Sample-Efficient Reinforcement Learning for POMDPs with Linear Function Approximations

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Abstract

Despite the success of reinforcement learning (RL) for Markov decision processes (MDPs) with function approximation, most RL algorithms easily fail if the agent only has partial observations of the state. Such a setting is often modeled as a partially observable Markov decision process (POMDP). Existing sample-efficient algorithms for POMDPs are restricted to the tabular setting where the state and observation spaces are finite. In this paper, we make the first attempt at tackling the tension between function approximation and partial observability. In specific, we focus on a class of undercomplete POMDPs with linear function approximations, which allows the state and observation spaces to be infinite. For such POMDPs, we show that the optimal policy and value function can be characterized by a sequence of finite-memory Bellman operators. We propose an RL algorithm that constructs optimistic estimators of these operators via reproducing kernel Hilbert space (RKHS) embedding. Moreover, we theoretically prove that the proposed algorithm finds an $\varepsilon$-optimal policy with $\tilde{O}(1/\varepsilon^2)$ episodes of exploration. Also, this sample complexity only depends on the intrinsic dimension of the POMDP polynomially and is independent of the size of the state and observation spaces. To our best knowledge, we develop the first provably sample-efficient algorithm for POMDPs with function approximation.

1 Introduction

Reinforcement learning has shown its strong power in solving difficult sequential decision-making problems. In particular, when combined with large-scale function approximators, deep reinforcement learning can learn action values in complicated and rapidly changing
environments to distinguish the best action from candidates and achieve the human-level intelligence (Mnih et al., 2015; Silver et al., 2016, 2017). However, most current successful applications of reinforcement learning are restricted in well-defined MDP environments, for example, video games, which are usually not the case for many real-world problems. The truly Markovian states are often unknown and can only be inferred by other observable information. For example, people’s preferences and intensions in a recommender system can only be inferred by their recent actions in the record. Therefore, to build reinforcement learning agents for solving real-world problems, we need to develop efficient algorithms that not only work for MDPs but also for POMDPs.

The decision-making in a POMDP is much more difficult (Vlassis et al., 2012) than that in an MDP. For any step of a POMDP, to find the optimal action, we need the entire history to complete the inference, whereas in an MDP we only need the current state. Such a setting raises both statistical and computational challenges in learning the optimal policy. On the statistical side, the model parameters of a POMDP can not be efficiently estimated, or even are not identifiable, from the interaction data, due to the latency of states. On the computational side, even when the model is known, each iteration of the dynamic programming procedure involves high dimensional integration due to the conditional expectation with a long history.

To develop efficient reinforcement learning algorithms for POMDPs, we start by focusing on the statistical efficiency. Recent studies have shown that reinforcement learning for MDPs is not significantly more difficult than bandit problems if the state distributions have finite intrinsic dimensions (Jin et al., 2020b; Ayoub et al., 2020). The claim is in the sense that the horizon of the process only increases the sample complexity of attaining the optimal policy by a polynomial factor. In contrast, similar results for POMDPs are established only when the observation and latent state spaces are finite (Jin et al., 2020a). Such a gap makes us wonder if it is possible to also establish sample efficiency reinforcement learning algorithms for POMDPs with infinite observations and latent state spaces, given their distributions are approximated by finite-dimensional function classes.

In this paper, we give a positive answer to the above question. We propose a new reinforcement learning algorithm for a special class of POMDPs with infinite state and observation spaces, which is guaranteed to obtain a near-optimal policy using minimal interaction data. Moreover, our analysis is based on a new variant of the Bellman operator designed for such POMDPs, inspired by the observable representation of hidden Markov models (Hsu et al., 2012), which avoids the computation of conditional expectation with respect to the entire history and thus implies computation efficiency. In detail, we consider POMDPs where the state and observation distributions are convex combinations of known distributions basis, and the observation distribution carries enough information about the belief of the latent state. We prove that, for any $\varepsilon > 0$, our algorithm obtains an $\varepsilon$-optimal policy after explorations in \(\text{poly}(H, A, d_s, d_o) \cdot \tilde{O}(1/\varepsilon^2)\) episodes, where $H$ is the maximal episode length, $A$ is
the number of actions, \( d_s \) and \( d_o \) are the numbers of basis functions in approximating the state and observation distributions, respectively.

1.1 Related Work

Our work is related to a line of recent work on the sample efficiency of reinforcement learning for POMDPs. In detail, Azizzadenesheli et al. (2016); Guo et al. (2016); Xiong et al. (2021) establish sample complexity guarantees for searching the optimal policy in POMDPs whose models are identifiable and can be estimated by spectral methods. However, Azizzadenesheli et al. (2016) and Guo et al. (2016) add extra assumptions such that efficient exploration of the POMDP can always be achieved by running arbitrary policies. In contrast, the upper bound confidence (UCB) method is used in Xiong et al. (2021) for adaptive exploration. The more related work is Jin et al. (2020a), which considers undercomplete POMDPs, in other words, the observations are more than the latent states. Their proposed algorithm can attain the optimal policy without estimating the exact model, but an observable component (Jaeger, 2000; Hsu et al., 2012), which is the same for our algorithm design, while only applies to tabular POMDPs.

In a broader context of reinforcement learning with partial observation, our work is related to several recent works on POMDPs with special structures. For example, Kwon et al. (2021) considers latent POMDPs, where each process has only one latent state, and the proposed algorithm efficiently infers the latent state using a short trajectory. Kozuno et al. (2021) considers POMDPs having tree-structured states with their positions in certain partitions being the observations. These special structures reduce the complexity of finding the optimal actions in a POMDP and thus are easier to be handled by techniques for MDPs. For both aforementioned literature, they only consider tabular POMDPs, which means that the state spaces and observation spaces are finite.

In the context of RL with function approximations, our work is also related to a vast body of recent progress (Yang and Wang, 2020; Jin et al., 2020b; Cai et al., 2020; Du et al., 2021; Kakade et al., 2020; Agarwal et al., 2020; Zhou et al., 2021; Ayoub et al., 2020) on the sample efficiency of RL for MDPs with linear function approximations. These works characterize the uncertainty in the regression for either the model or value function of an MDP and use the uncertainty as a bonus on rewards to encourage exploration. However, none of these approaches directly apply to POMDPs because the same type of regression analysis can not be performed without the data of latent states.

1.2 Notation

For any discrete or continuous set \( \mathcal{X} \) and \( p \in \mathbb{N} \), we denote by \( L^p(\mathcal{X}) \) the \( L^p \) space of functions over \( \mathcal{X} \) and \( \Delta(\mathcal{X}) \) the set of probability density functions over \( \mathcal{X} \) when \( \mathcal{X} \) is continuous or
probability mass functions when $X$ is discrete. For any $d \in \mathbb{N}$, we denote by $[d]$ the set of integers from 1 to $d$. For a vector $v$ and a matrix $M$, we denote by $[v]_i$ the $i$-th entry of $v$ and $[M]_{ij}$ the entry of $M$ at the $i$-th row and $j$-th column. We denote by $\| \cdot \|_p$ the $\ell^p$-norm of a vector or $L^p$-norm of a function. Also, for an operator $M$, we denote by $\|M\|_{p \to q}$ the operator norm of $M$ induced by the $\ell^p$-norm or $L^p$-norm of the domain and $\ell^q$-norm or $L^q$-norm of the range. We use the notation $\text{linspan}(\cdot)$ and $\text{conh}(\cdot)$ to represent the linear span and convex combination, respectively.

2 Preliminaries

2.1 Reinforcement Learning for POMDPs

We consider an episodic POMDP $(S, A, O, H, T, \mathcal{E}, \mu, r)$, where $S$, $A$, and $O$ are the (latent) state, action, and observation spaces, respectively, $H$ is the maximal length of each episode, $T$ is the state transition kernel from a state-action pair to the next state, $\mathcal{E}$ is the observation emission kernel from a state to its observation, $\mu$ is the initial state distribution, and $r : O \times A \to [0, 1]$ is the reward function defined on the observation and action for each step.

We consider the action space $A$ to have finite size $A \in \mathbb{Z}$, while the state space $S$ and observation space $O$ can be either finite or infinite. Also, we consider the non-homogeneous setting so that the state transition and observation emission kernels for each step can be different, and thus we use a subscript $h \in \mathbb{Z}$ to specify the step number. At the beginning of each episode, the agent receives the initial state $s_1$ sampled independently from $\mu$. Then, the agent interacts with the environment as follows. For any $h \in [H]$, at the $h$-th step, the agent receives the observation $o_h \sim \mathcal{E}_h(\cdot | s_h)$, takes an action $a_h$ based on the observation history

$$\tau_h = (o_1, \ldots, o_h),$$

and receives the reward $r_h = r(o_h, a_h)$. To select actions, any mapping $\pi$ from the observation history to the action is called a policy and we denote by $\Pi$ the set of all such mappings. We note that, if the policy $\pi$ is known and it chooses actions deterministically, then the historical actions do not provide additional information given the observation history defined in (2.1), and thus we do not need to include them in the policy input. Subsequently, the agent receives the next state $s_{h+1}$ following $s_{h+1} \sim T_h(\cdot | s_h, a_h)$.

In a reinforcement learning problem, the environment is unknown, which means that we do not know the state transition kernel $T$ and observation emission kernel $\mathcal{E}$. To proceed, we consider that we have a candidate class of them. In detail, we denote by $\{(T^\theta, \mathcal{E}^\theta) : \theta \in \Theta\}$ the candidate class of $T$ and $\mathcal{E}$, where $\theta$ represents the parameters and $\Theta$ is the feasible set of $\theta$. Note that our analysis does not require any concrete parametrization forms $T^\theta$ and

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\( \mathcal{E}^\theta \), as long as they satisfy our assumptions in Section 2.2. We assume that the realizability condition holds, that is, there exists \( \theta^* \in \Theta \) such that \( \mathcal{T} = \mathcal{T}^{\theta^*} \) and \( \mathcal{E} = \mathcal{E}^{\theta^*} \). Also, without loss of generality and for the ease of presentation, we assume that \( \mu, \mathcal{T}_1, \mathcal{E}_1, \text{ and } \mathcal{E}_2 \) are known, which account for the initialization of the POMDP. The objective of RL is to find the policy that maximizes the expected total reward. That is to say, we want to obtain 
\[
\pi^* = \arg\max_{\pi \in \Pi} J(\theta^*, \pi)
\]
for any \((\theta, \pi) \in \Theta \times \Pi\). Here, we write \( \theta \) and \( \pi \) as the subscripts of the expectation to represent that the parameters of the state transition kernel and observation emission kernel of the underlying POMDP take the value \( \theta \), and the actions are selected by policy \( \pi \), if not additionally specified.

**Additional Notation for POMDPs:** Recall that we denote by \( \Pi \) the set of all policies. For notational simplicity, we also denote by \( \overline{\Pi} \) the set of mixing policies, which mean that one policy is randomly selected from a set of policies following some distribution before the POMDP begins and is then fixed when running the POMDP. Moreover, for any \( h \in [H] \), we denote by \( \overline{\tau}_h \) the full history,
\[
\overline{\tau}_h = (o_1, a_1, \ldots, o_{h-1}, a_{h-1}, o_h)
\]
which, compared with the notation \( \tau_h \), additionally includes the historical actions before \( o_h \) is observed. We denote by \( \Gamma_h \) and \( \overline{\Gamma}_h \) the sets of all possible \( \tau_h \) and \( \overline{\tau}_h \), respectively. Throughout the paper, we use the bold font for states, actions, and observations to represent that they are random variables in one POMDP, whose model parameters and policy are specified in the context. While we use the regular font for them when they are deterministic variables.

### 2.2 Linear Function Approximations

In the following, we illustrate our requirement on the candidate set of the POMDP. We define the following two function classes, which involve the distribution functions of states,
\[
\mathcal{F}_s = \{p_\theta(s_h = \cdot \mid s_{h-1} = s, a_{h-1} = a) : (h, \theta, s, a) \in [H] \times \Theta \times \mathcal{S} \times \mathcal{A}\},
\]
\[
\mathcal{F}'_s = \{p_{\theta, \pi}(s_h = \cdot \mid o_{h+1} = o, a_h = a) : (h, \theta, a, o, \pi) \in [H] \times \Theta \times \mathcal{A} \times \mathcal{O} \times \overline{\Pi}\}.
\]
Here, \( p(\cdot) \) is the probability density function when the state space \( \mathcal{S} \) is continuous and is the probability mass function when \( \mathcal{S} \) is discrete, and the subscripts have the same meanings as those in (2.2). With a slight abuse of notation, the condition \( a_h = a \) means that the agent’s policy deterministically select action \( a \) as the \( h \)-th action regardless of the observation history, while other actions are selected by policy \( \pi \) specified in the subscript, if it is required
to define the probability. We keep using such notation in the rest of the paper. We note that $F_s$ corresponds to the distribution of the state conditional on the information of the past, while $F'_s$ corresponds to that of the future. Specially, we have $\mu \in F_s$ for the case $h = 1$, where the conditions are regarded as empty because $s_0$ and $a_0$ do not exist. Also, we define the following function class, which corresponds to the distribution functions of three contingent observations,

$$
F_o = \{ p_{\theta, \pi}(o_{h:h+2} = \cdot \mid a_h = a, a_{h+1} = a') : (h, \theta, \pi, a, a') \in [H - 1] \times \Theta \times \Pi \times \mathcal{A}^2 \},
$$

where the conditioning has a similar meaning as above. We have the following assumption, which says that the distribution function classes defined above fall in low-dimensional function classes.

**Assumption 2.1** (Linear Function Approximations). There exist $d_s, d_o \in \mathbb{N}$ and vector-valued functions

$$
\psi : S \to \mathbb{R}^{d_s}, \quad \phi : O^3 \to \mathbb{R}^{d_o},
$$

whose entries are denoted by $\{\psi_i\}_{i=1}^{d_s}$ and $\{\phi_i\}_{i=1}^{d_o}$, such that we have

1. $\psi_i \in \Delta(S)$ and $\phi_j \in \Delta(O^3)$ for $i \in [d_s], j \in [d_o]$,

2. $F_s, F'_s \subset \text{conh}(\psi)$ and $F_o \subset \text{conh}(\phi)$, where we regard $\psi$ and $\phi$ as sets of functions.

Assumption 2.1 requires that $F_s, F'_s$, and $F_o$ can be linearly approximated by known bases $\psi$ and $\phi$. Similar assumptions on state transition probabilities are also used in the MDP setting, for example, Du et al. (2021). The assumption can directly reduce to the tabular case where the state space and observation space are finite by choosing the corresponding indicator functions of state and observation spaces to form the bases $\psi$ and $\phi$.

Before we proceed to the algorithm, we have another assumption on the candidates of the observation emission kernel. For any $(h, \theta) \in [H] \times \Theta$, we define the linear operator

$$
\mathcal{O}^\theta_h : L^1(S) \to L^1(O)
$$

by

$$
(\mathcal{O}^\theta_h f)(o) = \int_S E^\theta_h(o \mid s) f(s) \, ds,
$$

for any $f \in L^1(S)$ and $o \in O$, which maps any distribution of the state $s_h$ to the distribution of its observation $o_h$ under the observation emission kernel $E^\theta_h$. Here the integral is the general notation for the summation over states in the state space $S$ for either discrete or continuous state space. We similarly use it for the summation over observations in the observation space $O$ and keep using the notation in the rest of the paper. We have the following assumption, which says that such a mapping is invertible.
Assumption 2.2 (Undercompleteness). For any \((h, \theta) \in [H] \times \Theta\), there exist a known function \(z_h^\theta : S \times O \rightarrow \mathbb{R}\) and a corresponding integral operator \(Z_h^\theta : L^1(O) \rightarrow L^1(S)\) defined by

\[
(Z_h^\theta f)(s) = \int_O z_h^\theta(s, o)f(o)\,do
\]

for any \(f \in L^1(O)\) and \(s \in S\), such that \(Z_h^\theta \mathcal{O}_h^\theta f = f\) for any \(f \in \text{linspan}(\psi)\) and \(\|Z_h^\theta\|_{1 \rightarrow 1} \leq \gamma\) for some constant \(\gamma > 0\).

Assumption 2.2 essentially only requires that, for any \((h, \theta) \in [H] \times \Theta\), the linear mapping \(\mathcal{O}_h^\theta\) restricted on the finite-dimensional function classes \(\text{linspan}(\psi)\) is injective, and thus its left inverse exists, whose domain can be naturally extended to the whole space \(L^1(O)\). In other words, the distribution of the observation carries full information of the distribution of its corresponding state. The term undercomplete represents that the observation space is larger compared with the state space. See more discussion in Section A, where we show that both Assumptions 2.1 and 2.2 hold if state transition and observation emission kernels themselves have certain linear structures, and we show the connection with tabular undercomplete POMDPs.

3 Algorithm

In this section, we first introduce the finite-memory Bellman operator in Section 3.1 and discuss its estimation in Section 3.2. Then, we present our algorithm, which combines the operator estimation and optimistic exploration, in Section 3.3.

3.1 The Finite-Memory Bellman Operator

The main challenge of reinforcement learning for POMDPs is that, if we want to treat the POMDP as an MDP to apply regular RL approaches, we have to aggregate the observations and actions in the entire history as an observable “state” to retrieve the Markov property. To be more specific, for any \((h, \theta) \in [H] \times \Theta\) and \(\pi \in \Pi\), we define the full-memory Bellman operator \(\mathcal{P}_{h, \pi}^\theta\) by

\[
(\mathcal{P}_{h, \pi}^\theta f)(\tau_h) = \mathbb{E}_{\theta, \pi}[f(\tau_{h+1}) | \tau_h = \tau_h]
\]

\[
= \int_O f(\tau_{h}, \pi(\tau_h), o_{h+1}) \cdot p_{\theta, \pi}(o_{h+1} = o_{h+1} | \tau_h = \tau_h)\,do_{h+1}
\]

for any function \(f\) defined on \(\overline{\Gamma}_{h+1}\) and history \(\tau_h \in \overline{\Gamma}_h\). Typically, here function \(f\) will be the expected total reward starting from any \((h + 1)\)-th step history \(\tau_{h+1} \in \overline{\Gamma}_{h+1}\), and the operator \(\mathcal{P}_{h, \pi}^\theta\) plays the role of mapping such a function to its \(h\)-th step correspondence, which
resembles the classical dynamic programming for MDPs. We denote by \( R : \Gamma_{H+1} \to [0, H] \) the function that calculates the exact total reward given a complete episode of observations and actions, that is

\[ R(\tau_{H+1}) = r(o_1, a_1) + \ldots + r(o_H, a_H), \quad (3.2) \]

for any \( \tau_{H+1} \in \Gamma_{H+1} \). Then, the expected total reward under \((\theta, \pi)\) satisfies the relation

\[ \mathbb{E}_{\theta, \pi} \left[ \sum_{h=1}^{H} r_h \mid \tau_h = \bar{\tau}_h \right] = (P_{h, \pi}^{\theta} \cdots P_{H}^{\theta} R)(\bar{\tau}_h) \quad (3.3) \]

for any \( h \in [H] \). Based on (3.3), either model-based or model-free reinforcement learning algorithms can be applied to approximately perform the calculation (3.1) and search for the optimal policy with respect to every single step in a recursive manner. However, such a direct method is extremely sample inefficient and never really used in practice. The conditional distribution function in (3.1) involves \( h \) observations and thus, in general, no accurate estimator to is unavailable because of the curse of dimensionality. In order to avoid such an issue, we note that the direct method does not utilize the independence between observations given the latent states.

In the sequel, we propose the finite-memory Bellman operator \( \mathbb{B}^{\theta, \pi}_h \), which is defined by

\[ (\mathbb{B}^{\theta, \pi}_h f)(\bar{\tau}_h) = \int_{\mathcal{O}_2} f(\tau_{h-1}, a_{h-1}, \bar{o}_h, a_h, o_{h+1}) \cdot \mathcal{B}^{\theta}_h(a_h, \bar{o}_h, o_{h+1}) d\bar{o}_h da_h, \quad (3.4) \]

where \( a_h = \pi(\tau_{h-1}, \bar{o}_h) \), \( f \) and \( \bar{\tau}_h \) are the same as in (3.1) and function \( \mathcal{B}^{\theta}_h(a) \) is defined by

\[ \mathcal{B}^{\theta}_h(a) = \int_{\mathcal{S}^2} \mathcal{E}^{\theta}_{h+1}(o' | s') \cdot \mathcal{T}^{\theta}_h(s' | s, a) \cdot \mathcal{E}^{\theta}_h(o' | s) \cdot z^{\theta}_h(s, o) ds ds' \quad (3.5) \]

for any \( o, o', o'' \in \mathcal{O} \) and \( a \in \mathcal{A} \). Here, the function \( z^{\theta}_h \) is defined in Assumption 2.2. The following lemma shows the desired property of such an operator.

**Lemma 3.1.** For any \((h, \pi, \theta) \in [H] \times \Pi \times \Theta \) and \( f : \Gamma_{h+1} \to \mathbb{R} \), we have

\[ \mathbb{E}_\theta[ (\mathbb{B}^{\theta, \pi}_h f)(\bar{\tau}_h) - (\mathbb{B}^{\theta, \pi}_h f)(\bar{\tau}_h) \mid \sigma_h ] = 0 \]

with the notation \( \sigma_h \) short for

\[ s_{h-1} = s_{h-1}, \bar{\tau}_{h-1} = \bar{\tau}_{h-1}, a_{h-1} = a_{h-1}. \]

Here, \( \bar{\tau}_{h-1} \in \Gamma_{h-1} \) and \((s_{h-1}, a_{h-1}) \in \mathcal{S} \times \mathcal{A} \) are also arbitrary.
By Lemma 3.1, we see that the finite-memory Bellman operator and full-memory Bellman operator have the same effect in calculating the expected total reward, given all historical information except for the last observation \( o_h \). However, we note that now the calculation in (3.5) only involves observations in a short window. This is because the new operator uses the undercompleteness condition (Assumption 2.2) to implicitly infer the posterior distribution of the hidden state \( s_h \), and thus the conditional independence between observations given the hidden states makes it no need to consider the earlier observations. Then, corresponding to (3.3), for any \( h \in [H] \), we define the value function

\[
V_{h}^{\theta,\pi} = \mathbb{E}_{h}^{\theta,\pi} \cdots \mathbb{E}_{H}^{\theta,\pi} R.
\]

(3.6)

The following corollary is a direct result of Lemma 3.1, which shows that the value function defined above computes the expected total rewards.

**Corollary 3.2.** For any \((h, \theta, \pi) \in [H] \times \Theta \times \Pi\), we have

\[
\mathbb{E}_{\theta,\pi}[V_{h}^{\theta,\pi}(\mathbb{T}_h) - \sum_{i=1}^{H} r_i \bigg| \sigma_h] = 0.
\]

(3.7)

where \( \sigma_h \) is defined the same as in Lemma 3.1. Specially, for the case of \( h = 1 \), we have

\[
J(\theta, \pi) = \mathbb{E}[V_{1}^{\theta,\pi}(o_1)].
\]

Corollary 3.7 shows that, to evaluate any policy, it suffices to know the finite-memory Bellman operator, instead of the full model. Later in Section 4.2, we will show how the value function defined in (3.6) helps us characterize the sample complexity of our algorithm.

### 3.2 Operator Estimation

Although the finite-memory Bellman operator \( \mathbb{F}_{h}^{\theta,\pi} \) defined in (3.4) does not involve observations \( o_{1:h-1} \), it is still unclear how to estimate it in a sample-efficient manner. To proceed, for any \((h, \theta) \in \{2, \ldots, H\} \times \Theta \) and \( a \in A \), we define the operator \( \mathbb{F}_{h,a}^{\theta} \) by

\[
(\mathbb{F}_{h,a}^{\theta} f)(o_{h-1}, o_h, o_{h+1})
\]

\[
= \int_{O} \mathcal{B}_{h,a}^{\theta}(\tilde{o}_h, o_h, o_{h+1}) \cdot f(o_{h-1}, \tilde{o}_h) d\tilde{o}_h
\]

(3.8)

for any \( f \in L^1(O^2) \) and \( o_{h-1}, o_h, o_{h+1} \in O \). We note that operators \( \mathbb{F}_{h,a}^{\theta} \) and \( \mathbb{B}_{h,a}^{\theta,\pi} \) are integral operators with the same integral kernel \( \mathcal{B}_{h,a}^{\theta} \), while their purposes are different. To distinguish the two operators, we call \( \mathbb{F}_{h,a}^{\theta} \) the forward Bellman operator, which maps the distribution of \( o_{h-1:h} \) to that of \( o_{h-1:h+1} \). In contrast, we call \( \mathbb{B}_{h}^{\theta,\pi} \) the backward Bellman operator, as it maps the \((h+1)\)-th step value function to the \( h \)-th step value function. Our algorithm for parameter estimation is based on the equation in the following lemma.
Lemma 3.3. For any \( h \in \{2, \ldots, H\} \) and \((\pi, a, a') \in \Pi \times A^2\), we have

\[
F_{h,a} \theta \ast \mathbb{P} = \mathbb{P} \tag{3.9}
\]

where \( \mathbb{P}^{(1)}_{h,a} \) and \( \mathbb{P}^{(2)}_{h,a,a'} \) are probability distribution functions of observations defined by

\[
P^{(1)}_{h,a}(o, o') = p^{\theta,\pi}(o_{h-1:h} = (o, o') \mid a_{h-1} = a) \tag{3.10}
\]

\[
P^{(2)}_{h,a,a'}(o, o', o'') = p^{\theta,\pi}(o_{h-1:h+1} = (o, o', o'') \mid a_{h-1} = a, a_h = a') \tag{3.11}
\]

for any \( o, o', o'' \in \mathcal{O} \).

Now, given an exploration policy \( \pi \) and any aforementioned \((h, a, a')\), suppose that we have a dataset \( \mathcal{D} \), whose data are collected by the following scheme. In each episode, we execute the exploration policy \( \pi \) for selecting actions \( a_1:h-2 \), select actions \( a_{h-1} = a \) and \( a_h = a' \) regardless of the observations, and add the observation tuple \((o_{h-1}, o_h, o_{h+1})\) into the dataset \( \mathcal{D} \). Then, we can use \( \mathcal{D} \) to estimate the distribution functions defined in (3.10) and (3.11). Subsequently, to match the two sides of the estimation equation (3.9), we estimate \( \theta^\ast \) by searching \( \theta \in \Theta \) to minimize

\[
\max_{(h,a,a') \in \{2, \ldots, H\} \times A^2} \| F_{h,a} \theta - \mathbb{P}^{(1)}_{h,a} - \mathbb{P}^{(2)}_{h,a,a'} \|_1,
\]

where \( \mathbb{P}^{(1)}_{h,a} \) and \( \mathbb{P}^{(2)}_{h,a,a'} \) are empirical estimators of \( P^{(1)}_{h,a} \) and \( P^{(2)}_{h,a,a'} \), respectively.

To concretely estimate the distributions from the dataset, we recall the linear approximation of observation distributions in Assumption 2.1 and use the reproducing kernel Hilbert space (RKHS) embedding (Smola et al., 2007). Let \( \mathcal{H} \) be an RKHS with the kernel \( K \) over \( \mathcal{O}^3 \) and the corresponding RKHS norm is denoted by \( \| \cdot \|_\mathcal{H} \). Then, we construct the estimator \( \mathbb{P}^{(2)}_{h,a,a'} \) as

\[
\mathbb{P}^{(2)}_{h,a,a'} = \arg\min_{p \in \text{span}(\phi)} \| Kp - \hat{K}\mathcal{D} \|_\mathcal{H} \tag{3.12}
\]

where \( Kp \) and \( \hat{K}\mathcal{D} \) represents embedding of distribution \( p \) and dataset \( \mathcal{D} \) into \( \mathcal{H} \), respectively, that is,

\[
(Kp)(x) = \mathbb{E}_{X \sim p}[K(X, x)], \quad (\hat{K}\mathcal{D})(x) = (1/|\mathcal{D}|) \cdot \sum_{y \in \mathcal{D}} K(y, x),
\]

for any \( x \in \mathcal{O}^3 \). Equivalently, we can also view \( \hat{K}\mathcal{D} \) as the embedding of the empirical distribution induced by the dataset \( \mathcal{D} \). We note that, in (3.12) we relax the feasible set of \( p \) from the convex combination to the linear span of \( \phi \), which contains elements that are not probability distribution functions. Then, the expectation in \( Kp \) is generalized to the same integral form if \( p \) is not a probability distribution function. Here, the RKHS norm
minimization in (3.12) can be solved by various approaches and we defer more details of the computation to Section 5. After we obtain the estimator \( \hat{P}_{h,a,a'}^{(2),\pi} \), by (3.10) and (3.11), it is natural for us to construct the estimator \( \hat{P}_{h,a}^{(1),\pi} \) by

\[
\hat{P}_{h,a}^{(1),\pi}(a, a') = \int_{O} \hat{P}_{h,a,a}^{(2),\pi}(a, a', o'') \, \text{d}o'',
\]

for any \( a, a' \in O \).

### 3.3 Optimistic Explorations

With the preparation in Sections 3.1 and 3.2, now we are ready to present our full algorithm. We start with an arbitrary policy \( \pi_0 \in \Pi \) and \( A^2(H - 1) \) empty datasets

\[
\{D_{h,a,a'}\}_{(h,a,a') \in \{2,\ldots,H\} \times A^2}
\]

and we update them for \( K \) iterations. Each iteration of the algorithm consists of an exploration phase and a planning phase. In the following, we illustrate details of the two phases in the \( k \)-th iteration for any \( k \in [K] \).

**Exploration Phase:** Given policy \( \pi_{k-1} \), for each tuple \( (h, a, a') \in \{2, \ldots, H\} \times A^2 \), we run one episode of the POMDP following the data collecting scheme defined in Section 3.2 to add one observation tuple into the dataset \( D_{h,a,a'} \), where the exploration policy is \( \pi_{k-1} \).

**Planning Phase:** After the exploration phase of the \( k \)-th iteration, there are \( k \) observation tuples in each dataset \( D_{h,a,a'} \). Although the data are collected following different exploration policies \( \pi_0, \ldots, \pi_{k-1} \) in historical iterations, we can equivalently regard the data in the dataset as collected by the mixing exploration policy

\[
\pi_k = \text{mixing}\{\pi_0, \ldots, \pi_{k-1}\}.
\]

where the sampling distribution of the mixing is the uniform distribution. Thus, we can apply the estimation method introduced in Section 3.2 to the dataset \( D_{h,a,a'} \) and construct a confidence set of the model parameters \( \theta \) as the level set

\[
\Theta_k = \left\{ \theta \in \Theta : L_k(\theta) \leq \beta \cdot k^{-1/2} \right\},
\]

for some constant \( \beta > 0 \), where \( L_k(\theta) \) is defined as

\[
L_k(\theta) = \max_{(h,a,a') \in \{2,\ldots,H\} \times A^2} \|P_{h,a}^{(1),\pi_k} - \hat{P}_{h,a,a'}^{(2),\pi_k}\|_1
\]

Here, the distribution function estimators \( P_{h,a,\pi_k}^{(1)} \) and \( P_{h,a,a',\pi_k}^{(2)} \) are defined in (3.12) and (3.13), respectively. Given the confidence set, we update the exploration policy by

\[
\pi_k = \arg\max_{\pi \in \Pi} \max_{\theta \in \Theta_k} J(\theta, \pi),
\]

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which is the optimal policy with respect to the most optimistic value estimate for the model parameters in the confidence set $\Theta_k$. Since our focus is the sample efficiency, we assume that (3.16) can be achieved by an optimization oracle with negligible computation error. The updated policy $\pi_k$ is then executed in the exploration phase of the $(k + 1)$-th iteration. We present the full algorithm in Algorithm 1.

**Algorithm 1** Optimistic Explorations

1: **Input:** number of iterations $K$, confidence set level $\beta$
2: **Initialization:** set $\pi_0$ as any deterministic policy
3: For $(h, a, a') \in \{2, \ldots, H\} \times A^2$ do
4: $\mathcal{D}_{h,a,a'} \leftarrow \emptyset$
5: For $k = 1$ to $K$ do
6: For $(h, a, a') \in \{2, \ldots, H\} \times A^2$ do
7: Start a new episode
8: Run policy $\pi_{k-1}$ to take the first $(h - 2)$ actions and observe $o_{h-1}$
9: Take action $a$ and observe $o_h$
10: Take action $a'$ and observe $o_{h+1}$
11: $\mathcal{D}_{h,a,a'} \leftarrow \mathcal{D}_{h,a,a'} \cup \{(o_{h-1}, o_h, o_{h+1})\}$
12: Construct the confidence set $\Theta_k$ by (3.15)
13: Update the policy by
$$\pi_k \leftarrow \arg\max_{\pi} \max_{\theta \in \Theta_k} J(\theta, \pi)$$
14: **Output:** Policies $\{\pi_1, \ldots, \pi_K\}$

4 Theoretical Results

In this section, we present the theoretical analysis of Algorithm 1. In Section 4.1, we show that the policies generated by Algorithm 1 converge to the optimal policy with polynomial sample complexity. In Section 4.2, we sketch the proof of the sample complexity by showing three main lemmas.

4.1 Sample Efficiency

Recall that in Sections 3.2 and 3.3 we use the RKHS embedding with kernel function $\mathcal{K}$ for the distribution estimation. We define random matrix $G \in \mathbb{R}^{d_o \times d_o}$ by
$$[G]_{i,j} = \mathcal{K}(X_i, X_j), \quad (4.1)$$
where $X_i \sim \phi_i$ for any $i, j \in [d_o]$. The following assumption specifies our regularity requirements on the kernel function $\mathcal{K}$ for learning distributions.
Assumption 4.1. The kernel $K$ is bounded, continuous, and positive definite. In particular, for any $x, y \in \mathcal{O}^3$, we have $|K(x, y)| \leq 1$, and there exists a constant $\alpha > 0$ such that $\sigma_{\text{min}}(\mathbb{E}[G]) > \alpha$.

As an example, when $K$ is the radial basis function (RBF) kernel (Schölkopf et al., 2002) with $\mathcal{O}^3$ embedded into a Euclidean space and $\phi$ being continuous, we have that Assumption 4.1 holds, since $K$ is bounded in $[0, 1]$ and the random matrix $G$ is positive definite with probability one. The following theorem is our main result of the paper.

Theorem 4.2. Under Assumptions 2.1, 2.2, and 4.1, for any $\delta > 0$, if we choose the confidence set level $\beta$ in Algorithm 1 to satisfy

$$\beta \geq (\gamma + 1)/\alpha \cdot \sqrt{8d_0^3 \cdot \log(2HA^2/\delta)}, \quad (4.2)$$

then, with probability at least $1 - \delta$, we have

$$\frac{1}{K} \sum_{k=1}^{K} (J(\theta^*, \pi^*) - J(\theta^*, \pi_k)) \leq 4d_3 \gamma^2 H^2 A^2 \cdot \log(K + 1) \cdot K^{-1/2} + 2d_3 \gamma H^2 \cdot K^{-1}. \quad (4.3)$$

We note that the first term on the right-hand side of (4.3) is the leading term for sufficiently large $K$. By Theorem 4.2, if we run Algorithm 1 for $K$ iterations and uniformly sample one from the generated policies, the expected suboptimality of the sampled policy converges to zero with a high probability at the rate of $K^{-1/2}$, regardless of logarithmic factors, and the orders on other factors are polynomial. In other words, to obtain an $\varepsilon$-optimal policy for any $\varepsilon > 0$, with a high probability, it suffices to run

$$\text{poly}(H, A, d_s, d_o, \gamma, 1/\alpha) \cdot \widetilde{O}(1/\varepsilon^2)$$

episodes of the POMDP to collect data. To our best knowledge, this is the first sample complexity upper bound for POMDPs that is independent of the number of states and observations, and the order of $\varepsilon$ is optimal even in the MDP setting (Ayoub et al., 2020), which is a special case of POMDPs.

4.2 Proof Sketch

In this section, we sketch the proof of Theorem 4.2. We show three lemmas as the main components of the proof. The following first lemma provides a decomposition of the difference of expected total rewards in two POMDPs when the model parameters are different and the policies are the same.
Lemma 4.3 (Decomposition). Under Assumptions 2.1 and 2.2, for any $\theta, \theta' \in \Theta$ and $\pi \in \Pi$, we have

$$J(\theta, \pi) - J(\theta', \pi) = \sum_{h=1}^{H} \mathbb{E}_{\theta', \pi}[(\mathbb{E}_{h}^{\theta, \pi}V_{h+1}^{\theta, \pi})(\mathbf{T}_h) - (\mathbb{E}_{h}^{\theta', \pi}V_{h+1}^{\theta', \pi})(\mathbf{T}_h)]$$

where the function $V_{h+1}^{\theta, \pi}$ is defined in (3.6) and we write $V_{H+1} = R$ with $R$ defined in (3.2).

For any $k \in [K]$, we denote by $\theta_k \in \Theta$ the selected model parameters in the planning phase (3.16) corresponding to the $k$-th iteration of Algorithm 1, that is, we have

$$(\theta_k, \pi_k) = \arg\max_{(\theta, \pi) \in \Theta \times \Pi} J(\theta, \pi). \quad (4.4)$$

And we define the following state-dependent error

$$e_h^k(s_{h-1}) = \mathbb{E}_{\theta^*, \pi_k}[e(\mathbf{T}_h) | s_{h-1} = s_{h-1}] \quad (4.5)$$

with $e(\mathbf{T}_h)$ short for

$$(\mathbb{E}_{h}^{\theta_k, \pi_k}V_{h+1}^{\theta_k, \pi_k})(\mathbf{T}_h) - (\mathbb{E}_{h}^{\theta^*, \pi_k}V_{h+1}^{\theta^*, \pi_k})(\mathbf{T}_h),$$

for any $(k, h, s_{h-1}) \in [K] \times [H] \times S$. Then, if it holds that $\theta^* \in \Theta_k$, by Lemma 4.3 we have

$$J(\theta^*, \pi^*) - J(\theta^*, \pi_k) \leq J(\theta_k, \pi_k) - J(\theta^*, \pi_k) \leq \sum_{h=1}^{H} \mathbb{E}_{\theta^*, \pi_k}[e_h^k(s_{h-1})]. \quad (4.6)$$

The following lemma characterizes the error expectations on the right-hand side of (4.6), when the underlying distribution of the state $s_{h-1}$ is replaced by the real data distribution, as well as showing that $\Theta_k$ is truly confidence set with high probability.

Lemma 4.4 (Accuracy). Under Assumptions 2.1, 2.2, and 4.1, for any $\delta > 0$, by choosing the confidence set level $\beta$ in Algorithm 1 to satisfy (4.2), with probability at least $1 - \delta$, it holds that

1. $\theta^* \in \Theta_k$,
2. $\mathbb{E}_{\theta^*, \pi_k}[e_h^k(s_{h-1})] \leq 2HA^2\gamma^2 \beta \cdot k^{-1/2}$,

for any $(k, h) \in [K] \times [H]$, where the mixing policy $\pi_k$ is defined in (3.14).

Thus, to characterize the right-hand side of (4.6), it remains to connect the error expectations with different underlying state distributions, which is shown by the following lemma.
Lemma 4.5 (Telescope of Errors). Under Assumptions 2.1 and 2.2, for any $h \in [H]$, we have

$$
\sum_{k=1}^{K} \mathbb{E}_{\theta, \pi_k} [e_h^k(s_{h-1})] \leq d_a \left( 2\gamma H + 2 \log(K + 1) \cdot \max_{k \in [K]} \{ k \cdot \mathbb{E}_{\theta, \pi_k} [e_h^k(s_{h-1})] \} \right).
$$

Combining the inequality (4.6) with Lemmas 4.4 and 4.5, we obtain the result in Theorem 4.2. See also Section C for a detailed proof.

5 Learning Distributions via RKHS embeddings

In this section, we show details of the computation for the minimization problem in (3.12).

Closed-form solution: For any dataset $D$ with data in $O^3$, we have that the solution $\hat{p}$ to (3.12) takes the form $\hat{p}(x) = \phi(x)^\top \hat{w}$ for any $x \in O^3$, where $\hat{w}$ satisfies

$$
\hat{w} = \text{argmin}_{w \in \mathbb{R}^{d_o}} \| (K\phi)^\top w - \hat{K}D \|_H.
$$

The minimization objective function of (5.1) can be further written as

$$
\| (K\phi)^\top w - \hat{K}D \|_H^2 = \langle (K\phi)^\top w, (K\phi)^\top w \rangle_H - 2 \langle (K\phi)^\top w, \hat{K}D \rangle_H + \| \hat{K}D \|_H^2
$$

$$
= w^\top Gw - 2U^\top w + \| \hat{K}D \|_H^2,
$$

which is a quadratic form of $w$. Here the matrix $G$ is defined in (4.1) and vector $U$ take the values

$$
[U]_i = \langle K\phi_i, \hat{K}D \rangle_H = \frac{1}{|D|} \sum_{y \in D} \mathbb{E}_{X_i \sim \phi_i} [K(X_i, y)],
$$

for any $i \in [d_o]$. Then, the vector $\hat{w}$ defined in (5.1) takes the form

$$
\hat{w} = G^{-1}U.
$$

We note that, if we want to make the estimate $\hat{p}$ always a probability distribution function, we only need to project the closed-form of $\hat{w}$ in (5.3) into the simplex $\Delta([d_o])$, that is, we can also let

$$
\hat{w} = \text{Proj}_{\Delta([d_o])}(G^{-1}U) = \text{argmin}_{w \in \Delta([d_o])} \| w - G^{-1}U \|_2.
$$

Both forms (5.3) and (5.4) apply to our theoretical analysis.

Randomized algorithm: We note that the computation of the vector $\hat{w}$ defined in (5.1) through the form (5.3) requires computing the inverse of the matrix $G$ with dimension $d_o$, which can be computationally expensive.
which might be computationally inefficient if $d_o$ is large. In the following, we introduce an alternative algorithm to obtain the vector $\hat{w}$ in a computationally efficient manner with the help of randomization.

We note that, for any $p \in \Delta(O^3)$, we have

$$
\|Kp - \hat{K}D\|_{\mathcal{H}} = \max_{f \in \mathcal{H}, \|f\|_{\mathcal{H}} \leq 1} \langle Kp - \hat{K}D, f \rangle_{\mathcal{H}}
$$

$$
= \max_{f \in \mathcal{H}, \|f\|_{\mathcal{H}} \leq 1} \left( \mathbb{E}_{X \sim p}[f(X)] - \frac{1}{|D|} \sum_{y \in D} f(y) \right).
$$

(5.5)

Here, for $p \in \text{linspan}(\phi)$ with the form $p(x) = \phi(x)^\top w$ for any $x \in O^3$, we can write

$$
\mathbb{E}_{X \sim p}[f(X)] = \sum_{i=1}^{d_o} \mathbb{E}_{X \sim \phi_i}[f(X)] \cdot [w]_i.
$$

Also, for a shift-invariant, continuous, and positive definite kernel $K$, by properly scaling we can write it in the random feature (Rahimi et al., 2007) form

$$
K(x, y) = \mathbb{E}_{\nu \sim \mathcal{P}_{\text{rf}}}[\rho(x; \nu)\rho(y; \nu)],
$$

where $\rho(\cdot; \nu)$ is the random feature with the distribution $\mathcal{P}_{\text{rf}}$ of the random parameter $\nu$. Then, by sampling $\{\nu_i\}_{i=1}^N$ independently from $\mathcal{P}_{\text{rf}}$, the RKHS ball $\{f \in \mathcal{H} : \|f\|_{\mathcal{H}} \leq 1\}$ can be approximated by the function class

$$
\hat{\mathcal{H}} = \left\{ f_\xi(\cdot) = \sum_{i=1}^N \rho(\cdot; \nu_i) \cdot [\xi]_i : \xi \in \mathbb{R}^N, \|\xi\|_2 \leq 1 \right\}.
$$

Thus, by (5.5), we can approximately obtain $\hat{w}$ in (5.1) by solving the following minimax problem,

$$
\hat{w} = \arg\min_{w \in \mathbb{R}^{d_o}} \max_{\xi \in \mathbb{R}^N : \|\xi\|_2 \leq 1} L(w, \xi),
$$

where $L(w, \xi)$ is short for

$$
\left( \sum_{i=1}^{d_o} \mathbb{E}_{X \sim \phi_i}[f_\xi(X)] \cdot [w]_i - \frac{1}{|D|} \sum_{y \in D} f_\xi(y) \right).
$$

This is similar to the training of the Wasserstein generative adversarial networks (Arjovsky et al., 2017). In particular, we can use the alternating stochastic gradient descent ascent algorithm to solve the problem, where we sample $X \sim \phi_i$ and $y \in D$ to estimate the gradient.
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A Examples: Linear Kernel POMDPs

In this section, we show examples of POMDPs that satisfy our assumptions in the main paper. In particular, we consider POMDPs satisfying the following assumption.

Assumption A.1. The state transition kernel $\mathcal{T}^g$ and observation emission kernel $\mathcal{E}^g$ take the form,

$$
\mathcal{T}^g_h(s' | s, a) = u(s')^\top M_{h,a}(\theta) v(s), \quad \mathcal{E}^g_h(o | s) = q(o)^\top g_h(s; \theta)
$$

for any $(s, s', a, o) \in \mathcal{S}^2 \times \mathcal{A} \times \mathcal{O}$ and $(h, \theta) \in [H] \times \Theta$, where vector-valued functions $u, v, q,$ and $g_h$ have dimensions $d_u, d_v, d_q,$ and $d_q$, respectively, and the matrix-valued function $M_{h,a}$ has dimensions $d_u$ and $d_v$. All functions have non-negative values and it holds that

$$
[u(\cdot)]_i \in \Delta(\mathcal{S}), \quad [q(\cdot)]_\ell \in \Delta(\mathcal{O})
$$

for any $i \in [d_v]$, and $\ell \in [d_q]$. Also, the initial state distribution $\mu$ satisfies $\mu \in \text{conh}([u(\cdot)]_{i=1}^{d_u})$.

We note that such a class of linear kernel POMDPs also includes tabular POMDPs, where each entry of $u$, as well as $v$, and $q$ is indicator function of each discrete state and observation, respectively. And, functions $M_{h,a}$ and $g_h$ satisfy

$$
[M_{h,a}(\theta)]_{s',s} = \mathcal{T}^g_h(s' | s, a), \quad [g_h(s; \theta)]_o = \mathcal{E}^g_h(o | s),
$$

for any $s, s' \in \mathcal{S}$ and $o \in \mathcal{O}$.

A.1 Verification of Assumption 2.1

Under Assumption A.1, the following lemma verifies Assumption 2.1 on the linear representation of state and observation distributions in Section 2.2.

Lemma A.2. Under Assumption A.1, there exists $\psi$ and $\phi$ such that Assumption 2.1 holds with

$$
d_s \leq d_u(d_v + 1) \quad \text{and} \quad d_o \leq d_q^3.
$$

Proof. We prove the lemma by constructing bases $\psi$ and $\phi$ satisfying Assumption 2.1. We first note that, to make $\mathcal{F}_s \in \text{conh}(\psi)$, it suffices to let the basis $\psi$ include the elements $
[u_i\}_i=1^{d_u}$. In the following, we show that $\mathcal{F}_s \in \text{conh}(\psi)$ if we add more elements to $\psi$.

For any policy $\pi$, $(h, \theta) \in [H] \times \Theta$ and $(s_h, a_h, o_{h+1}) \in \mathcal{S} \times \mathcal{A} \times \mathcal{O}$, we have

$$
p_{h,\pi}(s_h = s_h, o_{h+1} = o_{h+1} | a_h = a_h)
= \int_{\mathcal{S}} \mathcal{E}^g_{h+1}(o_{h+1} | s_{h+1}) \cdot \mathcal{T}^g_h(s_{h+1} | s_h, a_h) \cdot p_{h,\pi}(s_h = s_h) \, ds_{h+1}
= \left( \int_{\mathcal{S}} \mathcal{E}^g_{h+1}(o_{h+1} | s_{h+1}) \cdot u(s_{h+1})^\top M(\theta) \, ds_{h+1} \right) v_h(s_h, a_h) \cdot p_{h,\pi}(s_h = s_h), \quad (A.1)
$$

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where the second equality is by the linear form of $\mathcal{T}_{\theta}^*$ in Assumption A.1. Also, we have
\[
p_{\theta^*, \pi}(s_h = s_h) = \mathbb{E}_{\theta^*, \pi}[\mathcal{T}_{h-1}^{\theta^*}(s_h \mid s_{h-1}, a_{h-1})] \\
= u(s_h)\mathcal{T}_{h-1}^{\theta}(s_{h-1}, a_{h-1})
\] (A.2)
by the Markov property of the POMDP. For notational simplicity, we define the vectors
\[
\psi = \left\langle \cdot, \; \theta, \pi \left( s_h, o_{h+1}, a_h = a_h \right) \right\rangle
\]
where the second equality is by the linear form of $\mathcal{T}_{\theta}^*$ in Assumption A.1. Also, we have
\[
\zeta_1 = \left( \int_S \mathcal{E}^\theta_{h+1}(o_{h+1} \mid s_{h+1}) \cdot u(s_{h+1})^\top M(\theta) d s_{h+1} \right),
\]
\[
\zeta_2 = \mathbb{E}_{\theta, \pi}[M(\theta)v_{h-1}(s_{h-1}, a_{h-1})].
\] (A.3) (A.4)
Then, combining (A.1)-(A.4), we can write
\[
p_{\theta^*, \pi}(s_h = s_h \mid o_{h+1} = o_{h+1}, a_h = a_h) \\
= \frac{p_{\theta^*, \pi}(s_h = s_h, o_{h+1} = o_{h+1} \mid a_h = a_h)}{p_{\theta, \pi}(o_{h+1} = o_{h+1} \mid a_h = a_h)} = \frac{\zeta_1 v_h(s_h, a_h) u(s_h)^\top \zeta_2}{p_{\theta, \pi}(o_{h+1} = o_{h+1} \mid a_h = a_h)}.
\] (A.5)
We can rewrite (A.5) in a linear form,
\[
p_{\theta, \pi}(s_h = \cdot \mid o_{h+1} = o_{h+1}, a_h = a_h) = \left\langle (v(\cdot)u(\cdot))^\top, \frac{\zeta_2 \zeta_1^\top}{p_{\theta, \pi}(o_{h+1} = o_{h+1} \mid a_h = a_h)} \right\rangle_{\text{tr}},
\]
where $\left\langle \cdot, \cdot \right\rangle_{\text{tr}}$ represents the trace inner product of matrices. Therefore, we know that any function in $\mathcal{F}_*^\theta$ can be represented as a linear combination of the functions
\[
\{[u(\cdot)]_i \cdot [v(\cdot)]_j \}_{i \in [d_u], j \in [d_u]},
\] (A.6)
Thus, by normalizing each function in (A.6) as a probability distribution function, eliminating linearly dependent elements, and adding them into $\psi$, we have $\mathcal{F}_*^\theta \subset \text{conh}(\psi)$. In all, we have at most $d_u(d_o+1)$ basis probability distribution functions collected in $\psi$, which satisfies the conditions in Assumption 2.1.

In the following, we construct $\phi$ such that $\mathcal{F}_\phi \subset \text{conh}(\phi)$. Note that, for any $(h, \pi) \in [H - 1] \times \Theta, o_h, o_{h+1}, o_{h+2} \in \mathcal{O}$ and $a_h, a_{h+1} \in \mathcal{A}$, we have
\[
p_{\theta, \pi}(o_h = o_h, o_{h+1} = o_{h+1}, o_{h+2} = o_{h+2} \mid a_h = a_h, a_{h+1} = a_{h+1}) \\
= \int_{S^2} p_{\theta, \pi}(s_h = s_h) \cdot \mathcal{E}^\theta_{h}(o_h \mid s_h, a_h) \cdot \mathcal{T}^\theta_{h}(s_{h+1} \mid s_h, a_h) \cdot \mathcal{E}^\theta_{h+1}(o_{h+1} \mid s_{h+1}) \\
\cdot \mathcal{T}^\theta_{h+1}(s_{h+2} \mid s_{h+1}, a_{h+1}) \cdot \mathcal{E}^\theta_{h}(o_h \mid s_h) d s_h d s_{h+1} d s_{h+2} \\
= \sum_{i,j,\ell=1}^d \omega_{i,j,\ell} \cdot q_i(o_h) \cdot q_j(o_{h+1}) \cdot q_{\ell}(o_{h+2})
\]
20
where the scalars \( \{ \omega_{i,j,\ell} \}_{i,j,\ell \in [d_q]} \) are defined by

\[
\omega_{i,j,\ell} = \int_{\mathcal{S}^3} p_{\theta,\pi}(s_h = s_h) \cdot T_0^h(s_{h+1} \mid s_h, a_h) \cdot T_0^h(s_{h+2} \mid s_{h+1}, a_{h+1}) \cdot [g_h(s_h; \theta)]_i \cdot [g_h(s_{h+1}; \theta)]_j \cdot [g_h(s_{h+2}; \theta)]_\ell \, ds_h \, ds_{h+1} \, ds_{h+2}.
\]

Therefore, it suffices to let \( \phi \) contain the functions \( \{ [q]_i \cdot [q]_j \cdot [q]_\ell \}_{i,j,\ell \in [d_q]} \) to satisfy the conditions in Assumption 2.1, which concludes the proof of Lemma A.2. \( \square \)

### A.2 Verification of Assumption 2.2

Next, to make the linear kernel POMDP satisfy the undercompleteness assumption (Assumption 2.2), we have the following additional assumption.

**Assumption A.3.** For the functions defined in Assumption A.1, the following conditions hold.

1. There exists another \( d_q \)-dimensional vector-valued function \( q^* \) such that

\[
\int_{\mathcal{O}} [q(o)]_i \cdot [q^*(o)]_j \, do = \begin{cases} 
1 & \text{if } i = j, \\
0 & \text{if } i \neq j,
\end{cases}
\]

and \( \sup_{o \in \mathcal{O}} \sum_{i=1}^{d_q} ||q^*(o)||_i \leq \gamma_q \) for some constant \( \gamma_q > 0 \).

2. For the vector-valued function \( \psi \) we constructed in Lemma A.2, the matrix

\[ \Psi_\theta^h = \int_{\mathcal{S}} g_h(s; \theta) \psi(s)^\top \, ds \quad (A.7) \]

has full column rank for any \((h, \theta) \in [H] \times \Theta \). Moreover, the matrix operator norm of the left inverse of \( \Psi_\theta^h \),

\[
\| (\Psi_\theta^h)^+ \|_{1 \rightarrow 1} = \| ( (\Psi_\theta^h)^\top \Psi_\theta^h )^{-1} (\Psi_\theta^h)^\top \|_{1 \rightarrow 1},
\]

is upper bounded by some constant \( \gamma_u > 0 \).

We note that, to make the first condition in Assumption A.3 hold, it suffices to require \( \{ [q(\cdot)]_i \}_{i \in [d_q]} \) to be linearly independent in \( L^2(\mathcal{O}) \). In such a case, for any \( i \in [d_q] \), we can always find the satisfying function \( [q^*(\cdot)]_i \) in the orthogonal complement of \( \{ [q(\cdot)]_j \}_{j \in [d_q] \setminus \{i\}} \). When reduced to tabular POMDPs, Assumption A.3 is equivalent to the undercompleteness assumption for tabular POMDPs in Jin et al. (2020a). In such a case, matrix \( \Psi_\theta^h \) defined in (A.7) recovers the \( |\mathcal{O}| \times |\mathcal{S}| \) observation emission kernel matrix, which means we have

\[
[\Psi_\theta^h]_{o,s} = E_\theta^h(o \mid s)
\]

for any \( s \in \mathcal{S} \) and \( o \in \mathcal{O} \).

Under Assumption A.3, the following lemma verifies Assumption 2.2 on the undercompleteness of the POMDP.
Lemma A.4. Under Assumptions A.1 and A.3, we have that Assumption 2.2 holds with

\[ z_h^\theta(s, o) = \psi(s)^\top (\Psi_h^\theta)^\dagger q^*(o) \]

for any \((h, \theta) \in [H] \times \Theta\), and \(\gamma = \gamma_q \gamma_u\).

Proof. For any \(f \in \text{linspan}(\psi)\) with the coefficient \(w_f\), \((h, \theta) \in [H] \times \Theta\) and \(s \in S\), we have

\[
(Z_h^\theta \mathcal{O}_h^\theta f)(s) = \int_{S \times O} \psi(s)^\top (\Psi_h^\theta)^\dagger q^*(o) \cdot \mathcal{E}_h^\theta(o \mid s') \cdot \psi(s')^\top w_f \, do \, ds \]

\[
= \int_{S \times O} \psi(s)^\top (\Psi_h^\theta)^\dagger q^*(o) \cdot q(o)^\top g_h(s'; \theta) \cdot \psi(s')^\top w_f \, do \, ds. \tag{A.8}
\]

By Assumption A.3, we have

\[
\int_O q^*(o)q(o)^\top do = I_{d_v}, \quad (\Psi_h^\theta)^\dagger \int_S g_h(s'; \theta)\psi(s')^\top ds' = I_{d_v}. \tag{A.9}
\]

Plugging (A.9) into the right-hand side of (A.8), we obtain \((Z_h^\theta \mathcal{O}_h^\theta f)(s) = f(s)\). Also, for any \(f \in L^1(O)\) and \((h, \theta) \in [H] \times \Theta\), we have

\[
\|Z_h^\theta f\|_1 = \int_S \int_O \psi(s)^\top (\Psi_h^\theta)^\dagger q^*(o) \cdot f(o) \, do \, ds \leq \int_S \psi(s)^\top (\Psi_h^\theta)^\dagger \int_O q^*(o) \cdot f(o) \, do \, ds = \| (\Psi_h^\theta)^\dagger \int_O q^*(o) \cdot f(o) \, do \|_1, \tag{A.10}
\]

where we use the fact that elements of \(\psi\) are probability distribution functions by Lemma A.2. By Assumption A.3, we further have

\[
\left\| (\Psi_h^\theta)^\dagger \int_O q^*(o) \cdot f(o) \, do \right\|_1 \leq \gamma_v \cdot \left\| \int_O q^*(o) \cdot f(o) \, do \right\|_1 \leq \gamma_v \gamma_q \cdot \|f\|_1. \tag{A.11}
\]

Combining (A.10) and (A.11), we conclude the proof of Lemma A.4. \qed

## B Proofs for Section 3

In this section, we present the proofs for the results in Section 3.

### B.1 Proof of Lemma 3.1

Proof. For notational simplicity, we denote by \(\sigma\) the condition

\[
s_{h-1} = s_{h-1}, o_{h-1} = o_{h-1}, a_{h-1} = a_{h-1}.
\]
By the definition of $\mathbb{B}^\theta_{h,\pi}$ in Section 3, we can write

$$
\mathbb{E}_\theta(\mathbb{B}^\theta_{h,\pi}f)(\overline{\varphi}_h) | \sigma \\
= \int_{S^3 \times \mathcal{O}^3} f(\tau_{h-1}, a_{h-1}, \overline{o}_h, a_h, o_{h+1}) \cdot \mathcal{E}^\theta_{h+1}(o_{h+1} | s_{h+1}) \cdot T^\theta_h(s_{h+1} | \tilde{s}_h, a_h) \cdot \mathcal{E}^\theta_h(\overline{o}_h | \tilde{s}_h) \\
\cdot z^\theta_h(\tilde{s}_h, o_h) \cdot \mathcal{E}^\theta_h(o_h | s_h) \cdot p_\theta(s_h = s_h | \sigma) \, ds_h \, d\overline{s}_h \, ds_{h+1} \, do_h \, d\overline{o}_h \, do_{h+1}.
$$

(B.1)

where $a_h = \pi(\tau_{h-1}, \overline{o}_h)$. By Assumption 2.2, we have

$$
\int_{S^3 \times \mathcal{O}} z^\theta_h(\overline{s}_h, o_h) \cdot \mathcal{E}^\theta_h(o_h | s_h) \cdot p_\theta(s_h = s_h | \sigma) \, ds_h \, do_h = p_\theta(s_h = \overline{s}_h | \sigma).
$$

(B.2)

Also, note that we can write

$$
\int_{S^2} \mathcal{E}^\theta_{h+1}(o_{h+1} | s_{h+1}) \cdot T^\theta_h(s_{h+1} | \tilde{s}_h, a_h) \cdot \mathcal{E}^\theta_h(\overline{o}_h | \tilde{s}_h) \cdot p_\theta(s_h = \tilde{s}_h | \sigma) \, d\overline{s}_h \, ds_{h+1} \\
= p_\theta,\pi(o_{h+1} = o_{h+1}, o_h = \overline{o}_h | \sigma)
$$

(B.3)

Combining (B.1)-(B.3), we obtain

$$
\mathbb{E}_\theta(\mathbb{B}^\theta_{h,\pi}f)(\overline{\varphi}_h) | \sigma \\
= \int_{\mathcal{O}^2} f(\overline{\varphi}_{h-1}, a_{h-1}, \overline{o}_h, a_h, o_{h+1}) \cdot p_\theta,\pi(o_{h+1} = o_{h+1}, o_h = \overline{o}_h | \sigma) \, d\overline{o}_h \, do_{h+1} \\
= \mathbb{E}_\theta[f(\overline{\varphi}_{h+1}) | \sigma] = \mathbb{E}_\theta(\mathbb{B}^\theta_{h,\pi}f)(\overline{\varphi}_h) | \sigma,
$$

which concludes the proof of Lemma 3.1.

B.2 Proof of Corollary 3.2

Proof. For notational simplicity, we write $\sigma_{h-1}$ in short for the condition

$$s_{h-1} = s_{h-1}, \quad \overline{\varphi}_{h-1} = \overline{\varphi}_{h-1}, \quad a_{h-1} = a_{h-1}.$$

By our definition of the value function in (3.6), we can write

$$
\mathbb{E}_\theta\left[ V^\theta,\pi_{h}(\overline{\varphi}_h) \mid \sigma_{h-1} \right] = \mathbb{E}_\theta\left[ (\mathbb{B}^\theta,h \cdots \mathbb{B}^\theta,H R)(\overline{\varphi}_h) \mid \sigma_{h-1} \right]
$$

Invoking Lemma 3.1, we have

$$
\mathbb{E}_\theta\left[ (\mathbb{B}^\theta,h \cdots \mathbb{B}^\theta,H R)(\overline{\varphi}_h) \mid \sigma_{h-1} \right] \\
= \mathbb{E}_\theta\left[ (\mathbb{B}^\theta,h \mathbb{B}^\theta,h+1 \cdots \mathbb{B}^\theta,H R)(\overline{\varphi}_h) \mid \sigma_{h-1} \right] = \mathbb{E}_\theta,\pi \left[ (\mathbb{B}^\theta,h+1 \cdots \mathbb{B}^\theta,H R)(\overline{\varphi}_{h+1}) \mid \sigma_{h-1} \right]
$$

(B.4)
Using the tower property of the expectation, we can obtain
\[
\mathbb{E}_{\theta,\pi}[(\mathbb{E}_h^{0,\pi} \cdots \mathbb{E}_H^{0,\pi} R)(\mathcal{T}_{h+1}) | \sigma_{h-1}] = \mathbb{E}_{\theta,\pi}[\mathbb{E}_h^{0,\pi}[(\mathbb{E}_h^{0,\pi} \cdots \mathbb{E}_H^{0,\pi} R)(\mathcal{T}_{h+1} | s_h, \mathcal{T}_h) | \sigma_{h-1}] \\
= \mathbb{E}_{\theta,\pi}[(\mathbb{E}_h^{0,\pi} \cdots \mathbb{E}_H^{0,\pi} R)(\mathcal{T}_{h+2}) | s_h, \mathcal{T}_h) | \sigma_{h-1}] \\
= \mathbb{E}_{\theta,\pi}[(\mathbb{E}_h^{0,\pi} \cdots \mathbb{E}_H^{0,\pi} R)(\mathcal{T}_{h+2}) | \sigma_{h-1}],
\]
(E.5)
where the first equality omit the condition of \(s_{h-1}\) by the Markov property of the POMDP and the second equalities applies the same argument of (E.4) in the inner expectation. Then, by recursively using the same argument of (E.5), we obtain
\[
\mathbb{E}_{\theta}[(\mathbb{E}_h^{0,\pi} \cdots \mathbb{E}_H^{0,\pi} R)(\mathcal{T}_h) | \sigma_{h-1}] = \mathbb{E}_{\theta,\pi}[R(\mathcal{T}_{H+1}) | \sigma_{h-1}] = \mathbb{E}_{\theta,\pi}\left[ \sum_{i=1}^{H} T_i | \sigma_{h-1} \right],
\]
which concludes the proof of Corollary 3.2.

### B.3 Proof of Lemma 3.3

**Proof.** By the definition of \(P_{h,a}^{(1,\pi)}\) in (3.10), we can write
\[
P_{h,a}^{(1,\pi)}(o, o') = \int_{\mathcal{O}^2} \mathcal{E}_h(o' | s') \cdot \mathcal{T}_{h-1}(s' | s, a) \cdot \mathcal{E}_{h-1}(o | s) \cdot p_{\theta,\pi}(s_{h-1} = s) \, ds \, ds'.
\]
for any \(o, o' \in \mathcal{O}^2\). Then, by the definition of \(\mathbb{E}_{h,a}^{\theta_*}\) in (3.8), we have
\[
(\mathbb{E}_{h,a}^{\theta_*} P_{h,a}^{(1,\pi)})(o, o', o'') \\
= \int_{\mathcal{O} \times \mathcal{S}^2} \mathcal{E}_{h,a}^{\theta_*}(\bar{o}, o', o'') \cdot \mathcal{E}_{h}^{\theta_*}(\bar{o} | s') \cdot \mathcal{T}_{h-1}^{\theta_*}(s' | s, a) \cdot \mathcal{E}_{h-1}^{\theta_*}(o | s) \cdot p_{\theta,\pi}(s_{h-1} = s) \, d\bar{o} \, ds \, ds'
\]
\[
= \int_{\mathcal{O} \times \mathcal{S}^3} \mathcal{E}_{h+1}^{\theta_*}(o'' | s'') \cdot \mathcal{T}_{h}^{\theta_*}(s'' | \bar{s}, a') \cdot \mathcal{E}_{h}^{\theta_*}(o' | \bar{s}) \cdot z_{h}^{\theta_*}(\bar{s}, \bar{o}) \\
\cdot \mathcal{E}_{h}^{\theta_*}(\bar{o} | s') \cdot \mathcal{T}_{h-1}^{\theta_*}(s' | s, a) \cdot \mathcal{E}_{h-1}^{\theta_*}(o | s) \cdot p_{\theta,\pi}(s_{h-1} = s) \, d\bar{o} \, ds \, ds' \, d\bar{s} \, ds''.
\]
(E.6)
Note that, by Assumptions 2.1 and 2.2, we have
\[
\int_{\mathcal{S} \times \mathcal{O}} z_{h}^{\theta_*}(\bar{s}, \bar{o}) \cdot \mathcal{E}_{h}^{\theta_*}(\bar{o} | s') \cdot \mathcal{T}_{h-1}^{\theta_*}(s' | s, a) \, ds' \, d\bar{o} = \mathcal{T}_{h-1}^{\theta_*}(\bar{s} | s, a),
\]
plugging which into (E.6), we obtain
\[
(\mathbb{E}_{h,a}^{\theta_*} P_{h,a}^{(1,\pi)})(o, o', o'') \\
= \int_{\mathcal{S}^3} \mathcal{E}_{h+1}^{\theta_*}(o'' | s'') \cdot \mathcal{T}_{h}^{\theta_*}(s'' | \bar{s}, a') \cdot \mathcal{E}_{h}^{\theta_*}(o' | \bar{s}) \\
\cdot \mathcal{T}_{h-1}^{\theta_*}(\bar{s} | s, a) \cdot \mathcal{E}_{h-1}^{\theta_*}(o | s) \cdot p_{\theta,\pi}(s_{h-1} = s) \, ds \, d\bar{s} \, ds''
\]
\[
= P_{h,a}^{(2,\pi)}(o, o', o'').
\]
Thus, we conclude the proof of Lemma 3.3.  

\[\square\]
C Proof of Theorem 4.2

Proof. For any $\delta > 0$, by the definitions of $(\theta_k, \pi_k)$ in (4.4) and the first statement in Lemma 4.4, with probability at least $1 - \delta$, it holds that

$$J(\theta^*, \pi^*) - J(\theta^*, \pi_k) \leq J(\theta_k, \pi_k) - J(\theta^*, \pi_k)$$ (C.1)

for all $k \in [K]$. By further invoking Lemma 4.3 to the right-hand side of (C.1) and using the definition of the error function in (4.5), we obtain

$$J(\theta^*, \pi^*) - J(\theta^*, \pi_k) \leq \sum_{h=1}^{H} \mathbb{E}_{\theta^*, \pi_k}[e_h^k(s_h-1)],$$ (C.2)

where the equality uses the tower property of the expectation. Telescoping the both sides of (C.2) for $k \in [K]$ and applying Lemma 4.5, we obtain

$$\sum_{k=1}^{K} J(\theta^*, \pi^*) - J(\theta^*, \pi_k) \leq \sum_{h=1}^{H} \sum_{k=1}^{K} \mathbb{E}_{\theta^*, \pi_k}[e_h^k(s_h-1)]$$

$$\leq H d_s \left( 2\gamma H + 2 \log(K+1) \cdot \max_{k \in [K]} \left( k \cdot 2H A^2 A^2 \gamma^2 \beta \cdot k^{-1/2} \right) \right)$$ (C.3)

Applying the second statement of Lemma 4.4 to the right-hand side of (C.3), we further obtain

$$\sum_{k=1}^{K} J(\theta^*, \pi^*) - J(\theta^*, \pi_k) \leq H d_s \left( 2\gamma H + 2 \log(K+1) \cdot 2H A^2 A^2 \gamma^2 \beta \cdot K^{1/2} \right)$$

which concludes the proof of Theorem 4.2. □

D Proofs for Section 4.2

In this section, we present the proofs for the results in Section 4.2.
D.1 Proof of Lemma 4.3

Proof. Note that, by Corollary 3.2 and the definition of $V_{H+1}^{\theta,\pi}$, we can write

$$J(\theta, \pi) = \mathbb{E}_{\theta', \pi}[V_{1}^{\theta,\pi}(\bar{\tau}_1)], \quad J(\theta', \pi) = \mathbb{E}_{\theta', \pi}[V_{H+1}^{\theta,\pi}(\bar{\tau}_{H+1})],$$

which implies

$$J(\theta, \pi) - J(\theta', \pi) = \sum_{h=1}^{H} \mathbb{E}_{\theta', \pi}[V_{h}^{\theta,\pi}(\bar{\tau}_h)] - \mathbb{E}_{\theta', \pi}[V_{h+1}^{\theta,\pi}(\bar{\tau}_{h+1})]. \quad (D.1)$$

By the definition of $V_{h}^{\theta,\pi}$ in (3.6), we have

$$\mathbb{E}_{\theta', \pi}[V_{h}^{\theta,\pi}(\bar{\tau}_h)] = \mathbb{E}_{\theta', \pi}[(\mathbb{E}_{K, \pi, \theta} V_{h+1}^{\theta,\pi})(\bar{\tau}_h)], \quad (D.2)$$

and also, by Lemma 3.1, we have

$$\mathbb{E}_{\theta', \pi}[V_{h+1}^{\theta,\pi}(\bar{\tau}_{h+1})] = \mathbb{E}_{\theta', \pi}[(\mathbb{E}_{K, \pi, \theta} V_{h+1}^{\theta,\pi})(\bar{\tau}_{h+1})]. \quad (D.3)$$

Plugging (D.2) and (D.3) into the right-hand side of (D.1), we obtain

$$J(\theta, \pi) - J(\theta', \pi) = \sum_{h=1}^{H} \mathbb{E}_{\theta', \pi}[(\mathbb{E}_{K, \pi, \theta} V_{h+1}^{\theta,\pi})(\bar{\tau}_h) - (\mathbb{E}_{K, \pi, \theta} V_{h+1}^{\theta,\pi})(\bar{\tau}_{h+1})],$$

which concludes the proof of Lemma 4.3. □

D.2 Proof of Lemma 4.4

Proof. Invoking Lemma E.4 with $\delta_0 = \delta/(HK A^2)$, with probability at least $1 - \delta$, we have

$$\|\hat{P}_{h,a}^{(1),\pi_h} - P_{h,a}^{(1),\pi_h}\|_1 \leq \alpha^{-1} \cdot \sqrt{8d_0^3 \cdot \log(2HK A^2/\delta)} \cdot k^{-1/2}, \quad (D.4)$$

$$\|\hat{P}_{h,a,a'}^{(2),\pi_h} - P_{h,a,a'}^{(2),\pi_h}\|_1 \leq \alpha^{-1} \cdot \sqrt{8d_0^3 \cdot \log(2HK A^2/\delta)} \cdot k^{-1/2}, \quad (D.5)$$

for any $(k, h, a, a') \in [K] \times \{2, \ldots, H\} \times A^2$. In the following, we prove Lemma 4.4 by showing that the two statements in the lemma are true under (D.4) and (D.5).

**Proof of the first statement:** We first show $\theta^* \in \Theta_k$. Using the triangle inequality and (3.9), we have

$$\|\mathbb{E}_{h,a}^{\theta^*} \hat{P}_{h,a}^{(1),\pi_h} - \hat{P}_{h,a,a'}^{(1),\pi_h}\|_1 = \|\mathbb{E}_{h,a}^{\theta^*} \hat{P}_{h,a}^{(1),\pi_h} - \mathbb{E}_{h,a}^{\theta^*} P_{h,a}^{(1),\pi_h} + \mathbb{E}_{h,a}^{\theta^*} P_{h,a}^{(1),\pi_h} - \hat{P}_{h,a,a'}^{(1),\pi_h}\|_1 \leq \|\mathbb{E}_{h,a}^{\theta^*} \hat{P}_{h,a}^{(1),\pi_h} - \mathbb{E}_{h,a}^{\theta^*} P_{h,a}^{(1),\pi_h}\|_1 + \|P_{h,a}^{(1),\pi_h} - \hat{P}_{h,a,a'}^{(1),\pi_h}\|_1 \quad (D.6)$$

Combining (D.4), (D.5), and (D.6), and invoking Lemma E.2, we obtain

$$\|\mathbb{E}_{h,a}^{\theta^*} \hat{P}_{h,a}^{(1),\pi_h} - \hat{P}_{h,a,a'}^{(1),\pi_h}\|_1 \leq (\gamma + 1)/\alpha \cdot \sqrt{8d_0^3 \cdot \log(2HK A^2/\delta)} \cdot k^{-1/2} \leq \beta \cdot k^{-1/2},$$
which implies $\theta^* \in \Theta_k$ by our definition of $\Theta_k$.

**Proof of the second statement:** Since we assume that the model of the initial parts $\mu$, $\mathcal{T}_1$, $\mathcal{E}_1$, and $\mathcal{E}_2$ are known, we have that when $h = 1$ the error is zero for any $k \in [K]$. Thus, we only consider $h \geq 2$ in the following. For notational simplicity, we denote by $\sigma$ the conditions

$$s_{h-1} = s_{h-1}, \quad \mathcal{T}_{h-1} = \mathcal{T}_{h-1}, \quad a_{h-1} = a_{h-1}.$$ 

Rewriting the value function by Lemma E.1, we have

$$\mathbb{E}_{\theta^*} \left[ \left( (\mathbb{P}^{\theta_k, \pi_k}_h - \mathbb{P}^{\theta^*, \pi_k}_h) V^{\theta_k, \pi_k}_{h+1} \right)(\mathcal{T}_h) \mid \sigma \right] = \int \mathcal{O}^3 \times \mathcal{S} \mathcal{R}_{h+1} \cdot \mathcal{R}_{h+1} \cdot \Delta \mathcal{B}_{a_h}(o_h, \tilde{o}_h, o_{h+1}) \cdot p_{\theta^*}(o_h = o_h \mid \sigma) \, do_{h+1} \, do_h \, d\tilde{o}_h \, ds_{h+1},$$

where $a_h = \pi_k(\tau_{h-1}, \tilde{o}_h)$, $\mathcal{R}_{h+1}$ is short for the expectation

$$\mathcal{R}_{h+1} = \mathbb{E}_{\theta^*, \pi_k} \left[ \sum_{h=1}^{H} r_h \mid s_{h+1} = s_{h+1}, \mathcal{T}_{h-1} = \mathcal{T}_{h-1}, a_{h-1} = a_{h-1}, o_h = \tilde{o}_h, a_h = a_h \right],$$

and we denote

$$\Delta \mathcal{B}_a(o, o', o'') = \mathcal{B}^{\theta_k}_{h,a}(o, o', o'') - \mathcal{B}^{\theta^*}_{h,a}(o, o', o'').$$

Then, using the fact that $\mathcal{R}_{h+1} \in [0, H]$, we can upper bound the left-hand side of (D.7) by

$$\left| \mathbb{E}_{\theta^*} \left[ \left( (\mathbb{P}^{\theta_k, \pi_k}_h - \mathbb{P}^{\theta^*, \pi_k}_h) V^{\theta_k, \pi_k}_{h+1} \right)(\mathcal{T}_h) \mid \sigma \right] \right| \leq H \cdot \int \mathcal{O}^3 \times \mathcal{S} \left| \int \mathcal{O}^2 \cdot \mathcal{R}_{h+1} \cdot \Delta \mathcal{B}_{a_h}(o_h, \tilde{o}_h, o_{h+1}) \cdot p_{\theta^*}(o_h = o_h \mid \sigma) \, do_{h+1} \, do_h \, d\tilde{o}_h \, ds_{h+1} \right|. $$

By replacing the history-dependent actions $a_{h-1}$ and $a_h$ in the right-hand side of (D.8), where $a_{h-1}$ is hidden in $\sigma$, by all $a, a' \in A$, we have the inequality

$$\left| \mathbb{E}_{\theta^*} \left[ \left( (\mathbb{P}^{\theta_k, \pi_k}_h - \mathbb{P}^{\theta^*, \pi_k}_h) V^{\theta_k, \pi_k}_{h+1} \right)(\mathcal{T}_h) \mid \sigma \right] \right| \leq H \cdot \sum_{a, a' \in A} \int \mathcal{O}^3 \times \mathcal{S} \left| \int \mathcal{O}^2 \cdot \mathcal{R}_{h+1} \cdot \Delta \mathcal{B}_{a'}(o_h, \tilde{o}_h, o_{h+1}) \cdot p_{\theta^*}(o_h = o_h \mid s_{h-1} = s_{h-1}, a_{h-1} = a) \, do_{h+1} \, do_h \, d\tilde{o}_h \, ds_{h+1} \right| .$$

$$\leq H \gamma \cdot \sum_{a, a' \in A} \int \mathcal{O}^2 \left| \int \Delta \mathcal{B}_{a'}(o_h, \tilde{o}_h, o_{h+1}) \cdot p_{\theta^*}(o_h = o_h \mid s_{h-1} = s_{h-1}, a_{h-1} = a) \, do_h \, d\tilde{o}_{h+1} \right| .$$
where the last inequality uses the property of $z_{h+1}^{\theta_k}$ in Assumption 2.2. Note that the right-hand side of (D.9) is independent of $\overline{\tau}_{h-1}$ and $a_{h-1}$ in $\sigma$ on the left-hand side. Also, by the tower property of the expectation and Jensen’s inequality, we have the inequality

$$\left|\mathbb{E}_{\theta^*, \pi_k} \left[ \left( (\mathbb{B}_h^{\theta_k} - \mathbb{B}_h^{\theta^*}) V_{h+1}^{\theta_k, \pi_k} \right)(\overline{\tau}_h) \bigg| s_{h-1} = s_{h-1} \right] \right|$$

(D.10)

$$\leq \left| \mathbb{E}_{\theta^*, \pi_k} \left[ \mathbb{E}_{\theta^*} \left[ \left( (\mathbb{B}_h^{\theta_k} - \mathbb{B}_h^{\theta^*}) V_{h+1}^{\theta_k, \pi_k} \right)(\overline{\tau}_h) \bigg| s_{h-1} = s_{h-1}, \overline{\tau}_{h-1}, a_{h-1} \right] \bigg| s_{h-1} = s_{h-1} \right] \right|$$

$$\leq \mathbb{E}_{\theta^*, \pi_k} \left[ \left| \mathbb{E}_{\theta^*} \left[ \left( (\mathbb{B}_h^{\theta_k} - \mathbb{B}_h^{\theta^*}) V_{h+1}^{\theta_k, \pi_k} \right)(\overline{\tau}_h) \bigg| s_{h-1} = s_{h-1}, \overline{\tau}_{h-1}, a_{h-1} \right] \bigg| s_{h-1} = s_{h-1} \right] .$$

Then, plugging (D.9) into the right-hand side of (D.10), we obtain

$$\left| \mathbb{E}_{\theta^*, \pi_k} \left[ \left( (\mathbb{B}_h^{\theta_k} - \mathbb{B}_h^{\theta^*}) V_{h+1}^{\theta_k, \pi_k} \right)(\overline{\tau}_h) \bigg| s_{h-1} = s_{h-1} \right] \right|$$

(D.11)

$$\leq H \gamma \cdot \sum_{a, a' \in A} \int_{O^2} \left| \int_{O} \Delta B_{a'}(o_h, \overline{\theta}_h, \overline{o}_{h+1}) \right| p_{\theta^*}(o_h = o_h \big| s_{h-1} = s_{h-1}, a_{h-1} = a) \, do_h \, d\overline{\theta}_h \, d\overline{o}_{h+1}$$

$$= H \gamma \cdot \sum_{a, a' \in A} \int_{O^2} \left| \int_{S \times O} \Delta B_{a'}(o_h, \overline{\theta}_h, \overline{o}_{h+1}) \cdot \mathcal{E}_h^{\theta^*}(o_h \big| s_h) \cdot \mathcal{T}_{h-1}^{\theta^*}(s_h \big| s_{h-1}, a) \, ds_h \, do_h \right| \, d\overline{\theta}_h \, d\overline{o}_{h+1},$$

where, in the last equality, we use the expression

$$p_{\theta^*}(o_h = o_h \big| s_{h-1} = s_{h-1}, a_{h-1} = a) = \int_{S} \mathcal{E}_h^{\theta^*}(o_h \big| s_h) \cdot \mathcal{T}_{h-1}^{\theta^*}(s_h \big| s_{h-1}, a) \, ds_h.$$

For notational simplicity, we denote by $f$ the function

$$f(s_{h-1}, a, a', \overline{\theta}_h, \overline{o}_{h+1}) = \int_{S \times O} \Delta B_{a'}(o_h, \overline{\theta}_h, \overline{o}_{h+1}) \cdot \mathcal{E}_h^{\theta^*}(o_h \big| s_h) \cdot \mathcal{T}_{h-1}^{\theta^*}(s_h \big| s_{h-1}, a) \, ds_h \, do_h,$$

which enables us to simplify (D.11) as

$$e_k^h \leq H \gamma \cdot \sum_{a, a' \in A} \int_{O^2} |f(s_{h-1}, a, a', \overline{\theta}_h, \overline{o}_{h+1})| \, d\overline{\theta}_h \, d\overline{o}_{h+1}$$

(D.12)

Since our target is to upper bound $\mathbb{E}_{\theta^*, \pi_k}[e_k^h]$, in the following, we upper bound

$$\mathbb{E}_{\theta^*, \pi_k}[|f(s_{h-1}, a, a', \overline{\theta}_h, \overline{o}_{h+1})|]$$

$$= \int_{S} |f(s_{h-1}, a, a', \overline{\theta}_h, \overline{o}_{h+1})| \cdot p_{\theta^*, \pi_k}(s_{h-1} = s_{h-1}) \, ds_{h-1}.$$
We note that, by Assumption 2.1, we have
\[
\Delta B_{a'}(o_h, \tilde{o}_h, \tilde{o}_{h+1}) \cdot p_{\theta^*, \pi_k}(s_{h-1} = \cdot)
\]
\[
= \int_{\mathcal{O}} \Delta B_{a'}(o_h, \tilde{o}_h, \tilde{o}_{h+1}) \cdot p_{\theta^*, \pi_k}(o_h = o_h, s_{h-1} = \cdot | a_{h-1} = a) \, do_h
\]
\[
in \text{linspan}(\mathcal{F}_a') \subset \text{linspan}(\psi)
\]
for any \((a, a', \tilde{o}_h, \tilde{o}_{h+1}) \in \mathcal{A}^2 \times \mathcal{O}^2\). Thus, invoking Assumption 2.2, we have
\[
\int_{\mathcal{S}} |f(s_{h-1}, a, a', \tilde{o}_h, \tilde{o}_{h+1}) \cdot p_{\theta^*, \pi_k}(s_{h-1} = s_{h-1})| \, ds_{h-1}
\]
\[
= \int_{\mathcal{S}} \int_{\mathcal{S} \times \mathcal{O}} z_h^\theta (s_{h-1}, o_{h-1}) \cdot \mathcal{E}^\theta_{h-1}(o_{h-1} | \tilde{s}_{h-1})
\]
\[
\cdot f(\tilde{s}_{h-1}, a, a', \tilde{o}_h, \tilde{o}_{h+1}) \cdot p_{\theta^*, \pi_k}(s_{h-1} = \tilde{s}_{h-1}) \, d\tilde{s}_{h-1} \, do_{h-1} \bigg| ds_{h-1}
\]
\[
\leq \gamma \cdot \int_{\mathcal{O}} \int_{\mathcal{S}} \mathcal{E}^\theta_{h-1}(o_{h-1} | \tilde{s}_{h-1}) \cdot f(\tilde{s}_{h-1}, a, a', \tilde{o}_h, \tilde{o}_{h+1}) \cdot p_{\theta^*, \pi_k}(s_{h-1} = \tilde{s}_{h-1}) \, d\tilde{s}_{h-1} \, do_{h-1}.
\]
By the definition of \(f(\tilde{s}_{h-1}, a, a', \tilde{o}_h)\), we have
\[
\int_{\mathcal{S}} \mathcal{E}^\theta_{h-1}(o_{h-1} | \tilde{s}_{h-1}) \cdot f(\tilde{s}_{h-1}, a, a', \tilde{o}_h, \tilde{o}_{h+1}) \cdot p_{\theta^*, \pi_k}(s_{h-1} = \tilde{s}_{h-1}) \, d\tilde{s}_{h-1}
\]
\[
= \int_{\mathcal{S}^2 \times \mathcal{O}} \Delta B_{a'}(o_h, \tilde{o}_h, \tilde{o}_{h+1}) \cdot \mathcal{E}^\theta_{h}(o_h | s_h) \cdot T_{h}^\theta(s_h | \tilde{s}_{h-1}, a)
\]
\[
\cdot \mathcal{E}^\theta_{h-1}(o_{h-1} | \tilde{s}_{h-1}) \cdot p_{\theta^*, \pi_k}(s_{h-1} = \tilde{s}_{h-1}) \, ds_h \, d\tilde{s}_{h-1} \, do_h
\]
\[
= \int_{\mathcal{O}} \Delta B_{a'}(o_h, \tilde{o}_h, \tilde{o}_{h+1}) \cdot p_{\theta^*, \pi_k}(o_h = o_h, o_{h-1} = o_{h-1} | a_{h-1} = a) \, do_h.
\]
Using our notation in Section 3.2, we can rewrite the right-hand side of (D.14) as
\[
\int_{\mathcal{O}} \Delta B_{a'}(o_h, \tilde{o}_h, \tilde{o}_{h+1}) \cdot p_{\theta^*, \pi_k}(o_h = o_h, o_{h-1} = o_{h-1} | a_{h-1} = a) \, do_h
\]
\[
= (\mathbb{E}^\theta_{h,a'} P_{h,a}^{(1), \pi_k}(o_h = o_h, \tilde{o}_h, \tilde{o}_{h+1}) - (\mathbb{E}^\theta_{h,a'} P_{h,a}^{(1), \pi_k})(o_h = o_h, \tilde{o}_h, \tilde{o}_{h+1} + (\mathbb{E}^\theta_{h,a'} P_{h,a}^{(2), \pi_k} - P_{h,a}^{(2), \pi_k}))(o_h = o_h, \tilde{o}_h, \tilde{o}_{h+1})
\]
Combining (D.12), (D.13), (D.14), and (D.15), we obtain
\[
\mathbb{E}_{\theta, \pi_k}[e_{h}^{k}] \leq H \gamma^2 \cdot \sum_{a,a' \in A} \left\| \mathbb{E}^\theta_{h,a'} P_{h,a}^{(1), \pi_k} - P_{h,a}^{(2), \pi_k} \right\|_1.
\]
By the triangle inequality, we can write
\[
\left\| \mathbb{E}^\theta_{h,a'} P_{h,a}^{(1), \pi_k} - P_{h,a}^{(2), \pi_k} \right\|_1
\]
\[
= \left\| \mathbb{E}^\theta_{h,a'} P_{h,a}^{(1), \pi_k} - \mathbb{E}^\theta_{h,a'} \hat{P}_{h,a}^{(1), \pi_k} + \mathbb{E}^\theta_{h,a'} \hat{P}_{h,a}^{(1), \pi_k} - \hat{P}_{h,a,a'}^{(1), \pi_k} + \hat{P}_{h,a,a'}^{(1), \pi_k} - \hat{P}_{h,a,a'}^{(2), \pi_k} + \hat{P}_{h,a,a'}^{(2), \pi_k} \right\|_1
\]
\[
\leq \left\| \mathbb{E}^\theta_{h,a'} P_{h,a}^{(1), \pi_k} - \mathbb{E}^\theta_{h,a'} \hat{P}_{h,a}^{(1), \pi_k} \right\|_1 + \left\| \mathbb{E}^\theta_{h,a'} \hat{P}_{h,a}^{(1), \pi_k} - \hat{P}_{h,a,a'}^{(1), \pi_k} \right\|_1 + \left\| \hat{P}_{h,a,a'}^{(1), \pi_k} - \hat{P}_{h,a,a'}^{(2), \pi_k} \right\|_1.
By (D.4) and (D.5), and invoking Lemmas E.2, we have
\[
\| \mathbb{P}^{\theta_k}_{h,a^*} P^{(1), \pi_k}_{h,a} \mathbb{P}^{\theta_k}_{h,a} - \mathbb{P}^{\theta_k}_{h,a^*} \hat{P}^{(1), \pi_k}_{h,a} \|_1 \leq \gamma \cdot \| P^{(1), \pi_k}_{h,a} - \hat{P}^{(1), \pi_k}_{h,a} \|_1 \leq \gamma / \alpha \cdot \sqrt{8d_o^3 \cdot \log(2HKA^2 / \delta)} \cdot k^{-1/2}. \tag{D.18}
\]
and
\[
\| \hat{P}^{(2), \pi_k}_{h,a,a'} - P^{(2), \pi_k}_{h,a,a'} \|_1 \leq 1 / \alpha \cdot \sqrt{8d_o^3 \cdot \log(2HKA^2 / \delta)} \cdot k^{-1/2}. \tag{D.19}
\]
Also, by the definition of $\theta_k$ and $\Theta_k$, we have
\[
\| \mathbb{P}^{\theta_k}_{h,a} \hat{P}^{(1), \pi_k}_{h,a} - \hat{P}^{(2), \pi_k}_{h,a} \|_1 \leq \beta \cdot \frac{1}{k} \cdot \sum_{i=0}^{k-1} \mu^{\pi}_{h} \in \text{conh}(\psi).
\tag{D.20}
\]
Plugging (D.18)-(D.20) into the right-hand side of (D.17), we have
\[
\| \mathbb{P}^{\theta_k}_{h,a^*} P^{(1), \pi_k}_{h,a} - P^{(2), \pi_k}_{h,a,a'} \|_1 \leq 2 \beta \cdot k^{-1/2},
\]
combining which with (D.16), we obtain
\[
E_{\theta, \pi_k}[e^k_h] \leq 2HA^2 \gamma^2 \beta \cdot k^{-1/2}.
\]
Therefore, we conclude the proof of Lemma 4.4. \[ \square \]

### D.3 Proof of Lemma 4.5

**Proof.** For any $h \in [H]$ and $\pi \in \Pi$, we denote by $\mu^\pi_h$ the marginal distribution of $s_h$ under $(\theta^*, \pi)$. By Assumption 2.1, for any $(k, h) \in [K] \times [H]$, we have
\[
\mu^\pi_h \in \text{conh}(\psi), \quad \mu^\pi_h = \frac{1}{k} \sum_{i=0}^{k-1} \mu^\pi_{h,i} \in \text{conh}(\psi).
\]
Thus, there exists vectors $c^k_h, \overline{c}^k_h \in \Delta([d_s]) \subset \mathbb{R}^{d_s}$ such that
\[
\mu^\pi_h(\cdot) = \psi(\cdot)^T c^k_h, \quad \mu^\pi_h(\cdot) = \psi(\cdot)^T \overline{c}^k_h, \quad c^k_h = (1/k) \cdot \sum_{i=0}^{k-1} c^i_h.
\]
We define vector $b^k_h \in \mathbb{R}^{d_s}$ by
\[
[b^k_h]_i = E_{s_h \sim \psi_i}[e^k_{h+1}(s_h)], \text{ for any } i \in [d_s]. \tag{D.21}
\]
and it holds that
\[
E_{\theta, \pi^k}[e^k_{h+1}(s_h)] = (b^k_h)^T c^k_h, \quad E_{\theta, \pi^k}[e_{h+1}^k(s_h)] = (b^k_h)^T \overline{c}^k_h
\]
We note that \([b_h^k]_i\) is non-negative and upper bounded by \(2\gamma H\) for any \(i \in [d_u]\) because the error term in the expectation of (D.21) is upper bounded. The proof is deferred to Lemma E.3. With the above definitions, we have the following inequality

\[
\frac{[b_h^k]_i \cdot [c_h^k]_i}{\mathbb{E}_{\theta, \pi_h} [c_{h+1}^k(s_h)]} \leq \frac{[b_h^k]_i \cdot [c_h^k]_i}{\sum_{j=0}^{k-1} [c_h^j]_i} = k \cdot \frac{[c_h^k]_i}{\sum_{j=0}^{k-1} [c_h^j]_i} = \tag{D.22}
\]

for any \(i \in [d_u]\), where we use the fact that all entries of the vectors \(b_h^k\) and \(c_h^k\) are non-negative. The fraction in the right-hand side of (D.22) can be further upper bounded as

\[
\frac{[c_h^k]_i}{\sum_{j=0}^{k-1} [c_h^j]_i} \leq 2 \log \left(1 + \frac{[c_h^k]_i}{\sum_{j=0}^{k-1} [c_h^j]_i}\right) = 2 \log \sum_{j=1}^{k} [c_h^j]_i - 2 \log \sum_{j=0}^{k-1} [c_h^j]_i,  \tag{D.23}
\]

using the inequality \(x \leq 2 \log(1 + x)\) for \(x \in [0, 1]\). Thus, we can write

\[
\frac{[c_h^k]_i}{\sum_{j=0}^{k-1} [c_h^j]_i} \leq 2 \left(\log \sum_{j=0}^{k} [c_h^j]_i - \log \sum_{j=0}^{k-1} [c_h^j]_i\right) \tag{D.23}
\]

for any \(k \in \{k_0 + 1, \ldots, K\}\), where \(k_0\) is defined as

\[
k_0 = \max \left\{ k \in [K] : \sum_{j=0}^{k-1} [c_h^j]_i < 1 \right\}.  \tag{D.24}
\]

Then, by telescoping (D.23) for \(k \in \{k_0 + 1, \ldots, K\}\), we have

\[
\sum_{k=k_0+1}^{K} \frac{[c_h^k]_i}{\sum_{j=0}^{k-1} [c_h^j]_i} \leq \sum_{k=k_0+1}^{K} 2 \left(\log \sum_{j=0}^{k} [c_h^j]_i - \log \sum_{j=0}^{k-1} [c_h^j]_i\right) = 2 \left(\log \sum_{j=0}^{K} [c_h^j]_i - \log \sum_{j=1}^{k_0} [c_h^j]_i\right) \leq 2 \log \sum_{j=0}^{K} [c_h^j]_i \leq 2 \log(K + 1),
\]

combining which with (D.22), we obtain

\[
\sum_{k=k_0+1}^{K} [b_h^k]_i \cdot [c_h^k]_i \leq 2 \log K \cdot \left(\max_{k \in [K]} k \cdot \mathbb{E}_{\theta, \pi_h} [c_{h+1}^k(s_h)]\right).  \tag{D.25}
\]

Then, plugging (D.25) into the decomposition

\[
\sum_{k=1}^{K} \mathbb{E}_{\theta, \pi_h} [c_{h+1}^k(s_h)] = \sum_{i=1}^{d_u} \sum_{k=1}^{K} [b_h^k]_i \cdot [c_h^k]_i = \sum_{i=1}^{d_u} \sum_{k=k_0+1}^{K} [b_h^k]_i \cdot [c_h^k]_i + \sum_{k=k_0+1}^{K} [b_h^k]_i \cdot [c_h^k]_i
\]

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and using the fact
\[
\sum_{k=1}^{k_0} |b^k_h| \cdot |c^k_h| \leq (\max_{k \in [d_h]} |b^k_h|) \cdot \sum_{k=1}^{k_0} |c^k_h| \leq 2\gamma H \cdot 1 = 2\gamma H,
\]
by the definition of \(k_0\) in (D.24), we obtain
\[
\sum_{k=1}^{K} \mathbb{E}_{\theta,\pi_h}[e^k_{h+1}(s_h)] \leq d_s(2\gamma H + 2 \log K \cdot (\max_{k \in [K]} \mathbb{E}_{\theta,\pi_h}[e^k_{h+1}(s_h)])
\]
which concludes the proof of Lemma 4.5. \(\square\)

E Auxiliary Lemmas

In this section, we present the proofs for the auxiliary lemmas invoked in previous sections.

E.1 Properties of the Value Functions

**Lemma E.1.** For any \((h, \pi, \theta) \in [H] \times \Pi \times \Theta \) and \(\tau_h \in \Gamma_h\), it holds that

\[
V_{\theta, \pi}^h(\tau_h) = \int_{S} \mathbb{E}_{\theta,\pi} \left[ \sum_{h=1}^{H} r_h \bigg| s_h = s_h, \tau_{h-1} = \tau_{h-1}, a_{h-1} = a_{h-1} \right] \cdot z_{h}^{\theta}(s_h, o_h) \, ds_h. \tag{E.1}
\]

Here, we note that the variables \(\tau_{h-1}\) and \(a_{h-1}\) on the right-hand side of (E.1) are parts of \(\tau_h\).

**Proof.** We prove the lemma by induction. For \(h = H\), we directly have that (E.1) holds by applying the definitions of \(V_{H}^{\theta, \pi}, V_{H+1}^{\theta, \pi}\), and \(\mathbb{E}_{H, \pi, \theta}\) to obtain

\[
V_{H}^{\theta, \pi}(\tau_H) = (\mathbb{E}_{H, \pi, \theta} V_{H+1}^{\theta, \pi})(\tau_H)
\]

\[
= \int_{S} \left( r(o_H, \pi(\tau_h)) + \sum_{h=1}^{H-1} r(o_h, a_h) \right) \cdot z_{h}^{\theta}(s_H, o_H) \, ds_H,
\]

where we use the fact that the rewards are independent of \(o_{H+1}\).

Assume that the lemma holds for the value function of the \((h + 1)\)-th step. Then, we have

\[
V_{h}^{\theta, \pi}(\tau_h) = (\mathbb{E}_{h, \pi, \theta} V_{h+1}^{\theta, \pi})(\tau_h)
\]

\[
= \int_{S^3 \times O^2} \mathbb{E}_{\theta,\pi} \left[ \sum_{h=1}^{H} r_h \bigg| \sigma \right] \cdot z_{h+1}(\tilde{s}_{h+1}, o_{h+1}) \cdot z_{h+1}(s_{h+1} | s_h, a_h) \cdot \mathcal{E}_{h+1}(o_{h+1} | s_{h+1}) \cdot \mathcal{E}_{h+1}(s_{h+1} | s_h, a_h) \nonumber \\
\cdot \mathcal{E}_{h}(\tilde{o}_h | s_h) \cdot z_{h}(s_h, o_h) \, d\tilde{s}_{h+1} \, ds_h \, ds_{h+1} \, d\tilde{o}_h \, do_{h+1}, \tag{E.2}
\]

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where \( a_h = \pi(\tau_{h-1}, o_h) \) and \( \sigma \) is short for the condition

\[
s_{h+1} = \tilde{s}_{h+1}, \overline{\tau}_{h-1} = \tau_{h-1}, a_{h-1} = a_{h-1}, o_h = \tilde{o}_h.
\]

We note that, by Assumption 2.2, it holds that

\[
\int_{S^2} z^\theta_{h+1} (\tilde{s}_{h+1}, o_{h+1}) \cdot \mathcal{E}^\theta_{h+1} (o_{h+1} \mid s_{h+1}) \cdot T^\theta_h (s_{h+1} \mid s_h, a_h) \, ds_{h+1} \, do_{h+1} = T^\theta_h (\tilde{s}_{h+1} \mid s_h, a_h).
\]

Thus, we can rewrite (E.2) as

\[
V^\theta,\pi_h (\tau_h) = \int_{S^2 \times O} \mathbb{E}_{\theta,\pi} \left[ \sum_{h=1}^H r_h \, | \, s_{h+1} = \tilde{s}_{h+1}, \overline{\tau}_{h-1} = \tau_{h-1}, a_{h-1} = a_{h-1}, o_h = \tilde{o}_h \right] \cdot T^\theta_h (\tilde{s}_{h+1} \mid s_h, a_h) \cdot \mathcal{E}^\theta_h (\tilde{o}_h \mid s_h) \cdot z^\theta_h (s_h, o_h) \, d\tilde{s}_{h+1} \, ds_h \, d\tilde{o}_h.
\]

Note that we have

\[
T^\theta_h (\tilde{s}_{h+1} \mid s_h, a_h) \cdot \mathcal{E}^\theta_h (\tilde{o}_h \mid s_h) = p_\theta (s_{h+1} = \tilde{s}_{h+1}, o_h = \tilde{o}_h \mid s_h = s_h, a_h = a_h),
\]

and, by the independency between \( \{o_i\}_{i \geq h+1} \) and \( s_h \) conditional on \( s_{h+1} \), we have

\[
\mathbb{E}_{\theta,\pi} \left[ \sum_{h=1}^H r_h \, | \, s_h = s_h, \overline{\tau}_{h-1} = \tau_{h-1}, a_{h-1} = a_{h-1} \right] = \int_{S \times O} \mathbb{E}_{\theta,\pi} \left[ \sum_{h=1}^H r_h \, | \, s_{h+1} = \tilde{s}_{h+1}, \overline{\tau}_{h-1} = \tau_{h-1}, a_{h-1} = a_{h-1}, o_h = \tilde{o}_h \right] \cdot p_\theta (s_{h+1} = \tilde{s}_{h+1}, o_h = \tilde{o}_h \mid s_h = s_h, a_h = a_h) \, d\tilde{s}_{h+1} \, ds_h \, d\tilde{o}_h.
\]

Combining (E.3)-(E.5), we obtain

\[
V^\theta,\pi_h (\tau_h) = \int_S \mathbb{E}_{\theta,\pi} \left[ \sum_{h=1}^H r_h \, | \, s_h = s_h, \overline{\tau}_{h-1} = \tau_{h-1}, a_{h-1} = a_{h-1} \right] \cdot z^\theta_h (s_h, o_h) \, ds_h.
\]

Therefore, by induction, we conclude the proof of Lemma E.1. \( \square \)

### E.2 Useful Upper bounds

**Lemma E.2** (Operator Norm of \( F \)). For any \( f \in L_1(O^2) \) and \( (k, h, \theta) \in [K] \times [H] \times \Theta \), it holds that

\[
\| \mathbb{E}^\theta_{h,a} f \|_1 \leq \gamma \cdot \| f \|_1.
\]
Proof. By our definition of $\mathbb{F}_{h,a}^\theta$, we can write
\[
\|\mathbb{F}_{h,a}^\theta f\|_1 = \int_{\mathcal{O}^3} \left| \int_{\mathcal{O}^3} \mathcal{B}_{h,a}^\theta (o_{h+1}, \bar{o}_h, o_h) \cdot f(o_{h-1}, o_h) \, do_h \right| \, do_{h-1} \, do_{h+1}
\]
\[
= \int_{\mathcal{O}^3} \left| \int_{\mathcal{O}^3} \mathcal{P}_h (a_{h+1} = o_{h+1}, a_h = \bar{o}_h | s_h = s_h, a_h = a) \cdot z_h^\theta (s_h, o_h) \cdot f(o_{h-1}, o_h) \, ds_h \right| \, do_{h-1} \, do_{h+1}.
\]
By Jensen’s inequality, we have
\[
\|\mathbb{F}_{h,a}^\theta f\|_1 \leq \int_{\mathcal{O}^3} \left| \int_{\mathcal{O}^3} \mathcal{P}_h (a_{h+1} = o_{h+1}, a_h = \bar{o}_h | s_h = s_h, a_h = a) \cdot z_h^\theta (s_h, o_h) \cdot f(o_{h-1}, o_h) \, ds_h \right| \, do_{h-1} \, do_{h+1}
\]
\[
= \int_{\mathcal{O}^3} \left| \int_{\mathcal{O}^3} z_h^\theta (s_h, o_h) \cdot f(o_{h-1}, o_h) \, ds_h \right| \, do_{h-1} \, do_{h+1}
\]
\[
\leq \gamma \cdot \int_{\mathcal{O}^2} |f(o_{h-1}, o_h)| \, do_h \, do_{h-1} = \gamma \cdot \|f\|_1,
\]
where the second inequality is by Assumption 2.2. Thus, we conclude the proof of Lemma E.2.

**Lemma E.3.** For any $(k, h) \in [K] \times \{2, \ldots, H\}$ and $s_{h-1} \in \mathcal{S}$, we have
\[
e_{h}^k (s_{h-1}) \leq 2\gamma H.
\]

Proof. We prove the lemma by showing that
\[
\left| \mathbb{E}_\theta^* \left[ \left( (\mathbb{B}_{h,\pi_k,\theta_k} - \mathbb{B}_{h,\pi_k,\theta^*}) V_{h+1}^{\theta_k,\pi_k} \right) (\mathbf{f}_h) \mid s_{h-1} = s_{h-1}, \mathbf{f}_{h-1} = \mathbf{f}_{h-1}, a_{h-1} = a_{h-1} \right] \right| \leq 2\gamma H
\]
for any $\mathbf{f}_{h-1} \in \mathbf{f}_{h-1}$ and $(s_{h-1}, a_{h-1}) \in \mathcal{S} \times \mathcal{A}$. Then, the result of Lemma E.3 is obtained by averaging the realizations of $\mathbf{f}_{h-1}$ and $a_{h-1}$ and using Jensen’s inequality.

For notational simplicity, we denote by $\sigma$ the condition
\[
s_{h-1} = s_{h-1}, \mathbf{f}_{h-1} = \mathbf{f}_{h-1}, a_{h-1} = a_{h-1}.
\]
By our definition of $V_{h}^{\theta_k,\pi_k}$ and Lemma 3.1, we can write
\[
\mathbb{E}_\theta^* \left[ \left( (\mathbb{B}_{h,\pi_k,\theta_k} - \mathbb{B}_{h,\pi_k,\theta^*}) V_{h+1}^{\theta_k,\pi_k} \right) (\mathbf{f}_h) \mid \sigma \right]
\]
\[
= \mathbb{E}_\theta^* [V_{h}^{\theta_k,\pi_k} (\mathbf{f}_h) \mid \sigma] - \mathbb{E}_\theta^* \pi_k [V_{h+1}^{\theta_k,\pi_k} (\mathbf{f}_{h+1}) \mid \sigma]
\]
\[
\leq \left| \mathbb{E}_\theta^* [V_{h}^{\theta_k,\pi_k} (\mathbf{f}_h) \mid \sigma] \right| + \left| \mathbb{E}_\theta^* \pi_k [V_{h+1}^{\theta_k,\pi_k} (\mathbf{f}_{h+1}) \mid \sigma] \right|,
\]
(E.6)
where the inequality is by the triangle inequality. Here, the subscript $\pi_k$ in the second expectation is for indicating the selection of action $a_h$. In the following, we characterize the absolute values of the two expectations on the right-hand side of (E.6) one by one. By Lemma E.1, we can write

\[
\left|\mathbb{E}_{\theta^*} \left[ V_{\bar{h}, \pi_k} \left( \bar{G}_h \right) \mid \sigma \right] \right| = \left| \int_{S \times O} \mathbb{E}_{\theta_k, \pi_k} \left[ \sum_{h=1}^{H} r_h \mid s_h = s_h, \sigma \right] \cdot \theta_{s_h, o_h} \cdot p_{\theta^*} (o_h = o_h \mid \sigma) \, ds_h \, do_h \right| \leq H \cdot \left| \int_{S} \int_{O} \theta_{s_h, o_h} \cdot p_{\theta^*} (o_h = o_h \mid \sigma) \, do_h \right| \, ds_h \leq \gamma H. \tag{E.7}
\]

On the other hand, invoking Lemma E.1 again, we have

\[
\left|\mathbb{E}_{\theta^*, \pi_k} \left[ V_{\bar{h}, \pi_k} \left( \bar{G}_{h+1} \right) \mid \sigma \right] \right| \tag{E.8}
\]

\[
= \left| \int_{S \times O^2} \mathbb{E}_{\theta_k, \pi_k} \left[ \sum_{h=1}^{H} r_h \mid s_h = s_{h+1}, o_h = o_{h}, a_h = a_h, \sigma \right] \cdot \theta_{s_{h+1}, o_h} \cdot p_{\theta^*} (o_h = o_h \mid \sigma) \, ds_{h+1} \, do_h \, da_h \right| \leq H \cdot \left| \int_{S} \int_{O} \theta_{s_{h+1}, o_h} \cdot p_{\theta^*} (o_h = o_h \mid \sigma) \, do_h \right| \, ds_{h+1} \, da_h \leq \gamma H.
\]

Thus, plugging (E.7) and (E.8) into the right-hand side of (E.6), we conclude the proof of Lemma E.3.

\[\Box\]

### E.3 Concentration Inequalities

**Lemma E.4.** For any $\delta_0 > 0$ and $(k, h, a, a') \in [K] \times \{2, \ldots, H\} \times \mathcal{A}^2$, we have

\[
\max \left\{ \| \hat{P}^{(1), \pi_k}_{h,a} - P^{(1), \pi_k}_{h,a} \|_1, \| \hat{P}^{(2), \pi_k}_{h,a,a'} - P^{(2), \pi_k}_{h,a,a'} \|_1 \right\} \leq \alpha^{-1} \cdot \sqrt{8d_\theta^3 \cdot \log(2/\delta_0) \cdot k^{-1/2}},
\]

with probability at least $1 - \delta_0$.

**Proof.** For any $(k, h, a, a') \in [K] \times \{2, \ldots, H\} \times \mathcal{A}^2$, let \( \hat{w}^k_{h,a,a'}, \overline{w}^k_{h,a,a'} \in \mathbb{R}^{d_\theta} \) be the vectors such that

\[
\hat{P}^{(2), \pi_k}_{h,a,a'} = \phi^\top \hat{w}^k_{h,a,a'}, \quad \overline{P}^{(2), \pi_k}_{h,a,a'} = \phi^\top \overline{w}^k_{h,a,a'}. \tag{E.9}
\]

By the closed-form of \( \hat{w}^k_{h,a,a'} \) in Section 5 and Assumption 4.1, we have

\[
\| \hat{w}^k_{h,a,a'} - \overline{w}^k_{h,a,a'} \|_2 \leq \| G^{-1} U - G^{-1} \overline{G} \overline{w}^k_{h,a,a'} \|_2 = 1 / \alpha \cdot \| U - \overline{G} \overline{w}^k_{h,a,a'} \|_2. \tag{E.10}
\]

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where $G$ and $U$ are defined in (4.1) and (5.2). For any $i \in [d_0]$, by the linearity of $\mathbb{K}$, we have

$$
[Gw^k_{h,a,a'}]_i = \sum_{j=1}^{d_0} [G]_{i,j} \cdot [\pi^k_{h,a,a'}]_j
$$

$$
= \langle \mathbb{K} \phi_i, \mathbb{K} \left( \sum_{j=1}^{d_0} \phi_j \cdot [\pi^k_{h,a,a'}]_j \right) \rangle_{\mathcal{H}} = \langle \mathbb{K} \phi_i, \mathbb{K} P^{(2),\pi_k} \rangle_{\mathcal{H}}
$$

where the last equality uses the definition of $\pi^k_{h,a,a'}$ in (E.9). Thus, we can write

$$
[U - Gw^k_{h,a,a'}]_i = \langle \mathbb{K} \phi_i, \mathbb{K} D^k_{h,a,a'} - \mathbb{K} P^{(2),\pi_k} \rangle_{\mathcal{H}}
$$

(E.11)

where $D^k_{h,a,a'}$ represents the status of the dataset $D_{h,a,a'}$ at the planning phase of the $k$-th iteration. Note that, since entries of $\phi$ are distributions and $\mathbb{K}(\cdot, \cdot) \leq 1$, we have

$$
\|\mathbb{K} \phi_i\|^2_{\mathcal{H}} = \int_{O^3 \times O^3} \mathbb{K}(x, y) \phi_i(x) \phi_i(y) \, dx \, dy \leq 1.
$$

(E.12)

Also, we note that, when adapted to the data filtration of Algorithm 1,

$$
\left\{ \left( \frac{1}{k} \right) \cdot \left( \sum_{i=1}^{\min\{j,k\}} \mathbb{K}(y_i, \cdot) - \sum_{i=1}^{\min\{j,k\}} \mathbb{K} P^{(2),\pi_i} \right) \right\}_{j \geq 1}
$$

is a martingale in $\mathcal{H}$ with its total quadratic variation upper bounded by

$$
\sum_{i=1}^{k} \left( \frac{1}{k^2} \right) \cdot \|\mathbb{K}(y_i, \cdot) - \mathbb{K} P^{(2),\pi_i} \|^2_{\mathcal{H}} \leq \sum_{i=1}^{k} \left( \frac{1}{k^2} \right) \cdot 4 = \frac{4}{k},
$$

where the inequality uses the same argument of (E.12). Thus, invoking Lemma E.5 with $c^2 = 4/k$, with probability at least $1 - \delta_0$ for any $\delta_0 > 0$, it holds that

$$
\|\mathbb{K} D^k_{h,a,a'} - \mathbb{K} P^{(2),\pi_k} \|^2_{\mathcal{H}} \leq \sqrt{8 \log \left( \frac{2}{\delta_0} \right)} \cdot k^{-1/2},
$$

(E.14)

where, in order to apply the lemma, we note that the left-hand side of (E.14) is the RKHS norm of the $k$-th term of the martingale in (E.13). Combining (E.12) and (E.14) with (E.11), and using the Cauchy-Schwarz inequality, we obtain

$$
\|U - Gw^k_{h,a,a'}\|^2_2 = \sum_{i=1}^{d_0} \|\mathbb{K} \phi_i, \mathbb{K} D^k_{h,a,a'} - \mathbb{K} P^{(2),\pi_k} \|^2_{\mathcal{H}}
$$

$$
\leq \sum_{i=1}^{d_0} \|\mathbb{K} \phi_i\|^2_{\mathcal{H}} \cdot \|\mathbb{K} D^k_{h,a,a'} - \mathbb{K} P^{(2),\pi_k} \|^2_{\mathcal{H}} \leq d_o \cdot 8 \log \left( \frac{2}{\delta_0} \right) \cdot k^{-1}
$$

(E.15)
with probability at least $1 - \delta_0$. Combining (E.15) and (E.10), we obtain
\[
\|\hat{h}_{h,a,a'}^k - \overline{w}_{h,a,a'}^k\|_2 \leq \alpha^{-1} \cdot \|U - G\overline{w}_{h,a,a'}^k\|_2 \leq \alpha^{-1} \cdot \sqrt{8d_0 \log(2/\delta_0)} \cdot k^{-1/2} \tag{E.16}
\]
with probability at least $1 - \delta_0$.

In the following, we characterize the errors in the learning of distributions given the result in (E.16). By our definitions of the distributions $\hat{F}_{h,a,a'}^{(2)}$ and $P_{h,a,a'}^{(2)}$, we have
\[
\|\hat{F}_{h,a,a'}^{(2)} - P_{h,a,a'}^{(2)}\|_1
= \int_{\Omega^3} |\phi(o,o',o'')^\top \hat{w}_{h,a,a'}^k - \phi(o,o',o'')^\top \overline{w}_{h,a,a'}^k| \, dd'
\leq \int_{\Omega^3} \|\phi(o,o',o'')\|_2 \, dd' \cdot \|\hat{w}_{h,a,a'}^k - \overline{w}_{h,a,a'}^k\|_2
\leq d_0 \cdot \|\hat{w}_{h,a,a'}^k - \overline{w}_{h,a,a'}^k\|_2. \tag{E.17}
\]
where the last inequality is by
\[
\int_{\Omega^3} \|\phi(o,o',o'')\|_2 \, dd' \leq \int_{\Omega^3} \|\phi(o,o',o'')\|_1 \, dd' \leq d_0.
\]
Similarly, we have
\[
\|\hat{F}_{h,a}^{(1)} - P_{h,a}^{(1)}\|_1
= \int_{\Omega^2} \left| \int_{\Omega} \left(\phi(o,o',o'')^\top \hat{w}_{h,a,a'}^k - \phi(o,o',o'')^\top \overline{w}_{h,a,a'}^k\right) \, dd'' \right| \, dd'
\leq \int_{\Omega^3} |\phi(o,o',o'')^\top \hat{w}_{h,a,a'}^k - \phi(o,o',o'')^\top \overline{w}_{h,a,a'}^k| \, dd' \leq d_0 \cdot \|\hat{w}_{h,a,a'}^k - \overline{w}_{h,a,a'}^k\|_2. \tag{E.18}
\]
Combining (E.17) and (E.18) with (E.16), we conclude the proof of Lemma E.4.

**Lemma E.5.** Suppose that $\{M_t\}_{t \geq 1}$ is a martingale over an RKHS $H$ with norm $\| \cdot \|$, whose kernel is continuous and defined on a separable topological space. If we have
\[
\sum_{t=1}^{\infty} \text{ess sup} \|M_{t+1} - M_t\|^2 \leq c^2 \tag{E.19}
\]
for some $c > 0$, then, for any $\varepsilon > 0$, it holds that
\[
P\left(\text{sup}\{\|M_1\|, \|M_2\|, \|M_3\|, \ldots\} \geq \varepsilon\right) \leq 2 \exp\left\{-\frac{\varepsilon^2}{2c^2}\right\}.
\]

**Proof.** The lemma is a special case of Theorem 3.5 in Pinelis (1994) (see also, Theorem 3 in Pinelis (1992)), which is a more general result for martingales in Banach spaces. The result says that if $\{M_t\}_{t \geq 1}$ is a martingale over a $(2,D)$-smooth separable Banach space satisfying the condition in (E.19), it holds that
\[
P\left(\text{sup}\{\|M_1\|, \|M_2\|, \|M_3\|, \ldots\} \geq \varepsilon\right) \leq 2 \exp\left\{-\frac{\varepsilon^2}{2c^2D^2}\right\}. \tag{E.20}
\]
And, we have that any Hilbert space is $(2, 1)$-smooth (Pinelis, 1994). Also, because the kernel of $\mathcal{H}$ is continuous and defined on a separable space, we have that $\mathcal{H}$ is separable. Thus, by plugging $D = 1$ into (E.20), we conclude the proof of Lemma E.5. $\square$