Sample-Efficient Reinforcement Learning of Undercomplete POMDPs

Chi Jin Princeton University chij@princeton.edu

Akshay Krishnamurthy Microsoft Research, NYC akshaykr@microsoft.com Sham M. Kakade University of Washington Microsoft Research, NYC sham@cs.washington.edu

Qinghua Liu Princeton University qinghual@princeton.edu

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Abstract

Partial observability is a common challenge in many reinforcement learning applications, which requires an agent to maintain memory, infer latent states, and integrate this past information into exploration. This challenge leads to a number of computational and statistical hardness results for learning general Partially Observable Markov Decision Processes (POMDPs). This work shows that these hardness barriers do not preclude efficient reinforcement learning for rich and interesting subclasses of POMDPs. In particular, we present a sample-efficient algorithm, *OOM-UCB*, for episodic finite *undercomplete* POMDPs, where the number of observations is larger than the number of latent states and where exploration is essential for learning, thus distinguishing our results from prior works. *OOM-UCB* achieves an optimal sample complexity of $\tilde{C}(1/\epsilon^2)$ for finding an ε -optimal policy, along with being polynomial in all other relevant quantities. As an interesting special case, we also provide a computationally and statistically efficient algorithm for POMDPs with deterministic state transitions.

1 Introduction

In many sequential decision making settings, the agent lacks complete information about the underlying state of the system, a phenomenon known as *partial observability*. Partial observability significantly complicates the tasks of reinforcement learning and planning, because the non-Markovian nature of the observations forces the agent to maintain memory and reason about beliefs of the system state, all while exploring to collect information about the environment. For example, a robot may not be able to perceive all objects in the environment due to occlusions, and it must reason about how these objects may move to avoid collisions [10]. Similar reasoning problems arise in imperfect information games [8], medical diagnosis [13], and elsewhere [25]. Furthermore, from a theoretical perspective, well-known complexity-theoretic results show that learning and planning in partially observable environments is statistically and computationally intractable in general [23, 22, 30, 21].

The standard formulation for reinforcement learning with partial observability is the *Partially Observ*able Markov Decision Process (POMDP), in which an agent operating on noisy observations makes decisions that influence the evolution of a latent state. The complexity barriers apply for this model, but they are of a worst case nature, and they do not preclude efficient algorithms for interesting sub-classes of POMDPs. Thus we ask:

Can we develop efficient algorithms for reinforcement learning in large classes of POMDPs?

This question has been studied in recent works [3, 12], which incorporate a decision making component into a long line of work on "spectral methods" for estimation in latent variable models [14, 29, 1, 2], including the Hidden Markov Model. Briefly, these estimation results are based on the method of moments, showing that under certain assumptions the model parameters can be computed by a decomposition of a low-degree moment tensor. The works of Azizzadenesheli et al. [3] and Guo et al. [12] use tensor decompositions in the POMDP setting and obtain sample efficiency guarantees. Neither result considers a setting where strategic exploration is essential for information acquisition, and they do not address one of the central challenges in more general reinforcement learning problems.

Our contributions. In this work, we provide new sample-efficient algorithms for reinforcement learning in finite POMDPs in the *undercomplete* regime, where the number of observations is larger than the number of latent states. This assumption is quite standard in the literature on estimation in latent variable models [2]. Our main algorithm *OOM-UCB* uses the principle of optimism for exploration and uses the information gathered to estimate the *Observable Operators* induced by the environment. Our main result proves that *OOM-UCB* finds a near optimal policy for the POMDP using a number of samples that scales polynomially with all relevant parameters and additionally with the minimum singular value of the emission matrix. Notably, *OOM-UCB* finds an ε -optimal policy at the optimal rate of $\tilde{O}(1/\varepsilon^2)$.

While *OOM-UCB* is statistically efficient for this subclass of POMDPs, we should not expect it to be computationally efficient in general, as this would violate computational barriers for POMDPs. However, in our second contribution, we consider a further restricted subclass of POMDPs in which the latent dynamics are deterministic and where we provide *both* a computationally and statistically efficient algorithm. Notably, deterministic dynamics are still an interesting subclass due to that, while it avoids computational barriers, it still does not mitigate the need for strategic exploration. We prove that our second algorithm has sample complexity scaling with all the relevant parameters as well as the minimum ℓ_2 distance between emission distributions. This latter quantity replaces the minimum singular value in the guarantee for *OOM-UCB* and is a more favorable dependency.

We provide further motivation for our assumptions with two lower bounds: the first shows that the overcomplete setting is statistically intractable without additional assumptions, while the second necessitates the dependence on the minimum singular value of the emission matrix. In particular, under our assumptions, the agent must engage in strategic exploration for sample-efficiency. As such, the main conceptual advance in our line of inquiry over prior works is that our algorithms address exploration and partial observability in a provably efficient manner.

1.1 Related work

A number of computational barriers for POMDPs are known. If the parameters are known, it is PSPACEcomplete to compute the optimal policy, and, furthermore, it is NP-hard to compute the optimal memoryless policy [23, 30]. With regards to learning, Mossel and Roch [21] provided an average case computationally complexity result, showing that parameter estimation for a subclass of Hidden Markov Models (HMMs) is at least as hard as learning parity with noise. This directly implies the same hardness result for parameter estimation in POMDP models, due to that an HMM is just a POMDP with a fixed action sequence. On the other hand, for reinforcement learning in POMDPs (in particular, finding a near optimal policy), one may not need to estimate the model, so this lower bound need not directly imply that the RL problem is computational intractable. In this work, we do provide a lower bound showing that reinforcement learning in POMDPs is both statistically and computationally intractable (Propositions 1 and 2).

On the positive side, there is a long history of work on learning POMDPs. [11] studied POMDPs without resets, where the proposed algorithm has sample complexity scaling exponentially with a certain horizon time, which is not possible to relax without further restrictions. [26, 24] proposed to learn POMDPs using Bayesian methods; PAC or regret bounds are not known for these approaches. [18] studied policy gradient methods for learning POMDPs while they considered only Markovian policies and did not address exploration.

Closest to our work are POMDP algorithms based on spectral methods [12, 3], which were originally developed for learning latent variable models [14, 1, 2, 29, 28]. These works give PAC and regret bounds (respectively) for tractable subclasses of POMDPs, but, in contrast with our work, they make additional assumptions to mitigate the exploration challenge. In [12], it is assumed that all latent states can be reached with nontrivial probability with a constant number of random actions. This allows for estimating the *entire* model without sophisticated exploration. [3] consider a special class of memoryless policies in a setting where all of these policies visit every state and take every action with non-trivial probability. As with [12], this restriction guarantees that the entire model can be estimated regardless of the policy executed, so sophisticated exploration is not required. We also mention that [12, 3] assume that both the transition and observation matrices are full rank, which is stronger than our assumptions. We do not make any assumptions on the transition matrix.

Finally, the idea of representing the probability of a sequence as products of operators dates back to multiplicity automata [27, 9] and reappeared in the Observable Operator Model (OOMs) [16] and Predictive State Representations (PSRs) [20]. While spectral methods have been applied to PSRs [7], we are not aware of results with provable guarantees using this approach. It is also worth mentioning that any POMDP can be modeled as an Input-Output OOM [15].

2 Preliminaries

In this section, we define the partially observable Markov decision process, the observable operator model [16], and discuss their relationship.

Notation. For any natural number $n \in \mathbb{N}$, we use [n] to denote the set $\{1, 2, \ldots, n\}$. We use bold uppercase letters **B** to denote matrices and bold lower-case letters **b** to denote vectors. **B**_{*ij*} means the (i, j)th entry of matrix **B** and $(\mathbf{B})_i$ represents its *i*th column. For vectors we use $\|\cdot\|_p$ to denote the ℓ_p -norm, and for matrices we use $\|\cdot\|_1$, $\|\cdot\|_1$ and $\|\cdot\|_F$ to denote the spectral norm, entrywise ℓ_1 -norm and Frobenius norm respectively. We denote by $\|\mathbf{B}\|_{p\to q} = \max_{\|\mathbf{v}\|_p \leq 1} \|\mathbf{B}\mathbf{v}\|_q$ the *p*-to-*q* norm of **B**. For any matrix $\mathbf{B} \in \mathbb{R}^{m \times n}$, we use $\sigma_{\min}(\mathbf{B})$ to denote its smallest singular value, and $\mathbf{B}^{\dagger} \in \mathbb{R}^{n \times m}$ to denote its Moore-Penrose inverse. For vector $\mathbf{v} \in \mathbb{R}^n$, we denote diag $(\mathbf{v}) \in \mathbb{R}^{n \times n}$ as a diagonal matrix where $[\text{diag}(\mathbf{v})]_{ii} = \mathbf{v}_i$ for all $i \in [n]$. Finally, we use standard big-O and big-Omega notation $\mathcal{O}(\cdot), \Omega(\cdot)$ to hide only absolute constants which do not depend on any problem parameters, and notation $\tilde{\mathcal{O}}(\cdot), \tilde{\Omega}(\cdot)$ to hide only absolute constants and logarithmic factors.

2.1 Partially observable Markov decision processes

We consider an episodic tabular Partially Observable Markov Decision Process (POMDP), which can by specified as POMDP $(H, \mathscr{S}, \mathscr{A}, \mathscr{O}, \mathbb{T}, \mathbb{O}, r, \mu_1)$. Here H is the number of steps in each episode, \mathscr{S} is the set of states with $|\mathscr{S}| = S$, \mathscr{A} is the set of actions with $|\mathscr{A}| = A$, \mathscr{O} is the set of observations with $|\mathscr{O}| = O$, $\mathbb{T} = {\mathbb{T}_h}_{h=1}^H$ specify the transition dynamics such that $\mathbb{T}_h(\cdot|s, a)$ is the distribution over states if action a is taken from state s at step $h \in [H]$, $\mathbb{O} = {\mathbb{O}_h}_{h=1}^H$ are emissions such that $\mathbb{O}_h(\cdot|s)$ is the distribution over observations for state s at step $h \in [H]$, $r = {r_h : \mathscr{O} \to [0,1]}_{h=1}^H$ are the known deterministic reward functions¹, and $\mu_1(\cdot)$ is the initial distribution over states. Note that we consider nonstationary dynamics, observations, and rewards.

In a POMDP, states are hidden and unobserved to the learning agent. Instead, the agent is only able to see the observations and its own actions. At the beginning of each episode, an initial hidden state s_1 is sampled from initial distribution μ_1 . At each step $h \in [H]$, the agent first observes $o_h \in \mathcal{O}$ which is generated from the hidden state $s_h \in \mathscr{S}$ according to $\mathbb{O}_h(\cdot|s_h)$, and receives the reward $r_h(o_h)$, which can be computed from the observation o_h . Then, the agent picks an action $a_h \in \mathscr{A}$, which causes the environment to transition to hidden state s_{h+1} , that is drawn from the distribution $\mathbb{T}_h(\cdot|s_h, a_h)$. The episode ends when o_H is observed.

A policy π is a collection of H functions $\{\pi_h : \mathscr{T}_h \to \mathscr{A}\}_{h \in [H]}$, where $\mathscr{T}_h = (\mathscr{O} \times \mathscr{A})^{h-1} \times \mathscr{O}$ is the set of all possible histories of length h. We use $V^{\pi} \in \mathbb{R}$ to denote the value of policy π , so that V^{π} gives the expected cumulative reward received under policy π :

$$V^{\pi} := \mathbb{E}_{\pi} \left[\sum_{h=1}^{H} r_h(o_h) \right]$$

Since the state, action, observation spaces, and the horizon, are all finite, there always exists an optimal policy π^* which gives the optimal value $V^* = \sup_{\pi} V^{\pi}$. We remark that, in general, the optimal policy of a POMDP will select actions based the entire history, rather than just the recent observations and actions. This is one of the major differences between POMDPs and standard Markov Decision Processes (MDPs), where the optimal policies are functions of the most recently observed state. This difference makes POMDPs significantly more challenging to solve.

The POMDP learning objective. Our objective in this paper is to learn an ε -optimal policy $\hat{\pi}$ in the sense that $V^{\hat{\pi}} \ge V^* - \varepsilon$, using a polynomial number of samples.

2.2 The observable operator model

We have described the POMDP model via the transition and observation distributions \mathbb{T} , \mathbb{O} and the initial distribution μ_1 . While this parametrization is natural for describing the dynamics of the system, POMDPs can also be fully specified via a different set of parameters: a set of operators $\{\mathbf{B}_h(a, o) \in \mathbb{R}^{O \times O}\}_{h \in [H-1], a \in \mathcal{A}, o \in \mathcal{O}}$, and a vector $\mathbf{b}_0 \in \mathbb{R}^O$.

¹Since rewards are observable in most applications, it is natural to assume the reward is a known function of the observation. While we study deterministic reward functions for notational simplicity, our results generalize to randomized reward functions. Also, we assume the reward is in [0, 1] without loss of generality.

In the undercomplete setting where $S \leq O$ and where observation probability matrices $\{\mathbb{O}_h \in \mathbb{R}^{O \times S}\}_{h \in [H]}$ are all full column-rank, the operators $\{\mathbf{B}_h(a, o)\}_{h, a, o}$ and vector \mathbf{b}_0 can be expressed in terms of $(\mathbb{T}, \mathbb{O}, \mu_1)$ as follows:

$$\mathbf{B}_{h}(a,o) = \mathbb{O}_{h+1}\mathbb{T}_{h}(a)\operatorname{diag}(\mathbb{O}_{h}(o|\cdot))\mathbb{O}_{h}^{\dagger}, \qquad \mathbf{b}_{0} = \mathbb{O}_{1}\mu_{1}.$$
(1)

where we use the matrix and vector notation for $\mathbb{O}_h \in \mathbb{R}^{O \times S}$ and $\mu_1 \in \mathbb{R}^S$ here, such that $[\mathbb{O}_h]_{o,s} = \mathbb{O}_h(o|s)$ and $[\mu_1]_s = \mu_1(s)$. $\mathbb{T}_h(a) \in \mathbb{R}^{S \times S}$ denotes the transition matrix given action $a \in \mathscr{A}$ where $[\mathbb{T}_h(a)]_{s',s} = \mathbb{T}_h(s'|s,a)$, and $\mathbb{O}_h(o|\cdot) \in \mathbb{R}^S$ denotes the *o*-th row in matrix \mathbb{O}_h with $[\mathbb{O}_h(o|\cdot)]_s = \mathbb{O}_h(o|s)$. Note that the matices defined in (1) have rank at most S. Using these matrices \mathbf{B}_h , it can be shown that (Appendix E.1), for any sequence of $(o_H, \ldots, a_1, o_1) \in \mathscr{O} \times (\mathscr{A} \times \mathscr{O})^{H-1}$, we have:

$$\mathbb{P}(o_H,\ldots,o_1|a_{H-1},\ldots,a_1) = \mathbf{e}_{o_H}^\top \cdot \mathbf{B}_{H-1}(a_{H-1},o_{H-1})\cdots \mathbf{B}_1(a_1,o_1)\cdot \mathbf{b}_0.$$
 (2)

Describing these conditional probabilities for every sequence is sufficient to fully specify the entire dynamical system. Therefore, as an alternative to directly learning \mathbb{T} , \mathbb{O} and μ_1 , it is also sufficient to learn operators $\{\mathbf{B}_h(a, o)\}_{h,a,o}$ and vector \mathbf{b}_0 in order to learn the optimal policy. The latter approach enjoys the advantage that (2) does not explicitly involve latent variables. It refers only to observable quantities—actions and observations.

We remark that the operator model introduced in this section (which is parameterized by $\{\mathbf{B}_h(a, o)\}_{h,a,o}$ and \mathbf{b}_0) bears significant similarity to Jaeger's Input-Output Observable Operator Model (IO-OOM) [16], except a few minor technical differences.² With some abuse of terminology, we also refer to our model as Observable Operator Model (OOM) in this paper. It is worth noting that Jaeger's IO-OOMs are strictly more general than POMDPs [16] and also includes overcomplete POMDPs via a relation different from (1). Since our focus is on undercomplete POMDPs, we refer the reader to [16] for more details.

3 Main Results

We first state our main assumptions, which we motivate with corresponding hardness results in their absence. We then present our main algorithm, *OOM-UCB*, along with its sample efficiency guarantee.

3.1 Assumptions

In this paper, we make the following assumptions.

Assumption 1. We assume the POMDP is undercomplete, i.e. $S \leq O$. We also assume the minimum singular value of the observation probability matrices $\sigma_{\min}(\mathbb{O}_h) \geq \alpha > 0$ for all $h \in [H]$.

Both assumptions are standard in the literature on learning Hidden Markov Models (HMMs)—an uncontrolled version of POMDP [see e.g., 1]. The second assumption that $\sigma_{\min}(\mathbb{O}_h)$ is lower-bounded is a robust version of the assumption that $\mathbb{O}_h \in \mathbb{R}^{O \times S}$ is full column-rank, which is equivalent to $\sigma_{\min}(\mathbb{O}_h) > 0$. Together, these assumption ensure that the observations will contain a reasonable amount of information about the latent states.

We do not assume that the initial distribution μ_1 has full support, nor do we assume the transition probability matrices \mathbb{T}_h are full rank. In fact, Assumption 1 is *not* sufficient for identification of the system,

²Jaeger's IO-OOM further requires the column-sums of operators to be 1.

Algorithm 1 Observable Operator Model with Upper Confidence Bound (OOM-UCB)

- 1: Initialize: set all entries in a vector of counts $\mathbf{n} \in \mathbb{N}^O$, and in matrices of counts $\mathbf{N}_h(a, \tilde{a}) \in \mathbb{N}^{O \times O}$, $\mathbf{M}_h(o, a, \tilde{a}) \in \mathbb{N}^{O \times O}$ to be zero for all $(o, a, \tilde{a}) \in \mathscr{O} \times \mathscr{A}^2$ 2: set confidence set $\Theta_1 \leftarrow \bigcap_{h \in [H]} \{\hat{\theta} \mid \sigma_{\min}(\hat{\mathbb{O}}_h) \ge \alpha\}.$
- 3: for k = 1, 2, ..., K do
- compute the optimistic policy $\pi_k \leftarrow \operatorname{argmax}_{\pi} \operatorname{max}_{\hat{\theta} \in \Theta_k} V^{\pi}(\hat{\theta}).$ 4:
- observe o_1 , and set $\mathbf{n} \leftarrow \mathbf{n} + \mathbf{e}_{o_1}$ 5:

 $\mathfrak{b} \leftarrow (\cap_{h \in [H]} \{ \hat{\theta} \mid \sigma_{\min}(\hat{\mathbb{O}}_h) \geq \alpha \}) \cap \{ \hat{\theta} \mid \|k \cdot \mathbf{b}_0(\hat{\theta}) - \mathbf{n}\|_2 \leq \beta_k \}.$ for $(h, a, \tilde{a}) \in [H - 1] \times \mathscr{A}^2$ do 6:

- 7:
- execute policy π_k from step 1 to step h 2. 8:
- take action \tilde{a} at step h 1, and action a at step h respectively. 9:
- observe (o_{h-1}, o_h, o_{h+1}) , and set $\mathbf{N}_h(a, \tilde{a}) \leftarrow \mathbf{N}_h(a, \tilde{a}) + \mathbf{e}_{o_h} \mathbf{e}_{o_{h-1}}^\top$. 10:

set $\mathbf{M}_h(o_h, a, \tilde{a}) \leftarrow \mathbf{M}_h(o_h, a, \tilde{a}) + \mathbf{e}_{o_{h+1}} \mathbf{e}_{o_{h-1}}^\top$. 11:

- $\mathfrak{B}_h(a,\tilde{a}) \leftarrow \bigcap_{o \in \mathscr{O}} \{ \hat{\theta} \mid \| \mathbf{B}_h(a,o;\hat{\theta}) \mathbf{N}_h(a,\tilde{a}) \mathbf{M}_h(o,a,\tilde{a}) \|_F \le \gamma_k \}.$ 12:
- construct the confidence set $\Theta_{k+1} \leftarrow [\cap_{(h,a,\tilde{a})\in [H-1]\times\mathscr{A}^2} \mathfrak{B}_h(a,\tilde{a})] \cap \mathfrak{b}.$ 13:
- 14: **Output:** π_k where k is sampled uniformly from [K].

i.e. recovering parameters $\mathbb{T}, \mathbb{O}, \mu_1$ in total-variance distance. Exploration is crucial to find a near-optimal policy in our setting.

We motivate both assumptions above by showing that, with absence of either one, learning a POMDP is statistically intractable. That is, it would require an exponential number of samples for any algorithm to learn a near-optimal policy with constant probability.

Proposition 1. For any algorithm \mathfrak{A} , there exists an overcomplete POMDP (S > O) with S and O being small constants, which satisfies $\sigma_{\min}(\mathbb{O}_h) = 1$ for all $h \in [H]$, such that algorithm \mathfrak{A} requires at least $\Omega(A^{H-1})$ samples to ensure learning a (1/4)-optimal policy with probability at least 1/2.

Proposition 2. For any algorithm \mathfrak{A} , there exists an undercomplete POMDP ($S \leq O$) with S and O being small constants, such that algorithm \mathfrak{A} requires at least $\Omega(A^{H-1})$ samples to ensure learning a (1/4)optimal policy with probability at least 1/2.

Proposition 1 and 2 are both proved by constructing hard instances, which are modifications of classical combinatorial locks for MDPs [19]. We refer readers to Appendix B for more details.

Algorithm 3.2

We are now ready to describe our algorithm. Assumption 1 enables the representation of the POMDP using OOM with relation specified as in Equation (1). Our algorithm, Observable Operator Model with Upper Confidence Bound (OOM-UCB, algorithm 1), is an optimistic algorithm which heavily exploits the OOM representation to obtain valid uncertainty estimates of the parameters of the underlying model.

To condense notation in Algorithm 1, we denote the parameters of a POMDP as $\theta = (\mathbb{T}, \mathbb{O}, \mu_1)$. We denote $V^{\pi}(\theta)$ as the value of policy π if the underlying POMDP has parameter θ . We also write the parameters of the OOM $(\mathbf{b}_0(\theta), \mathbf{B}_h(a, o; \theta))$ as a function of parameter θ , where the dependency is specified as in (1). We adopt the convention that at the 0-th step, the observation o_0 and state s_0 are always set to be some fixed

dummy observation and state, and, starting from s_0 , the environment transitions to s_1 with distribution μ_1 regardless of what action a_0 is taken.

At a high level, Algorithm 1 is an iterative algorithm that, in each iteration, (a) computes an optimistic policy and model by maximizing the value (Line 4) subject to a given confidence set constraint, (b) collects data using the optimistic policy, and (c) incorporates the data into an updated confidence set for the OOM parameters (Line 5-13). The first two parts are straightforward, so we focus the discussion on computing the confidence set. We remark that in general the optimization in Line 4 may not be solved in polynomial time (see discussions of the computational complexity after Theorem 3).

First, since b_0 in (1) is simply the probability over observations at the first step, our confidence set for b_0 in Line 6 is simply based on counting the number of times each observation appears in the first step and Hoeffding's concentration inequality.

Our construction of the confidence sets for the operators $\{\mathbf{B}_h(a, o)\}_{h,a,o}$ is inspired by the method-ofmoments estimator in HMM literature [14]. Consider two fixed actions a, \tilde{a} , and an arbitrary distribution over s_{h-1} . Let $\mathbf{P}_h(a, \tilde{a}), \mathbf{Q}_h(o, a, \tilde{a}) \in \mathbb{R}^{O \times O}$ be the probability matrices such that

$$[\mathbf{P}_{h}(a,\tilde{a})]_{o',o''} = \mathbb{P}(o_{h} = o', o_{h-1} = o''|a_{h} = a, a_{h-1} = \tilde{a}),$$

$$[\mathbf{Q}_{h}(o,a,\tilde{a})]_{o',o''} = \mathbb{P}(o_{h+1} = o', o_{h} = o, o_{h-1} = o''|a_{h} = a, a_{h-1} = \tilde{a}).$$
 (3)

It can be verified that $\mathbf{B}_h(a, o)\mathbf{P}_h(a, \tilde{a}) = \mathbf{Q}_h(o, a, \tilde{a})$ (Fact 17 in the appendix). Our confidence set construction (Line 12 in Algorithm 1) is based on this fact: we replace the probability matrices \mathbf{P}, \mathbf{Q} by empirical estimates \mathbf{N}, \mathbf{M} , and we use concentration inequalities to determine the width of the confidence set. Finally, our overall confidence set for the parameters θ is simply the intersection of the confidence sets for all induced operators and \mathbf{b}_0 , additionally incorporating the constraint on $\sigma_{\min}(\mathbb{O}_h)$ from Assumption 1.

3.3 Theoretical guarantees

Our OOM-UCB algorithm enjoys the following sample complexity guarantee.

Theorem 3. For any $\varepsilon \in (0, H]$, there exists $K_{\max} = \text{poly}(H, S, A, O, \alpha^{-1})/\varepsilon^2$ and an absolute constant c_1 , such that for any POMDP that satisfies Assumption 1, if we set hyperparameters $\beta_k = c_1 \sqrt{k \log(KAOH)}$, $\gamma_k = \sqrt{S}\beta_k/\alpha$, and $K \ge K_{\max}$, then the output policy $\hat{\pi}$ of Algorithm 1 will be ε -optimal with probability at least 2/3.

Theorem 3 claims that in polynomially many iterations of the outer loop, Algorithm 1 learns a nearoptimal policy for any undercomplete POMDP that satisfies Assumption 1. Since our algorithm only uses $O(H^2A^2)$ samples per iteration of the outer loop, this implies that the sample complexity is also $poly(H, S, A, O, \alpha^{-1})/\varepsilon^2$. We remark that the $1/\varepsilon^2$ dependence is optimal, which follows from standard concentration arguments. To the best of our knowledge, this is the first sample efficiency result for learning a class of POMDPs where exploration is essential.³

While Theorem 3 does guarantee sample efficiency, Algorithm 1 is not computationally efficient due to that the computation of the optimistic policy (Line 4) may not admit a polynomial time implementation, which should be expected given the aforementioned computational complexity results. We now turn to a further restricted (and interesting) subclass of POMDPs where we can address *both* the computational and statistical challenges.

³See Appendix C.4 for the explicit polynomial dependence of sample complexity; here, the success probability is a constant, but one can make it arbitrarily close to 1 by a standard boosting trick (see Appendix E.3).

4 Results for POMDPs with Deterministic Transition

In this section, we complement our main result by investigating the class of POMDPs with deterministic transitions, where both computational and statistical efficiency can be achieved. We say a POMDP is of *deterministic transition* if both its transition and initial distribution are deterministic, i.e, if the entries of matrices $\{\mathbb{T}_h\}_h$ and vector μ_1 are either 0 or 1. We remark that while deterministic dynamics avoids computational barriers, it does not mitigate the need for exploration.

Instead of Assumption 1, for the deterministic transition case, we require that the columns of the observation matrices \mathbb{O}_h are well-separated.

Assumption 2. For any $h \in [H]$, $\min_{s \neq s'} \|\mathbb{O}_h(\cdot|s) - \mathbb{O}_h(\cdot|s')\| \ge \xi$.

Assumption 2 guarantees that observation distributions for different states are sufficiently different, by at least ξ in Euclidean norm. It does not require that the POMDP is undercomplete, and, in fact, is strictly weaker than Assumption 1. In particular, for undercomplete models, $\min_{s\neq s'} \|\mathbb{O}_h(\cdot|s) - \mathbb{O}_h(\cdot|s')\| \ge \sqrt{2\sigma_{\min}(\mathbb{O}_h)}$, and so Assumption 1 implies Assumption 2 for $\xi = \sqrt{2\alpha}$.

Leveraging deterministic transitions, we can design a specialized algorithm (Algorithm 2 in the appendix) that learns an ε -optimal policy using polynomially many samples and in polynomial time. We present the formal theorem here, and refer readers to Appendix D for more details.

Theorem 4. For any $p \in (0, 1]$, there exists an algorithm such that for any deterministic transition POMDP satisfying Assumption 2, within $\mathcal{O}\left(H^2SA\log(HSA/p)/(\min\{\varepsilon/(\sqrt{O}H),\xi\})^2\right)$ samples and computations, the output policy of the algorithm is ε -optimal with probability at least 1 - p.

5 Analysis Overview

In this section, we provide an overview of the proof of our main result—Theorem 3. Please refer to Appendix C for the full proof.

We start our analysis by noticing that the output policy $\hat{\pi}$ of Algorithm 1 is uniformly sampled from $\{\pi_k\}_{k=1}^K$ computed in the algorithm. If we can show that

$$(1/K)\sum_{k=1}^{K} V^{\star} - V^{\pi_k} \le \varepsilon/10,$$
 (4)

then at least a 2/3 fraction of the policies in $\{\pi_k\}_{k=1}^K$ must be ε -optimal, and uniform sampling would find such a policy with probability at least 2/3. Therefore, our proof focuses on achieving (4).

We begin by conditioning on the event that for each iteration k, our constructed confidence set Θ_k in fact contains the true parameters $\theta^* = (\mathbb{T}, \mathbb{O}, \mu_1)$ of the POMDP. This holds with high probability and is achieved by setting the widths β_k and γ_k appropriately (see Lemma 14 in the appendix).

5.1 Bounding suboptimality in value by error in density estimation

Line 4 of Algorithm 1 computes the greedy policy $\pi_k \leftarrow \operatorname{argmax}_{\pi} \operatorname{max}_{\hat{\theta} \in \Theta_k} V^{\pi}(\hat{\theta})$ with respect to the current confidence set Θ_k . Let θ_k denote the maximizing model parameters in the k-th iteration. As (π_k, θ_k) are optimistic, we have $V^* \equiv V^*(\theta^*) \leq V^{\pi_k}(\theta_k)$ for all $k \in [K]$. Thus, for any $k \in [K]$:

$$V^{\star} - V^{\pi_{k}} \leq V^{\pi_{k}}(\theta_{k}) - V^{\pi_{k}}(\theta^{\star}) \leq H \sum_{o_{H},...,o_{1}} |\mathbb{P}_{\theta_{k}}^{\pi_{k}}(o_{H},...,o_{1}) - \mathbb{P}_{\theta^{\star}}^{\pi_{k}}(o_{H},...,o_{1})|,$$
(5)

where $\mathbb{P}^{\pi}_{\theta}$ denotes the probability measure over observations under policy π for POMDP with parameters θ . The second inequality holds because the cumulative reward is a function of observations (o_H, \ldots, o_1) and is upper bounded by H. This upper bounds the suboptimality in value by the total variation distance between the H-step observation distributions.

Next, note that we can always choose the greedy policy π_k to be deterministic, i.e., the probability to take any action given a history is either 0 or 1. This allows us to define the following set for any deterministic policy π :

$$\Gamma(\pi, H) := \{ \tau_H = (o_H, \dots, a_1, o_1) \mid \pi(a_{H-1}, \dots, a_1 \mid o_H, \dots, o_1) = 1 \}.$$

In words, $\Gamma(\pi, H)$ is a set of all the observation and action sequences of length H that could occur under the π . For any deterministic policy π , there is a one-to-one correspondence between \mathcal{O}^H and $\Gamma(\pi, H)$ and moreover, for any sequence $\tau_H = (o_H, \ldots, a_1, o_1) \in \Gamma(\pi, H)$, we have:

$$p(\tau_H;\theta) := \mathbb{P}_{\theta}(o_H, \dots, o_1 | a_{H-1}, \dots, a_1) = \mathbb{P}_{\theta}^{\pi}(o_H, \dots, o_1).$$
(6)

The derivation of equation (6) can be found in Appendix E.2. Combining this with (5) and summing over all episodes, we conclude that:

$$\sum_{k=1}^{K} (V^{\star} - V^{\pi_k}) \le H \sum_{k=1}^{K} \sum_{\tau_H \in \Gamma(\pi_k, H)} |p(\tau_H; \theta_k) - p(\tau_H; \theta^{\star})|.$$

This upper bounds the suboptimality in value by errors in estimating the conditional probabilities.

5.2 Bounding error in density estimation by error in estimating operators

For the next step, we leverage the OOM representation to bound the difference between the conditional probabilities $p(\tau_H; \theta_k)$ and $p(\tau_H; \theta^*)$. Recall that from (2), the conditional probability can be written as a product of the observable operators for each step and \mathbf{b}_0 . Therefore, for any two parameters $\hat{\theta}$ and θ , we have following relation for any sequence $\tau_H = (o_H, \ldots, a_1, o_1)$:

$$p(\tau_{H};\hat{\theta}) - p(\tau_{H};\theta) = \mathbf{e}_{o_{H}}^{\top} \cdot \mathbf{B}_{H-1}(a_{H-1}, o_{H-1};\hat{\theta}) \cdots \mathbf{B}_{1}(a_{1}, o_{1};\hat{\theta}) \cdot [\mathbf{b}_{0}(\hat{\theta}) - \mathbf{b}_{0}(\theta)]$$
$$+ \sum_{h=1}^{H-1} \mathbf{e}_{o_{H}}^{\top} \cdot \mathbf{B}_{H-1}(a_{H-1}, o_{H-1};\hat{\theta}) \cdots [\mathbf{B}_{h}(a_{h}, o_{h};\hat{\theta}) - \mathbf{B}_{h}(a_{h}, o_{h};\theta)] \cdots \mathbf{B}_{1}(a_{1}, o_{1};\theta) \cdot \mathbf{b}_{0}(\theta)$$

This relates the difference $p(\tau_H; \hat{\theta}) - p(\tau_H; \theta)$ to the differences in operators and \mathbf{b}_0 . Formally, with further relaxation and summation over all sequence in $\Gamma(\pi, H)$, we have the following lemma (also see Lemma 10 in Appendix C).

Lemma 5. Given a deterministic policy π and two sets of undercomplete POMDP parameters $\theta = (\mathbb{O}, \mathbb{T}, \mu_1)$ and $\hat{\theta} = (\hat{\mathbb{O}}, \hat{\mathbb{T}}, \hat{\mu}_1)$ with $\sigma_{\min}(\hat{\mathbb{O}}) \ge \alpha$, we have

$$\sum_{\tau_{H}\in\Gamma(\pi,H)} |p(\tau_{H};\hat{\theta}) - p(\tau_{H};\theta)| \leq \frac{\sqrt{S}}{\alpha} \left(\|\mathbf{b}_{0}(\hat{\theta}) - \mathbf{b}_{0}(\theta)\|_{1} + \sum_{(a,o)\in\mathscr{A}\times\mathscr{O}} \|[\mathbf{B}_{1}(a,o;\hat{\theta}) - \mathbf{B}_{1}(a,o;\theta)]\mathbf{b}_{0}(\theta)\|_{1} + \sum_{h=2}^{H-1} \sum_{(a,\tilde{a},o)\in\mathscr{A}\times\mathscr{O}} \sum_{s=1}^{S} \|\left(\mathbf{B}_{h}(a,o;\hat{\theta}) - \mathbf{B}_{h}(a,o;\theta)\right) \mathbb{O}_{h}\mathbb{T}_{h-1}(\tilde{a})\mathbf{e}_{s}\|_{1} \mathbb{P}_{\theta}^{\pi}(s_{h-1}=s)\right).$$
(7)

This lemma suggests that if we could estimate the operators accurately, we would have small value suboptimality. However, Assumption 1 is not sufficient for parameter recovery. It is possible that in some step h, there exists a state s_h that can be reached with only very small probability no matter what policy is used. Since we cannot collect many samples from s_h , it is not possible to estimate the corresponding component in the operator B_h . In other words, we cannot hope to make $\|\mathbf{B}_h(a, o; \hat{\theta}) - \mathbf{B}_h(a, o; \theta)\|_1$ small in our setting.

To proceed, it is crucial to observe that the third term on the RHS of (7), is in fact the operator error $\mathbf{B}_h(a, o; \hat{\theta}) - \mathbf{B}_h(a, o; \theta)$ projected onto the direction $\mathbb{O}_h \mathbb{T}_{h-1}(\tilde{a})\mathbf{e}_s$ and additionally reweighted by the probability of visiting state *s* in step h-1. Therefore, if *s* is hard to reach, the weighting probability will be very small, which means that even though we cannot estimate $\mathbf{B}_h(a, o; \theta)$ accurately in the corresponding direction, it has a negligible contribution to the density estimation error (LHS of (7)).

5.3 Bounding error in estimating operators by OOM-UCB algorithm

By Lemma 5, we only need to bound the error in operators reweighted by visitation probability. This is achieved by a careful design of the confidence sets in the OOM-UCB algorithm. This construction is based on the method of moments, which heavily exploits the undercompleteness of the POMDP. To showcase the main idea, we focus on bounding the third term on the RHS of (7).

Consider a fixed (o, a, \tilde{a}) tuple, a fixed step $h \in [H]$, and a fixed iteration $k \in [K]$. We define moment matrices $\mathbf{P}_h(a, \tilde{a}), \mathbf{Q}_h(o, a, \tilde{a}) \in \mathbb{R}^{O \times O}$ as in (3) for distribution on s_{h-1} that equals $(1/k) \cdot \sum_{t=1}^k \mathbb{P}_{\theta^*}^{\pi_t}(s_{h-1} = \cdot)$. We also denote $\hat{\mathbf{P}}_h(a, \tilde{a}) = \mathbf{N}_h(a, \tilde{a})/k$, $\hat{\mathbf{Q}}_h(o, a, \tilde{a}) = \mathbf{M}_h(o, a, \tilde{a})/k$ for $\mathbf{N}_h, \mathbf{M}_h$ matrices after the update in the k-th iteration of Algorithm 1. By martingale concentration, it is not hard to show that with high probability:

$$\|\mathbf{P}_h(a,\tilde{a}) - \hat{\mathbf{P}}_h(a,\tilde{a})\|_F \le \tilde{\mathcal{O}}(1/\sqrt{k}), \qquad \|\mathbf{Q}_h(o,a,\tilde{a}) - \hat{\mathbf{Q}}_h(o,a,\tilde{a})\|_F \le \tilde{\mathcal{O}}(1/\sqrt{k}).$$

Additionally, we can show that for the true operator and the true moments, we have $\mathbf{B}_h(a, o; \theta^*)\mathbf{P}_h(a, \tilde{a}) = \mathbf{Q}_h(o, a, \tilde{a})$. Meanwhile, by the construction of our confidence set Θ_{k+1} , we know that for any $\hat{\theta} \in \Theta_{k+1}$, we have

$$\|\mathbf{B}_h(a,o;\theta)\mathbf{\hat{P}}_h(a,\tilde{a}) - \mathbf{\hat{Q}}_h(o,a,\tilde{a})\|_F \le \gamma_k/k.$$

Combining all relations above, we see that $\mathbf{B}_h(a, o; \hat{\theta})$ is accurate in the directions spanned by $\mathbf{P}_h(a, \tilde{a})$, which, by definition, are directions frequently visited by the previous policies $\{\pi_t\}_{t=1}^k$. Formally, we have the following lemma, which allows us to bound the third term on the RHS of (7) using the algebraic transformation in Lemma 16.

Lemma 6. With probability at least $1 - \delta$, for all $k \in [K]$, for any $\hat{\theta} = (\hat{\mathbb{O}}, \hat{\mathbb{T}}, \hat{\mu}_1) \in \Theta_{k+1}$ and $(o, a, \tilde{a}, h) \in \mathcal{O} \times \mathscr{A}^2 \times \{2, \ldots, H-1\}$, and $\iota = \log(KAOH/\delta)$, we have

$$\sum_{s=1}^{S} \left\| \left(\mathbf{B}_{h}(a,o;\hat{\theta}) - \mathbf{B}_{h}(a,o;\theta^{\star}) \right) \mathbb{O}_{h} \mathbb{T}_{h-1}(\tilde{a}) \mathbf{e}_{s} \right\|_{1} \sum_{t=1}^{k} \mathbb{P}_{\theta^{\star}}^{\pi_{t}}(s_{h-1}=s) \le \mathcal{O}\left(\sqrt{\frac{kS^{2}O\iota}{\alpha^{4}}}\right)$$

6 Conclusion

In this paper, we give a sample efficient algorithm for reinforcement learning in undercomplete POMDPs. Our results leverage a connection to the observable operator model and employ a refined error analysis. To our knowledge, this gives the first provably efficient algorithm for strategic exploration in partially observable environments.

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Notation A

 $\mathbb{P}^{\pi}_{\theta}(s_h = s)$

 $\mathbf{1}(x=y)$

 \mathbf{e}_o

 $(\mathbf{X})_o$

 \mathbf{I}_n

 $C_{\rm poly}$

L

notation	definition
\mathbf{n}^k	value of n after the update in the k^{th} iteration of Algorithm 1
$\mathbf{N}_{h}^{k}(a,\tilde{a})$	value of $N_h(a, \tilde{a})$ after the update in the k^{th} iteration of Algorithm 1
$\mathbf{M}_{h}^{k}(o,a,\tilde{a})$	value of $\mathbf{M}_h(o, a, \tilde{a})$ after the update in the k^{th} iteration of Algorithm 1
heta	a parameter triple $(\mathbb{T}, \mathbb{O}, \mu_1)$ of a POMDP
$ heta^{\star}$	the groundtruth POMDP parameter triple
$\text{POMDP}(\theta)$	$\operatorname{POMDP}(H, \mathscr{S}, \mathscr{A}, \mathscr{O}, \mathbb{T}, \mathbb{O}, r, \mu_1)$
${\tau_h}^4$	a length-h trajectory: $\tau_h = [a_h, o_h, \dots, a_1, o_1] \in (\mathscr{A} \times \mathscr{O})^h$
$\Gamma(\pi,h)^5$	$\{\tau_h = (a_h, o_h, \dots, a_1, o_1) \mid \pi(a_h, \dots, a_1 o_h, \dots, o_1) = 1\}.$
$\mathbf{b}(au_h; heta)$	$\mathbf{B}_h(a_h,o_h; heta)\cdots \mathbf{B}_1(a_1,o_1; heta)\cdot \mathbf{b}_0(heta)$

Below, we introduce some notations that will be used in appendices.

 $\log(AOHK/\delta)$ Let $\mathbf{x} \in \mathbb{R}^{n_x}$, $\mathbf{y} \in \mathbb{R}^{n_y}$ and $\mathbf{z} \in \mathbb{R}^{n_z}$. We denote by $\mathbf{x} \otimes \mathbf{y} \otimes \mathbf{z}$ the tensor product of vectors \mathbf{x} , \mathbf{y} and \mathbf{z} , an $n_x \times n_y \times n_z$ tensor with $(i, j, k)^{\text{th}}$ entry equal to $\mathbf{x}_i \mathbf{y}_j \mathbf{z}_k$. Let $\mathbf{X} \in \mathbb{R}^{n_X \times m}$, $\mathbf{Y} \in \mathbb{R}^{n_Y \times m}$ and $\mathbf{Z} \in \mathbb{R}^{n_Z \times m}$. We generalize the notation of tensor product to matrices by defining $\mathbf{X} \otimes \mathbf{Y} \otimes \mathbf{Z} = \sum_{l=1}^{m} (\mathbf{X})_l \otimes (\mathbf{Y})_l \otimes (\mathbf{Z})_l$, which is an $n_X \times n_Y \times n_Z$ tensor with $(i, j, k)^{\text{th}}$ entry equal to $\sum_{l=1}^m \mathbf{X}_{il} \mathbf{Y}_{jl} \mathbf{Z}_{kl}$.

probability of visiting state s at h^{th} step when executing policy π

on POMDP(θ)

equal to 1 if x = y and 0 otherwise.

an O-dimensional vector with $(\mathbf{e}_o)_i = \mathbf{1}(o=i)$

the o^{th} column of matrix **X**

 $n \times n$ identity matrix

 $\operatorname{poly}(S, O, A, H, 1/\alpha, \log(1/\delta))$

Let X be a random variable taking value in [m], we denote by $\mathbb{P}(X = \cdot)$ an m-dimensional vector whose i^{th} entry is $\mathbb{P}(X = i)$.

³Note that this definition is *different* from the one used in Section 5, where $\tau_h = [o_h, \ldots, a_1, o_1] \in \mathcal{O} \times (\mathscr{A} \times \mathscr{O})^{h-1}$ does not include the action a_h at h^{th} step.

⁴WLOG, all the polices considered in this paper are *deterministic*. Also note that the trajectory in $\Gamma(\pi, h)$ contains a_h , which is different from the definition in Section 5

B Proof of Hardness Results

The hard examples constructed below are variants of the ones used in [19].

Proposition 1. For any algorithm \mathfrak{A} , there exists an overcomplete POMDP (S > O) with S and O being small constants, which satisfies $\sigma_{\min}(\mathbb{O}_h) = 1$ for all $h \in [H]$, such that algorithm \mathfrak{A} requires at least $\Omega(A^{H-1})$ samples to ensure learning a (1/4)-optimal policy with probability at least 1/2.

Proof. Consider the following *H*-step nonstationary POMDP:

- 1. STATE There are four states: two good states g_1 and g_2 and two bad states b_1 and b_2 . The initial state is picked uniformly at random.
- 2. OBSERVATION There are only two different observations u_1 and u_2 . At step $h \in [H-1]$, we always observe u_1 at g_1 and b_1 , and observe u_2 at g_2 and b_2 . At step H, we always observe u_1 at good states and u_2 at bad states. It's direct to verify $\sigma_{\min}(\mathbb{O}_h) = 1$ for all $h \in [H]$.
- 3. REWARD There is no reward at the fist H 1 steps (i.e. $r_h = 0$ for all $h \in [H 1]$). At step H, we receive reward 1 if we observe u_1 and no reward otherwise (i.e. $r_H(o) = \mathbf{1}(o = u_1)$).
- 4. TRANSITION There is one good action a_h^* and A 1 bad actions for each $h \in [H 1]$. At step $h \in [H 1]$, suppose we are at a good state $(g_1 \text{ or } g_2)$, then we will transfer to g_1 or g_2 uniformly at random if we take a_h^* and otherwise transfer to b_1 or b_2 uniformly at random. In contrast, if we are at a bad state $(b_1 \text{ or } b_2)$, we will always transfer to b_1 or b_2 uniformly at random no matter what action we take. Note that two good (bad) states are equivalent in terms of transition.

We have the following key observations:

- 1. Once we are at bad states, we always stay at bad states.
- 2. We have

$$\mathbb{P}(o_{1:H-1} = z \mid a_{1:H-1}, o_H) = \frac{1}{2^{H-1}}$$

for any $z \in \{u_1, u_2\}^{H-1}$ and $(a_{1:H-1}, o_H) \in [A]^{H-1} \times \{u_1, u_2\}$

Therefore, the observations at the first H - 1 steps provide no information about the underlying transition. The only useful information is the last observation o_H which tells us whether we end in good states or not.

3. The optimal policy is unique and is to execute the good action sequence $(a_1^*, \ldots, a_{H-1}^*)$ regardless of the observations.

Based on the observations above, this is equivalent to a multi-arm bandits problem with A^{H-1} arms. Therefore, we cannot do better than Brute-force search, which has sample complexity at least $\Omega(A^{H-1})$.

Proposition 2. For any algorithm \mathfrak{A} , there exists an undercomplete POMDP ($S \leq O$) with S and O being small constants, such that algorithm \mathfrak{A} requires at least $\Omega(A^{H-1})$ samples to ensure learning a (1/4)-optimal policy with probability at least 1/2.

Proof. We continue to use the POMDP constructed in Proposition 1 and slightly modify it by splitting u_2 into another 4 different observations $\{q_1, q_2, q_3, q_4\}$, so in the new POMDP (O = 5 > S = 4), we will observe a q_i picked uniformly at random from $\{q_1, q_2, q_3, q_4\}$ when we are 'supposed' to observe u_2 . It's easy to see the modification does not change its hardness.

C Analysis of OMM-UCB

Throughout the proof, we use τ_h to denote a length-*h* trajectory: $[a_h, o_h, \ldots, a_1, o_1] \in (\mathscr{A} \times \mathscr{O})^h$. Note that this definition is *different* from the one used in Section 5, where $\tau_h = [o_h, \ldots, a_1, o_1] \in \mathscr{O} \times (\mathscr{A} \times \mathscr{O})^{h-1}$ does not include the action a_h at h^{th} step. Besides, we define

$$\Gamma(\pi, h) = \{ \tau_h = (a_h, o_h, \dots, a_1, o_1) \mid \pi(a_h, \dots, a_1 \mid o_h, \dots, o_1) = 1 \},\$$

which is also *different* from the definition in Section 5 where a_h is not included.

Please refer to Appendix A for definitions of frequently used notations.

C.1 Bounding the error in belief states

In this subsection, we will bound the error in (unnormalized) belief states, i.e., $\mathbf{b}(\tau_h; \theta) - \mathbf{b}(\tau_h; \hat{\theta})$ by the error in operators reweighed by the probability distribution of visited states.

We start by proving the following lemma that helps us decompose the error in belief states inductively.

Lemma 7. Given a deterministic policy π and two set of POMDP parameters $\hat{\theta} = (\hat{\mathbb{O}}, \hat{\mathbb{T}}, \hat{\mu}_1)$ and $\theta = (\mathbb{O}, \mathbb{T}, \mu_1)$, for all $h \ge 1$ and $\mathbf{X} \in \{\mathbf{I}_O, \hat{\mathbb{O}}_{h+1}^{\dagger}\}$, we have

$$\sum_{\tau_{h}\in\Gamma(\pi,h)} \left\| \mathbf{X} \left(\mathbf{b}(\tau_{h};\theta) - \mathbf{b}(\tau_{h};\hat{\theta}) \right) \right\|_{1} \leq \sum_{\tau_{h-1}\in\Gamma(\pi,h-1)} \left\| \hat{\mathbb{O}}_{h}^{\dagger} \left(\mathbf{b}(\tau_{h-1};\theta) - \mathbf{b}(\tau_{h-1};\hat{\theta}) \right) \right\|_{1} + \sum_{\tau_{h}\in\Gamma(\pi,h)} \left\| \mathbf{X} \left(\mathbf{B}_{h}(a_{h},o_{h};\hat{\theta}) - \mathbf{B}_{h}(a_{h},o_{h};\theta) \right) \mathbf{b}(\tau_{h-1};\theta) \right\|_{1}.$$

Proof. By the definition of $\mathbf{b}(\tau_h; \theta)$ and $\mathbf{b}(\tau_h; \hat{\theta})$,

$$\sum_{\tau_h \in \Gamma(\pi,h)} \| \mathbf{X} \left(\mathbf{b}(\tau_h; \theta) - \mathbf{b}(\tau_h; \hat{\theta}) \right) \|_1$$

=
$$\sum_{\tau_h \in \Gamma(\pi,h)} \| \mathbf{X} \left(\mathbf{B}_h(a_h, o_h; \theta) \mathbf{b}(\tau_{h-1}; \theta) - \mathbf{B}_h(a_h, o_h; \hat{\theta}) \mathbf{b}(\tau_{h-1}; \hat{\theta}) \right) \|_1$$

$$\leq \sum_{\tau_h \in \Gamma(\pi,h)} \| \mathbf{X} \mathbf{B}_h(a_h, o_h; \hat{\theta}) \left(\mathbf{b}(\tau_{h-1}; \theta) - \mathbf{b}(\tau_{h-1}; \hat{\theta}) \right) \|_1$$

+
$$\sum_{\tau_h \in \Gamma(\pi,h)} \| \mathbf{X} \left(\mathbf{B}_h(a_h, o_h; \hat{\theta}) - \mathbf{B}_h(a_h, o_h; \theta) \right) \mathbf{b}(\tau_{h-1}; \theta) \|_1.$$

The first term can be bounded as following,

$$\begin{split} &\sum_{\tau_{h}\in\Gamma(\pi,h)} \|\mathbf{X}\mathbf{B}_{h}(a_{h},o_{h};\hat{\theta})(\mathbf{b}(\tau_{h-1};\theta)-\mathbf{b}(\tau_{h-1};\hat{\theta}))\|_{1} \\ &=\sum_{\tau_{h}\in\Gamma(\pi,h)} \|\mathbf{X}\hat{\mathbb{O}}_{h+1}\hat{\mathbb{T}}_{h}(a_{h})\operatorname{diag}(\hat{\mathbb{O}}_{h}(o_{h}\mid\cdot))\hat{\mathbb{O}}_{h}^{\dagger}\left(\mathbf{b}(\tau_{h-1};\theta)-\mathbf{b}(\tau_{h-1};\hat{\theta})\right)\|_{1} \\ &\leq \sum_{\tau_{h}\in\Gamma(\pi,h)} \sum_{i} \left\|\left(\mathbf{X}\hat{\mathbb{O}}_{h+1}\hat{\mathbb{T}}_{h}(a_{h})\operatorname{diag}(\hat{\mathbb{O}}_{h}(o_{h}\mid\cdot))\right)_{i}\right\|_{1} \left|\left(\hat{\mathbb{O}}_{h}^{\dagger}\left(\mathbf{b}(\tau_{h-1};\theta)-\mathbf{b}(\tau_{h-1};\hat{\theta})\right)\right)_{i}\right| \\ &=\sum_{\tau_{h}\in\Gamma(\pi,h)} \sum_{i} \left\|\left(\mathbf{X}\hat{\mathbb{O}}_{h+1}\hat{\mathbb{T}}_{h}(a_{h})\right)_{i}\right\|_{1} \hat{\mathbb{O}}_{h}(o_{h}\mid i) \left|\left(\hat{\mathbb{O}}_{h}^{\dagger}\left(\mathbf{b}(\tau_{h-1};\theta)-\mathbf{b}(\tau_{h-1};\hat{\theta})\right)\right)_{i}\right| \\ &=\sum_{\tau_{h}\in\Gamma(\pi,h)} \sum_{i} \hat{\mathbb{O}}_{h}(o_{h}\mid i) \left|\left(\hat{\mathbb{O}}_{h}^{\dagger}\left(\mathbf{b}(\tau_{h-1};\theta)-\mathbf{b}(\tau_{h-1};\hat{\theta})\right)\right)_{i}\right|, \end{split}$$

where the inequality is by triangle inequality, and the last identity follows from $\hat{\mathbb{T}}_h(a_h)$ (when $\mathbf{X} = \hat{\mathbb{O}}_{h+1}^{\dagger}$) and $\hat{\mathbb{O}}_{h+1}\hat{\mathbb{T}}_h(a_h)$ (when $\mathbf{X} = \mathbf{I}_O$) having columns with ℓ_1 -norm equal to 1.

As π is deterministic, a_h is unique given τ_{h-1} and o_h . Therefore,

$$\begin{split} &\sum_{\tau_{h}\in\Gamma(\pi,h)}\sum_{i}\hat{\mathbb{O}}_{h}(o_{h}\mid i)\left|\left(\hat{\mathbb{O}}_{h}^{\dagger}\left(\mathbf{b}(\tau_{h-1};\theta)-\mathbf{b}(\tau_{h-1};\hat{\theta})\right)\right)_{i}\right|\\ &=\sum_{\tau_{h-1}\in\Gamma(\pi,h-1)}\sum_{o_{h}}\sum_{i}\hat{\mathbb{O}}_{h}(o_{h}\mid i)\left|\left(\hat{\mathbb{O}}_{h}^{\dagger}\left(\mathbf{b}(\tau_{h-1};\theta)-\mathbf{b}(\tau_{h-1};\hat{\theta})\right)\right)_{i}\right|\\ &=\sum_{\tau_{h-1}\in\Gamma(\pi,h-1)}\sum_{i}\sum_{o_{h}}\hat{\mathbb{O}}_{h}(o_{h}\mid i)\left|\left(\hat{\mathbb{O}}_{h}^{\dagger}\left(\mathbf{b}(\tau_{h-1};\theta)-\mathbf{b}(\tau_{h-1};\hat{\theta})\right)\right)_{i}\right|\\ &=\sum_{\tau_{h-1}\in\Gamma(\pi,h-1)}\sum_{i}\left|\left(\hat{\mathbb{O}}_{h}^{\dagger}\left(\mathbf{b}(\tau_{h-1};\theta)-\mathbf{b}(\tau_{h-1};\hat{\theta})\right)\right)_{i}\right|\\ &=\sum_{\tau_{h-1}\in\Gamma(\pi,h-1)}\left\|\hat{\mathbb{O}}_{h}^{\dagger}\left(\mathbf{b}(\tau_{h-1};\theta)-\mathbf{b}(\tau_{h-1};\hat{\theta})\right)\right\|_{1},\end{split}$$

which completes the proof.

By applying Lemma 7 inductively, we can bound the error in belief states by the projection of errors in operators on preceding belief states.

Lemma 8. Given a deterministic policy π and two sets of undercomplete POMDP parameters $\theta = (\mathbb{O}, \mathbb{T}, \mu_1)$ and $\hat{\theta} = (\hat{\mathbb{O}}, \hat{\mathbb{T}}, \hat{\mu}_1)$ with $\sigma_{\min}(\hat{\mathbb{O}}) \ge \alpha$, for all $h \ge 1$, we have

$$\sum_{\tau_h \in \Gamma(\pi,h)} \left\| \mathbf{b}(\tau_h;\theta) - \mathbf{b}(\tau_h;\hat{\theta}) \right\|_1$$

$$\leq \frac{\sqrt{S}}{\alpha} \sum_{j=1}^h \sum_{\tau_j \in \Gamma(\pi,j)} \left\| \left(\mathbf{B}_j(a_j,o_j;\hat{\theta}) - \mathbf{B}_j(a_j,o_j;\theta) \right) \mathbf{b}(\tau_{j-1};\theta) \right\|_1 + \frac{\sqrt{S}}{\alpha} \left\| \mathbf{b}_0(\theta) - \mathbf{b}_0(\hat{\theta}) \right\|_1.$$

Proof. Invoking Lemma 7 with $\mathbf{X} = \hat{\mathbb{O}}_{j+1}^{\dagger}$, we have

$$\sum_{\tau_{j}\in\Gamma(\pi,j)} \|\hat{\mathbb{O}}_{j+1}^{\dagger}\left(\mathbf{b}(\tau_{j};\theta)-\mathbf{b}(\tau_{j};\hat{\theta})\right)\|_{1} \leq \sum_{\tau_{j-1}\in\Gamma(\pi,j-1)} \left\|\hat{\mathbb{O}}_{j}^{\dagger}\left(\mathbf{b}(\tau_{j-1};\theta)-\mathbf{b}(\tau_{j-1};\hat{\theta})\right)\right\|_{1} + \sum_{\tau_{j}\in\Gamma(\pi,j)} \|\hat{\mathbb{O}}_{j+1}^{\dagger}\left(\mathbf{B}_{j}(a_{j},o_{j};\hat{\theta})-\mathbf{B}_{j}(a_{j},o_{j};\theta)\right)\mathbf{b}(\tau_{j-1};\theta)\|_{1}.$$
(8)

Summing (8) over $j = 1, \ldots, h - 1$, we obtain

$$\sum_{\tau_{h-1}\in\Gamma(\pi,h-1)} \|\hat{\mathbb{O}}_{h}^{\dagger}\left(\mathbf{b}(\tau_{h-1};\theta) - \mathbf{b}(\tau_{h-1};\hat{\theta})\right)\|_{1}$$

$$\leq \sum_{j=1}^{h-1} \sum_{\tau_{j}\in\Gamma(\pi,j)} \left\|\hat{\mathbb{O}}_{j+1}^{\dagger}\left(\mathbf{B}_{j}(a_{j},o_{j};\hat{\theta}) - \mathbf{B}_{j}(a_{j},o_{j};\theta)\right)\mathbf{b}(\tau_{j-1};\theta)\right\|_{1} + \left\|\hat{\mathbb{O}}_{1}^{\dagger}\left(\mathbf{b}_{0}(\theta) - \mathbf{b}_{0}(\hat{\theta})\right)\right\|_{1}.$$
(9)

Again, invoking Lemma 7 with $\mathbf{X} = \mathbf{I}_O$ gives

$$\sum_{\tau_{h}\in\Gamma(\pi,h)} \|\mathbf{b}(\tau_{h};\theta) - \mathbf{b}(\tau_{h};\hat{\theta})\|_{1} \leq \sum_{\tau_{h-1}\in\Gamma(\pi,h-1)} \|\hat{\mathbb{O}}_{h}^{\dagger}(\mathbf{b}(\tau_{h-1};\theta) - \mathbf{b}(\tau_{h-1};\hat{\theta}))\|_{1} + \sum_{\tau_{h}\in\Gamma(\pi,h)} \|\left(\mathbf{B}_{h}(a_{h},o_{h};\hat{\theta}) - \mathbf{B}_{h}(a_{h},o_{h};\theta)\right)\mathbf{b}(\tau_{h-1};\theta)\|_{1}.$$
 (10)

Plugging (9) into (10), and using the fact that $\|\hat{\mathbb{O}}_h^{\dagger}\|_{1\to 1} \leq \sqrt{S} \|\hat{\mathbb{O}}_h^{\dagger}\|_2 \leq \frac{\sqrt{S}}{\alpha}$ complete the proof.

The following lemma bounds the projection of any vector on belief states by its projection on the product of the observation matrix and the transition matrix, reweighed by the visitation probability of states.

Lemma 9. For any deterministic policy π , fixed $a_{h+1} \in \mathscr{A}$, $\mathbf{u} \in \mathbb{R}^O$, and $h \ge 0$, we have

$$\sum_{o_{h+1} \in \mathscr{O}} \sum_{\tau_h \in \Gamma(\pi,h)} \left| \mathbf{u}^\top \mathbf{b}([a_{h+1}, o_{h+1}, \tau_h]; \theta) \right| \le \sum_{s=1}^S |\mathbf{u}^\top (\mathbb{O}_{h+2} \mathbb{T}_{h+1}(a_{h+1}))_s| \mathbb{P}_{\theta}^{\pi}(s_{h+1} = s).$$

Proof. By definition, for any $[a_{h+1}, o_{h+1}, \tau_h] \in \mathscr{A} \times \mathscr{O} \times \Gamma(\pi, h)$, we have

$$\mathbf{b}([a_{h+1}, o_{h+1}, \tau_h]; \theta) = \mathbb{O}_{h+2} \mathbb{T}_{h+1}(a_{h+1}) \mathbb{P}_{\theta}^{\pi}(s_{h+1} = \cdot, [o_{h+1}, \tau_h]),$$

where $\mathbb{P}_{\theta}^{\pi}(s_{h+1} = \cdot, [o_{h+1}, \tau_h])$ is an *s*-dimensional vector, whose *i*th entry is equal to the probability of observing $[o_{h+1}, \tau_h]$ and reaching state *i* at step h + 1 when executing policy π in POMDP(θ).

Therefore,

$$\begin{split} &\sum_{\tau_{h}\in\Gamma(\pi,h)}\sum_{o_{h+1}\in\mathcal{O}}|\mathbf{u}^{\top}\mathbf{b}([a_{h+1},o_{h+1},\tau_{h}];\theta)|\\ &=\sum_{\tau_{h}\in\Gamma(\pi,h)}\sum_{o_{h+1}\in\mathcal{O}}|\mathbf{u}^{\top}\mathbb{O}_{h+2}\mathbb{T}_{h+1}(a_{h+1})\mathbb{P}_{\theta}^{\pi}(s_{h+1}=\cdot,[o_{h+1},\tau_{h}])|\\ &\leq\sum_{\tau_{h}\in\Gamma(\pi,h)}\sum_{o_{h+1}\in\mathcal{O}}\sum_{s=1}^{S}|\mathbf{u}^{\top}(\mathbb{O}_{h+2}\mathbb{T}_{h+1}(a_{h+1}))_{s}|\mathbb{P}_{\theta}^{\pi}(s_{h+1}=s,[o_{h+1},\tau_{h}])\\ &=\sum_{s=1}^{S}|\mathbf{u}^{\top}(\mathbb{O}_{h+2}\mathbb{T}_{h+1}(a_{h+1}))_{s}|\left(\sum_{\tau_{h}\in\Gamma(\pi,h)}\sum_{o_{h+1}\in\mathcal{O}}\mathbb{P}_{\theta}^{\pi}(s_{h+1}=s,[o_{h+1},\tau_{h}])\right)\\ &=\sum_{s=1}^{S}|\mathbf{u}^{\top}(\mathbb{O}_{h+2}\mathbb{T}_{h+1}(a_{h+1}))_{s}|\mathbb{P}_{\theta}^{\pi}(s_{h+1}=s). \end{split}$$

Combining Lemma 8 and Lemma 9, we obtain the target bound.

Lemma 10. Given a deterministic policy π and two sets of undercomplete POMDP parameters $\theta = (\mathbb{O}, \mathbb{T}, \mu_1)$ and $\hat{\theta} = (\hat{\mathbb{O}}, \hat{\mathbb{T}}, \hat{\mu}_1)$ with $\sigma_{\min}(\hat{\mathbb{O}}) \ge \alpha$, for all $h \ge 1$, we have

$$\sum_{\substack{\tau_h \in \Gamma(\pi,h) \\ \leq \frac{\sqrt{S}}{\alpha} \left\| \mathbf{b}_0(\theta) - \mathbf{b}_0(\hat{\theta}) \right\|_1 + \frac{\sqrt{S}}{\alpha} \sum_{(a,o) \in \mathscr{A} \times \mathscr{O}} \left\| \left(\mathbf{B}_1(a,o;\hat{\theta}) - \mathbf{B}_1(a,o;\theta) \right) \mathbf{b}_0(\theta) \right\|_1 \\ + \frac{\sqrt{S}}{\alpha} \sum_{j=2}^h \sum_{(a,\tilde{a},o) \in \mathscr{A}^2 \times \mathscr{O}} \sum_{s=1}^S \left\| \left(\mathbf{B}_j(a,o;\hat{\theta}) - \mathbf{B}_j(a,o;\theta) \right) (\mathbb{O}_j \mathbb{T}_{j-1}(\tilde{a}))_s \right\|_1 \mathbb{P}_{\theta}^{\pi}(s_{j-1} = s).$$

Proof. By Lemma 8,

$$\sum_{\tau_{h}\in\Gamma(\pi,h)} \|\mathbf{b}(\tau_{h};\theta) - \mathbf{b}(\tau_{h};\hat{\theta})\|_{1}$$

$$\leq \frac{\sqrt{S}}{\alpha} \sum_{j=2}^{h} \sum_{\tau_{j}\in\Gamma(\pi,j)} \left\| \left(\mathbf{B}_{j}(a_{j},o_{j};\hat{\theta}) - \mathbf{B}_{j}(a_{j},o_{j};\theta) \right) \mathbf{b}(\tau_{j-1};\theta) \right\|_{1}$$

$$+ \frac{\sqrt{S}}{\alpha} \sum_{\tau_{1}\in\Gamma(\pi,1)} \left\| \left(\mathbf{B}_{1}(a_{1},o_{1};\hat{\theta}) - \mathbf{B}_{1}(a_{1},o_{1};\hat{\theta}) \right) \mathbf{b}_{0}(\theta) \right\|_{1} + \frac{\sqrt{S}}{\alpha} \left\| \mathbf{b}_{0}(\theta) - \mathbf{b}_{0}(\hat{\theta}) \right\|_{1}.$$
(11)

Bounding the first term: note that $\Gamma(\pi, j) \subseteq \Gamma(\pi, j-2) \times (\mathscr{O} \times \mathscr{A})^2$, so we have

$$\sum_{\tau_{j}\in\Gamma(\pi,j)} \| \left(\mathbf{B}_{j}(a_{j},o_{j};\hat{\theta}) - \mathbf{B}_{j}(a_{j},o_{j};\theta) \right) \mathbf{b}(\tau_{j-1};\theta) \|_{1}$$

$$\leq \sum_{\tau_{j-2}\in\Gamma(\pi,j-2)} \sum_{o_{j-1}\in\mathscr{O}} \sum_{a_{j-1}\in\mathscr{A}} \sum_{o_{j}\in\mathscr{O}} \sum_{a_{j}\in\mathscr{A}} \| \left(\mathbf{B}_{j}(a_{j},o_{j};\hat{\theta}) - \mathbf{B}_{j}(a_{j},o_{j};\theta) \right) \mathbf{b}([a_{j-1},o_{j-1},\tau_{j-2}];\theta) \|_{1}$$

$$= \sum_{\substack{(a_{j},a_{j-1},o_{j})\in\mathscr{A}^{2}\times\mathscr{O} \\ \sum_{\tau_{j-2}\in\Gamma(\pi,j-2)} \sum_{o_{j-1}\in\mathscr{O}} \| \left(\mathbf{B}_{j}(a_{j},o_{j};\hat{\theta}) - \mathbf{B}_{j}(a_{j},o_{j};\theta) \right) \mathbf{b}([a_{j-1},o_{j-1},\tau_{j-2}];\theta) \|_{1}.$$
(12)

We can bound (\diamond) by Lemma 9 and obtain,

$$\sum_{\tau_{j}\in\Gamma(\pi,j)} \| \left(\mathbf{B}_{j}(a_{j},o_{j};\hat{\theta}) - \mathbf{B}_{j}(a_{j},o_{j};\theta) \right) \mathbf{b}(\tau_{j-1};\theta) \|_{1}$$

$$\leq \sum_{(a_{j},a_{j-1},o_{j})\in\mathscr{A}^{2}\times\mathscr{O}} \sum_{s=1}^{S} \| \left(\mathbf{B}_{j}(a_{j},o_{j};\hat{\theta}) - \mathbf{B}_{j}(a_{j},o_{j};\theta) \right) (\mathbb{O}_{j}\mathbb{T}_{j-1}(a_{j-1}))_{s} \|_{1}\mathbb{P}_{\theta}^{\pi}(s_{j-1}=s)$$

$$= \sum_{(a,\tilde{a},o)\in\mathscr{A}^{2}\times\mathscr{O}} \sum_{s=1}^{S} \| \left(\mathbf{B}_{j}(a,o;\hat{\theta}) - \mathbf{B}_{j}(a,o;\theta) \right) (\mathbb{O}_{j}\mathbb{T}_{j-1}(\tilde{a}))_{s} \|_{1}\mathbb{P}_{\theta}^{\pi}(s_{j-1}=s), \quad (13)$$

where the identity only changes the notations $(a_j, a_{j-1}, o_j) \rightarrow (a, \tilde{a}, o)$ to make the expression cleaner.

Bounding the second term: note that $\Gamma(\pi, 1) \subseteq \mathscr{O} \times \mathscr{A}$, we have

$$\sum_{\tau_1 \in \Gamma(\pi, 1)} \left\| \left(\mathbf{B}_1(a_1, o_1; \theta) - \mathbf{B}_1(a_1, o_1; \hat{\theta}) \right) \mathbf{b}_0(\theta) \right\|_1$$

$$\leq \sum_{(a, o) \in \mathscr{A} \times \mathscr{O}} \left\| \left(\mathbf{B}_1(a, o; \theta) - \mathbf{B}_1(a, o; \hat{\theta}) \right) \mathbf{b}_0(\theta) \right\|_1.$$
(14)

Plugging (13) and (14) into (11) completes the proof.

C.2 A hammer for studying confidence sets

In this subsection, we develop a martingale concentration result, which forms the basis of analyzing confidence sets.

We start by giving the following basic fact about POMDP. The proof is just some basic algebraic calculation so we omit it here.

Fact 11. In POMDP(θ), suppose s_{h-1} is sampled from μ_{h-1} , fix $a_{h-1} \equiv \tilde{a}$, and $a_h \equiv a$. Then the joint distribution of (o_{h+1}, o_h, o_{h-1}) is

$$\mathbb{P}(o_{h+1} = \cdot, o_h = \cdot, o_{h-1} = \cdot) = (\mathbb{O}_{h+1}\mathbb{T}_h(a)) \otimes \mathbb{O}_h \otimes (\mathbb{O}_{h-1}\operatorname{diag}(\mu_{h-1})\mathbb{T}_{h-1}(\tilde{a})^\top).$$

By slicing the tensor, we can further obtain

$$\begin{cases} \mathbb{P}(o_{h-1} = \cdot) = \mathbb{O}_{h-1}\mu_{h-1}, \\ \mathbb{P}(o_h = \cdot, o_{h-1} = \cdot) = \mathbb{O}_h \mathbb{T}_{h-1}(\tilde{a}) \operatorname{diag}(\mu_{h-1}) \mathbb{O}_{h-1}^\top, \\ \mathbb{P}(o_{h+1} = \cdot, o_h = o, o_{h-1} = \cdot) = \mathbb{O}_{h+1} \mathbb{T}_h(a) \operatorname{diag}(\mathbb{O}_h(o \mid \cdot)) \mathbb{T}_{h-1}(\tilde{a}) \operatorname{diag}(\mu_{h-1}) \mathbb{O}_{h-1}^\top \end{cases}$$

A simple implication of Fact 11 is that if we execute policy π from step 1 to step h - 2, take \tilde{a} and a at step h - 1 and h respectively, then the joint distribution of (o_{h+1}, o_h, o_{h-1}) is the same as above except for replacing μ_{h-1} with $\mathbb{P}^{\pi}_{\theta}(s_{h-1} = \cdot)$.

Suppose we are given a set of sequential data $\{(o_{h+1}^{(t)}, o_h^{(t)}, o_{h-1}^{(t)})\}_{t=1}^N$ generated from POMDP(θ) in the following way: at time t, execute policy π_t from step 1 to step h-2, take action \tilde{a} at step h-1, and action a at step h respectively, and observe $(o_{h+1}^{(t)}, o_h^{(t)}, o_{h-1}^{(t)})$. Here, we allow the policy π_t to be *adversarial*, in the sense that π_t can be chosen based on $\{(\pi_i, o_{h+1}^{(i)}, o_h^{(i)}, o_{h-1}^{(i)})\}_{i=1}^{t-1}$. Define $\mu_{h-1}^{adv} = \frac{1}{N} \sum_{t=1}^N \mathbb{P}_{\theta}^{\pi_t}(s_{h-1} = \cdot)$. Based on Fact 11, we define the following probability vector, matrices and tensor,

$$\begin{cases} P_{h-1} = \mathbb{O}_{h-1} \mu_{h-1}^{adv}, \\ P_{h,h-1} = \mathbb{O}_{h} \mathbb{T}_{h-1}(\tilde{a}) \operatorname{diag}(\mu_{h-1}^{adv}) \mathbb{O}_{h-1}^{\top}, \\ P_{h+1,h,h-1} = (\mathbb{O}_{h+1} \mathbb{T}_{h}(a)) \otimes \mathbb{O}_{h} \otimes (\mathbb{O}_{h-1} \operatorname{diag}(\mu_{h-1}^{adv}) \mathbb{T}_{h-1}(\tilde{a})^{\top}) \\ P_{h+1,o,h-1} = \mathbb{O}_{h+1} \mathbb{T}_{h}(a) \operatorname{diag}(\mathbb{O}_{h}(o \mid \cdot)) \mathbb{T}_{h-1}(\tilde{a}) \operatorname{diag}(\mu_{h-1}^{adv}) \mathbb{O}_{h-1}^{\top}, \quad o \in \mathscr{O}. \end{cases}$$

Accordingly, we define their empirical estimates as below

$$\begin{cases} \hat{P}_{h-1} = \frac{1}{N} \sum_{t=1}^{N} \mathbf{e}_{o_{h-1}^{(t)}}, \\ \hat{P}_{h,h-1} = \frac{1}{N} \sum_{t=1}^{N} \mathbf{e}_{o_{h}^{(t)}} \otimes \mathbf{e}_{o_{h-1}^{(t)}}, \\ \hat{P}_{h+1,h,h-1} = \frac{1}{N} \sum_{t=1}^{N} \mathbf{e}_{o_{h+1}^{(t)}} \otimes \mathbf{e}_{o_{h}^{(t)}} \otimes \mathbf{e}_{o_{h-1}^{(t)}}, \\ \hat{P}_{h+1,o,h-1} = \frac{1}{N} \sum_{t=1}^{N} \mathbf{e}_{o_{h+1}^{(t)}} \otimes \mathbf{e}_{o_{h-1}^{(t)}} \mathbf{1}(o_{h}^{(t)} = o), \quad o \in \mathscr{O}. \end{cases}$$

Lemma 12. There exists an absolute constant c_1 , s.t. the following concentration bound holds with probability at least $1 - \delta$

$$\max\left\{ \|\hat{P}_{h+1,h,h-1} - P_{h+1,h,h-1}\|_{F}, \|\hat{P}_{h,h-1} - P_{h,h-1}\|_{F}, \\ \max_{o \in \mathscr{O}} \|\hat{P}_{h+1,o,h-1} - P_{h+1,o,h-1}\|_{F}, \|\hat{P}_{h-1} - P_{h-1}\|_{2} \right\} \le c_{1}\sqrt{\frac{\log(ON/\delta)}{N}}.$$

Proof. We start with proving that with probability at least $1 - \delta/2$,

$$\|\hat{P}_{h+1,h,h-1} - P_{h+1,h,h-1}\|_F \le c_1 \sqrt{\frac{\log(ON/\delta)}{N}}$$

Let \mathcal{F}_t be the σ -algebra generated by $\left\{ \{\pi_i\}_{i=1}^{t+1}, \{(o_{h+1}^{(i)}, o_h^{(i)}, o_{h-1}^{(i)})\}_{i=1}^t \right\}$. (\mathcal{F}_t) is a filtration. Define

$$X_t = e_{o_{h+1}^{(t)}} \otimes e_{o_h^{(t)}} \otimes e_{o_{h-1}^{(t)}} - (\mathbb{O}_{h+1}\mathbb{T}_h(a)) \otimes \mathbb{O}_h \otimes (\mathbb{O}_{h-1}\operatorname{diag}(\mathbb{P}_{\theta}^{\pi_t}(s_{h-1}=\cdot))\mathbb{T}_{h-1}(\tilde{a})^{\top}).$$

We have $X_t \in \mathcal{F}_t$ and $\mathbb{E}[X_t | \mathcal{F}_{t-1}] = \mathbb{E}[X_t | \pi_t] = 0$, where the second identity follows from Fact 11. Moreover,

$$\|X_t\|_F \le \|X_t\|_1 \le \|e_{o_{h+1}^{(t)}} \otimes e_{o_h^{(t)}} \otimes e_{o_{h-1}^{(t)}}\|_1 + \|(\mathbb{O}_{h+1}\mathbb{T}_h(a)) \otimes \mathbb{O}_h \otimes (\mathbb{O}_{h-1}\text{diag}(\mathbb{P}_{\theta}^{\pi_t}(s_{h-1}=\cdot))\mathbb{T}_{h-1}(\tilde{a})^{\top})\|_1 = 2,$$
(15)

where $\|\cdot\|_1$ denotes the entry-wise ℓ_1 -norm of the tensor.

Now, we can bound $\|\hat{P}_{h+1,h,h-1} - P_{h+1,h,h-1}\|_F$ by writing $\hat{P}_{h+1,h,h-1} - P_{h+1,h,h-1}$ as the sum of a sequence of tensor-valued martingale difference, vectorizing the tensors, and applying the standard vector-valued martingale concentration inequality (e.g. see Corollary 7 in [17]):

$$\begin{split} \|\hat{P}_{h+1,h,h-1} - P_{h+1,h,h-1}\|_{F} \\ = \|\frac{1}{N} \sum_{t=1}^{N} \left(e_{o_{h+1}^{(t)}} \otimes e_{o_{h}^{(t)}} \otimes e_{o_{h-1}^{(t)}} - \\ (\mathbb{O}_{h+1}\mathbb{T}_{h}(a)) \otimes \mathbb{O}_{h} \otimes (\mathbb{O}_{h-1}\text{diag}(\mathbb{P}_{\theta}^{\pi_{t}}(s_{h-1} = \cdot))\mathbb{T}_{h-1}(\tilde{a})^{\top}) \right)\|_{F} \\ = \|\frac{1}{N} \sum_{t=1}^{N} X_{t}\|_{F} \leq \mathcal{O}\left(\sqrt{\frac{\log(ON/\delta)}{N}}\right), \end{split}$$

with probability at least $1 - \delta/2$. We remark that when vectoring a tensor, its Frobenius norm will become the ℓ_2 -norm the vector. So the upper bound of the norm of the vectorized martingales directly follows from (15).

Similarly, we can show that with probability at least $1 - \delta/2$,

$$\|\hat{P}_{h,h-1} - P_{h,h-1}\|_F \le \mathcal{O}\left(\sqrt{\frac{\log(ON/\delta)}{N}}\right) \quad \text{and} \quad \|\hat{P}_{h-1} - P_{h-1}\|_F \le \mathcal{O}\left(\sqrt{\frac{\log(ON/\delta)}{N}}\right)$$

Using the fact $\|\hat{P}_{h+1,o,h-1} - P_{h+1,o,h-1}\|_F \le \|\hat{P}_{h+1,h,h-1} - P_{h+1,h,h-1}\|_F$ completes the whole proof. \Box

C.3 Properties of confidence sets

For convenience of discussion, we divide the constraints in Θ_k into three categories as following

Type-0 constraint:

$$\|k \cdot \mathbf{b}_0(\hat{\theta}) - \mathbf{n}^k\|_2 \le \beta_k\}$$

Type-I constraint:

$$\|\mathbf{B}_1(a,o;\hat{\theta})\mathbf{N}_1^k(a,\tilde{a}) - \mathbf{M}_1^k(o,a,\tilde{a})\|_F \le \gamma_k$$

where \mathbf{M}_1^k and \mathbf{N}_1^k are actually equivalent to *O*-dimensional counting vectors because there is no observation (or only a dummy observation) at step 0, which implies each of them has only one non-zero column. With slight abuse of notation, we use \mathbf{M}_1^k and \mathbf{N}_1^k to denote their non-zero columns in the following proof. **Type-II constraint:** for $2 \le h \le H - 1$,

$$\|\mathbf{B}_{h}(a,o;\hat{\theta})\mathbf{N}_{h}^{k}(a,\tilde{a}) - \mathbf{M}_{h}^{k}(o,a,\tilde{a})\|_{F} \leq \gamma_{k}$$

Recalling the definition of $\mathbf{n}^k(\theta)$, $\mathbf{N}^k_h(a, \tilde{a})$ and $\mathbf{M}^k_h(o, a, \tilde{a})$ and applying Lemma 12, we get the following concentration results.

Corollary 13. Let $\theta^* = (\mathbb{T}, \mathbb{O}, \mu_1)$. By applying Lemma 12 directly, with probability at least $1 - \delta$, for all $k \in [K]$ and $(o, a, \tilde{a}) \in \mathcal{O} \times \mathscr{A}^2$, we have

$$\begin{split} \left\{ \begin{aligned} \left\| \frac{1}{k} \mathbf{n}^{k} - \mathbb{O}_{1} \mu_{1} \right\|_{2} &\leq \mathcal{O}\left(\sqrt{\frac{\iota}{k}}\right), \\ \left\| \frac{1}{k} \mathbf{N}_{1}^{k}(a, \tilde{a}) - \mathbb{O}_{1} \mu_{1} \right\|_{2} &\leq \mathcal{O}\left(\sqrt{\frac{\iota}{k}}\right), \\ \left\| \frac{1}{k} \mathbf{M}_{1}^{k}(o, a, \tilde{a}) - \left(\mathbb{O}_{2} \mathbb{T}_{1}(\tilde{a}) \operatorname{diag}(\mu_{1}) \mathbb{O}_{1}^{\top}\right)_{o} \right\|_{2} &\leq \mathcal{O}\left(\sqrt{\frac{\iota}{k}}\right), \\ \left\| \frac{1}{k} \mathbf{N}_{h}^{k}(a, \tilde{a}) - \underbrace{\mathbb{O}_{h} \mathbb{T}_{h-1}(\tilde{a}) \operatorname{diag}(\mu_{h-1}^{k}) \mathbb{O}_{h-1}^{\top}}_{\mathbf{V}} \right\|_{F} &\leq \mathcal{O}\left(\sqrt{\frac{\iota}{k}}\right), \\ \left\| \frac{1}{k} \mathbf{M}_{h}^{k}(o, a, \tilde{a}) - \underbrace{\mathbb{O}_{h+1} \mathbb{T}_{h}(a) \operatorname{diag}(\mathbb{O}_{h}(o \mid \cdot)) \mathbb{T}_{h-1}(\tilde{a}) \operatorname{diag}(\mu_{h-1}^{k}) \mathbb{O}_{h-1}^{\top}}_{\mathbf{W}} \right\|_{F} &\leq \mathcal{O}\left(\sqrt{\frac{\iota}{k}}\right), \end{aligned}\right.$$

where

$$\iota = \log(KAOH/\delta)$$
 and $\mu_{h-1}^k = \frac{1}{k} \sum_{t=1}^k \mathbb{P}_{\theta^*}^{\pi_t}(s_{h-1} = \cdot)$ $2 \le h \le H - 1.$

Note that for all $k \in [K]$ *,* $\mu_1^k = \mu_1$ *independent of* π_1, \ldots, π_k *.*

Now, with Corollary 13, we can prove the true parameter θ^* always lies in the confidence sets for $k \in [K]$ with high probability.

Lemma 14. Denote by $\theta^* = (\mathbb{T}, \mathbb{O}, \mu_1)$ the the ground truth parameters of the POMDP. With probability at least $1 - \delta$, we have $\theta^* \in \Theta_k$ for all $k \in [K]$.

Proof. By the definition of $\mathbf{b}_0(\theta^*)$ and $\mathbf{B}_h(a, o; \theta^*)$, we have

$$(*) \begin{cases} \mathbf{b}_{0}(\theta^{\star}) = \mathbb{O}_{1}\mu_{1}, \\ \left(\mathbb{O}_{2}\mathbb{T}_{1}(\tilde{a})\operatorname{diag}(\mu_{1})\mathbb{O}_{1}^{\top}\right)_{o} = \mathbf{B}_{1}(\tilde{a}, o; \theta^{\star})\mathbb{O}_{1}\mu_{1}, \\ \mathbf{W} = \mathbf{B}_{h}(a, o; \theta^{\star}) \cdot \mathbf{V}, \quad h \geq 2, \end{cases}$$

where W and V are shorthands defined in Corollary 13.

It's easy to see (*) and Corollary13 directly imply $\|\mathbf{n}^k - \mathbf{b}_0(\theta^*)\|_2 \leq \mathcal{O}(\sqrt{k\iota})$ and thus θ^* satisfies Type-0 constraint. For other constraints, we have

Type-I constraint:

$$\begin{split} \|\mathbf{M}_{1}^{k}(o, a, \tilde{a}) - \mathbf{B}_{1}(\tilde{a}, o; \theta^{\star})\mathbf{N}_{1}^{k}(a, \tilde{a})\|_{2} \\ \leq \|\mathbf{M}_{1}^{k}(o, a, \tilde{a}) - k\left(\mathbb{O}_{2}\mathbb{T}_{1}(\tilde{a})\mathrm{diag}(\mu_{1})\mathbb{O}_{1}^{\top}\right)_{o}\|_{2} + \|\mathbf{B}_{1}(\tilde{a}, o; \theta^{\star})(k\mathbb{O}_{1}\mu_{1} - \mathbf{N}_{1}^{k}(a, \tilde{a}))\|_{2} \\ + k\|\left(\mathbb{O}_{2}\mathbb{T}_{1}(\tilde{a})\mathrm{diag}(\mu_{1})\mathbb{O}_{1}^{\top}\right)_{o} - \mathbf{B}_{1}(\tilde{a}, o; \theta^{\star})\mathbb{O}_{1}\mu_{1}\|_{2} \\ = \|\mathbf{M}_{1}^{k}(o, a, \tilde{a}) - k\left(\mathbb{O}_{2}\mathbb{T}_{1}(\tilde{a})\mathrm{diag}(\mu_{1})\mathbb{O}_{1}^{\top}\right)_{o}\|_{2} + \|\mathbf{B}_{1}(\tilde{a}, o; \theta^{\star})(k\mathbb{O}_{1}\mu_{1} - \mathbf{N}_{1}^{k}(a, \tilde{a}))\|_{2} \\ \leq \|\mathbf{M}_{1}^{k}(o, a, \tilde{a}) - k\left(\mathbb{O}_{2}\mathbb{T}_{1}(\tilde{a})\mathrm{diag}(\mu_{1})\mathbb{O}_{1}^{\top}\right)_{o}\|_{2} + \|\mathbf{B}_{1}(\tilde{a}, o; \theta^{\star})\|_{2}\|k\mathbb{O}_{1}\mu_{1} - \mathbf{N}_{1}^{k}(a, \tilde{a})\|_{2} \\ \leq \mathcal{O}\left(\frac{\sqrt{kS\iota}}{\alpha}\right) \end{split}$$

where the identity follows from (*), and the last inequality follows from Corollary13 and

$$\begin{split} \|\mathbf{B}_{h}(a,o;\theta^{\star})\|_{2} &= \|\mathbb{O}_{h+1}\mathbb{T}_{h}(a)\mathrm{diag}(\mathbb{O}_{h}(o|\cdot))\mathbb{O}_{h}^{\dagger}\|_{2} \\ &\leq \frac{1}{\alpha}\|\mathbb{O}_{h+1}\mathbb{T}_{h}(a)\mathrm{diag}(\mathbb{O}_{h}(o|\cdot))\|_{2} \\ &\leq \frac{\sqrt{S}}{\alpha}\|\mathbb{O}_{h+1}\mathbb{T}_{h}(a)\mathrm{diag}(\mathbb{O}_{h}(o|\cdot))\|_{1\to 1} \leq \frac{\sqrt{S}}{\alpha}. \end{split}$$

Type-II constraint: similarly, for $h \ge 2$, we have

$$\begin{split} \|\mathbf{B}_{h}(a,o;\theta^{\star})\mathbf{N}_{h}^{k}(a,\tilde{a}) - \mathbf{M}_{h}^{k}(o,a,\tilde{a})\|_{F} \\ \leq & k\|\mathbf{B}_{h}(a,o;\theta^{\star})\cdot\mathbf{V} - \mathbf{W}\|_{F} + \|\mathbf{B}_{h}(a,o;\theta^{\star})(\mathbf{N}_{h}^{k}(a,\tilde{a}) - k\mathbf{V})\|_{F} + \|k\mathbf{W} - \mathbf{M}_{h}^{k}(o,a,\tilde{a})\|_{F} \\ = & \|\mathbf{B}_{h}(a,o;\theta^{\star})(\mathbf{N}_{h}^{k}(a,\tilde{a}) - k\mathbf{V})\|_{F} + \|k\mathbf{W} - \mathbf{M}_{h}^{k}(o,a,\tilde{a})\|_{F} \\ \leq & \|\mathbf{B}_{h}(a,o;\theta^{\star})\|_{2}\|\mathbf{N}_{h}^{k}(a,\tilde{a}) - k\mathbf{V}\|_{F} + \|k\mathbf{W} - \mathbf{M}_{h}^{k}(o,a,\tilde{a})\|_{F} \\ \leq & \mathcal{O}\left(\frac{\sqrt{kS\iota}}{\alpha}\right), \end{split}$$

Therefore, we conclude that $\theta^* \in \Theta_k$ for all $k \in [K]$ with probability at least $1 - \delta$.

Furthermore, with Corollary 13, we can prove the following bound for operator error.

Lemma 15. With probability at least $1 - \delta$, for all $k \in [K]$, $\hat{\theta} = (\hat{\mathbb{O}}, \hat{\mathbb{T}}, \hat{\mu}_1) \in \Theta_{k+1}$ and $(o, a, \tilde{a}, h) \in \mathcal{O} \times \mathscr{A}^2 \times \{2, \ldots, H-1\}$, we have

$$\begin{cases} \left\| \mathbf{b}_{0}(\theta^{\star}) - \mathbf{b}_{0}(\hat{\theta}) \right\|_{2} \leq \mathcal{O}\left(\sqrt{\frac{\iota}{k}}\right), \\ \left\| \left(\mathbf{B}_{1}(\tilde{a}, o; \hat{\theta}) - \mathbf{B}_{1}(\tilde{a}, o; \theta^{\star}) \right) \mathbf{b}_{0}(\theta^{\star}) \right\|_{2} \leq \mathcal{O}\left(\sqrt{\frac{S\iota}{k\alpha^{2}}}\right), \\ \sum_{s=1}^{S} \left\| \left(\mathbf{B}_{h}(a, o; \hat{\theta}) - \mathbf{B}_{h}(a, o; \theta^{\star}) \right) (\mathbb{O}_{h} \mathbb{T}_{h-1}(\tilde{a}))_{s} \right\|_{1} \sum_{t=1}^{k} \mathbb{P}_{\theta^{\star}}^{\pi_{t}}(s_{h-1} = s) \leq \mathcal{O}\left(\sqrt{\frac{kS^{2}O\iota}{\alpha^{4}}}\right), \end{cases}$$

where $\iota = \log(KAOH/\delta)$.

Proof. For readability, we copy the following set of identities from Lemma 14 here,

$$(*) \begin{cases} \mathbf{b}_{0}(\theta^{\star}) = \mathbb{O}_{1}\mu_{1}, \\ \left(\mathbb{O}_{2}\mathbb{T}_{1}(\tilde{a})\operatorname{diag}(\mu_{1})\mathbb{O}_{1}^{\top}\right)_{o} = \mathbf{B}_{1}(\tilde{a}, o; \theta^{\star})\mathbb{O}_{1}\mu_{1}, \\ \mathbf{W} = \mathbf{B}_{h}(a, o; \theta^{\star}) \cdot \mathbf{V}, \quad h \geq 2. \end{cases}$$

Type-0 closeness:

$$\left\|\mathbf{b}_{0}(\theta^{\star})-\mathbf{b}_{0}(\hat{\theta})\right\|_{2} \leq \left\|\frac{1}{k}\mathbf{n}^{k}-\mathbf{b}_{0}(\theta^{\star})\right\|_{2}+\left\|\frac{1}{k}\mathbf{n}^{k}-\mathbf{b}_{0}(\hat{\theta})\right\|_{2} \leq \mathcal{O}\left(\sqrt{\frac{\iota}{k}}\right),$$

where the last inequality follows from (*), Corollary13 and $\hat{\theta} \in \Theta_{k+1}$.

Type-I closeness: similarly, we have

$$\begin{split} & \left\| \left(\mathbf{B}_{1}(\tilde{a}, o; \hat{\theta}) - \mathbf{B}_{1}(\tilde{a}, o; \theta^{\star}) \right) \mathbf{b}_{0}(\theta^{\star}) \right\|_{2} \\ & \leq \left\| \left(\mathbb{O}_{2} \mathbb{T}_{1}(\tilde{a}) \operatorname{diag}(\mu_{1}) \mathbb{O}_{1}^{\top} \right)_{o} - \mathbf{B}_{1}(\tilde{a}, o; \theta^{\star}) \mathbf{b}_{0}(\theta^{\star}) \right\|_{2} \\ & + \left\| \left(\mathbb{O}_{2} \mathbb{T}_{1}(\tilde{a}) \operatorname{diag}(\mu_{1}) \mathbb{O}_{1}^{\top} \right)_{o} - \mathbf{B}_{1}(\tilde{a}, o; \hat{\theta}) \mathbf{b}_{0}(\theta^{\star}) \right\|_{2} \\ & = \left\| \left(\mathbb{O}_{2} \mathbb{T}_{1}(\tilde{a}) \operatorname{diag}(\mu_{1}) \mathbb{O}_{1}^{\top} \right)_{o} - \mathbf{B}_{1}(\tilde{a}, o; \hat{\theta}) \mathbf{b}_{0}(\theta^{\star}) \right\|_{2} \\ & \leq \left\| \left(\mathbb{O}_{2} \mathbb{T}_{1}(\tilde{a}) \operatorname{diag}(\mu_{1}) \mathbb{O}_{1}^{\top} \right)_{o} - \frac{1}{k} \mathbf{M}_{1}^{k}(o, a, \tilde{a}) \right\|_{2} + \frac{1}{k} \left\| \mathbf{M}_{1}^{k}(o, a, \tilde{a}) - \mathbf{B}_{1}(\tilde{a}, o; \hat{\theta}) \mathbf{N}_{1}^{k}(a, \tilde{a}) \right\|_{2} \\ & + \left\| \mathbf{B}_{1}(\tilde{a}, o; \hat{\theta}) \left(\frac{1}{k} \mathbf{N}_{1}^{k}(a, \tilde{a}) - \mathbf{b}_{0}(\theta^{\star}) \right) \right\|_{2} \\ & \leq \left\| \left(\mathbb{O}_{2} \mathbb{T}_{1}(\tilde{a}) \operatorname{diag}(\mu_{1}) \mathbb{O}_{1}^{\top} \right)_{o} - \frac{1}{k} \mathbf{M}_{1}^{k}(o, a, \tilde{a}) \right\|_{2} + \frac{1}{k} \left\| \mathbf{M}_{1}^{k}(o, a, \tilde{a}) - \mathbf{B}_{1}(\tilde{a}, o; \hat{\theta}) \mathbf{N}_{1}^{k}(a, \tilde{a}) \right\|_{2} \\ & + \left\| \mathbf{B}_{1}(\tilde{a}, o; \hat{\theta}) \right\|_{2} \left\| \frac{1}{k} \mathbf{N}_{1}^{k}(a, \tilde{a}) - \mathbb{O}_{1} \mu_{1} \right\|_{2} \\ & \leq \mathcal{O} \left(\sqrt{\frac{S\iota}{k\alpha^{2}}} \right), \end{split}$$

where the identity follows from (*) and the last inequality follows from Corollary13 and $\hat{\theta} \in \Theta_{k+1}$.

Type-II closeness: we continue to use the same proof strategy, for $h \ge 2$

$$\begin{aligned} \left\| \left(\mathbf{B}_{h}(a,o;\hat{\theta}) - \mathbf{B}_{h}(a,o;\theta^{\star}) \right) \mathbf{V} \right\|_{F} \\ \leq \left\| \mathbf{W} - \mathbf{B}_{h}(a,o;\theta^{\star}) \mathbf{V} \right\|_{F} + \left\| \frac{1}{k} \mathbf{M}_{h}^{k}(o,a,\tilde{a}) - \mathbf{W} \right\|_{F} \\ + \frac{1}{k} \left\| \mathbf{B}_{h}(a,o;\hat{\theta}) \mathbf{N}_{h}^{k}(a,\tilde{a}) - \mathbf{M}_{h}^{k}(o,a,\tilde{a}) \right\|_{F} + \left\| \mathbf{B}_{h}(a,o;\hat{\theta}) \left(\mathbf{V} - \frac{1}{k} \mathbf{N}_{h}^{k}(a,\tilde{a}) \right) \right\|_{F} \\ = \left\| \frac{1}{k} \mathbf{M}_{h}^{k}(o,a,\tilde{a}) - \mathbf{W} \right\|_{F} + \frac{1}{k} \left\| \mathbf{B}_{h}(a,o;\hat{\theta}) \mathbf{N}_{h}^{k}(a,\tilde{a}) - \mathbf{M}_{h}^{k}(o,a,\tilde{a}) \right\|_{F} \\ + \left\| \mathbf{B}_{h}(a,o;\hat{\theta}) \left(\mathbf{V} - \frac{1}{k} \mathbf{N}_{h}^{k}(a,\tilde{a}) \right) \right\|_{F} \\ \leq \mathcal{O} \left(\sqrt{\frac{S\iota}{k\alpha^{2}}} \right), \end{aligned}$$
(16)

where the identity follows from (*) and the last inequality follows from Corollary13 and $\hat{\theta} \in \Theta_{k+1}$.

Recall $\mathbf{V} = \mathbb{O}_h \mathbb{T}_{h-1}(\tilde{a}) \operatorname{diag}(\mu_{h-1}^k) \mathbb{O}_{h-1}^\top$ and utilize Assumption 1,

$$\begin{split} & \left\| \left(\mathbf{B}_{h}(a,o;\hat{\theta}) - \mathbf{B}_{h}(a,o;\theta^{\star}) \right) \mathbf{V} \right\|_{F} \\ \geq & \alpha \left\| \left(\mathbf{B}_{h}(a,o;\hat{\theta}) - \mathbf{B}_{h}(a,o;\theta^{\star}) \right) \mathbb{O}_{h} \mathbb{T}_{h-1}(\tilde{a}) \operatorname{diag}(\mu_{h-1}^{k}) \right\|_{F} \\ \geq & \frac{\alpha}{\sqrt{SO}} \left\| \left(\mathbf{B}_{h}(a,o;\hat{\theta}) - \mathbf{B}_{h}(a,o;\theta^{\star}) \right) \mathbb{O}_{h} \mathbb{T}_{h-1}(\tilde{a}) \operatorname{diag}(\mu_{h-1}^{k}) \right\|_{1} \\ = & \frac{\alpha}{k\sqrt{SO}} \sum_{s=1}^{S} \left\| \left(\mathbf{B}_{h}(a,o;\hat{\theta}) - \mathbf{B}_{h}(a,o;\theta^{\star}) \right) (\mathbb{O}_{h} \mathbb{T}_{h-1}(\tilde{a}))_{s} \right\|_{1} \sum_{t=1}^{k} \mathbb{P}_{\theta^{\star}}^{\pi_{t}}(s_{h-1} = s). \end{split}$$

Plugging it back into (16) completes the whole proof.

C.4 Proof of Theorem 3

In order to utilize Lemma 15 to bound the operator error in Lemma 10, we need the following algebraic transformation. Its proof is postponed to Appendix E.

Lemma 16. Let $z_k \in [0, C_z]$ and $w_k \in [0, C_w]$ for $k \in \mathbb{N}$. Define $S_k = \sum_{j=1}^k w_j$ and $S_0 = 0$. If $z_k S_{k-1} \leq C_z C_w C_0 \sqrt{k}$ for any $k \in [K]$, we have

$$\sum_{k=1}^{K} z_k w_k \le 2C_z C_w (C_0 + 1)\sqrt{K} \log(K).$$

Moreover, there exists some hard case where we have a almost matching lower bound $O\left(C_z C_w C_0 \sqrt{K}\right)$.

Now, we are ready to prove the main theorem based on Lemma 10, Lemma 15 and Lemma 16.

Theorem 3. For any $\varepsilon \in (0, H]$, there exists $K_{\max} = \text{poly}(H, S, A, O, \alpha^{-1})/\varepsilon^2$ and an absolute constant c_1 , such that for any POMDP that satisfies Assumption 1, if we set hyperparameters $\beta_k = c_1 \sqrt{k \log(KAOH)}$, $\gamma_k = \sqrt{S}\beta_k/\alpha$, and $K \ge K_{\max}$, then the output policy $\hat{\pi}$ of Algorithm 1 will be ε -optimal with probability at least 2/3.

Proof. There always exist an optimal deterministic policy π^* for the ground truth POMDP(θ^*), i.e., $V^*(\theta^*) = V^{\pi^*}(\theta^*)$. WLOG, we can always choose the greedy policy π_k to be deterministic, i.e., the probability to take any action given a history is either 0 or 1.

By Lemma 14, we have $\theta^* \in \Theta_k$ for all $k \in [K]$ with probability at least $1 - \delta$. Recall that $(\pi_k, \theta_k) =$

 $\arg \max_{\pi,\theta\in\Theta_k} V^{\pi}(\theta)$, so with probability at least $1-\delta$, we have

$$\sum_{k=1}^{K} \left(V^{\pi^{\star}}(\theta^{\star}) - V^{\pi_{k}}(\theta^{\star}) \right)$$

$$\leq \sum_{k=1}^{K} \left(V^{\pi_{k}}(\theta_{k}) - V^{\pi_{k}}(\theta^{\star}) \right)$$

$$\leq H \sum_{k=1}^{K} \sum_{[o_{H}, \tau_{H-1}] \in \mathscr{O} \times \Gamma(\pi_{k}, H-1)} \|\mathbb{P}_{\theta^{\star}}^{\pi_{k}}([o_{H}, \tau_{H-1}]) - \mathbb{P}_{\theta_{k}}^{\pi_{k}}([o_{H}, \tau_{H-1}])\|_{1}$$

$$= H \sum_{k=1}^{K} \sum_{\tau_{H-1} \in \Gamma(\pi_{k}, H-1)} \|\mathbf{b}(\tau_{H-1}; \theta^{\star}) - \mathbf{b}(\tau_{H-1}; \theta_{k})\|_{1}, \qquad (17)$$

where the identity follows from Fact 18.

Applying Lemma 10, we have

$$\sum_{\substack{\tau_{H-1}\in\Gamma(\pi_k,H-1)\\\leq\frac{\sqrt{S}}{\alpha}\|\mathbf{b}_0(\theta^{\star})-\mathbf{b}_0(\theta_k)\|_1+\frac{\sqrt{S}}{\alpha}\sum_{\substack{(a,o)\in\mathscr{A}\times\mathscr{O}\\J_k}}\|(\mathbf{B}_1(a,o;\theta_k)-\mathbf{B}_1(a,o;\theta^{\star}))\mathbf{b}_0(\theta^{\star})\|_1}{J_k}} + \frac{\sqrt{S}}{\alpha}\sum_{h=2}^{H-1}\sum_{(a,\tilde{a},o)\in\mathscr{A}\times\mathscr{O}}\sum_{s=1}^{S}\|(\mathbf{B}_h(a,o;\theta_k)-\mathbf{B}_h(a,o;\theta^{\star}))(\mathbb{O}_h\mathbb{T}_{h-1}(\tilde{a}))_s\|_1\mathbb{P}_{\theta^{\star}}^{\pi_k}(s_{h-1}=s).$$
(18)

We can bound the first two terms by Lemma 15, and obtain that with probability at least $1 - \delta$,

$$H\sum_{k=1}^{K} J_k \le \mathcal{O}\left(\frac{HSAO}{\alpha^2}\sqrt{K\iota}\right).$$
(19)

Plugging (18) and (19) into (17), we obtain

$$\sum_{k=1}^{K} \left(V^{\pi^{\star}}(\theta^{\star}) - V^{\pi_{k}}(\theta^{\star}) \right) \leq \mathcal{O}\left(\frac{HSAO}{\alpha^{2}}\sqrt{K\iota}\right) + \frac{H^{2}S^{1.5}A^{2}O}{\alpha} \max_{s,o,a,\tilde{a},h} \sum_{k=1}^{K} \left\| \left(\mathbf{B}_{h}(a,o;\theta_{k}) - \mathbf{B}_{h}(a,o;\theta^{\star}) \right) \left(\mathbb{O}_{h}\mathbb{T}_{h-1}(\tilde{a}) \right)_{s} \right\|_{1} \mathbb{P}_{\theta^{\star}}^{\pi_{k}}(s_{h-1}=s). \quad (20)$$

It remains to bound the second term.

By Lemma 15, with probability at least $1 - \delta$, for all $k \in [K]$, $\theta_k \in \Theta_k$ and $(s, o, a, \tilde{a}, h) \in \mathscr{S} \times \mathscr{O} \times \mathscr{A}^2 \times \{2, \ldots, H - 1\}$, we have

$$\underbrace{\|(\mathbf{B}_{h}(a,o;\theta_{k})-\mathbf{B}_{h}(a,o;\theta^{\star}))(\mathbb{O}_{h}\mathbb{T}_{h-1}(\tilde{a}))_{s}\|_{1}}_{Z_{k}}\sum_{t=1}^{k-1}\underbrace{\mathbb{P}_{\theta^{\star}}^{\pi_{t}}(s_{h-1}=s)}_{W_{t}} \leq \mathcal{O}\left(\sqrt{\frac{kS^{2}O\iota}{\alpha^{4}}}\right).$$
 (21)

By simple calculation, we have $z_k \leq \sqrt{S}/\alpha$. Invoking Lemma 16 with (21), we obtain

$$\sum_{k=1}^{K} w_k z_k \le \mathcal{O}\left(\frac{\sqrt{S^3 O\iota}}{\alpha^3} \sqrt{K} \log(K)\right).$$
(22)

Plugging (22) back into (20) gives

$$\sum_{k=1}^{K} \left(V^{\pi^{\star}}(\theta^{\star}) - V^{\pi_{k}}(\theta^{\star}) \right) \leq \mathcal{O}\left(\frac{H^{2}S^{3}A^{2}O^{1.5}\sqrt{\iota}}{\alpha^{4}}\sqrt{K}\log(K) \right).$$
(23)

Finally, choosing

$$K_{\max} = \mathcal{O}\left(\frac{H^4 S^6 A^4 O^3 \log(HSAO/\varepsilon)}{\alpha^8 \varepsilon^2}\right),$$

and outputting a policy from $\{\pi_1, \ldots, \pi_K\}$ uniformly at random complete the proof.

D Learning POMDPs with Deterministic Transition

In this section, we introduce a computationally and statistically efficient algorithm for POMDPs with deterministic transition. A sketched proof is provided.

We comment that some previous works have studied POMDPs with deterministic transitions or deterministic emission process assuming the model is *known* (e.g. [4, 5, 6]); their results mainly focus on the planning aspect. In contrast, we assume *unknown* models which requires to learn the transition and emission process first. It is also worth mentioning that the (quasi)-deterministic POMDPs defined in these works are not exactly the same as ours. For example, the deterministic POMDPs in [6] refer to those with stochastic initial state but deterministic emission process, while we assume deterministic initial state but stochastic emission process. Therefore, their computational hardness results do not conflict with the efficient algorithm in this section.

Algorithm 2 Learning POMDPs with Deterministic Transition

1: initialize
$$N = C \log(HSA/p)/(\min\{\epsilon/(\sqrt{OH}), \xi\})^2$$
, $n_h = \mathbf{1}(h = 1)$ for all $h \in [H]$.
2: for $h = 1, \ldots, H - 1$ do
3: for $(s, a) \in [n_h] \times \mathscr{A}$ do
4: Reset $z \leftarrow \mathbf{0}_{O \times 1}$ and $t \leftarrow n_{h+1} + 1$
5: for $i \in [N]$ do
6: execute policy $\pi_h(s)$ from step 1 to step $h - 1$, take action a at h^{th} step and observe o_{h+1}
8: for $s' \in [n_{h+1}]$ do
9: if $\|\phi_{h+1,s'} - z\|_2 \le 0.5\xi$ then
10: $t \leftarrow s'$
11: if $t = n_{h+1} + 1$ then
12: $n_{h+1} \leftarrow n_{h+1} + 1$
13: $\phi_{h+1,n_{h+1}} \leftarrow z$ and $\pi_{h+1}(n_{h+1}) \leftarrow a \circ \pi_h(s)$
14: Set the s^{th} column of $\hat{\mathbb{T}}_{h,a}$ to be e_t
15: output $\hat{\mu}_0 = e_1$ and $\{n_h, \{\hat{\mathbb{T}}_{h,a}\}_{a \in \mathscr{A}}$ and $\{\phi_{h,i}\}_{i \in [n_h]}$: $h \in [H]\}$

Theorem 4. For any $p \in (0, 1]$, there exists an algorithm such that for any deterministic transition POMDP satisfying Assumption 2, within $\mathcal{O}\left(H^2SA\log(HSA/p)/(\min\{\varepsilon/(\sqrt{O}H),\xi\})^2\right)$ samples and computations, the output policy of the algorithm is ε -optimal with probability at least 1 - p.

Proof. The algorithm works by inductively finding all the states we can reach at each step, utilizing the property of deterministic transition and good separation between different observation vectors. We sketch a proof based on induction below.

We say a state s is h-step reachable if there exists a policy π s.t. $\mathbb{P}^{\pi}(s_h = s) = 1$. In our algorithm, we use n_h to denote the number of h-step reachable states. All the policies mentioned below is a sequence of fixed actions (independent of observations).

Suppose at step h, there are n_h h-step reachable states and we can reach the s^{th} one of them at the h^{th} step by executing a *known* policy $\pi_h(s)$. Note that for every state s' that is (h + 1)-step reachable, there must exist some state s and action a s.t. s is h-step reachable and $\mathbb{T}_h(s' \mid s, a) = 1$. Therefore, based on our induction assumption, we can reach all the (h + 1)-step reachable states by executing all $a \circ \pi_h(s)$ for $(a, s) \in \mathscr{A} \times [n_h]$.

Now the problem is how to tell if we reach the same state by executing two different $a \circ \pi_h(s)$'s. The solution is to look at the distribution of o_{h+1} . Because the POMDP has deterministic transition, we always reach the same state when executing the same $a \circ \pi_h(s)$ and hence the distribution of o_{h+1} is exactly the distribution of observation corresponding to that state. By Hoeffding's inequality, for each fixed $a \circ \pi_h(s)$, we can estimate the distribution of o_{h+1} with ℓ_2 -error smaller than $\xi/8$ with high probability using $N \ge \tilde{\Omega}(1/\xi^2)$ samples. Since the observation distributions of two different states have ℓ_2 -separation no smaller than ξ , we can tell if two different $a \circ \pi_h(s)$'s reach the same state by looking at the distance between their distributions of o_{h+1} . For those policies reaching the same state, we only need to keep one of them, so there are at most S policies kept $(n_{h+1} \le S)$.

By repeating the argument inductively from h = 1 to h = H, we can recover the exact transition dynamics $\mathbb{T}_h(\cdot | s, a)$ and get an high-accuary estimate of $\mathbb{O}_h(\cdot | s)$ for every *h*-step reachable state *s* and all $(h, a) \in [H] \times \mathscr{A}$ up to permutation of states. Since the POMDP has deterministic transition, we can easily find the optimal policy of the estimated model by dynamic programming.

The ϵ -optimality simply follows from the fact that when $N \geq \tilde{\Omega}(H^2O/\epsilon^2)$, we have the estimated distribution of observation for each state being $\mathcal{O}(\epsilon/H)$ accurate in ℓ_1 -distance for all reachable states. This implies that the optimal policy of the estimated model is at most $\mathcal{O}(\epsilon/H) \times H = \mathcal{O}(\epsilon)$ suboptimal. The overall sample complexity follows from our requirement $N \geq \max{\{\tilde{\Omega}(H^2O/\epsilon^2), \tilde{\Omega}(1/\xi^2)\}}$, and the fact we need to run N episodes for each $h \in [H], s \in \mathcal{S}, a \in \mathcal{A}$.

E Auxiliary Results

E.1 Derivation of equation (2)

When conditioning on a fixed action sequence $\{a_{H-1}, \ldots, a_1\}$, a POMDP will reduce to a non-stationary HMM, whose transition matrix and observation matrix at h^{th} step are $\mathbb{T}_h(a_h)$ and \mathbb{O}_h , respectively. So $\mathbb{P}(o_H, \ldots, o_1 | a_{H-1}, \ldots, a_1)$ is equal to the probability of observing $\{o_H, \ldots, o_1 | a_{H-1}, \ldots, a_1\}$ in this particular HMM. Using the basic properties of HMMs, we can easily express $\mathbb{P}(o_H, \ldots, o_1 | a_{H-1}, \ldots, a_1)$ in terms of the

transition and observation matrices

$$\mathbb{O}_{H}(o_{H}|\cdot) \cdot [\mathbb{T}_{H-1}(a_{H-1})\operatorname{diag}(\mathbb{O}_{H-1}(o_{H-1}|\cdot))] \cdots [\mathbb{T}_{1}(a_{1})\operatorname{diag}(\mathbb{O}_{1}(o_{1}|\cdot))] \cdot \mu_{1}$$

Recall the definition of operators

$$\mathbf{B}_{h}(a,o) = \mathbb{O}_{h+1}\mathbb{T}_{h}(a)\operatorname{diag}(\mathbb{O}_{h}(o|\cdot))\mathbb{O}_{h}^{\dagger}, \qquad \mathbf{b}_{0} = \mathbb{O}_{1}\mu_{1},$$

and $\mathbb{O}_{h}^{\dagger}\mathbb{O}_{h} = \mathbf{I}_{S}$, we conclude that

$$\mathbb{P}(o_H, \dots, o_1 | a_{H-1}, \dots, a_1) = \mathbf{e}_{o_H}^\top \cdot \mathbf{B}_{H-1}(a_{H-1}, o_{H-1}) \cdots \mathbf{B}_1(a_1, o_1) \cdot \mathbf{b}_0.$$

E.2 Derivation of equation (6)

Note that π is a deterministic policy and $\Gamma(\pi, H)$ is a set of all the observation and action sequences of length H that could occur under policy π , i.e., for any $\tau_H = (o_H, \ldots, a_1, o_1) \in \Gamma(\pi, H)$, we have $\pi(a_{H-1}, \ldots, a_1 \mid o_H, \ldots, o_1) = 1$, and $\pi(a'_{H-1}, \ldots, a'_1 \mid o_H, \ldots, o_1) = 0$ for any action sequence $(a'_{H-1}, \ldots, a'_1) \neq (a_{H-1}, \ldots, a_1)$. Therefore, for $\tau_H \in \Gamma(\pi, H)$, we have:

$$\begin{split} \mathbb{P}_{\theta}^{\pi}(o_{H},\ldots,o_{1}) &= \sum_{a_{H-1}'\in\mathscr{A}} \cdots \sum_{a_{1}'\in\mathscr{A}} \mathbb{P}_{\theta}^{\pi}(o_{H},a_{H-1}',\ldots,a_{1}',o_{1}) \\ &= \mathbb{P}_{\theta}^{\pi}(o_{H},a_{H-1},\ldots,a_{1},o_{1}) \\ &= \left[\prod_{h=1}^{H-1} \pi(a_{h} \mid o_{h},a_{h-1},\ldots,a_{1},o_{1})\right] \cdot \left[\prod_{h=1}^{H} \mathbb{P}_{\theta}(o_{h} \mid a_{h-1},o_{h-1},\ldots,a_{1},o_{1})\right] \\ &= \prod_{h=1}^{H} \mathbb{P}_{\theta}(o_{h} \mid a_{h-1},o_{h-1},\ldots,a_{1},o_{1}) \\ &= \mathbb{P}_{\theta}(o_{H},\ldots,o_{1} \mid a_{H-1},\ldots,a_{1}). \end{split}$$

E.3 Boosting the success probability

We can run Algorithm 1 independently for $n = O(\log(1/\delta))$ times and obtain n policies. Each policy is independent of others and is ε -optimal with probability at least 2/3. So with probability at least $1 - \delta/2$, at least one of them will be ε -optimal. In order to evaluate their performance, it suffices to run each policy for $O(\log(n/\delta)H^2/\varepsilon^2)$ episodes and use the empirical average of the cumulative reward as an estimate. By standard concentration argument, with probability at least $1 - \delta/2$, the estimation error for each policy is smaller than ε . Therefore, if we pick the policy with the best empirical performance, then with probability at least $1 - \delta$, it is 3ε -optimal. Rescaling ε gives the desired accuracy. It is direct to see that the boosting procedure will only incur an additional polylog $(1/\delta)$ factor in the final sample complexity, and thus will not hurt the optimal dependence on ε .

E.4 Basic facts about POMDPs and the operators

In this section, we provide some useful facts about POMDPs. Since their proofs are quite straightforward, we omit them here.

The following fact gives two linear equations the operators always satisfy. Its proof simply follows from the definition of the operators and Fact 11.

Fact 17. In the same setting as Fact 11, suppose Assumption 1 holds, then we have

$$\begin{cases} \mathbb{P}(o_h = \cdot, o_{h-1} = \cdot) \mathbf{e}_o = \mathbf{B}_h(\tilde{a}, o; \theta) \mathbb{P}(o_{h-1} = \cdot), \\ \mathbb{P}(o_{h+1} = \cdot, o_h = o, o_{h-1} = \cdot) = \mathbf{B}_h(a, o; \theta) \mathbb{P}(o_h = \cdot, o_{h-1} = \cdot) \end{cases}$$

The following fact relates (unnormalized) belief states to distributions of observable sequences. Its proof follows from simple computation using conditional probability formula and $\mathbb{O}_{h}^{\dagger}\mathbb{O}_{h} = \mathbf{I}_{S}$.

Fact 18. For any POMDP(θ) satisfying Assumption 1, deterministic policy π and $[o_h, \tau_{h-1}] \in \mathscr{O} \times \Gamma(\pi, h-1)$, we have

$$\mathbf{e}_{o_h}^{\top} \mathbf{b}(\tau_{h-1}; \theta) = \mathbb{P}_{\theta}^{\pi}([o_h, \tau_{h-1}]),$$

where $\mathbb{P}^{\pi}_{\theta}([o_h, \tau_{h-1}])$ is the probability of observing $[o_h, \tau_{h-1}]$ when executing policy π in POMDP(θ).

E.5 Proof of Lemma 16

Proof. WLOG, assume $C_z = C_w = 1$. Let $n = \min\{k \in [K] : S_k \ge 1\}$. We have

$$\sum_{k=1}^{K} z_k w_k = \sum_{k=1}^{n} z_k w_k + \sum_{k=n+1}^{K} z_k w_k \le \sum_{k=1}^{n} w_k + \sum_{k=n+1}^{K} z_k w_k$$
$$= S_n + \sum_{k=n+1}^{K} z_k w_k$$
$$\le 2 + \sum_{k=n+1}^{K} z_k w_k.$$

It remains to bound the second term. Using the condition that $z_k S_{k-1} \leq C_0 \sqrt{k}$ for all $k \in [K]$, we have $z_k \leq \frac{C_0 \sqrt{k}}{S_{k-1}}$ for all $k \in [K]$ and $i \in [m]$. Therefore,

$$\begin{split} \sum_{k=n+1}^{K} z_k w_k &\leq \sum_{k=n+1}^{K} C_0 \sqrt{k} \frac{w_k}{S_{k-1}} \\ &\leq C_0 \sqrt{K} \sum_{k=n+1}^{K} \frac{w_k}{S_{k-1}} \\ &\stackrel{(a)}{\leq} 2C_0 \sqrt{K} \sum_{k=n+1}^{K} \log(\frac{S_k}{S_{k-1}}) \\ &= 2C_0 \sqrt{K} \log(\frac{S_K}{S_n}) \leq 2C_0 \sqrt{K} \log(K), \end{split}$$

where (a) follows from $x \le 2\log(x+1)$ for $x \in [0,1]$.