3 and Proposition 3.2, it holds for all $(s_h, a_h) \in \mathcal{S}\times\mathcal{A}$ that

$$R_h(s_h, a_h) = \mathbb{E}\big[r_h \,\big|\, s_h, \mathrm{do}(a_h)\big] = \mathbb{E}_{u_h\sim\widetilde{\mathcal{P}}_h(\cdot\,|\,s_h)}\big[\phi_h(s_h, a_h, u_h)^\top\theta_h\big] = \psi_h(s_h, a_h)^\top\theta_h.$$

Hence, following from the Bellman equations in (3.3) and (3.4), the action-value functions Q_h^π and Q_h^* are linear in the backdoor-adjusted feature ψ_h for all π. Thus, we complete the proof of Proposition 3.4. $\square$

F.2 Proof of Proposition A.4

Proof. It holds for all $h \in [H]$ and $(s_{h+1}, s_h, a_h, m_h) \in \mathcal{S} \times \mathcal{S} \times \mathcal{A} \times \mathcal{M}$ that

$$
\begin{aligned}
&\mathbb{P}(s_{h+1}, s_h, a_h, m_h) \\
&\quad = \int_{\mathcal{W}} \mathcal{P}_h(s_{h+1} \,|\, s_h, a_u, w_h) \cdot \nu_h(a_h \,|\, s_h, w_h) \cdot \widetilde{\mathcal{P}}_h(w_h \,|\, s_h) \cdot \breve{\mathcal{P}}_h(m_h \,|\, s_h, a_h) \cdot \mathbb{P}(s_h) \mathrm{d}w_h.
\end{aligned}
$$

Meanwhile, it holds for all $h \in [H]$ and $(s_h, a_h, m_h) \in \mathcal{S} \times \mathcal{A} \times \mathcal{M}$ that

$$
\mathbb{P}(s_h, a_h, m_h) = \int_{\mathcal{W}} \nu_h(a_h \,|\, s_h, w_h) \cdot \widetilde{\mathcal{P}}_h(w_h \,|\, s_h) \cdot \breve{\mathcal{P}}_h(m_h \,|\, s_h, a_h) \cdot \mathbb{P}(s_h) \mathrm{d}w_h.
$$

Hence, we have

$$
\begin{aligned}
\mathbb{P}(s_{h+1} \,|\, s_h, a_h, m_h) &= \frac{\mathbb{P}(s_{h+1}, s_h, a_h, m_h)}{\mathbb{P}(s_h, a_h, m_h)} \\
&= \frac{\int_{\mathcal{W}} \mathcal{P}_h(s_{h+1} \,|\, s_h, a_u, w_h) \cdot \nu_h(a_h \,|\, s_h, w_h) \cdot \widetilde{\mathcal{P}}_h(w_h \,|\, s_h) \mathrm{d}w_h}{\int_{\mathcal{W}} \nu_h(a_h \,|\, s_h, w_h) \cdot \widetilde{\mathcal{P}}_h(w_h \,|\, s_h) \mathrm{d}w_h}. \qquad \text{(F.1)}
\end{aligned}
$$

Meanwhile, following from Assumption A.3, we have

$$
\mathcal{P}_h(s_{h+1} \,|\, s_h, a_h, w_h) = \langle \rho_h(s_h, a_h, w_h), \mu_h(s_{h+1}) \rangle. \qquad \text{(F.2)}
$$

Recall that we define $\widetilde{\nu}_h(a_h \,|\, s_h) = \mathbb{E}_{w_h \sim \widetilde{\mathcal{P}}_h(\cdot \,|\, s_h)}[\pi(a_h \,|\, s_h, u_h)]$. Hence, by plugging (F.2) into (F.1), we obtain that

$$
\mathbb{P}(s_{h+1} \,|\, s_h, a_h, m_h) = \langle \phi_h(s_h, a_h, m_h), \mu_h(s_{h+1}) \rangle,
$$

where we define for all $h \in [H]$ and $(s_h, a_h, m_h) \in \mathcal{S} \times \mathcal{A} \times \mathcal{M}$ that

$$
\begin{aligned}
\phi_h(s_h, a_h, m_h) &= \frac{\int_{\mathcal{W}} \rho_h(s_h, a_u, w_h) \cdot \nu_h(a_h \,|\, s_h, w_h) \cdot \widetilde{\mathcal{P}}_h(w_h \,|\, s_h) \mathrm{d}w_h}{\int_{\mathcal{W}} \nu_h(a_h \,|\, s_h, w_h) \cdot \widetilde{\mathcal{P}}_h(w_h \,|\, s_h) \mathrm{d}w_h} \\
&= \frac{\mathbb{E}_{w_h \sim \widetilde{\mathcal{P}}_h(\cdot \,|\, s_h)} \big[\rho_h(s_h, m_h, w_h) \cdot \nu_h(a_h \,|\, s_h, w_h)\big]}{\widetilde{\nu}_h(a_h \,|\, s_h)}.
\end{aligned}
$$

Thus, we complete the proof of Proposition A.4. □

F.3 Proof of Theorem 3.5

Proof. We first define for all $(k, h) \in [K] \times [H]$ the model prediction error ι_h^k as follows,

$$
\iota_h^k(s_h, a_h) = -Q_h^k(s_h, a_h) + R_h(s_h, a_h) + (\mathbb{P}_h V_{h+1}^k)(s_h, a_h), \quad \forall (s_h, a_h) \in \mathcal{S} \times \mathcal{A}. \qquad \text{(F.3)}
$$

We define the filtrations associated with Algorithm 1 as follows.

Definition F.1 (Filtration). For all $(k, h) \in [K] \times [H]$, we define $\mathcal{F}_{k,h,1}$ the σ-algebra generated by the following set,

$$
\begin{aligned}
B_{k,h,1} = &\big\{(s_h^i, a_h^i, u_h^i, r_h^i)\big\}_{(i,h) \in [n] \times [H]} \cup \big\{(s_j^\tau, a_j^\tau, r_j^\tau)\big\}_{(\tau,j) \in [k-1] \times [H]} \\
&\cup \big\{(s_j^k, a_j^k, r_j^k)\big\}_{j \in [h-1]} \cup \big\{(s_h^k, a_h^k)\big\}. \qquad \text{(F.4)}
\end{aligned}
$$

Similarly, we define $\mathcal{F}_{k,h,2}$ the σ-algebra generated by the following set,

$$
B_{k,h,2} = B_{k,h,1} \cup \{s_{h+1}^k\} \cup \{r_h^k\}. \qquad \text{(F.5)}
$$

Moreover, we define $\mathcal{F}_{0,h,2}$ the σ-algebra generated by the set $\{(s_h^i, a_h^i, u_h^i, r_h^i)\}_{(i,h) \in [n] \times [H]}$ for all $h \in [H]$. We define the timestep index as follows,

$$
t(k, h, m) = 2H \cdot k + 2(h-1) + m. \qquad \text{(F.6)}
$$

It then holds for $t(k, h, m) \leq t(k', h', m')$ that $\mathcal{F}_{k,h,m} \subseteq \mathcal{F}_{k',h',m'}$. Hence, the set of σ-algebra $\{\mathcal{F}_{k,h,m}\}_{(k,h,m) \in [K] \times [H] \times [2]}$ is a filtration with the timestep index $t(\cdot, \cdot, \cdot)$ defined in (F.6).

The following lemma characterizes the model prediction errors defined in (F.3).

Lemma F.2. Let $\beta = CdH\sqrt{\log(d(T+nH)/\zeta)}$ and $\zeta \in (0,1]$. Under Assumption 3.3, it holds with probability at least $1-2\zeta$ that

$$-2\Gamma_h^k(s_h,a_h) \le \iota_h^k(s_h,a_h) \le 0, \quad \forall (k,h) \in [K]\times[H],\ (s_h,a_h) \in \mathcal{S}\times\mathcal{A}.$$

Proof. See §G.1 for a detailed proof. □

In the sequel, we define the following operators,

$$(\mathbb{J}_h f)(s) = \langle f(s,\cdot), \pi_h^*(\cdot\,|\,s)\rangle_{\mathcal{A}}, \qquad (\mathbb{J}_{k,h} f)(s) = \langle f(s,\cdot), \pi_h^k(\cdot\,|\,s)\rangle_{\mathcal{A}}, \quad \forall s \in \mathcal{S}.$$

Meanwhile, recall that we define

$$(\mathbb{P}_h V)(s_h,a_h) = \mathbb{E}_{s_{h+1}\sim\mathbb{P}(\cdot\,|\,s_h,\mathrm{do}(a_h))}\big[V(s_{h+1})\big], \quad \forall (s_h,a_h)\in\mathcal{S}\times\mathcal{A}.$$

We define the following martingale adapted to the filtration $\{\mathcal{F}_{k,h,m}\}_{(k,h,m)\in[K]\times[H]\times[2]}$,

$$M_{k,h,m} = \sum_{\substack{(\tau,i,\ell)\in[K]\times[H]\times[2]\\ t(\tau,i,\ell)\le t(k,h,m)}} D_{\tau,i,\ell},$$

where

$$D_{k,h,1} = \big(\mathbb{J}_{k,h}(Q_h^k - Q_h^{\pi^k,k})\big)(s_h^k) - (Q_h^k - Q_h^{\pi^k,k})\big)(s_h^k,a_h^k), \quad \forall (k,h)\in[K]\times[H],$$
$$D_{k,h,2} = \big(\mathbb{P}_h(V_{h+1}^k - V_{h+1}^{\pi^k,k})\big)(s_h^k,a_h^k) - (V_{h+1}^k - V_{h+1}^{\pi^k,k})(s_{h+1}^k), \quad \forall (k,h)\in[K]\times[H].$$

The following lemma is adapted from [7].

Lemma F.3 (Lemma 4.2 of [7])**.** It holds that

$$\begin{aligned}
\mathrm{Regret}(T) &= \sum_{k=1}^K V_1^{\pi^*}(x_1^k) - V_1^{\pi_k}(x_1^k)\\
&= Y + \mathcal{M}_{K,H,2} + \sum_{k=1}^K\sum_{h=1}^H\Big(\mathbb{E}_{\pi^*}\big[\iota_h^k(s_h,a_h)\,\big|\,s_1=s_1^k\big] - \iota_h^k(s_h^k,a_h^k)\Big),
\end{aligned} \tag{F.7}$$

where

$$Y = \sum_{k=1}^K\sum_{h=1}^H \mathbb{E}_{\pi^*}\big[\langle Q_h^k(s_h,\cdot), \pi_h^*(\cdot\,|\,s_h) - \pi_h^k(\cdot\,|\,s_h)\rangle\,\big|\,s_1 = s_1^k\big]. \tag{F.8}$$

Proof. See [7] for a detailed proof. □

In what follows, we upper bound the right-hand side of (F.7) in Lemma F.3. By Algorithm 1, it holds that π_h^k is the greedy policy with respect to the action-value function Q_h^k. Hence, for Y defined in (F.8) of Lemma F.3, we have

$$Y = \sum_{k=1}^K\sum_{h=1}^H \mathbb{E}_{\pi^*}\big[\langle Q_h^k(s_h,\cdot), \pi_h^*(\cdot\,|\,s_h) - \pi_h^k(\cdot\,|\,s_h)\rangle\,\big|\,s_1 = s_1^k\big] \le 0. \tag{F.9}$$

Meanwhile, following from the proof of Theorem 3.1 in [7], it holds with probability at least $1-\zeta/2$ that

$$M_{K,H,2} \le C_0 \cdot \sqrt{d^3H^3T}\cdot\sqrt{\log(1/\zeta)}, \tag{F.10}$$

where $C_0 > 0$ is an absolute constant. In addition, following from Lemma F.2, it holds with probability at least $1-2\zeta$ that

$$\sum_{k=1}^K\sum_{h=1}^H\Big(\mathbb{E}_{\pi^*}\big[\iota_h^k(s_h,a_h)\,\big|\,s_1=s_1^k\big] - \iota_h^k(s_h^k,a_h^k)\Big) \le 2\sum_{k=1}^K\sum_{h=1}^H \Gamma_h^k(s_h^k,a_h^k). \tag{F.11}$$

Recall that for all $(s_h, a_h) \in \mathcal{S} \times \mathcal{A}$, we define

$$\Gamma_h^k(s_h, a_h) = \beta \cdot \Big(\log\det\big(\Lambda_h^k + \psi_h(s_h, a_h)\psi_h(s_h, a_h)^\top\big) - \log\det(\Lambda_h^k)\Big)^{1/2}. \tag{F.12}$$

Hence, by the Cauchy-Schwartz inequality, we obtain that

$$\begin{aligned}\sum_{k=1}^K \sum_{h=1}^H \Gamma_h^k(s_h^k, a_h^k) &= \beta \sum_{k=1}^K \sum_{h=1}^H \Big(\log\det\big(\Lambda_h^k + \psi_h(s_h^k, a_h^k)\psi_h(s_h^k, a_h^k)^\top\big) - \log\det(\Lambda_h^k)\Big)^{1/2} \\ &\le \beta \sum_{h=1}^H \bigg(K \sum_{k=1}^K \big(\log\det(\Lambda_h^{k+1}) - \log\det(\Lambda_h^k)\big)\bigg)^{1/2} \\ &= \beta\sqrt{K} \sum_{h=1}^H \big(\log\det(\Lambda_h^{K+1}) - \log\det(\Lambda_h^1)\big)^{1/2}. \end{aligned} \tag{F.13}$$

In what follows, we define

$$\Delta_H = \frac{1}{\sqrt{dH^2}} \sum_{h=1}^H \big(\log\det(\Lambda_h^{K+1}) - \log\det(\Lambda_h^1)\big)^{1/2}. \tag{F.14}$$

Thus, by plugging (F.14) and $\beta = CdH \cdot \sqrt{\log(d(T+nH)/\zeta)}$ into (F.13), it holds with probability at least $1 - 2\zeta$ that,

$$\sum_{k=1}^K \sum_{h=1}^H \Gamma_h^k(s_h^k, a_h^k) \le C \cdot \Delta_H \cdot \sqrt{d^3H^3T} \cdot \sqrt{\log\big(d(T+nH)/\zeta\big)}, \tag{F.15}$$

where recall that we define $T = HK$. By further plugging (F.15) into (F.11), it holds with probability at least $1 - 2\zeta$ that,

$$\begin{aligned}&\sum_{k=1}^K \sum_{h=1}^H \Big(\mathbb{E}_{\pi^*}\big[\iota_h^k(s_h, a_h) \,\big|\, s_1 = s_1^k\big] - \iota_h^k(s_h^k, a_h^k)\Big) \\ &\qquad \le 2C \cdot \Delta_H \cdot \sqrt{d^3H^3T} \cdot \sqrt{\log\big(d(T+nH)/\zeta\big)}. \end{aligned} \tag{F.16}$$

Finally, combining Lemma F.3, (F.9), (F.10), and (F.16), it holds with probability at least $1 - 5\zeta/2$ that

$$\text{Regret}(T) \le C' \cdot \Delta_H \cdot \sqrt{d^3H^3T} \cdot \sqrt{\log\big(d(T+nH)/\zeta\big)},$$

where $C' > 0$ is an absolute constant and

$$\Delta_H = \frac{1}{\sqrt{dH^2}} \sum_{h=1}^H \big(\log\det(\Lambda_h^{K+1}) - \log\det(\Lambda_h^1)\big)^{1/2}.$$

Thus, we complete the proof of Theorem 3.5. □

F.4 Proof of Theorem A.5

Proof. In the sequel, we define the following operators,

$$(\mathbb{J}_h f)(s) = \langle f(s, \cdot), \pi_h^*(\cdot \,|\, s)\rangle_{\mathcal{A}}, \qquad (\mathbb{J}_{k,h} f)(s) = \langle f(s, \cdot), \pi_h^k(\cdot \,|\, s)\rangle_{\mathcal{A}}. \tag{F.17}$$

Meanwhile, recall that we define the following transition operators,

$$\mathbb{P}_{h+1/2} V(s_h, m_h) = \mathbb{E}\Big[V(s_{h+1}) \,\Big|\, s_{h+1} \sim \mathbb{P}\big(\cdot \,\big|\, s_h, \mathrm{do}(m_h)\big)\Big], \quad \forall V : \mathcal{S} \mapsto \mathbb{R},\ (s_h, m_h) \in \mathcal{S} \times \mathcal{M}.$$

$$\mathbb{P}_h V'(s_h, a_h) = \mathbb{E}\big[V'(s_h, m_h) \,\big|\, m_h \sim \breve{\mathcal{P}}_h(\cdot \,|\, s, a)\big], \quad \forall V' : \mathcal{S} \times \mathcal{M} \mapsto \mathbb{R},\ (s_h, a_h) \in \mathcal{S} \times \mathcal{A}.$$

We further define for all $(k, h) \in [K] \times [H]$ the following transition operator,

$$\widetilde{\mathbb{P}}_{h+1/2} V(s_h, a_h, m_h) = \mathbb{E}\big[V(s_{h+1}) \,\big|\, s_{h+1} \sim \mathbb{P}(\cdot \,|\, s_h, a_h, m_h)\big], \quad \forall V : \mathcal{S} \mapsto \mathbb{R},\ (s_h, a_h, m_h) \in \mathcal{S} \times \mathcal{A} \times \mathcal{M}.$$

We define the following model prediction errors,

$$\iota_h^k(s_h,a_h) = -Q_h^k(s_h,a_h) + r_h(s_h,a_h) + (\mathbb{P}_h V_{h+1/2}^k)(s_h,a_h), \quad \forall (s_h,a_h)\in\mathcal{S}\times\mathcal{A},$$
$$\iota_{h+1/2}^k(s_h,m_h) = -V_{h+1/2}^k(s_h,m_h) + (\mathbb{P}_{h+1/2} V_{h+1}^k)(s_h,m_h), \quad \forall (s_h,m_h)\in\mathcal{S}\times\mathcal{M}. \quad \text{(F.18)}$$

In parallel to Definition F.1, we define the following filtrations that correspond to Algorithm 2.

Definition F.4 (Filtration)**.** For $(k,h)\in[K]\times[H]$, we define $\mathcal{F}'_{k,h,1}$ the σ-algebra generated by the following set,

$$B'_{k,h,1} = \big\{(s_h^i,a_h^i,m_h^i,r_h^i)\big\}_{(i,h)\in[n]\times[H]} \cup \big\{(s_j^\tau,a_j^\tau,m_j^\tau,r_j^\tau)\big\}_{(\tau,j)\in[k-1]\times[H]}$$
$$\cup \big\{(s_j^k,a_j^k,m_j^k,r_j^k)\big\}_{j\in[h-1]} \cup \big\{(s_h^k,a_h^k)\big\}. \quad \text{(F.19)}$$

Similarly, we define $\mathcal{F}'_{k,h,2}$ the σ-algebra generated by the following set,

$$B'_{k,h,2} = B'_{k,h,1} \cup \{m_h^k\} \cup \{r_h^k\}, \quad \text{(F.20)}$$

and we define $\mathcal{F}'_{k,h,3}$ the σ-algebra generated by the following set,

$$B'_{k,h,3} = B'_{k,h,2} \cup \{s_{h+1}^k\}, \quad \text{(F.21)}$$

Moreover, we define $\mathcal{F}'_{0,h,3}$ the σ-algebra generated by the set $\{(s_h^i,a_h^i,m_h^i,r_h^i)\}_{(i,h)\in[n]\times[H]}$ for all $h\in[H]$. We define the timestep index as follows,

$$t'(k,h,m) = 3H\cdot k + 3(h-1) + m. \quad \text{(F.22)}$$

It then holds for $t'(k,h,m)\le t'(k',h',m')$ that $\mathcal{F}'_{k,h,m}\subseteq\mathcal{F}'_{k',h',m'}$. Hence, the set of σ-algebra $\{\mathcal{F}'_{k,h,m}\}_{(k,h,m)\in[K]\times[H]\times[3]}$ is a filtration with the timestep index $t'(\cdot,\cdot,\cdot)$ defined in (F.22).

The following lemma characterizes the model prediction errors defined in (F.18).

Lemma F.5. Let $\beta = CdH\sqrt{\log(d(T+nH)/\zeta)}$ and $\zeta\in(0,1]$. Under Assumption A.3, it holds with probability at least $1-4\zeta$ that

$$-2\Gamma_{h+1/2}^k(s_h,m_h) \le \iota_{h+1/2}^k(s_h,m_h) \le 0,\ \forall (k,h)\in[K]\times[H],\ (s_h,m_h)\in\mathcal{S}\times\mathcal{M}, \quad \text{(F.23)}$$
$$-2\Gamma_h^k(s_h,a_h) \le \iota_h^k(s_h,a_h) \le 0, \quad \forall (k,h)\in[K]\times[H],\ (s_h,a_h)\in\mathcal{S}\times\mathcal{A}. \quad \text{(F.24)}$$

Proof. See §G.2 for a detailed proof. □

Our goal is to upper bound the regret, which takes the following form,

$$\begin{aligned}\text{Regret}(T) &= \sum_{k=1}^K V_1^{\pi^*}(s_1^k) - V_1^{\pi^k}(s_1^k)\\ &= \underbrace{\sum_{k=1}^K \big(V_1^{\pi^*}(s_1^k) - V_1^k(x_1^k)\big)}_{\text{(i)}} + \underbrace{\sum_{k=1}^K \big(V_1^k(s_1^k) - V_1^{\pi^k}(x_1^k)\big)}_{\text{(ii)}},\end{aligned} \quad \text{(F.25)}$$

where $\{V_h^k\}_{(k,h)\in[K]\times[H]}$ is the output of Algorithm 2. In what follows, we calculate terms (i) and (ii) on the right-hand side of (F.25) separately.

Term (i). We now calculate term (i) on the right-hand side of (F.25). By (F.17), for all $h\in[H]$, it holds that

$$V_h^{\pi^*} - V_h^k = \mathbb{J}_h Q_h^{\pi^*} + \mathbb{J}_{k,h} Q_h^k = \mathbb{J}_h(Q_h^{\pi^*} - Q_h^k) + (\mathbb{J}_h - \mathbb{J}_{k,h})Q_h^k. \quad \text{(F.26)}$$

We first calculate the term $Q_h^{\pi^*} - Q_h^k$ on the right-hand side of (F.26). Recall that we define

$$\iota_h^k = -Q_h^k + r_h + \mathbb{P}_h V_{h+1/2}^k, \qquad \iota_{h+1/2}^k = -V_{h+1/2}^k + \mathbb{P}_{h+1/2} V_{h+1}^k.$$

Meanwhile, following from the Bellman equation in (A.2), we obtain that

$$Q_h^{\pi^*} = r_h + \mathbb{P}_h V_{h+1/2}^{\pi^*}, \qquad V_{h+1/2}^{\pi^*} = \mathbb{P}_{h+1/2} V_{h+1}^{\pi^*}.$$

Thus, it holds that

$$Q_h^{\pi^*} - Q_h^k = \iota_h^k + \mathbb{P}_h (V_{h+1/2}^{\pi^*} - V_{h+1/2}^k) = \iota_h^k + \mathbb{P}_h \iota_{h+1/2}^k + \mathbb{P}_h \mathbb{P}_{h+1/2} (V_{h+1}^{\pi^*} - V_{h+1}^k). \tag{F.27}$$

Recall that we set $V_{H+1}^{\pi^*} = V_{H+1}^k = 0$. Hence, upon recursion, we obtain from (F.26) and (F.27) that

$$\begin{aligned}
V_1^{\pi^*} - V_1^k &= \Big(\prod_{h=1}^{H} \mathbb{J}_h \mathbb{P}_h \mathbb{P}_{h+1/2}\Big)(V_{H+1}^{\pi^*} - V_{H+1}^k) + \sum_{h=1}^{H} \Big(\prod_{i=1}^{h-1} \mathbb{J}_i \mathbb{P}_i \mathbb{P}_{i+1/2}\Big) \mathbb{J}_h \iota_h^k \\
&\quad + \sum_{h=1}^{H} \Big(\prod_{i=1}^{h-1} \mathbb{J}_i \mathbb{P}_i \mathbb{P}_{i+1/2}\Big) \mathbb{J}_h \mathbb{P}_h \iota_{h+1/2}^k + \sum_{h=1}^{H} \Big(\prod_{i=1}^{h-1} \mathbb{J}_i \mathbb{P}_i \mathbb{P}_{i+1/2}\Big) (\mathbb{J}_h - \mathbb{J}_{k,h}) Q_h^k \\
&= \sum_{h=1}^{H} \Big(\prod_{i=1}^{h-1} \mathbb{J}_i \mathbb{P}_i \mathbb{P}_{i+1/2}\Big) (\mathbb{J}_h \iota_h^k + \mathbb{J}_h \mathbb{P}_h \iota_{h+1/2}^k) + \sum_{h=1}^{H} \Big(\prod_{i=1}^{h-1} \mathbb{J}_i \mathbb{P}_i \mathbb{P}_{i+1/2}\Big) (\mathbb{J}_h - \mathbb{J}_{k,h}) Q_h^k.
\end{aligned} \tag{F.28}$$

By the definition of $\mathbb{J}_h$ and $\mathbb{J}_{k,h}$ in (F.17), we further obtain from (F.28) that

$$\begin{aligned}
\sum_{k=1}^{K} \big(V_1^{\pi^*}(s_1^k) - V_1^k(s_1^k)\big) &= \sum_{k=1}^{K} \sum_{h=1}^{H} \mathbb{E}_{\pi^*} \big[\iota_h^k(s_h, a_h) + \iota_{h+1/2}^k(s_h, m_h) \,\big|\, s_1 = s_1^k\big] \\
&\quad + \sum_{k=1}^{K} \sum_{h=1}^{H} \mathbb{E}_{\pi^*} \big[\langle Q_h^k(s_h, \cdot), \pi_h^*(\cdot \,|\, s_h) - \pi_h^k(\cdot \,|\, s_h) \,\big|\, s_1 = s_1^k\big],
\end{aligned} \tag{F.29}$$

which completes the calculation of term (i) on the right-hand side of (F.25).

Term (ii). We now calculate term (ii) on the right-hand side of (F.25). By (F.17), for all $h \in [H]$, we have

$$V_h^k(s_h^k) - V_h^{\pi^k}(s_h^k) = \big(\mathbb{J}_{k,h}(Q_h^k - Q_h^{\pi^k})\big)(s_h^k). \tag{F.30}$$

Meanwhile, by (F.18) it holds that

$$\begin{aligned}
\iota_h^k(s_h^k, a_h^k) &= r_h(s_h^k, a_h^k) + (\mathbb{P}_h V_{h+1/2}^k)(s_h^k, a_h^k) - Q_h^k(s_h^k, a_h^k) \\
&= r_h(s_h^k, a_h^k) - Q_h^{\pi^k}(s_h^k, a_h^k) + \mathbb{P}_h V_{h+1/2}^k(s_h^k, a_h^k) + (Q_h^{\pi^k} - Q_h^k)(s_h^k, a_h^k)(s_h^k, a_h^k) \\
&= \big(\mathbb{P}_h (V_{h+1/2}^k - V_{h+1/2}^{\pi^k})\big)(s_h^k, a_h^k) - (Q_h^k - Q_h^{\pi^k})(s_h^k, a_h^k),
\end{aligned} \tag{F.31}$$

where the second equality follows from the Bellman equation $Q_h^{\pi^k}(s_h, a_h) = r_h(s_h, a_h) + (\mathbb{P}_h V_{h+1/2}^{\pi^k})(s_h, a_h)$. Similarly, we have

$$\iota_{h+1/2}^k(s_h^k, m_h^k) = \big(\mathbb{P}_{h+1/2}(V_{h+1}^k - V_{h+1}^{\pi^k})\big)(s_h^k, m_h^k) - (V_{h+1/2}^k - V_{h+1/2}^{\pi^k})(s_h^k, m_h^k). \tag{F.32}$$

Thus, by combining (F.30), (F.31), and (F.32), we have

$$\begin{aligned}
&(V_h^k - V_h^{\pi^k})(s_h^k) + \iota_h^k(s_h^k, a_h^k) + \iota_{h+1/2}^k(s_h^k, m_h^k) \\
&\quad = (V_{h+1}^k - V_{h+1}^{\pi^k})(s_{h+1}^k) + \underbrace{\big(\mathbb{J}_{k,h}(Q_h^k - Q_h^{\pi^k})\big)(s_h^k) - (Q_h^k - Q_h^{\pi^k})(s_h^k, a_h^k)}_{D_{k,h,1}} \\
&\qquad + \underbrace{\big(\mathbb{P}_h (V_{h+1/2}^k - V_{h+1/2}^{\pi^k})\big)(s_h^k, a_h^k) - (V_{h+1/2}^k - V_{h+1/2}^{\pi^k})(s_h^k, m_h^k)}_{D_{k,h,2}} \\
&\qquad + \underbrace{\big(\mathbb{P}_{h+1/2}(V_{h+1}^k - V_{h+1}^{\pi^k})\big)(s_h^k, m_h^k) - (V_{h+1}^k - V_{h+1}^{\pi^k})(s_{h+1}^k)}_{D_{k,h,3}}.
\end{aligned} \tag{F.33}$$

Meanwhile, note that $V_{H+1}^{\pi^k} = V_{H+1}^k = 0$. Hence, by recursively applying (F.33), we obtain that

$$
\begin{aligned}
&(V_1^k - V_1^{\pi^k})(s_1^k) \\
&\quad = \sum_{h=1}^{H} (D_{k,h,1} + D_{k,h,2} + D_{k,h,3}) - \sum_{h=1}^{H} \big(\iota_h^k(s_h^k, a_h^k) + \iota_{h+1/2}^k(s_h^k, m_h^k) \big).
\end{aligned} \tag{F.34}
$$

By the definition of filtration in (F.4), for the terms $D_{k,h,1}$, $D_{k,h,2}$ and $D_{k,h,3}$ on the right-hand side of (F.33), it holds for all $(k, h) \in [K] \times [H]$ that

$$
D_{k,h,1} \in \mathcal{F}_{k,h,1}, \quad D_{k,h,2} \in \mathcal{F}_{k,h,2}, \quad D_{k,h,3} \in \mathcal{F}_{k,h,3}.
$$

Moreover, it holds that

$$
\mathbb{E}[D_{k,h,1} \,|\, \mathcal{F}_{k,h-1,3}] = \mathbb{E}[D_{k,h,2} \,|\, \mathcal{F}_{k,h,1}] = \mathbb{E}[D_{k,h,3} \,|\, \mathcal{F}_{k,h,2}] = 0.
$$

Hence, the terms $D_{k,h,1}$, $D_{k,h,2}$ and $D_{k,h,3}$ defines a martingale $M'_{k,h,m}$ with respect to the timestep index $t'(\cdot, \cdot, \cdot)$ as follows,

$$
M'_{k,h,m} = \sum_{\substack{(\tau,i,\ell) \in [K]\times[H]\times[3] \\ t'(\tau,i,\ell) \le t'(k,h,m)}} D_{\tau,i,\ell}, \tag{F.35}
$$

where $t'(\cdot, \cdot, \cdot)$ is defined in (F.22) of Definition F.4. In specific, we have

$$
M'_{K,H,3} = \sum_{k=1}^{K} \sum_{h=1}^{H} (D_{k,h,1} + D_{k,h,2} + D_{k,h,3}). \tag{F.36}
$$

By further taking sum of (F.34) over $k \in [K]$, we obtain from (F.36) that

$$
\sum_{k=1}^{K} (V_1^k - V_1^{\pi^k})(s_1^k) = M'_{K,H,3} - \sum_{k=1}^{K} \sum_{h=1}^{H} \big(\iota_h^k(s_h^k, a_h^k) + \iota_{h+1/2}^k(s_h^k, m_h^k) \big), \tag{F.37}
$$

which completes the calculation of term (ii) on the right-hand side of (F.25).

Finally, by plugging (F.29) and (F.37) into (F.25), we conclude that

$$
\begin{aligned}
\mathrm{Regret}(T) = &\sum_{k=1}^{K} \sum_{h=1}^{H} \mathbb{E}_{\pi^*} \big[\langle Q_h^k(s_h, \cdot), \pi_h^*(\cdot \,|\, s_h) - \pi_h^k(\cdot \,|\, s_h) \,\big|\, s_1 = s_1^k \big] + M'_{K,H,3} \\
&+ \sum_{k=1}^{K} \sum_{h=1}^{H} \mathbb{E}_{\pi^*} \big[\iota_h^k(s_h, a_h) + \iota_{h+1/2}^k(s_h, m_h) \,\big|\, s_1 = s_1^k \big] \\
&- \sum_{k=1}^{K} \sum_{h=1}^{H} \big(\iota_h^k(s_h^k, a_h^k) + \iota_{h+1/2}^k(s_h^k, m_h^k) \big),
\end{aligned} \tag{F.38}
$$

where $M'_{K,H,3}$ is defined in (F.36).

We now upper bound the right-hand side of (F.38). The following proof is similar to that of Theorem 3.5 in §F.3. In the sequel, we define

$$
\begin{aligned}
Y' &= \sum_{k=1}^{K} \sum_{h=1}^{H} \mathbb{E}_{\pi^*} \big[\langle Q_h^k(s_h, \cdot), \pi_h^*(\cdot \,|\, s_h) - \pi_h^k(\cdot \,|\, s_h) \,\big|\, s_1 = s_1^k \big], \\
Z' &= \sum_{k=1}^{K} \sum_{h=1}^{H} \mathbb{E}_{\pi^*} \big[\iota_h^k(s_h, a_h) + \iota_{h+1/2}^k(s_h, m_h) \,\big|\, s_1 = s_1^k \big] - \sum_{k=1}^{K} \sum_{h=1}^{H} \big(\iota_h^k(s_h^k, a_h^k) + \iota_{h+1/2}^k(s_h^k, m_h^k) \big).
\end{aligned}
$$

It then follows from (F.38) that

$$
\mathrm{Regret}(T) = Y' + M'_{K,H,3} + Z'. \tag{F.39}
$$

Recall that we set π_h^k to be the greedy policy with respect to the action-value function Q_h^k. Thus, it holds that

$$Y' = \sum_{k=1}^{K}\sum_{h=1}^{H} \mathbb{E}_{\pi^*}\big[\langle Q_h^k(s_h,\cdot), \pi_h^*(\cdot\,|\,s_h) - \pi_h^k(\cdot\,|\,s_h)\,\big|\, s_1 = s_1^k\big] \le 0. \tag{F.40}$$

Meanwhile, following from the truncation of Q_h^k in Algorithm 2 and the assumption that $r_h \in [0,1]$, for terms $D_{k,h,i}$ defined in (F.33), we have

$$|D_{k,h,i}| \le 2H, \quad \forall (k,h,i) \in [K]\times[H]\times[3].$$

Hence, by the Azumas-Hoeffding lemma, it holds with probability at least $1-\zeta$ that

$$M'_{K,H,3} \le C_1 \cdot \sqrt{d^3H^3T}\cdot\sqrt{\log(dT/\zeta)}, \tag{F.41}$$

where $M'_{K,H,3}$ is the martingale defined in (F.35), $C_1 > 0$ is an absolute constant, and $T = HK$. Following from Lemma F.5, it holds with probability at least $1-4\zeta$ that

$$Z' \le 2\sum_{k=1}^{K}\sum_{h=1}^{H}\Gamma_{h+1/2}^k(s_h^k, m_h^k) + 2\sum_{k=1}^{K}\sum_{h=1}^{H}\Gamma_h^k(s_h^k, a_h^k). \tag{F.42}$$

Following from the definition of $\Gamma_{h+1/2}^k$ in (A.12), we obtain that

$$\begin{aligned}\sum_{k=1}^{K}\sum_{h=1}^{H}\Gamma_{h+1/2}^k(s_h^k, m_h^k) &= 2\beta\sum_{k=1}^{K}\sum_{h=1}^{H}\Big(\log\det\big(\Lambda_{1,h}^k + \psi_h(s_h^k, m_h^k)\psi_h(s_h,m_h)^\top\big) - \log\det(\Lambda_{1,h}^k)\Big)^{1/2} \\ &= 2\beta\sum_{k=1}^{K}\sum_{h=1}^{H}\big(\log\det(\Lambda_{1,h}^{k+1}) - \log\det(\Lambda_{1,h}^k)\big)^{1/2}.\end{aligned} \tag{F.43}$$

Thus, by the Cauchy-Schwartz inequality, we obtain from (F.43) that

$$\begin{aligned}\sum_{k=1}^{K}\sum_{h=1}^{H}\Gamma_{h+1/2}^k(s_h^k, m_h^k) &\le \beta\sum_{h=1}^{H}\bigg(K\cdot\sum_{k=1}^{K}\big(\log\det(\Lambda_{1,h}^{k+1}) - \log\det(\Lambda_{1,h}^1)\big)\bigg)^{1/2} \\ &\le \beta\cdot\sqrt{K}\sum_{h=1}^{H}\big(\log\det(\Lambda_{1,h}^{K+1}) - \log\det(\Lambda_{1,h}^1)\big)^{1/2}.\end{aligned} \tag{F.44}$$

Similarly, we obtain that

$$\sum_{k=1}^{K}\sum_{h=1}^{H}\Gamma_h^k(s_h^k, a_h^k) \le \beta\cdot\sqrt{K}\sum_{h=1}^{H}\big(\log\det(\Lambda_{2,h}^{k+1}) - \log\det(\Lambda_{2,h}^1)\big)^{1/2}. \tag{F.45}$$

In what follows, we define

$$\begin{aligned}\Delta_{1,H} &= \frac{1}{\sqrt{dH^2}}\sum_{h=1}^{H}\big(\log\det(\Lambda_{1,h}^{K+1}) - \log\det(\Lambda_{1,h}^1)\big)^{1/2}, \\ \Delta_{2,H} &= \frac{1}{\sqrt{dH^2}}\sum_{h=1}^{H}\big(\log\det(\Lambda_{2,h}^{k+1}) - \log\det(\Lambda_{2,h}^1)\big)^{1/2}.\end{aligned}$$

By plugging (F.44), (F.45), and $\beta = CdH\cdot\sqrt{\log(d(T+nH)/\zeta)}$ into (F.42), we obtain that

$$Z' \le 2C\cdot(\Delta_{1,H}+\Delta_{2,H})\cdot\sqrt{d^3H^3T}\cdot\sqrt{\log\big(d(T+nH)/\zeta\big)}, \tag{F.46}$$

which holds with probability at least $1-4\zeta$. Here recall that we define $T = HK$. Finally, by plugging (F.40), (F.41), and (F.46) into (F.39), it holds with probability at least $1-5\zeta$ that

$$\mathrm{Regret}(T) \le C'\cdot(\Delta_{1,H}+\Delta_{2,H})\cdot\sqrt{d^3H^3T}\cdot\sqrt{\log\big(d(T+nH)/\zeta\big)},$$

where $C' > 0$ is an absolute constant. Thus, we complete the proof of Theorem A.5. $\square$

G Proof of Auxiliary Result

G.1 Proof of Lemma F.2

Proof. Recall that we define

$$
\begin{aligned}
(\mathbb{P}_h V)(s_h, a_h) &= \mathbb{E}\Big[V(s_{h+1}) \,\Big|\, s_{h+1} \sim \mathbb{P}\big(\cdot \,\big|\, s_h, \mathrm{do}(a_h)\big)\Big] \\
&= \mathbb{E}\big[V(s_{h+1}) \,\big|\, s_{h+1} \sim \mathcal{P}_h(\cdot \,|\, s_h, a_h, u_h), u_h \sim \widetilde{\mathcal{P}}_h(\cdot \,|\, s_h)\big],
\end{aligned}
$$

where the second equality follows from Proposition 3.2. In the sequel, we define

$$
(\widetilde{\mathbb{P}}_h V)(s_h, a_h, u_h) = \mathbb{E}\Big[V(s_{h+1}) \,\Big|\, s_{h+1} \sim \mathcal{P}_h\big(\cdot \,\big|\, s_h, a_h, u_h\big)\Big].
$$

By Assumption 3.3, we obtain that

$$
\mathbb{P}_h V_{h+1}^k = \psi_h^\top \langle \mu_h, V_{h+1}^k \rangle = \psi_h^\top (\Lambda_h^k)^{-1} \Lambda_h^k \langle \mu_h, V_{h+1}^k \rangle, \quad \widetilde{\mathbb{P}}_h V_{h+1}^k = \phi_h^\top \langle \mu_h, V_{h+1}^k \rangle. \tag{G.1}
$$

Recall that

$$
\Lambda_h^k = \sum_{\tau=1}^{k-1} \psi_h(s_h^\tau, a_h^\tau) \psi_h(s_h^\tau, a_h^\tau)^\top + \sum_{i=1}^{n} \phi_h(s_h^i, a_h^i, u_h^i) \phi_h(s_h^i, a_h^i, u_h^i)^\top + \lambda I.
$$

Therefore, by (G.1), we obtain that

$$
\begin{aligned}
(\mathbb{P}_h V_{h+1}^k)(\cdot, \cdot) &= \psi_h(\cdot, \cdot)^\top (\Lambda_h^k)^{-1} \bigg(\sum_{\tau=1}^{k-1} \psi_h(s_h^\tau, a_h^\tau) \psi_h(s_h^\tau, a_h^\tau)^\top \langle \mu_h, V_{h+1}^k \rangle + \lambda \cdot \langle \mu_h, V_{h+1}^k \rangle \\
&\qquad + \sum_{i=1}^{n} \phi_h(s_h^i, a_h^i, u_h^i) \phi_h(s_h^i, a_h^i, u_h^i)^\top \langle \mu_h, V_{h+1}^k \rangle \bigg) \\
&= \psi_h(\cdot, \cdot)^\top (\Lambda_h^k)^{-1} \bigg(\sum_{\tau=1}^{k-1} \psi_h(s_h^\tau, a_h^\tau) \cdot (\mathbb{P}_h V_{h+1}^k)(s_h^\tau, a_h^\tau) + \lambda \cdot \langle \mu_h, V_{h+1}^k \rangle \\
&\qquad + \sum_{i=1}^{n} \phi_h(s_h^i, a_h^i, u_h^i) \cdot (\widetilde{\mathbb{P}}_h V_{h+1}^k)(s_h^i, a_h^i, u_h^i) \bigg).
\end{aligned} \tag{G.2}
$$

Recall that we define the counterfactual reward as follows,

$$
R_h(s_h, a_h) = \mathbb{E}_{u_h}\big[r(s_h, a_h, u_h) \,\big|\, S_h = s_h\big], \quad \forall (s_h, a_h) \in \mathcal{S} \times \mathcal{A}. \tag{G.3}
$$

It then follows from Assumption 3.3 and Proposition 3.4 that $R_h(\cdot, \cdot) = \psi_h(\cdot, \cdot)^\top \theta_h$. Hence, it holds for all $h \in [H]$ that

$$
\begin{aligned}
r_h(\cdot, \cdot, \cdot) &= \phi_h(\cdot, \cdot, \cdot)^\top \theta_h = \phi_h(\cdot, \cdot, \cdot)^\top (\Lambda_h^k)^{-1} \Lambda_h^k \theta_h \\
&= \phi_h(\cdot, \cdot, \cdot)^\top (\Lambda_h^k)^{-1} \bigg(\sum_{\tau=1}^{k-1} \psi_h(s_h^\tau, a_h^\tau) \psi_h(s_h^\tau, a_h^\tau)^\top \theta_h + \lambda \cdot \langle \mu_h, V_{h+1}^k \rangle \\
&\qquad + \sum_{i=1}^{n} \phi_h(s_h^i, a_h^i, u_h^i) \phi_h(s_h^i, a_h^i, u_h^i)^\top \theta_h \bigg) \\
&= \phi_h(\cdot, \cdot, \cdot)^\top (\Lambda_h^k)^{-1} \bigg(\sum_{\tau=1}^{k-1} \psi_h(s_h^\tau, a_h^\tau) \cdot R_h(s_h^\tau, a_h^\tau) + \lambda \cdot \theta_h \\
&\qquad + \sum_{i=1}^{n} \phi_h(s_h^i, a_h^i, u_h^i) \cdot \mathbb{E}[r_h \,|\, s_h^i, a_h^i, u_h^i] \bigg).
\end{aligned} \tag{G.4}
$$

Meanwhile, following from the explicit update of ω_h^k in (3.9), we obtain that

$$
\begin{aligned}
\psi_h(\cdot, \cdot)^\top \omega_h^k = \psi_h(\cdot, \cdot)^\top (\Lambda_h^k)^{-1} \bigg(&\sum_{\tau=1}^{k-1} \psi_h(s_h^\tau, a_h^\tau) \cdot \big(V_{h+1}^k(s_{h+1}^\tau) + r_h^\tau\big) \\
&+ \sum_{i=1}^{n} \phi_h(s_h^i, a_h^i, u_h^i) \cdot \big(V_{h+1}^k(s_{h+1}^i) + r_h^i\big) \bigg).
\end{aligned} \tag{G.5}
$$

Hence, combining (G.2), (G.4), and (G.5), we obtain that

$$
\begin{aligned}
&\psi_h(\cdot,\cdot)^\top \omega_h^k - R_h(\cdot,\cdot) - (\mathbb{P}_h V_{h+1}^k)(\cdot,\cdot) \\
&\quad = \psi_h(\cdot,\cdot)^\top (\Lambda_h^k)^{-1}(S_{1,h} + S_{2,h} + S_{3,h} + S_{4,h}) - \psi_h(\cdot,\cdot)^\top \lambda \cdot \big(\langle \mu_h, V_{h+1}^k\rangle + \theta_h\big), \qquad (G.6)
\end{aligned}
$$

where we define

$$
\begin{aligned}
S_{1,h} &= \sum_{\tau=1}^{k-1} \psi_h(s_h^\tau, a_h^\tau) \cdot \big(V_{h+1}^k(s_{h+1}^\tau) - (\mathbb{P}_h V_{h+1}^k)(s_h^\tau, a_h^\tau)\big), \qquad (G.7)\\
S_{2,h} &= \sum_{i=1}^{n} \phi_h(s_h^i, a_h^i, u_h^i) \cdot \big(V_{h+1}^k(s_{h+1}^i) - (\widetilde{\mathbb{P}}_h V_{h+1}^k)(s_h^i, a_h^i, u_h^i)\big),\\
S_{3,h} &= \sum_{\tau=1}^{k-1} \psi_h(s_h^\tau, a_h^\tau) \cdot \big(r_h^\tau - R(s_h^\tau, a_h^\tau)\big), \quad \text{and} \quad S_{4,h} = \sum_{i=1}^{n} \phi_h(s_h^i, a_h^i, u_h^i) \cdot \big(r_h^i - \mathbb{E}[r_h \,|\, s_h^i, a_h^i, u_h^i]\big).
\end{aligned}
$$

In what follows, we upper bound the right-hand side of (G.6). By the Cauchy-Schwartz inequality, we obtain that

$$
\begin{aligned}
&|\psi_h(\cdot,\cdot)^\top \omega_h^k - R_h(\cdot,\cdot) - (\mathbb{P}_h V_{h+1}^k)(\cdot,\cdot)| \qquad (G.8)\\
&\quad \le \big(\psi_h(\cdot,\cdot)^\top (\Lambda_h^k)^{-1} \psi_h(\cdot,\cdot)\big)^{1/2} \cdot \Bigg(\bigg\| \sum_{\ell=1}^{4} S_{\ell,h} \bigg\|_{(\Lambda_h^k)^{-1}} + \lambda \cdot \big(\|\langle \mu_h, V_{h+1}^k\rangle\|_{(\Lambda_h^k)^{-1}} + \|\theta_h\|_{(\Lambda_h^k)^{-1}} \big) \Bigg),
\end{aligned}
$$

where $S_{1,h}$, $S_{2,h}$, $S_{3,h}$, and $S_{4,h}$ are defined in (G.7). By Lemma H.6, for $\lambda = 1$, it holds with probability at least $1 - 2\zeta$ that

$$
\bigg\| \sum_{\ell=1}^{4} S_{\ell,h} \bigg\|_{(\Lambda_h^k)^{-1}} \le C' d H \sqrt{\log\big(2(C+1)d(T+nH)/\zeta\big)}, \qquad (G.9)
$$

where $C > 0$ and $C' > 0$ are absolute constants. Meanwhile, by Assumption 3.3, it holds that

$$
\begin{aligned}
\|\langle \mu_h, V_{h+1}^k\rangle\|_{(\Lambda_h^k)^{-1}} &\le \|\langle \mu_h, V_{h+1}^k\rangle\|_2 / \sqrt{\lambda}\\
&\le \bigg(\sum_{\ell=1}^{d} \|\mu_{\ell,h}\|_1^2 \bigg)^{1/2} \cdot \|V_{k+1}^h\|_\infty / \sqrt{\lambda} \le H\sqrt{d/\lambda}, \qquad (G.10)
\end{aligned}
$$

where the first inequality follows from the fact that $\Lambda_h^k \succeq \lambda I$, the second inequality follows from the Hölder's inequality, and the third inequality follows from Assumption 3.3 and the fact that $V_{k+1}^h \le H$. Similarly, it holds from Assumption 3.3 that

$$
\|\theta_h\|_{(\Lambda_h^k)^{-1}} \le \|\theta_h\|_2/\sqrt{\lambda} \le \sqrt{d/\lambda}. \qquad (G.11)
$$

Finally, by plugging (G.9), (G.10), and (G.11) into (G.8) with $\lambda = 1$, it holds with probability at least $1 - 2\zeta$ that

$$
|\psi_h(\cdot,\cdot)^\top \omega_h^k - R_h(\cdot,\cdot) - (\mathbb{P}_h V_{h+1}^k)(\cdot,\cdot)| \le \beta/\sqrt{2} \cdot \big(\psi_h(\cdot,\cdot)^\top (\Lambda_h^k)^{-1} \psi_h(\cdot,\cdot)\big)^{1/2}, \qquad (G.12)
$$

where we set $\beta = C'' d H \sqrt{\log(d(T+nH)/\zeta)}$ for a sufficiently large absolute constant $C'' > 0$. By further applying Lemma H.7 to (G.12), for $\lambda = 1$, it holds with probability at least $1 - 2\zeta$ that

$$
\begin{aligned}
&|\psi_h(\cdot,\cdot)^\top \omega_h^k - R_h(\cdot,\cdot) - (\mathbb{P}_h V_{h+1}^k)(\cdot,\cdot)|\\
&\quad \le \beta \cdot \Big(\log\det\big(\Lambda_h^k + \psi_h(\cdot,\cdot)\psi_h(\cdot,\cdot)^\top\big) - \log\det(\Lambda_h^k) \Big)^{1/2} = \Gamma_h^k(\cdot,\cdot). \qquad (G.13)
\end{aligned}
$$

Recall that we set

$$
Q_h^k(\cdot,\cdot) = \min\big\{\psi_h(\cdot,\cdot)^\top \omega_h^k + \Gamma_h^k(\cdot,\cdot), H - h\big\}.
$$

Hence, by (G.13), it holds with probability at least $1 - 2\zeta$ that

$$
\begin{aligned}
-\iota_h^k(\cdot,\cdot) &= Q_h^k(\cdot,\cdot) - R_h(\cdot,\cdot) - (\mathbb{P}_h V_{h+1}^k)(\cdot,\cdot)\\
&\le \psi_h(\cdot,\cdot)^\top \omega_h^k + \Gamma_h^k(\cdot,\cdot) - R_h(\cdot,\cdot) - (\mathbb{P}_h V_{h+1}^k)(\cdot,\cdot) \le 2\Gamma_h^k(\cdot,\cdot),
\end{aligned}
$$

and

$$\iota_h^k(\cdot,\cdot) = -Q_h^k(\cdot,\cdot) + R_h(\cdot,\cdot) + (\mathbb{P}_h V_{h+1}^k)(\cdot,\cdot)$$
$$\leq \max\bigl\{(\mathbb{P}_h V_{h+1}^k)(\cdot,\cdot) + R_h(\cdot,\cdot) - \psi_h(\cdot,\cdot)^\top \omega_h^k - \Gamma_h^k, R_h(\cdot,\cdot) + (\mathbb{P}_h V_{h+1}^k)(\cdot,\cdot) - H + h\bigr\} \leq 0,$$

where the second inequality follows from (G.13) the facts that $V_{h+1}^k \leq H - h - 1$ and $R_h \leq 1$. In conclusion, it holds with probability at least $1 - 2\zeta$ that

$$-2\Gamma_h^k(\cdot,\cdot) \leq \iota_h^k(\cdot,\cdot) \leq 0,$$

which concludes the proof of Lemma F.2. □

G.2 Proof of Lemma F.5

Proof. Recall that we define the following transition operators,

$$\mathbb{P}_{h+1/2} V(s_h, m_h) = \mathbb{E}\Bigl[V(s_{h+1}) \,\Big|\, s_{h+1} \sim \mathbb{P}\bigl(\cdot \,\big|\, s_h, \mathrm{do}(m_h)\bigr)\Bigr]$$
$$\widetilde{\mathbb{P}}_{h+1/2} V(s_h, a_h, m_h) = \mathbb{E}\bigl[V(s_{h+1}) \,\big|\, s_{h+1} \sim \mathbb{P}(\cdot \,|\, s_h, a_h, m_h)\bigr]. \quad \text{(G.14)}$$

Following from Assumption A.3 and (A.7), we have

$$\mathbb{P}_{h+1/2} V_{h+1}^k = \psi_h^\top \langle \mu_h, V_{h+1}^k \rangle = \psi_h^\top (\Lambda_{1,h}^k)^{-1} \Lambda_{1,h}^k \langle \mu_h, V_{h+1}^k \rangle, \quad \text{(G.15)}$$
$$\widetilde{\mathbb{P}}_{h+1/2} V_{h+1}^k = \phi_h^\top \langle \mu_h, V_{h+1}^k \rangle, \quad \text{(G.16)}$$

where we define

$$\Lambda_{1,h}^k = \sum_{\tau=1}^{k-1} \psi_h(s_h^\tau, m_h^\tau) \psi(s_h^\tau, m_h^\tau)^\top + \sum_{i=1}^{n} \phi_h(s_h^i, a_h^i, m_h^i) \phi_h(s_h^i, a_h^i, m_h^i)^\top + \lambda I. \quad \text{(G.17)}$$

Hence, following from (G.15), it holds for all $(s_h, m_h) \in \mathcal{S} \times \mathcal{M}$ that

$$\mathbb{P}_{h+1/2} V_{h+1}^k(s_h, m_h)$$
$$= \psi_h(s_h, m_h)^\top (\Lambda_{1,h}^k)^{-1} \biggl(\sum_{\tau=1}^{k-1} \psi_h(s_h^\tau, m_h^\tau) \psi(s_h^\tau, m_h^\tau)^\top \langle \mu_h, V_{h+1}^k \rangle + \lambda \cdot \langle \mu_h, V_{h+1}^k \rangle \quad \text{(G.18)}$$
$$+ \sum_{i=1}^{n} \phi_h(s_h^i, a_h^i, m_h^i) \phi_h(s_h^i, a_h^i, m_h^i)^\top \langle \mu_h, V_{h+1}^k \rangle \biggr).$$

By plugging (G.15) and (G.16) into (G.18), we further obtain that

$$\mathbb{P}_{h+1/2} V_{h+1}^k(s_h, m_h)$$
$$= \psi_h(s_h, m_h)^\top (\Lambda_{1,h}^k)^{-1} \biggl(\sum_{\tau=1}^{k-1} \psi_h(s_h^\tau, m_h^\tau) \cdot (\mathbb{P}_{h+1/2} V_{h+1}^k)(s_h^\tau, m_h^\tau) + \lambda \cdot \langle \mu_h, V_{h+1}^k \rangle \quad \text{(G.19)}$$
$$+ \sum_{i=1}^{n} \phi_h(s_h^i, a_h^i, m_h^i) \cdot (\widetilde{\mathbb{P}}_{h+1/2} V_{h+1}^k)(s_h^i, a_h^i, m_h^i) \biggr).$$

Following from the update of $\omega_{1,h}^k$ in (A.10), it holds for all $h \in [H]$ and $(s_h, m_h) \in \mathcal{S} \times \mathcal{M}$ that

$$\psi_h(s_h, m_h)^\top \omega_{1,h}^k = \psi_h(s_h, m_h)^\top (\Lambda_{1,h}^k)^{-1} \biggl(\sum_{\tau=1}^{k-1} \psi_h(s_h^\tau, m_h^\tau) \cdot V_{h+1}^k(s_{h+1}^\tau) \quad \text{(G.20)}$$
$$+ \sum_{i=1}^{n} \phi_h(s_h^i, a_h^i, m_h^i) \cdot V_{h+1}^k(s_{h+1}^i) \biggr).$$

Hence, combining (G.19) and (G.20), we obtain for all $h \in [H]$ and $(s_h, m_h) \in \mathcal{S} \times \mathcal{M}$ that

$$\psi_h(s_h, m_h)^\top \omega_{1,h}^k - \mathbb{P}_{h+1/2} V_{h+1}^k(s_h, m_h)$$
$$= \psi_h(s_h, m_h)^\top (\Lambda_{1,h}^k)^{-1} (S'_{1,h} + S'_{2,h}) + \lambda \cdot \psi_h(s, m)^\top \langle \mu_h, V_{h+1}^k \rangle, \quad \text{(G.21)}$$

where we define

$$S'_{1,h} = \sum_{\tau=1}^{k-1} \psi_h(s_h^\tau, m_h^\tau) \cdot \big(V_{h+1}^k(s_{h+1}^\tau) - (\mathbb{P}_{h+1/2} V_{h+1}^k)(s_h^\tau, m_h^\tau)\big),$$
$$S'_{2,h} = \phi_h(s_h^i, a_h^i, m_h^i) \cdot \big(V_{h+1}^k(s_{h+1}^i) - (\widetilde{\mathbb{P}}_{h+1/2} V_{h+1}^k)(s_h^i, a_h^i, m_h^i)\big).$$

We now upper bound the right-hand side of (G.21). By the Cauchy-Schwartz inequality, we obtain from (G.21) that

$$|\psi_h^\top \omega_{1,h}^k - \mathbb{P}_{h+1/2} V_{h+1}^k| \\ \leq \big(\psi_h^\top (\Lambda_{1,h}^k)^{-1} \psi_h\big)^{1/2} \cdot \big(\|S'_{1,h} + S'_{2,h}\|_{(\Lambda_h^k)^{-1}} + \lambda \cdot \|\langle \mu_h, V_{h+1}^k \rangle\|_{(\Lambda_h^k)^{-1}}\big). \tag{G.22}$$

Following from similar analysis to the proof of Lemma H.6 in §H, for $\lambda = 1$, it holds with probability at least $1 - 2\zeta$ that

$$\|S'_{1,h} + S'_{2,h}\|_{(\Lambda_h^k)^{-1}} \leq C' dH \sqrt{\log\big(2(C+1)d(T+nH)/\zeta\big)}. \tag{G.23}$$

Meanwhile, by Assumption A.3, we have

$$\|\langle \mu_h, V_{h+1}^k \rangle\|_{(\Lambda_h^k)^{-1}} \leq \|\langle \mu_h, V_{h+1}^k \rangle\|_2 / \sqrt{\lambda} \\ \leq \bigg(\sum_{\ell=1}^d \|\mu_{\ell,h}\|_1^2\bigg)^{1/2} \cdot \|V_{k+1}^h\|_\infty / \sqrt{\lambda} \leq H\sqrt{d/\lambda}, \tag{G.24}$$

where the first inequality follows from the fact that $\Lambda_{1,h}^k \succeq \lambda I$, the second inequality follows from the Hölder's inequality, and the third inequality follows from Assumption A.3 and the fact that $V_{k+1}^h \leq H$. Finally, by plugging (G.23) and (G.24) into (G.22), we obtain for all $(s_h, m_h) \in \mathcal{S} \times \mathcal{M}$ that

$$|\psi_h(s_h, m_h)^\top \omega_{1,h}^k - (\mathbb{P}_{h+1/2} V_{h+1}^k)(s_h, m_h)| \\ \leq \beta/\sqrt{2} \cdot \big(\psi_h(s_h, m_h)^\top (\Lambda_{1,h}^k)^{-1} \psi_h(s_h, m_h)\big)^{1/2} \\ \leq \beta \cdot \Big(\log\det\big(\Lambda_{1,h}^k + \psi_h(s_h, m_h)\psi_h(s_h, m_h)^\top\big) - \log\det(\Lambda_{1,h}^k)\Big)^{1/2} \\ = \Gamma_{h+1/2}^k(s_h, m_h), \tag{G.25}$$

where we set $\beta = C'' dH \sqrt{\log(d(T+nH)/\zeta)}$ for a sufficiently large absolute constant $C'' > 0$ and the last inequality follows from Lemma H.7. Here $\Gamma_{h+1/2}^k$ is the UCB defined in (A.12). Recall that for all $(s_h, m_h) \in \mathcal{S} \times \mathcal{M}$, we define

$$V_{h+1/2}^k(s_h, m_h) = \min\big\{\psi_h(s_h, m_h)^\top \omega_{1,h}^k + \Gamma_{h+1/2}^k(s_h, m_h), H - h\big\}.$$

Hence, by (G.25), for all $(s_h, m_h) \in \mathcal{S} \times \mathcal{M}$, it holds with probability at least $1 - 2\zeta$ that

$$-\iota_{h+1/2}^k(s_h, m_h) = V_{h+1/2}^k(s_h, m_h) - (\mathbb{P}_{h+1/2} V_{h+1}^k)(s_h, m_h) \\ \leq \psi_h(s_h, m_h)^\top \omega_h^k + \Gamma_{h+1/2}^k(s_h, m_h) - (\mathbb{P}_{h+1/2} V_{h+1}^k)(s_h, m_h) \leq 2\Gamma_{h+1/2}^k(s_h, m_h),$$

and

$$\iota_{h+1/2}^k(s_h, m_h) = -V_{h+1/2}^k(s_h, m_h) + (\mathbb{P}_{h+1/2} V_{h+1}^k)(s_h, m_h) \\ \leq \max\big\{(\mathbb{P}_{h+1/2} V_{h+1}^k)(s_h, m_h) - \psi_h(s_h, m_h)^\top \omega_{1,h}^k - \Gamma_{h+1/2}^k(s_h, m_h), \\ (\mathbb{P}_{h+1/2} V_{h+1}^k)(s_h, m_h) - H + h\big\} \leq 0,$$

where the second inequality follows from (G.25) and the fact that $V_{h+1}^k \leq H - h - 1$. In conclusion, it holds with probability at least $1 - 2\zeta$ that

$$-2\Gamma_{h+1/2}^k(s_h, m_h) \leq \iota_{h+1/2}^k(s_h, m_h) \leq 0.$$

Similarly, following from the proof of Lemma F.2 with Lemma H.5 in place of Lemma H.4, the reward r_h in place of R_h, and the feature γ_h in place of both ψ_h and ϕ_h, for all $(s_h, a_h) \in \mathcal{S} \times \mathcal{A}$, it holds with probability at least $1 - 2\zeta$ that

$$-2\Gamma_h^k(s_h, a_h) \leq \iota_h^k(s_h, a_h) \leq 0.$$

Thus, we complete the proof of Lemma F.5. □

H Auxiliary Lemma

Lemma H.1 (Concentration of Self-Normalized Process [1, 16]). Let $\{\epsilon_t\}_{t=1}^{\infty}$ be a real-valued stochastic process adapted to the filtration $\{\mathcal{F}_t\}_{t=0}^{\infty}$. Let $\epsilon_t \mid \mathcal{F}_{t-1}$ be zero-mean and σ-sub-Gaussian. Let $\{\psi_t\}_{t=0}^{\infty}$ be an $\mathbb{R}^d$-valued stochastic process with $\psi_t \in \mathcal{F}_{t-1}$. Let $\overline{\Lambda}_t = \overline{\Lambda}_0 + \sum_{\tau=1}^{t} \psi_\tau \psi_\tau^\top$, where $\overline{\Lambda}_0$ is a positive definite matrix. Let $\delta > 0$ be an absolute constant. It then holds with probability at least $1-\delta$ that

$$\Big\| \sum_{\tau=1}^{t} \psi_\tau \cdot \epsilon_\tau \Big\|_{\overline{\Lambda}_t^{-1}}^2 \le 2\sigma^2 \cdot \log\Big(\sqrt{\det(\overline{\Lambda}_t)/\det(\overline{\Lambda}_0)} \cdot \delta^{-1} \Big), \quad \forall t \ge 0.$$

Proof. See [1] for a detailed proof. □

Lemma H.2 (Lemma D.4 of [16]). Let $\{s_t\}_{t=1}^{\infty}$ and $\{\psi_t\}_{t=1}^{\infty}$ with $\|\psi_t\|_2 \le 1$ be $\mathcal{S}$-valued and $\mathbb{R}^d$-valued stochastic processes adopted to the filtration $\{\mathcal{F}_t\}_{t=0}^{\infty}$, respectively. Let $\overline{\Lambda}_t = \overline{\Lambda}_0 + \sum_{\tau=1}^{t} \psi_\tau \psi_\tau^\top$, where $\overline{\Lambda}_0 \succeq \lambda I$ is a positive definite matrix. Let $\sup_{s\in\mathcal{S}} |V(s)| \le H$ for all $V \in \mathcal{V}$. Let $\delta > 0$ be an absolute constant. It then holds with probability at least $1-\delta$ that

$$\begin{aligned}
&\Big\| \sum_{\tau=1}^{t} \psi_\tau \cdot \Big(V(s_\tau) - \mathbb{E}\big[V(s_\tau) \mid \mathcal{F}_{\tau-1}\big] \Big) \Big\|_{\overline{\Lambda}_t^{-1}}^2 \\
&\qquad \le 4H^2 \cdot \Big(d/2 \cdot \log\big(\det(\overline{\Lambda}_t)/\det(\overline{\Lambda}_0)\big) + \log(\mathcal{N}_\epsilon/\delta) \Big) + 8t^2\epsilon^2/\lambda.
\end{aligned}$$

Here $\mathcal{N}_\epsilon$ is the ϵ-covering number of $\mathcal{V}$ with respect to the metric $d(V, V') = \sup_{s\in\mathcal{S}} |V(s) - V'(s)|$ for all $V, V' \in \mathcal{V}$.

Proof. The proof technique is similar to that of Lemma D.4 by [16]. For all $V \in \mathcal{V}$, there exist an element $\widetilde{V}$ in the ϵ-covering of $\mathcal{V}$ satisfying

$$d(V, \widetilde{V}) = \sup_{s\in\mathcal{S}} |V(s) - \widetilde{V}(s)| \le \epsilon. \tag{H.1}$$

In the sequel, we define

$$\Delta_V(\cdot) = V(\cdot) - \widetilde{V}(\cdot). \tag{H.2}$$

It then holds that

$$\begin{aligned}
&\Big\| \sum_{\tau=1}^{t} \psi_\tau \cdot \Big(V(s_\tau) - \mathbb{E}\big[V(s_\tau) \mid \mathcal{F}_{\tau-1}\big] \Big) \Big\|_{\overline{\Lambda}_t^{-1}}^2 \\
&\quad \le 2\Big\| \sum_{\tau=1}^{t} \psi_\tau \cdot \Big(\widetilde{V}(s_\tau) - \mathbb{E}\big[\widetilde{V}(s_\tau) \mid \mathcal{F}_{\tau-1}\big] \Big) \Big\|_{\overline{\Lambda}_t^{-1}}^2 \\
&\qquad + 2\Big\| \sum_{\tau=1}^{t} \psi_\tau \cdot \Big(\Delta_V(s_\tau) - \mathbb{E}\big[\Delta_V(s_\tau) \mid \mathcal{F}_{\tau-1}\big] \Big) \Big\|_{\overline{\Lambda}_t^{-1}}^2.
\end{aligned} \tag{H.3}$$

Note that $|\widetilde{V}(s)| \le H$ for all $s \in \mathcal{S}$. Hence, following from Lemma H.1 and a union bound argument, it holds with probability at least $1-\delta$ that

$$\begin{aligned}
&2\Big\| \sum_{\tau=1}^{t} \psi_\tau \cdot \Big(\widetilde{V}(s_\tau) - \mathbb{E}\big[\widetilde{V}(s_\tau) \mid \mathcal{F}_{\tau-1}\big] \Big) \Big\|_{\overline{\Lambda}_t^{-1}}^2 \\
&\qquad \le 4H^2 \cdot \Big(d/2 \cdot \log\big(\det(\overline{\Lambda}_t)/\det(\overline{\Lambda}_0)\big) + \log(\mathcal{N}_\epsilon/\delta) \Big),
\end{aligned} \tag{H.4}$$

where $\mathcal{N}_\epsilon$ is the ϵ-covering number of $\mathcal{V}$. Meanwhile, it follows from (H.1) and (H.2) that $|\Delta_V(s)| \le \epsilon$ for all $s \in \mathcal{S}$. Hence, we have

$$2\Big\| \sum_{\tau=1}^{t} \psi_\tau \cdot \Big(\Delta_V(s_\tau) - \mathbb{E}\big[\Delta_V(s_\tau) \mid \mathcal{F}_{\tau-1}\big] \Big) \Big\|_{\overline{\Lambda}_t^{-1}}^2 \le 8t^2\epsilon^2/\lambda, \tag{H.5}$$

where the inequality follows from the fact that $\overline{\Lambda}_t \succeq \lambda I$. By plugging (H.4) and (H.5) into (H.3), it holds with probability at least $1-\delta$ that

$$\Big\|\sum_{\tau=1}^{t} \psi_\tau \cdot \Big(V(s_\tau) - \mathbb{E}\big[V(s_\tau) \,\big|\, \mathcal{F}_{\tau-1}\big]\Big)\Big\|^2_{\overline{\Lambda}_t^{-1}}$$
$$\le 4H^2 \cdot \Big(d/2 \cdot \log\big(\det(\overline{\Lambda}_t)/\det(\overline{\Lambda}_0)\big) + \log(\mathcal{N}_\epsilon/\delta)\Big) + 8t^2\epsilon^2/\lambda,$$

which concludes the proof of Lemma H.2. $\square$

Lemma H.3 (Upper Bound of Parameter [16])**.** Under Assumption 3.3, It holds that

$$\|\omega_h^k\|_2 \le H\big(d(k+n)/\lambda\big)^{1/2}, \quad \forall (k,h) \in [K]\times[H]. \tag{H.6}$$

Proof. See [16] for a detailed proof. $\square$

Lemma H.4 (Covering Number of $\mathcal{V}$ [16])**.** Let $\mathcal{V}$ be a class of functions V satisfying

$$V(\cdot) = \min\big\{\max_{a\in\mathcal{A}} \psi(\cdot,a)^\top\omega + \Gamma(\cdot,a), H-h\big\}, \tag{H.7}$$

where

$$\Gamma(\cdot,\cdot) = \sqrt{2}\beta \cdot \Big(\log\det\big(\Lambda + \psi(\cdot,\cdot)\psi(\cdot,\cdot)^\top\big) - \log\det(\Lambda)\Big)^{1/2}. \tag{H.8}$$

Here the function V is parameterized by (ω,Λ) and the parameter β is fixed. Let $\psi(\cdot,\cdot)$ be an $\mathbb{R}^d$-valued function and $\Lambda \in \mathbb{R}^{d\times d}$. Let $\|\psi(s,a)\|_2 \le 1$ for all $(s,a)\in\mathcal{S}\times\mathcal{A}$. For $\|\omega\|_2 \le L$, $\Lambda \succeq \lambda I$, $\beta\in[0,B]$, and $\epsilon>0$, there exist an ϵ-covering of $\mathcal{V}$ with respect to the metric $d(V,V') = \sup_{s\in\mathcal{S}}|V(s)-V'(s)|$, such that the covering number $\mathcal{N}_\epsilon$ is upper bounded as follows,

$$\log\mathcal{N}_\epsilon \le d\cdot\log(1+4L/\epsilon) + d^2\cdot\log\big(1+16B^2d^{1/2}/(\epsilon^2\lambda)\big).$$

Proof. The proof technique is similar to that of Lemma D.6 by [16]. Let V_1 and V_2 be the functions defined in (H.7), which are parameterized by (ω_1,Λ_1) and (ω_2,Λ_2), respectively. Note that

$$\begin{aligned} d(V_1,V_2) &\le \sup_{s\in\mathcal{S}}\Big|\min\big\{\max_{a\in\mathcal{A}}\psi(s,a)^\top\omega_1 + \Gamma_1(s,a), H-h\big\} \\ &\qquad\qquad - \min\big\{\max_{a\in\mathcal{A}}\psi(s,a)^\top\omega_2 + \Gamma_2(s,a), H-h\big\}\Big| \\ &\le \sup_{(s,a)\in\mathcal{S}\times\mathcal{A}} |\psi(s,a)^\top(\omega_1-\omega_2) + \Gamma_1(s,a) - \Gamma_2(s,a)|, \end{aligned} \tag{H.9}$$

where the second inequality follows from the fact that $\min\{\cdot, H-h\}$ and $\max_{a\in\mathcal{A}}$ are contraction mappings. Here we define Γ_1 and Γ_2 in (H.8) with $\Lambda=\Lambda_1$ and $\Lambda=\Lambda_2$, respectively. Meanwhile, following from the matrix determinant lemma, we have

$$\begin{aligned} \Gamma_1(s,a) &= \sqrt{2}\beta\cdot\Big(\log\det\big(\Lambda_1 + \psi(s,a)\psi(s,a)^\top\big) - \log\det(\Lambda_1)\Big)^{1/2} \\ &= \sqrt{2}\beta\cdot\Big(\log\big(1+\psi(s,a)^\top\Lambda_1^{-1}\psi(s,a)\big)\Big)^{1/2}, \quad \forall (s,a)\in\mathcal{S}\times\mathcal{A}. \end{aligned}$$

Thus, following from the inequalities $|\sqrt{x}-\sqrt{y}| \le \sqrt{|x-y|}$ and $|\log(1+x)-\log(1+y)| \le |x-y|$ for all $x,y\ge 0$, we have

$$\begin{aligned} |\Gamma_1(s,a)-\Gamma_2(s,a)| &\le \sqrt{2}\beta\cdot\Big(\big|\log\big(1+\psi(s,a)^\top\Lambda_1^{-1}\psi(s,a)\big) - \log\big(1+\psi(s,a)^\top\Lambda_2^{-1}\psi(s,a)\big)\big|\Big)^{1/2} \\ &\le \sqrt{2}\beta\cdot\Big(\big|\psi(s,a)^\top(\Lambda_1^{-1}-\Lambda_2^{-1})\psi(s,a)\big|\Big)^{1/2}. \end{aligned} \tag{H.10}$$

Combining (H.14) and (H.10), we have

$$\begin{aligned} d(V_1,V_2) &\le \sup_{(s,a)\in\mathcal{S}\times\mathcal{A}} |\psi(s,a)^\top(\omega_1-\omega_2) + \Gamma_1(s,a)-\Gamma_2(s,a)| \\ &\le \sup_{\|\psi\|_2\le 1}|\psi^\top(\omega_1-\omega_2)| + \sqrt{2}\beta\cdot\sup_{\|\psi\|_2\le1}\big(|\psi^\top(\Lambda_1^{-1}-\Lambda_2^{-1})\psi|\big)^{1/2} \\ &= \|\omega_1-\omega_2\|_2 + \|2\beta^2\cdot\Lambda_1^{-1} - 2\beta^2\cdot\Lambda_2^{-1}\|_{\mathrm{OP}}^{1/2} \\ &\le \|\omega_1-\omega_2\|_2 + \|2\beta^2\cdot\Lambda_1^{-1} - 2\beta^2\cdot\Lambda_2^{-1}\|_{\mathrm{F}}^{1/2}, \end{aligned} \tag{H.11}$$

where we denote by $\|\cdot\|_{\mathrm{OP}}$ and $\|\cdot\|_{\mathrm{F}}$ the operator norm and Frobenius norm, respectively. For $\Lambda \succeq \lambda I$ and $\beta \in [0, B]$, it holds that $\|2\beta^2 \cdot \Lambda^{-1}\|_{\mathrm{F}} \le 2B^2 d^{1/2} \lambda^{-1}$. Meanwhile, let $\mathcal{N}_{\omega,\epsilon}$ be the $\epsilon/2$-covering number of $\{\omega \in \mathbb{R}^d : \|\omega\|_2 \le L\}$, and $\mathcal{N}_{A,\epsilon}$ be the $\epsilon^2/4$-covering number of $\{A \in \mathbb{R}^{d\times d} : \|A\|_{\mathrm{F}} \le 2B^2 d^{1/2}\lambda^{-1}\}$. It is known that [41]

$$\mathcal{N}_{\omega,\epsilon} \le (1 + 4L/\epsilon)^d, \qquad \mathcal{N}_{A,\epsilon} \le \bigl(1 + 16B^2 d^{1/2}/(\lambda\epsilon^2)\bigr)^{d^2}.$$

Hence, by (H.11), we obtain that

$$\log \mathcal{N}_\epsilon \le \log(\mathcal{N}_{\omega,\epsilon} \cdot \mathcal{N}_{A,\epsilon}) \le d \cdot \log(1 + 4L/\epsilon) + d^2 \cdot \log\bigl(1 + 16B^2 d^{1/2}/(\epsilon^2\lambda)\bigr),$$

which concludes the proof of Lemma H.4. □

Lemma H.5 (Covering Number of Q [16])**.** Let $\mathcal{Q}$ be a class of functions Q satisfying

$$Q(\cdot,\cdot) = \min\bigl\{\psi(\cdot,\cdot)^\top \omega + \Gamma(\cdot,\cdot), H - h\bigr\}, \tag{H.12}$$

where

$$\Gamma(\cdot,\cdot) = \sqrt{2}\beta \cdot \Bigl(\log\det\bigl(\Lambda + \psi(\cdot,\cdot)\psi(\cdot,\cdot)^\top\bigr) - \log\det(\Lambda)\Bigr)^{1/2}. \tag{H.13}$$

Here the function Q is parameterized by (ω, Λ) and the parameter β is fixed. Let $\psi(\cdot,\cdot)$ be an $\mathbb{R}^d$-valued function and $\Lambda \in \mathbb{R}^{d\times d}$. Let $\|\psi(s,m)\|_2 \le 1$ for all $(s,m) \in \mathcal{S}\times\mathcal{M}$. For $\|\omega\|_2 \le L$, $\Lambda \succeq \lambda I$, $\beta \in [0, B]$, and $\epsilon > 0$, there exist an ϵ-covering of $\mathcal{Q}$ with respect to the metric $d(V, V') = \sup_{(s,m)\in\mathcal{S}\times\mathcal{M}} |Q(s,m) - Q'(s,m)|$, such that the covering number $\mathcal{N}_\epsilon$ is upper bounded as follows,

$$\log \mathcal{N}_\epsilon \le d \cdot \log(1 + 4L/\epsilon) + d^2 \cdot \log\bigl(1 + 16B^2 d^{1/2}/(\epsilon^2\lambda)\bigr).$$

Proof. The proof is similar to that of Lemma H.4. Let Q_1 and Q_2 be the functions defined in (H.12), which are parameterized by (ω_1, Λ_1) and (ω_2, Λ_2), respectively. Note that

$$\begin{aligned} d(Q_1, Q_2) \le \sup_{\min\{(s,m)\in\mathcal{S}\times\mathcal{M}} &\bigl|\psi(s,m)^\top\omega_1 + \Gamma_1(s,m), H - h\bigr\} \\ &\quad - \min\bigl\{\psi(s,m)^\top\omega_2 + \Gamma_2(s,m), H - h\bigr\}\bigr| \\ \le \sup_{(s,m)\in\mathcal{S}\times\mathcal{M}} &|\psi(s,m)^\top(\omega_1 - \omega_2) + \Gamma_1(s,m) - \Gamma_2(s,m)|, \end{aligned} \tag{H.14}$$

where the second inequality follows from the fact that $\min\{\cdot, H - h\}$ is a contraction mapping. Here we define Γ_1 and Γ_2 in (H.13) with $\Lambda = \Lambda_1$ and $\Lambda = \Lambda_2$, respectively. The rest of the proof is the same as that of Lemma H.4. We omit the proof and refer to the proof of Lemma H.4 for the details. □

Lemma H.6 (Concentration of Self-Normalized Process)**.** Let $\lambda = 1$ and $\beta = CdH\sqrt{\log(d(T + nH)/\zeta)}$. Let $\zeta > 0$ be an absolute constant. It holds with probability at least $1 - 2\zeta$ that

$$\Bigl\|\sum_{\ell=1}^4 S_{\ell,h}\Bigr\|_{(\Lambda_h^k)^{-1}} \le C' dH \sqrt{\log\bigl(2(C+1)d(T + nH)/\zeta\bigr)}, \quad \forall (k,h) \in [K]\times[H].$$

where C and C' are positive absolute constants and C' is independent of C.

Proof. Recall that we define

$$S_{1,h} = \sum_{\tau=1}^{k-1} \psi_h(s_h^\tau, a_h^\tau) \cdot \bigl(V_{h+1}^k(s_{h+1}^\tau) - (\mathbb{P}_h V_{h+1}^k)(s_h^\tau, a_h^\tau)\bigr),$$

$$S_{2,h} = \sum_{i=1}^{n} \phi_h(s_h^i, a_h^i, u_h^i) \cdot \bigl(V_{h+1}^k(s_{h+1}^i) - (\widetilde{\mathbb{P}}_h V_{h+1}^k)(s_h^i, a_h^i, u_h^i)\bigr),$$

$$S_{3,h} = \sum_{\tau=1}^{k-1} \psi_h(s_h^\tau, a_h^\tau) \cdot \bigl(r_h^\tau - R(s_h^\tau, a_h^\tau)\bigr), \quad S_{4,h} = \sum_{i=1}^{n} \phi_h(s_h^i, a_h^i, u_h^i) \cdot \bigl(r_h^i - \mathbb{E}[r_h \mid s_h^i, a_h^i, u_h^i]\bigr).$$

We define $\mathcal{F}_{-n+i}$ the σ-algebra generated by the set $\{(s_h^\ell, a_h^\ell, u_h^\ell, r_h^\ell)\}_{(\ell,h)\in[i]\times[H]}$ with timestep index $-n+i$. The set of σ-algebra $\{\mathcal{F}_{-n+i}\}_{i\in[n]}$ captures the data generation process in the offline setting. We attach $\{\mathcal{F}_{-n+i}\}_{i\in[n]}$ to the σ-algebra $\{\mathcal{F}_{k,h,m}\}_{(k,h,m)\in[K,H,2]}$ with timestep index t defined in Definition F.1 to obtain the complete filtration. By Lemma H.1 with such a complete filtration, it holds with probability at least $1-\zeta$ that

$$\begin{aligned}&\|S_{1,h}+S_{2,h}\|_{(\Lambda_h^k)^{-1}}\\&\qquad\le 4H^2\cdot\Big(d/2\cdot\log\big(\det(\Lambda_h^k)/\det(\Lambda_0)\big)+\log(2\mathcal{N}_\epsilon/\zeta)\Big)+8(n+k)^2\epsilon^2/\lambda,\end{aligned}\tag{H.15}$$

where $\Lambda_0=\lambda I$ and

$$\Lambda_h^k=\sum_{\tau=1}^{k-1}\psi_h(s_h^\tau,a_h^\tau)\psi_h(s_h^\tau,a_h^\tau)^\top+\sum_{i=1}^{n}\phi_h(s_h^i,a_h^i,u_h^i)\phi_h(s_h^i,a_h^i,u_h^i)^\top+\lambda I.$$

Similarly, by Lemma H.1, it holds with probability at least $1-\zeta$ that

$$\|S_{3,h}+S_{4,h}\|_{(\Lambda_h^k)^{-1}}\le 4H^2\cdot\Big(d/2\cdot\log\big(\det(\Lambda_h^k)/\det(\Lambda_0)\big)\Big).\tag{H.16}$$

Note that

$$\begin{aligned}\Lambda_h^k&=\sum_{\tau=1}^{k-1}\psi_h(s_h^\tau,a_h^\tau)\psi_h(s_h^\tau,a_h^\tau)^\top+\sum_{i=1}^{n}\phi_h(s_h^i,a_h^i,u_h^i)\phi_h(s_h^i,a_h^i,u_h^i)^\top+\lambda I\\&\preceq(k+n+\lambda)I.\end{aligned}$$

Meanwhile, recall that $\Lambda_0=\lambda I$. Thus, we obtain that

$$\det(\Lambda_h^k)/\det(\Lambda_0)\le(k+n+\lambda)/\lambda.\tag{H.17}$$

On the other hand, we obtain from Lemma H.3 and Lemma H.4 that

$$\log\mathcal{N}_\epsilon\le d\cdot\big(1+4H\sqrt{d(n+k)}/(\epsilon\sqrt{\lambda})\big)+d^2\cdot\log\big(1+16\beta^2\sqrt{d}/(\epsilon^2\lambda)\big),\tag{H.18}$$

where we set $\beta=CdH\sqrt{\log(d(T+nH)/\zeta)}$. Finally, by setting $\epsilon=dH/(n+k)$ in (H.15), plugging (H.17) and (H.18) into (H.15) and (H.16), respectively, and setting $\lambda=1$, we obtain that

$$\begin{aligned}\Big\|\sum_{\ell=1}^4 S_{\ell,h}\Big\|_{(\Lambda_h^k)^{-1}}&\le\|S_{1,h}+S_{2,h}\|_{(\Lambda_h^k)^{-1}}+\|S_{3,h}+S_{4,h}\|_{(\Lambda_h^k)^{-1}}\\&\le C'dH\sqrt{\log\big(2(C+1)d(T+nH)/\zeta\big)},\end{aligned}$$

which holds with probability at least $1-2\zeta$. Here $T=HK$ and C,C' are absolute constants, where C' is independent of C. Thus, we complete the proof of Lemma H.6. $\square$

Lemma H.7. Let $\Lambda_t\in\mathbb{R}^{d\times d}$ be a positive definite matrix satisfying $\Lambda_t\succeq I$. Let $\psi_t(\cdot,\cdot)$ be a $\mathbb{R}^d$-valued function such that $\|\psi_t(\cdot,\cdot)\|_2\le 1$. Let $\Lambda_{t+1}(\cdot,\cdot)=\Lambda_t+\psi_t(\cdot,\cdot)\psi_t(\cdot,\cdot)^\top$. It then holds that

$$\psi_t(\cdot,\cdot)^\top(\Lambda_t)^{-1}\psi_t(\cdot,\cdot)\le 2\log\det\big(\Lambda_{t+1}(\cdot,\cdot)\big)-2\log\det(\Lambda_t).$$

Proof. Note that $\Lambda_t\succeq I$. Thus, it holds that

$$0\le\psi_t(\cdot,\cdot)^\top(\Lambda_t)^{-1}\psi_t(\cdot,\cdot)\le\|\psi_t(\cdot,\cdot)\|_2^2\le 1.$$

It then follows from the inequality $x\le 2\log(1+x)$ for all $x\in[0,1]$ that

$$\psi_t(\cdot,\cdot)^\top(\Lambda_t)^{-1}\psi_t(\cdot,\cdot)\le 2\log\big(1+\psi_t(\cdot,\cdot)^\top(\Lambda_t)^{-1}\psi_t(\cdot,\cdot)\big).\tag{H.19}$$

Meanwhile, it follows from the matrix determinant lemma that

$$\det\big(\Lambda_{t+1}(\cdot,\cdot)\big)=\det(\Lambda_t)\cdot\big(1+\psi_t(\cdot,\cdot)^\top(\Lambda_t)^{-1}\psi_t(\cdot,\cdot)\big).\tag{H.20}$$

Finally, combining (H.19) and (H.20), we conclude that

$$\psi_t(\cdot,\cdot)^\top(\Lambda_t)^{-1}\psi_t(\cdot,\cdot)\le 2\log\det\big(\Lambda_{t+1}(\cdot,\cdot)\big)-2\log\det(\Lambda_t),$$

which concludes the proof of Lemma H.7. $\square$