Model-Based Reinforcement Learning in Contextual Decision Processes

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Abstract

We study the sample complexity of model-based reinforcement learning in general contextual decision processes. We design new algorithms for RL with an abstract model class and analyze their statistical properties. Our algorithms have sample complexity governed by a new structural parameter called the \textit{witness rank}, which we show to be small in several settings of interest, including Factored MDPs and reactive POMDPs. We also show that the witness rank of a problem is never larger than the recently proposed \textit{Bellman rank} parameter governing the sample complexity of the model-free algorithm $\text{O}_{\text{LIVE}}$ (Jiang et al., 2017), the only other provably sample efficient algorithm at this level of generality. Focusing on the special case of Factored MDPs, we prove an exponential lower bound for all model-free approaches, including $\text{O}_{\text{LIVE}}$, which when combined with our algorithmic results demonstrates exponential separation between model-based and model-free RL in some rich-observation settings.

1 Introduction

Algorithms for reinforcement learning can be broadly categorized into model-based and model-free methods. Methods in the former family explicitly model the environment dynamics and then use planning techniques to find a near-optimal policy. In contrast, the latter family models much less, typically only what is needed to succinctly represent an optimal policy and its reward. Algorithms from both families have seen substantial empirical success, but we lack a rigorous understanding of the tradeoffs between them, making algorithm selection difficult for practitioners. This paper provides a new understanding of these tradeoffs, via a comparative analysis between model-based and model-free methods in general RL environments.

Conventional wisdom and intuition suggests that model-based methods are more sample-efficient than model-free methods, since they leverage more supervision. This argument is supported by classical control-theoretic settings like the linear-quadratic regulator, where state-of-the-art model-based methods have better dimension dependence than contemporary model-free ones (although no formal separation is known). On the other hand, since models typically have more degrees of freedom (e.g., parameters) and can waste effort on unimportant elements of the environment, one might suspect that model-free methods have better statistical properties. Indeed, recent work in tabular Markov Decision Processes (MDPs) suggest that there is almost no sample-efficiency gap between the two families (Jin et al., 2018). Even worse, in the rich environments of interest, where function approximation is essential, the only algorithms with sample-complexity guarantees are model-free (Jiang et al., 2017). In such environments, which of these competing perspectives applies?

To answer this question, we study model-based reinforcement learning in general episodic contextual decision processes (CDPs) where a rich high-dimensional observation is used for decision making (Jiang et al., 2017).
et al., 2017). We assume the algorithm is given access to a class \( \mathcal{M} \) of models of the environment and that the true environment dynamics are representable by the class. Under such assumptions our main thesis is:

*Model-based methods rely on stronger function-approximation capabilities but can be exponentially more sample efficient than model-free counterparts.*

Our contributions provide evidence for this thesis and can be summarized as follows:

1. We show that there exist MDPs where (1) all model-free methods must suffer \( \Omega(\exp(H)) \) sample complexity, where \( H \) is the horizon, and (2) there exist model-based methods with polynomial sample complexity. In fact, these MDPs belong to the well-studied class of Factored MDPs (Kearns and Koller, 1999), which we use as a running example throughout the paper.

2. We design a new model-based algorithm for general CDPs and analyze its sample complexity. We show that the algorithm has sample complexity governed by a new structural parameter, the *witness rank*, which we further show to be small in many concrete settings, including tabular and low rank MDPs, reactive POMDPs, and reactive PSRs, among others. This algorithm is the first provably-efficient model-based algorithm that does not rely on tabular representations or highly structured control-theoretic settings.

3. We compare our new algorithm and the witness rank with the model-free algorithm OLIVE (Jiang et al., 2017) and the Bellman rank, the only available algorithm and structural parameter at this level of generality. We show that the witness rank is never larger than the Bellman rank, but that it can be much smaller. In particular, our algorithm has polynomial sample complexity in Factored MDPs, which represents an exponential improvement over OLIVE and any model-free algorithm.

The caveat in our thesis is that model-based methods rely on strong realizability assumptions. In the rich environments we study, where function approximation is essential, some form of realizability is necessary (see Proposition 1 in Krishnamurthy et al. (2016)), but our model-based realizability assumption (See Assumption 1) is strictly stronger than prior value-based analogs (Antos et al., 2008; Krishnamurthy et al., 2016; Jiang et al., 2017). On the other hand, our sample complexity bounds precisely quantify the tradeoffs between model-based and model-free approaches, which may guide empirical efforts.

### 2 Related Work

A number of sample-efficient RL approaches exist for tabular MDPs (Kearns and Singh, 2002; Jaksch et al., 2010; Dann and Brunskill, 2015; Szita and Szepesvári, 2010; Azar et al., 2017; Jin et al., 2018), and while most of these algorithms are model-based, model-free methods also exist (e.g., Strehl et al., 2006). Indeed, recently Jin et al. (2018) showed that a variant of Q-learning with optimistic initialization — a model-free algorithm — has regret that is at most a \( \sqrt{H} \)-factor worse than the information-theoretic limit, demonstrating that the two algorithmic families can differ by at most this small factor. Our work departs from this line in that we focus on more realistic rich-observation settings.\(^1\)

Turning to MDPs with large or continuous state spaces, the results diverge considerably. With linear function approximation, Parr et al. (2008) show an equivalence between model-free and model-based RL from an approximation perspective (i.e., without realizability), but they focus on the batch setting and do not address exploration issues, which is our focus. For Factored MDPs, Kearns and Koller (1999) and later Osband and Van Roy (2014b) obtain polynomial sample complexity via model-based methods, and, as we show here, no provably-efficient model-free algorithms can exist. For the Linear Quadratic Regulator,

\(^1\)In fact, our information-theoretic definition of model-free methods (Definition 1 below) is not interesting in the tabular setting.
model-based algorithms (Abbasi-Yadkori and Szepesvári, 2011; Dean et al., 2018) are polynomially better
than the best known model-free methods (Tu and Recht, 2017; Abbasi-Yadkori et al., 2018), but there is
no lower bound separating these families of algorithms. Finally, for Lipschitz-continuous MDPs in general
metric spaces, all known algorithms are model based (Kakade et al., 2003; Ortner and Ryabko, 2012; Pazis
and Parr, 2013; Lakshmanan et al., 2015). Our work provides several new results for specific models: (1) we
formally show statistical separation between model-based and model free methods for Factored MDPs, (2)
we expect that our algorithm or natural variants have polynomial sample complexity in many of these specific
settings.

In more abstract settings, on the model-free side, Wen and Van Roy (2013); Krishnamurthy et al.
(2016); Dann et al. (2018) obtain sample-efficient algorithms for environments with rich high-dimensional
observations but with some determinism in the transition dynamics. Jiang et al. (2017) address a more general
class of environments — all CDPs (whose dynamics may be fully stochastic) with low Bellman rank — and
propose a model-free algorithm with sample complexity scaling quadratically with the Bellman rank. Our
work can be seen as a model-based analog to Jiang et al. (2017), and, in addition, we provide a rigorous
comparison between model-based and model-free methods in general rich-observation settings.

On the model-based side, Lattimore et al. (2013) and Osband and Van Roy (2014a) obtain sample
complexity guarantees; the former makes no assumptions but the guarantee scales linearly with the model
class size, and the latter makes continuity assumptions and scales with the eluder dimension, which is only
known to be small for specific function classes. In comparison, we introduce a natural structural measure,
the witness rank, which is small in many settings, and our bounds scale with standard statistical complexity
notions.

On the empirical side, models are often used to speed up learning (see e.g., Aboaf et al., 1989; Deisenroth
et al., 2011, for classical references in robotics). Such results provide empirical evidence that models can be
statistically valuable, which complement our theoretical results.

Finally, it is worth mentioning two recent papers on model-based RL with some technical similarities to
our work. Farahmand et al. (2017) use a definition similar to our witnessed model misfit, but their analysis is
restricted to test functions that form a ball in an Reproducing Kernel Hilbert Space (RKHS), and they do
not obtain a sample-efficient algorithm. Xu et al. (2018) use average Bellman error to detect discrepancy
between a candidate model and the truth, as we also do in Algorithm 1, but their algorithm involves local
policy improvement and cannot find a globally optimal policy in a sample-efficient manner. In contrast, we
derive sample-efficient algorithms with global optimality guarantees in very general settings.

3 Preliminaries

We study Contextual Decision Processes (CDPs), a general sequential decision making setting where the agent
optimizes long-term reward by learning a policy that directly maps from rich observations (e.g., raw-pixel
images) to actions. The term CDP was originally proposed by Krishnamurthy et al. (2016) and extended by
Jiang et al. (2017), where the authors show that CDPs capture a broad class of RL problems which allow very
rich observation spaces while still allowing for tractable solutions, including (Partially Observable) Markov
Decision Processes, Predictive State Representations, and Linear Quadratic Regulators. Please see Jiang et al.
(2017) for further background.

Notation. For $N \in \mathbb{N}$ we use $[N] \triangleq \{1, \ldots, N\}$. For a set $S$, $\Delta(S)$ denotes the set of distributions over $S$, and $U(S)$ is the uniform distribution over $S$. For a function $f : S \to \mathbb{R}$, $\|f\|_\infty$ denotes $\sup_{s \in S} |f(s)|$.  

3
3.1 Basic Definitions

Let $H \in \mathbb{N}$ denote a time horizon and let $\mathcal{X}$ be a large context space of unbounded size, partitioned into subsets $\mathcal{X}_1, \ldots, \mathcal{X}_H$. A finite horizon episodic CDP is a tuple $(\mathcal{X}, \mathcal{A}, R, P)$ consisting of a (partitioned) context space $\mathcal{X}$, an action space $\mathcal{A}$, a transition operator $P : \{\bot\} \cup (\mathcal{X} \times \mathcal{A}) \to \Delta(\mathcal{X})$, and a reward function $R : \mathcal{X} \times \mathcal{A} \to \Delta(\mathcal{R})$ with $\mathcal{R} \subseteq [0, 1]$. We assume a layered Markovian structure, so that for any $h \in [H - 1]$, $x_h \in \mathcal{X}_h$ and $a \in \mathcal{A}$, the future context and the reward distributions are characterized by $x_h, a$ and moreover $P_{x_h,a} \triangleq P(x_h, a) \in \Delta(\mathcal{X}_{h+1})$. We use $P_0 \triangleq P(\bot) \in \Delta(\mathcal{X}_1)$ to denote the initial context distribution, and we assume $|\mathcal{A}| = K$ throughout.\footnote{Note that partitioning the context space by time allows us to capture more general time-dependent dynamics, reward, and policy.}

A policy $\pi : \mathcal{X} \to \Delta(\mathcal{A})$ maps each context to a distribution over actions. By executing this policy in the CDP for $h - 1$ steps, we naturally induce a distribution over $\mathcal{X}_h$, and we use $\mathbb{E}_{x_h \sim \pi}[:,]$ to denote the expectation with respect to this distribution. A policy $\pi$ has associated value and action-value functions $V^\pi : \mathcal{X} \to \mathbb{R}^+$ and $Q^\pi : \mathcal{X} \times \mathcal{A} \to \mathbb{R}^+$, defined as

$$\forall h \in [H], \forall x \in \mathcal{X}_h : V^\pi(x) \triangleq \mathbb{E}_{\pi} \left[ \sum_{t=h}^{H} r_t | x_h = x \right], \quad Q^\pi(x, a) \triangleq \mathbb{E}_{r \sim R(x,a)} [r] + \mathbb{E}_{x' \sim P_{x,a}} [V^\pi(x')] ,$$

Here, the expectation is over randomness in the environment and the policy, with all actions sampled by $\pi$. Note that we do not index $V$ and $Q$ by the time point, since it is always encoded in the context. The value of a policy $\pi$ is $v^\pi \triangleq \mathbb{E}_{x \sim P_0} [V^\pi(x)]$ and the goal is to find a policy $\pi$ that maximizes $v^\pi$.

For regularity, we assume that almost surely $\sum_{h=1}^{H} r_h \leq 1$.

Running Example. As a running example, we consider Factored MDPs (Kearns and Koller, 1999). Let $d \in \mathbb{N}$ and let $\mathcal{O}$ be a small finite set. Define the context space $\mathcal{X} \triangleq [H] \times \mathcal{O}^d$, with the natural partition by time. For a state $x \in \mathcal{X}$ we use $x[i]$ for $i \in [d]$ to denote the value of $x$ on the $i$th state variable (ignoring the time step $h$), and similar notation for a subset of state variables. For each state variable $i \in [d]$, the parents of $i$, $\text{pa}_i \subseteq [d]$ are the subset of state variables that directly influence $i$. In Factored MDPs, the transition dynamics $P$ factorize according to the parent relationships:

$$\forall h, x \in \mathcal{X}_h, x' \in \mathcal{X}_{h+1}, a \in \mathcal{A}, \quad P(x' | x, a) = \prod_{i=1}^{d} P^{(i)}[x'[i] | x[\text{pa}_i], a, h]$$ \hspace{1cm} (1)

for conditional distributions $\{P^{(i)}\}_{i=1}^{d}$ of the appropriate dimensions. Note that we always condition on the time point $h$ to allow for non-stationary transitions. This factored transition operator has $L \triangleq \sum_{i=1}^{d} HK \cdot |\mathcal{O}|^{1+|\text{pa}_i|}$ parameters, which can be much smaller than $dHK|\mathcal{O}|^{1+d}$ for an unfactored process on $|\mathcal{O}|^d$ states.\footnote{Actually the full unfactored process has $HK|\mathcal{O}|^{2d}$ parameters. Here we are assuming that the state variables are conditionally independent given the previous state and action.} As such when $|\text{pa}_i|$ is small for all $i$, we can expect algorithms with low-sample complexity. Indeed Kearns and Koller (1999) show that Factored MDPs can be PAC learned with $\text{poly}(H, K, L, \epsilon, \log(1/\delta))$ samples.

3.2 Model Class

Since we are interested in general CDPs with large state spaces, we equip model-based algorithms with a class $\mathcal{M}$ consisting of a large but finite number of models.\footnote{As we will see, extensions to infinite classes with bounded statistical complexity are straightforward.} Each model $M \triangleq (R, P)$ consists of an instantaneous reward function: $R : \mathcal{X} \times \mathcal{A} \to \Delta(\mathcal{R})$, and transition dynamics $P : \{\bot\} \cup \mathcal{X} \times \mathcal{A} \to \Delta(\mathcal{X})$. The environment reward and dynamics are called the true model and denoted $M^* \triangleq (R^*, P^*)$. For any model...
$M \in \mathcal{M}$, $\pi_M$, $V_M$, $Q_M$, and $v_M$ are the optimal policy, value function, action-value function, and value \textit{in the model} $M$, respectively. These objects can all be computed directly from $M$, without any interaction from the environment. For the true model $M^*$, these quantities are denoted $\pi^*$, $V^*$, $Q^*$, $v^*$, suppressing subscripts. For $M \triangleq (R, P)$, we denote $(r, x') \sim M_{a,a}$ as sampling a reward and next context from model $M$: $r \sim R(x, a), x' \sim P_{x,a}$. We use $x_h \sim \pi$ to denote a state being sampled by executing $\pi$ in the true environment $M^*$ for $h - 1$ steps.

We use $\mathcal{OP}$ (for Optimal Planning) to represent the operator that maps from a model $M$ to its optimal $Q$ function, that is $\mathcal{OP}(M) \triangleq Q_M$. We denote $\mathcal{OP}(\mathcal{M})$ as the set of $Q$ functions derived from the class $\mathcal{M}$:

$$\mathcal{OP}(\mathcal{M}) = \{Q: \exists M \in \mathcal{M} \text{ s.t. } \mathcal{OP}(M) = Q\}.$$ 

Throughout the paper, when we compare model-based approaches to model-free methods, we use $\mathcal{M}$ as input for former and $\mathcal{OP}(\mathcal{M})$ for the latter.

We assume the model class satisfies a natural realizability condition.

\textbf{Assumption 1 (Realizability of $\mathcal{M}$).} We assume the model class $\mathcal{M}$ contains the true model $M^*$.

\textbf{Running Example.} For Factored MDPs, it is standard to further assume the factorization, formally $p_{i,a}$ for all $i \in [d]$, and the reward function are known (Kearns and Koller, 1999). Thus all models in $\mathcal{M}$ share the same reward, and the natural model class $\mathcal{M}$ is just the set of all transition dynamics of the form (1), which obey the factorization. While this class is infinite, it admits an $\ell_\infty$ cover at scale $\varepsilon$ of size $\varepsilon^{-L}$, so it can be effectively treated as a finite class (See, e.g., Chapter 27 in Shalev-Shwartz and Ben-David, 2014).

\section{Why Model-based RL?}

This section contains our first main result, which establishes that model-based methods can be \textit{exponentially} more sample-efficient than model-free ones. To our knowledge, this is the first result of this form.

To show such separation, we must prove a lower bound against all model-free methods, and, to do so, we first formally define this class of algorithms. Strehl et al. (2006) define model-free algorithms to be those with $O(|X|^2|A|)$ space, but this definition is specialized to the tabular setting and provides little insight for algorithms employing function approximation. In contrast, our definition is information-theoretic: Intuitively, a model-free algorithm does not operate on the context $x$ directly, but rather through the evaluations of an action-value function class $\mathcal{Q}$. Formally:

\textbf{Definition 1 (Model-free algorithm).} \textit{Given a (finite) function class $\mathcal{Q}: (X \times A) \rightarrow \mathbb{R}$, define the $Q$-projection $\Phi_\mathcal{Q}: X \rightarrow \mathbb{R}^{|\mathcal{Q}| \times |A|}$ by $\Phi_\mathcal{Q}(x) \rightarrow [Q(x, a)]_{Q \in \mathcal{Q}, a \in A}$. An algorithm is model-free using $\mathcal{Q}$ if it accesses $x$ exclusively through $\Phi_\mathcal{Q}(x)$ for all $x \in X$ during its entire execution.}

This definition agrees with an intuitive notion of model-free algorithms, and captures algorithms such as OLIVE (Jiang et al., 2017), optimistic $Q$-learning (Jin et al., 2018), and Delayed $Q$-learning (Strehl et al., 2006). In fact, in Appendix E, we show that for tabular environments with a fully expressive $\mathcal{Q}$ class, the underlying context/state can be recovered from the $Q$-projection, and hence Definition 1 introduces no restriction whatsoever in this setting. However, beyond tabular settings, the $Q$-projection can obfuscate the true context from the agent and may even introduce partial observability. This can lead to a significant loss of information, which can have a dramatic effect on the sample complexity of RL. Such information loss is formalized in the following theorem.

\textbf{Theorem 1.} Fix $\delta, \varepsilon \in (0, 1]$. There exists a family of CDPs with horizon $H$, all with the same reward function, and a class of models $\mathcal{M}$ with $|\mathcal{M}| \leq 2^H$, such that for each CDP, $M^* \in \mathcal{M}$ and
1. For any CDP in the family, with probability at least \(1 - \delta\), a model-based algorithm (namely Algorithm 3, in Appendix C) outputs a policy \(\hat{\pi}\) satisfying \(v_\hat{\pi} \geq v^* - \epsilon\) using at most \(\text{poly}(H, 1/\epsilon, \log(1/\delta))\) samples.

2. With \(Q = \mathcal{O}(\mathcal{M})\) as the Q-function class, any model-free algorithm using \(o(2^H)\) trajectories outputs a policy \(\hat{\pi}\) with \(v_\hat{\pi} < v^* - 1/2\) with probability at least 1/3.

See Appendix D.2 for the proof. Informally, the result shows that model-based methods can be exponentially more sample-efficient than any model-free method. To our knowledge, this is the first separation result for these families of algorithms. Indeed, even the definition of model-free methods is new here.

Note that since \(M^* \in \mathcal{M}\) for each CDP in the family, we also have \(Q^* \in \mathcal{O}(\mathcal{M})\). This latter value-function realizability assumption is standard in model-free reinforcement learning with function approximation (Jiang et al., 2017; Antos et al., 2008), but the model-based analog, that \(M^* \in \mathcal{M}\), can be substantially stronger. As such, model-based methods operating under this realizability notion typically require more powerful function approximation than model-free methods. Thus, while Theorem 1 formalizes an argument in favor of model-based methods, realizability considerations provide an important caveat.

Running Example. The construction in the proof of Theorem 1 is a simple Factored MDP with \(d = H\), \(|\mathcal{O}| = 4\), \(|p_{a,x}| = 1\) for all \(i\), and deterministic dynamics. As we will see, our algorithm has polynomial sample complexity in all Factored MDPs (and a broad class of other environments).

On the other hand, the theorem shows that model-free methods cannot succeed in Factored MDPs. To our knowledge, no information theoretic lower bounds are known for Factored MDPs, but the result does agree with existing computational and representational barriers, namely (a) that \(Q^*\) and \(\pi^*\) may not factorize (Guestrin et al., 2003), (b) that planning in factored MDPs is NP-hard (Mundhenk et al., 2000), and (c) that the optimal policy \(\pi^*\) cannot be represented by a polynomially sized Boolean circuit (Allender et al., 2003). Our result provides a new form of hardness, namely statistical complexity, for model-free RL in Factored MDPs.

5 Witnessed Model Misfit

In this section we introduce witnessed model misfit, a measure of model error, which we will later use to eliminate candidate models in our algorithm.

To verify the validity of a candidate model, a natural idea is to compare the samples from the environment with synthetic samples generated from a model \(M\). To formalize this comparison approach, we use Integral Probability Metrics (IPM) (Müller, 1997): for two probability distributions \(P_1, P_2 \in \Delta(\mathcal{X})\) and a function class \(\mathcal{F} : \mathcal{X} \to \mathbb{R}\) that is symmetric (i.e. if \(f \in \mathcal{F}\) then \(-f \in \mathcal{F}\) also holds), the IPM with respect \(\mathcal{F}\) is

\[
\sup_{f \in \mathcal{F}} \mathbb{E}_{x \sim P_1}[f(x)] - \mathbb{E}_{x \sim P_2}[f(x)].
\]

In words, we search for a test function from \(\mathcal{F}\) whose expectation under \(P_1\) is maximally different from the expectation under \(P_2\). We use IPMs to define witnessed model misfit.

Definition 2 (Witnessed Model Misfit). For a class \(\mathcal{F} : \mathcal{X} \times \mathcal{A} \times \mathcal{R} \times \mathcal{X} \to \mathbb{R}\), two models \(M, M' \in \mathcal{M}\) and a time step \(h \in [H]\), the Witnessed Model Misfit of \(M'\) as witnessed by \(M\) at level \(h\) is:

\[
\mathcal{W}(M, M', h) \triangleq \max_{f \in \mathcal{F}} \mathbb{E}_{x_h \sim p_M, a_h \sim \pi_M} \left[ \mathbb{E}_{(r,x') \sim M_h}[f(x_h, a_h, r, x')] - \mathbb{E}_{(r,x') \sim M'_h}[f(x_h, a_h, r, x')] \right],
\]

where for model \(M = (R, P)\), \((r, x') \sim M_h\) is shorthand for \(r \sim R_{x_h, a_h}, x' \sim P_{x_h, a_h}\).
The IPM (Gretton et al., 2012; Sriperumbudur et al., 2012).

In this case, witnessed model misfit reduces to Maximum Mean Discrepancy (MMD)—a special instance of IPM (Gretton et al., 2012; Sriperumbudur et al., 2012).

**Example** (Total Variation). When $\mathcal{F} = \{f : \|f\|_\infty \leq 1\}$, the witnessed model misfit becomes

$$W(M, M', h) = \mathbb{E} \left[ \left\| P'_{x,h,a_h} \circ R'_{x,h,a_h} - P^*_{x,h,a_h} \circ R^*_{x,h,a_h} \right\|_{TV} \mid x_h \sim \pi_M, a_h \sim \pi_M' \right] ,$$

(3)

where $P_{x,a} \circ R_{x,a}$ is the distribution over $\mathcal{X} \times \mathcal{R}$ with $x' \sim P_{x,a}, r \sim R_{x,a}$ independently. This is just the total variation distance\(^5\) between $P' \circ R'$ and $P^* \circ R^*$, averaged over context-action pairs $x \sim \pi_M, a \sim \pi_M' (\cdot | x)$ sampled from the environment.

**Example** (Exponential Family). Suppose the models $M \triangleq (R, P)$ are from a conditional exponential family: conditioned on $(x, a) \in \mathcal{X} \times \mathcal{A}$, we have $P_{x,a} \circ R_{x,a} \triangleq \exp \left( \left( \theta_{x,a}, T(r, x') \right) \right) / Z(\theta_{x,a})$ for parameters $\theta_{x,a} \in \Theta \triangleq \{\theta : \|\theta\| \leq 1\} \subset \mathbb{R}^m$ with partition function $Z(\theta_{x,a})$ and sufficient statistics $T : \mathcal{R} \times \mathcal{X} \rightarrow \mathbb{R}^m$.

With $\mathcal{G} = \{g : \mathcal{X} \times \mathcal{A} \rightarrow \Theta\}$, we design $\mathcal{F} = \{(x, a, r, x') \mapsto (g(x, a), T(r, x')) : g \in \mathcal{G}\}$. In this setting, witnessed model misfit is

$$\mathbb{E}_{x_h \sim \pi_M, a_h \sim \pi_M'} \left[ \left\| \mathbb{E}_{(r, x') \sim M_h} [T(r, x')] - \mathbb{E}_{(r, x') \sim M_h} [T(r, x')] \right\|_\ast \right] ,$$

with $\|x\|_\ast \triangleq \sup \{\|x, \theta\| : \|\theta\| \leq 1\}$. In this case, we measure distance, in the dual norm, between the expected sufficient statistics of $(r, x')$ sampled from $M'$ and the true model $M^*$. See Appendix G for more details.

**Example** (Maximum Mean Discrepancy). The third example is when $\mathcal{F} = \{f : \|f\|_H \leq 1\}$ is the unit ball in a Reproducing Kernel Hilbert Space (RKHS) $\mathcal{H}$ with kernel $k : \mathcal{Z} \times \mathcal{Z} \rightarrow [0, 1]$ with $\mathcal{Z} \triangleq \mathcal{X} \times \mathcal{A} \times \mathcal{R} \times \mathcal{X}$.

In this case, witnessed model misfit reduces to Maximum Mean Discrepancy (MMD)—a special instance of IPM (Gretton et al., 2012; Sriperumbudur et al., 2012).

### 5.1 Connections with Bellman error

Witnessed model misfit is also closely related to the average Bellman error, introduced by Jiang et al. (2017). Given two $Q$ functions, $Q$ and $Q'$, the average Bellman error (Jiang et al., 2017) at time step $h$ is defined as:

$$E_B(Q, Q', h) \triangleq \mathbb{E} \left[ Q'(x_h, a_h) - r_h - Q'(x_{h+1}, a_{h+1}) \mid x_h \sim \pi_Q, a_{h:h+1} \sim \pi_{Q'}, r_h \sim R^*_{x,h,a_h} \right]$$

(4)

where $\pi_Q$ is the greedy policy associated with $Q$, i.e., $\pi_Q(a|x) = 1\{a = \arg\max_{a'} Q(x, a')\}$, and all other randomness is from the true environment.

When the class of $Q$ functions is derived from a model class, meaning that $Q = \mathcal{OP}(M)$, we can extend the above definition to any pair of models $M, M' \in \mathcal{M}$, using $Q_M$ and $Q_{M'}$. The following fact shows that this extension is closely related to witnessed model misfit.

**Fact 1.** For any two models $M, M'$, the Bellman error of $Q$ and $Q'$ can be written as

$$E_B(M, M', h) \triangleq E_B(Q_M, Q_{M'}, h)$$

$$= \mathbb{E}_{x_h \sim \pi_M, a_h \sim \pi_M'} \left[ \mathbb{E}_{(r, x') \sim M_h} [r + V_{M'}(x')] - \mathbb{E}_{(r, x') \sim M_h} [r + V_M(x')] \right] .$$

(5)

\(^5\)Throughout the paper, we simply define $\|P_1 - P_2\|_{TV} = \sum_{x \in \mathcal{X}} |P_1(x) - P_2(x)|$, ignoring the constant factor.
Thus, the average Bellman error can be understood in terms of a special test function $f_{M'}(x, a, r, x') \triangleq r + V_{M'}(x')$. Our main assumption on $\mathcal{F}$ is that it contains these special functions $f_M$, for each $M \in \mathcal{M}$.

**Assumption 2** (Expressivity and Capacity of $\mathcal{F}$). Assume $\mathcal{F}$ is expressive enough that $\forall M \in \mathcal{M}$, there exists $f_M \in \mathcal{F}$ such that $f_M(x, a, r, x') \triangleq r + V_M(x')$ for all tuples $(x, a, r, x')$. Further assume that $\mathcal{F}$ is symmetric and finite in size.\(^6\)

This assumption implies that the witnessed model misfit always dominates the average Bellman error.

**Fact 2** (Bellman Domination). Under **Assumption 2**, for any pair of models $M, M'$ and $h \in [H]$, we have:

$$\mathcal{E}_B(M, M', h) \leq \mathcal{W}(M, M', h).$$

## 6 A Model-based Algorithm

In this section, we present our main algorithm and sample complexity results. We start by describing the algorithm. Then, working toward a statistical analysis, we introduce the witness rank, a new structural complexity measure. We end this section with the main sample complexity bounds.

### 6.1 Algorithm

Since we do not have access to $M^*$, we must estimate the witnessed model misfit from samples. Given a dataset $\mathcal{D} = \{(x^{(n)}_h, a^{(n)}_h, r^{(n)}_h, x^{(n)}_{h+1})\}_{n=1}^N$ with

$$x^{(n)}_h \sim \pi_M, \ a^{(n)}_h \sim U(A), \ (r^{(n)}_h, x^{(n)}_{h+1}) \sim M^*_h,$$

denote the importance weight $\rho^{(n)} \triangleq K \pi_{M'}(a^{(n)}_h | x^{(n)}_h)$. We simply use the empirical model misfit:

$$\hat{\mathcal{W}}(M, M', h) \triangleq \max_{f \in \mathcal{F}} \frac{1}{N} \left( \sum_{n=1}^N \rho^{(n)} \left( \mathbb{E}_{(r,x') \sim M'_h} [f(x^{(n)}_h, a^{(n)}_h, r, x')] - f(x^{(n)}_h, a^{(n)}_h, r^{(n)}_h, x^{(n)}_{h+1}) \right) \right). \quad (6)$$

Here the importance weight $\rho^{(n)}$ accounts for distribution mismatch, since we are sampling from $U(A)$ instead of $\pi_{M'}$. Via standard uniform convergence arguments (in Appendix A) we show that $\hat{\mathcal{W}}(M, M', h)$ provides a high-quality estimate of $\mathcal{W}(M, M', h)$ under **Assumption 2**.

We also require an estimator for the average Bellman error $\hat{\mathcal{E}}_B(M, M, h)$. Given a data set $\{(x^{(n)}_h, a^{(n)}_h, r^{(n)}_h, x^{(n)}_{h+1})\}_{n=1}^N$ where $x^{(n)}_h \sim \pi_M, a^{(n)}_h \sim \pi_M$, and $(r^{(n)}_h, x^{(n)}_{h+1}) \sim M^*_h$, we may use **Fact 1** to form an unbiased estimate of $\mathcal{E}_B(M, M, h)$ as

$$\hat{\mathcal{E}}_B(M, M, h) \triangleq \frac{1}{N} \sum_{n=1}^N \left[ Q_M(x^{(n)}_h, a^{(n)}_h) - \left[ r^{(n)}_h + V_M(x^{(n)}_{h+1}) \right] \right]. \quad (7)$$

Here $V_M, Q_M$ are obtained through a query to $\mathcal{OP}$ using model $M$.

Our algorithm is summarized in **Algorithm 1**. The algorithm is round-based, maintaining a version space of models and eliminating a model from the version space when the discrepancy between the model and the ground truth $M^*$ is witnessed. The witness distributions are selected using a form of optimism: at each round, we select, from all surviving models, the one with the highest predicted value, and we use the associated policy for data collection. If the policy achieves a high value in the environment, we simply return

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\(^6\)As before, our results extend to the case where $\mathcal{F}$ has bounded statistical complexity, for example any Glivenko-Cantelli class.
it. Otherwise we estimate the witnessed model misfit on the context distributions induced by the policy, and we shrink the version space by eliminating all incorrect models. Then we proceed to the next iteration.

Intuitively, if $M^t$ is the optimistic model at round $t$ and we do not terminate, then there must exist a time step $h_t$ (Line 9) where the average Bellman error is large. Using Fact 2, this also implies that the witness model misfit for $M^t$ witnessed by $M^t$ itself must be large. Thus, if $t$ is a non-terminal round, we ensure that $M^t$ and potentially many other models will be eliminated.

The algorithm is similar to OLIVE (Jiang et al., 2017), which uses average Bellman error instead of witnessed model misfit to shrink the version space. However, by appealing to Fact 2, witness model misfit provides a more aggressive elimination criterion, since a large average Bellman error on a distribution immediately implies a large witnessed model misfit on the same distribution, but the opposite direction does not necessarily hold. Since the algorithm uses an aggressive elimination rule, it often requires fewer iterations than OLIVE, as discussed below.

### 6.2 A structural complexity measure

In our development so far, we have imposed a realizability assumption (Assumption 1) on model class $\mathcal{M}$. Unfortunately, this assumption alone does not enable tractable reinforcement learning with polynomial sample complexity, as verified by the following simple lower bound.

**Proposition 1.** Fix $H, K \in \mathbb{N}^+$ with $K \geq 2$ and $\epsilon \in (0, \sqrt{1/8})$. There exists a class of MDPs, a realizable model class $\mathcal{M}$ with $|\mathcal{M}| = K^{H-1}$, and a constant $c > 0$, such that any model-based algorithm using $T \leq cK^{H-1}/\epsilon^2$ episodes outputs a policy $\hat{\pi}$ with $v^\pi < v^* - \epsilon$ with probability at least $1/3$.

The proof, provided in Appendix D.1, uses a construction from Krishnamurthy et al. (2016) for showing that value-based realizability is insufficient for model-free algorithms. The result suggests that we must introduce further structure to obtain polynomial sample complexity guarantees. We do so with a new structural complexity measure, the *witness rank*.

For any matrix $B \in \mathbb{R}^{n \times n}$, define $\text{rank}(B, \beta)$ to be the smallest integer $k$ such that $B = UV^\top$ with $U, V \in \mathbb{R}^{n \times k}$ and for every pair of rows $u_i, v_j$, we have $\|u_i\|_2 \cdot \|v_j\|_2 \leq \beta$. This generalizes the standard definition of matrix rank, with a condition on the row norms of the factorization. We now turn to the definition.
We define the witness rank as

\[ W(\kappa, \beta, \mathcal{M}, \mathcal{F}, h) \triangleq \min_{A \in \mathcal{N}_{\kappa, h}} \text{rank}(A, \beta). \]

We typically suppress the dependence on \( \beta \) in the definition because it appears only logarithmically in our sample complexity bound. Any choice of \( \beta \) that is polynomial in the other parameters (\( K, H \) and the rank itself) suffices.

To build intuition for the definition, first consider the extreme where \( A = W \in \mathbb{R}^{|\mathcal{M}| \times |\mathcal{M}|} \). The rank of this matrix corresponds to the number of context distributions on which we can verify non-zero witnessed model misfit for all incorrect models. This follows from the fact that that there are at most \( \text{rank}(W) \) linearly independent rows (context distributions), so any non-zero column (an incorrect model) must have a non-zero in at least one of these rows. Algorithmically, if we can find the policies \( \pi_M \) corresponding to these rows, we can eliminate all incorrect models to find \( M^* \) and hence \( \pi^* \).

The other extreme, where \( A = \mathcal{E}_B \in \mathbb{R}^{|\mathcal{M}| \times |\mathcal{M}|} \), is the Bellman error matrix introduced by Jiang et al. (2017), who show that the Bellman rank, \( \text{rank}(\mathcal{E}_B, \beta) \), governs the sample complexity of the model-free algorithm \texttt{OLIVE}. They further show that many natural RL settings, including tabular MDPs, reactive POMDPs, and reactive PSRs, admit Bellman rank that is polynomial in the natural parameters for these settings (See Section 2 of Jiang et al. (2017) for details). Since \( \mathcal{N}_{\kappa, h} \) always includes the Bellman error matrix, we know that \( W(\kappa, \mathcal{M}, \mathcal{F}, h) \) is never larger than the Bellman rank, and the aforementioned scenarios with low Bellman rank also yield low witness rank.

In between these extremes, one recipe for constructing a matrix \( A \) is to use a restricted class of test functions \( \mathcal{G} \subset \mathcal{F} \), possibly varying the restriction per entry of the matrix. For any function class \( \mathcal{G}_M \) satisfying \( \{ f_M(x, a, r, x') \mapsto r + V_M(x') \} \subset \mathcal{G}_M \subset \mathcal{F} \) we know by Fact 1 that the IPM induced by \( \mathcal{G}_M \) is sandwiched between \( \mathcal{E}_B(\cdot, M, h) \) and \( W(\cdot, M, h) \). Hence, one way to upper bound \( W \) is to carefully choose the test functions \( \mathcal{G} \) for each pair \( (M, M') \) to minimize the rank of the corresponding matrix. In Section 7 we study Factored MDPs, and we follows this recipe to construct a low rank matrix sandwiched between Bellman error (scaled by \( \kappa \)) and witness model misfit matrices. This example demonstrates the flexibility of the witness rank definition.

### 6.3 Sample complexity results

We analyze the sample complexity of Algorithm 1 using the witness rank. Denote \( W_\kappa \triangleq \max_{h \in [H]} W(\kappa, \beta, \mathcal{M}, \mathcal{F}, h) \).

The main guarantee for Algorithm 1 is the following theorem.

**Theorem 2.** Under Assumption 1 and Assumption 2, for any \( \epsilon, \delta, \kappa \in (0, 1] \), set \( \phi = \frac{\kappa \epsilon}{48H\sqrt{W_\kappa}} \), and denote \( T = HW_\kappa \log(\beta/2\phi) / \log(5/3) \), run Algorithm 1 with inputs \((\mathcal{M}, \mathcal{F}, n_\epsilon, n, \epsilon, \delta, \phi)\), where

\[ n_\epsilon = \Theta \left( \frac{H^2 \log(HT/\delta)}{\epsilon^2} \right), \quad n = \Theta \left( \frac{H^2 K W_\kappa \log(T |\mathcal{M}| |\mathcal{F}| / \delta)}{\kappa^2 \epsilon^2} \right), \]

then with probability at least \( 1 - \delta \), Algorithm 1 outputs a policy \( \pi \) such that \( v^\pi \geq v^* - \epsilon \). The number of trajectories collected is at most

\[ \tilde{O} \left( \frac{H^3 W^2 K}{\kappa^2 \epsilon^2} \log \left( \frac{T |\mathcal{F}| |\mathcal{M}|}{\delta} \right) \right). \]
The proof of the above theorem is included in Appendix A. Since, as we have discussed, many popular RL models admit low Bellman rank and hence low witness rank, Theorem 2 verifies that Algorithm 1 has polynomial sample complexity in all of these settings. A noteworthy case that does not have small Bellman rank but does have small witness rank is the Factored MDP, which we discuss further in Section 7.

Comparison with OLIVE. From the theorem, the minimum sample complexity is achieved at $\inf \kappa W_\kappa/\kappa$, which is never larger than Bellman rank. In fact when $\kappa = 1$, the sample complexity bounds match in all terms except (a) we replace Bellman rank with witness rank, and (b) we have a dependence on model and test-function complexity $\log(|M||F|)$ instead of $Q$-function complexity $\log|OP(M)|$. The witness rank is never larger than the Bellman rank and it can be substantially smaller, which is favorable for Algorithm 1. However, we always have $\log |M| \geq \log |OP(M)|$ and since we require realizability, the model class can be much larger than the induced $Q$-function class. Thus the two results are in general incomparable, but for problems where modeling the environment is not much harder than modeling the optimal $Q$-function (in other words $\log(|M||F|) \approx \log |OP(M)|$), Algorithm 1 can be substantially more sample-efficient than OLIVE.

Remark. Note for Theorem 2, the algorithm must know the value of $\kappa$ and $W_\kappa$ (unless we set $\kappa = 1$), as it appears in the parameters $\phi$ and $n$. In Appendix F, we show that a standard doubling trick using Algorithm 1 as a subroutine yields an algorithm that adapts to $\kappa$ and $W_\kappa$. This algorithm has sample complexity $\tilde{O}(H^3W_\kappa^2K/((\kappa^*\epsilon)^2)\log(|M||F|/\delta))$, where $\kappa^* = \arg\min_{\kappa \in (0,1]} W_\kappa/\kappa$ minimizes the sample complexity from Theorem 2. A similar technique was used by Jiang et al. (2017) to adapt to unknown Bellman rank.

Theorem 2 as stated assumes that $M$ and $F$ are finite classes, but since the proof involves standard uniform convergence arguments, the result extends naturally to function class with bounded statistical complexity (e.g., VC Dimension, Rademacher Complexity). However, it is desirable to move beyond classes with bounded statistical complexity, in particular for the test function class $F$. For example, we would like to handle the total variation distance, which is the IPM induced by the class $F = \{ f : \|f\|_\infty \leq 1 \}$. This class does not admit uniform convergence, so our analysis for Theorem 2 does not apply. To handle such rich classes, we borrow ideas from the Scheffé estimator and tournament of Devroye and Lugosi (2012), and extend the method to handle conditional distributions and IPMs induced by an arbitrary class. The analysis here covers the total-variation based witnessed model misfit defined in (3) as a special case.

Theorem 3. Under Assumption 1 and Assumption 2, with no restriction on the size of $F$, there exists an algorithm with the following guarantee: For any $\epsilon, \delta \in (0, 1]$, with probability at least $1 - \delta$ the algorithm outputs a policy $\pi$ such that $v^\pi \geq v^* - \epsilon$ and the number of trajectories collected is at most

$$\hat{O}\left(\frac{H^3W_\kappa^2K}{\kappa^2\epsilon^2} \log\left(\frac{T|M|}{\delta}\right)\right),$$

where $T = HW_\kappa \log(\beta/2\phi)/\log(5/3)$.

The algorithm is a modification to Algorithm 1 incorporating the Scheffé estimator in lieu of (6). We defer a precise description of the algorithm (Algorithm 2) and proof details to Appendix B. The main improvement over Theorem 2 is that the sample complexity here has no dependence on $F$, so we may use test function classes with unbounded statistical complexity.

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\footnote{The classical Scheffé tournament targets the following problem: given a set of distributions $\{ P_i \}_{i=1}^N$ over $X$, and a set of i.i.d samples $\{ x_i \}_{i=1}^N$ from $P^* \in \Delta(X)$, approximate the minimizer $\arg\min_{i \in [K]} \| P_i - P^* \|_{TV}$.}
7 Case Study on MDPs with Factored Transition

In this section, we study the Factored MDP running example in detail. Recall the definition of factored transition dynamics in (1). Following the formulation of Kearns and Koller (1999), we assume the reward distribution $R^*$ is known and shared by all models in $\mathcal{M}$, so that models only disagree on the transition dynamics. For this setting, we have the following guarantee.

**Theorem 4.** For MDPs with factored transitions and for any $\epsilon, \delta \in (0, 1]$, with probability at least $1 - \delta$ a modification of Algorithm 1 (Algorithm 3 in Appendix C) outputs a policy $\pi$ with $v^\pi \geq v^* - \epsilon$ using at most \(\tilde{O}(H^3L^3d^2K^2 \log(1/(\epsilon\delta))/\epsilon^2)\) trajectories.

This result should be contrasted with the $\Omega(2^H)$ lower bound from Theorem 1 that actually applies precisely to this setting. Combining the two results we have demonstrated exponential separation between model-based and model-free algorithms for MDPs with factored transitions.

**Corollary 1.** For MDPs with factored transitions, the sample complexity of model-based methods is polynomial in all parameters, while all model-free methods must incur $\Omega(2^H)$ sample complexity.

Theorem 4 involves a slight modification to Algorithm 1, which uses a different notion of witnessed model misfit, defined as

$$\mathcal{W}_U(M, M', h) = \mathbb{E} \left[ \|P'_{x_h,a_h} - P'^*_{x_h,a_h}\|_{TV} \mid x_h \sim \pi_M, a_h \sim U(A) \right].$$

(8)

The main difference with (3) is that $a_h$ is sampled from $U(A)$ rather than $\pi_M'$. This modification is crucial to obtain a low witness rank, since $\pi_M'$ is in general not guaranteed to be factored. At the same time, the modification introduces no complications to our analysis, which we provide for completeness in Appendix C.

The key to Theorem 4 is that we find a low-rank matrix $A$ sandwiched between $\mathcal{E}_B/(Kd)$ and $\mathcal{W}_U$. This matrix is based on a natural factored test function class $\mathcal{G} = \{g_1 + \ldots + g_d : g_i \in \mathcal{G}_i\}$ with $\mathcal{G}_i = \{g : O[^{pa_i}] \times A \times O \to \mathbb{R}, \|g\|_\infty \leq 1\}$ as the function class that acts only on the $i$th factor. The IPM induced by $\mathcal{G}_i$ is the total variation distance on just the $i$th factor, and so the IPM induced by $\mathcal{G}$ is the sum of the TV-distances across all factors. Analyzing this matrix is much simpler and yields the bound in Theorem 4.

8 Discussion

In this paper, we study model-based reinforcement learning in general contextual decision processes. We derive an algorithm for general CDPs and prove that it has sample complexity upper-bounded by a new structural notion called the witness rank, which is small in many settings of interest. Comparing model-based and model-free methods, we show that model-based methods can be exponentially more sample efficient in some settings, but they also require stronger function-approximation capabilities, which can result in worse sample complexity in other cases. Comparing the guarantees here with those derived by Jiang et al. (2017) precisely quantifies these tradeoffs, which we hope will guide future design of RL algorithms.

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\[8\text{Note that since all models share the same unknown reward distribution, } \|P'_{x,a}R_{x,a} - P^*_{x,a}R^*_{x,a}\|_{TV} = \|P_{x,a} - P^*_{x,a}\|_{TV}.\]
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A Proof of Theorem 2

We first present several lemmas that are useful for proving Theorem 2.

**Lemma 1** (Lemma 11 of Jiang et al. (2017)). Consider a closed and bounded set \( V \subset \mathbb{R}^d \) and a vector \( p \in \mathbb{R}^d \). Let \( B \) be any origin-centered enclosing ellipsoid of \( V \). Suppose there exists \( v \in V \) such that \( p^T v \geq \kappa \) and define \( B_+ \) as the minimum volume enclosing ellipsoid of \( \{ v \in B : |p^T v| \leq \frac{\kappa}{3\sqrt{d}} \} \). With \( \text{vol}(\cdot) \) denoting the (Lebesgue) volume, we have:

\[
\frac{\text{vol}(B)}{\text{vol}(B_+)} \leq \frac{3}{5}.
\]

Recall that \( V_M, \pi_M \) denote the optimal value function and policy derived from model \( M \), and that \( v_M \) denotes \( \pi_M \)'s value in \( M \). For any policy \( \pi, v^\pi \) denotes the policy \( \pi \)'s value in the true environment.

**Lemma 2** (Simulation Lemma). Fix a model \( M \). Under Assumption 2, we have

\[
v_M - v^{\pi_M} = \sum_{h=1}^{H} \mathcal{E}_B(M, M, h), \quad \text{and} \quad v_M - v^{\pi_M} \leq \sum_{h=1}^{H} \mathcal{W}(M, M, h).
\]

**Proof.** Start at time step \( h = 1 \),

\[
\mathbb{E}_{x_1 \sim P_0} [V_M(x_1) - V^{\pi_M}(x_1)]
= \mathbb{E}_{x_1 \sim P_0, a_1 \sim \pi_M} \left[ \mathbb{E}_{(r,x_2) \sim M_{x_1,a_1}} [r + V_M(x_2)] - \mathbb{E}_{(r,x_2) \sim M_{x_1,a_1}} [r + V^{\pi_M}(x_2)] \right]
= \mathbb{E}_{x_1 \sim P_0, a_1 \sim \pi_M} \left[ \mathbb{E}_{(r,x_2) \sim M_{x_1,a_1}} [r + V_M(x_2)] - \mathbb{E}_{(r,x_2) \sim M_{x_1,a_1}} [r + V_M(x_2)] \right]
+ \mathbb{E}_{x_1 \sim P_0, a_1 \sim \pi_M} \left[ \mathbb{E}_{(r,x_2) \sim M_{x_1,a_1}} [V_M(x_2)] - \mathbb{E}_{(r,x_2) \sim M_{x_1,a_1}} [V^{\pi_M}(x_2)] \right],
\]

where the first equality is based on applying Bellman’s equation to \( V_M \) in \( M \) and \( V^{\pi_M} \) in \( M^* \). Now, by Fact 1, the first term above is exactly \( \mathcal{E}_B(M, M, 1) \). The second term can be expressed as

\[
\mathbb{E} [V_M(x_2) - V^{\pi_M}(x_2) | x_2 \sim \pi_M],
\]

which we can further expand by applying the same argument recursively to obtain the identity involving the average Bellman errors. For the bound involving the witness model misfit, since \( V_M \in \mathcal{F} \), we simply observe that \( \mathcal{E}_B(M, M, h) \leq \mathcal{W}(M, M, h) \).
Next, we present several concentration results.

**Lemma 3.** Fix a policy \( \pi \), and fix \( \epsilon, \delta \in (0, 1) \). Sample \( n_e = \frac{\log(2/\delta)}{(2e)^2} \) trajectories \( \{(x_h^{(i)}, a_h^{(i)}, r_h^{(i)})_{h=1}^H\}_{i=1}^{n_e} \) by executing \( \pi \) and set \( \hat{v}^\pi = \frac{1}{n_e} \sum_{i=1}^{n_e} \sum_{h=1}^{H} r_h^{(i)}. \) With probability at least \( 1 - \delta \), we have \( |\hat{v}^\pi - v^\pi| \leq \epsilon. \)

The proof is a direct application of Hoeffding’s inequality on the random variables \( \sum_{h=1}^{H} r_h^{(i)} \).

Recall the definitions of \( \hat{W} \) and \( \hat{E}_B \) from (6) and (7), and the shorthand notation \( (r, x') \sim M_h \), which means \( (r, x') \sim M_{x,a} \) and is clear from context.

**Lemma 4 (Deviation Bound for \( \hat{E}_M \)).** Fix \( h \) and model \( M \in \mathcal{M} \). Sample a dataset \( \mathcal{D} = \{((x_h^{(i)}, a_h^{(i)}, r_h^{(i)}, x_{h+1}^{(i)}))_{i=1}^{N} \) with \( x_h^{(i)} \sim \pi_M, a_h^{(i)} \sim U(\mathcal{A}), (r_h^{(i)}, x_{h+1}^{(i)}) \sim M_h^* \) of size \( N \). Then with probability at least \( 1 - \delta \), we have for all \( M' \in \mathcal{M} \):

\[
\left| \hat{W}(M, M', h) - W(M, M', h) \right| \leq \sqrt{\frac{2K \log(2|\mathcal{M}||\mathcal{F}|/\delta)}{N}} + \frac{2K \log(2|\mathcal{M}||\mathcal{F}|/\delta)}{3N}.
\]

**Proof.** Fix \( M' \in \mathcal{M} \) and \( f \in \mathcal{F} \), define the random variable \( z_i(M', f) \) as:

\[
z_i(M', f) = K \pi_{M'}(a_h^{(i)}|x_h^{(i)}) \left( \mathbb{E}_{(r, x') \sim M_h^*} f(x_h^{(i)}, a_h^{(i)}, r, x') - f(x_h^{(i)}, a_h^{(i)}, r_h^{(i)}, x_{h+1}^{(i)}) \right).
\]

The expectation of \( z_i(M', f) \) is

\[
\mathbb{E}[z_i(M', f)] = \mathbb{E}_{x_h \sim \pi_M, a_h \sim \pi_M}[\mathbb{E}_{(r, x') \sim M_h^*}[f(x_h, a_h, r, x')] - \mathbb{E}_{(r, x') \sim M_h^*}[f(x_h, a_h, r, x')]],
\]

and it is easy to verify that \( \text{Var}(z_i(M', f)) \leq 4K \). Hence, we can apply Bernstein’s inequality, so that with probability at least \( 1 - \delta \), we have

\[
\left| \frac{1}{N} \sum_{i=1}^{N} z_i(M', f) - d(M', M^*, f) \right| \leq \sqrt{\frac{2K \log(2/\delta)}{N}} + \frac{2K \log(2/\delta)}{3N}.
\]

Via a union bound over \( \mathcal{M} \) and \( \mathcal{F} \), we have that for all pairs \( M' \in \mathcal{M}, f \in \mathcal{F} \), with probability at least \( 1 - \delta \):

\[
\left| \frac{1}{N} \sum_{i=1}^{N} z_i(M', f) - d(M', M^*, f) \right| \leq \sqrt{\frac{2K \log(2|\mathcal{M}||\mathcal{F}|/\delta)}{N}} + \frac{2K \log(2|\mathcal{M}||\mathcal{F}|/\delta)}{3N}.
\]

(9)

For fixed \( M' \), we have shown uniform convergence over \( \mathcal{F} \), and this implies that the empirical and the population maxima must be similarly close, which yields the result.

**Lemma 5 (Deviation Bound on \( \hat{E}_B \)).** Fix model \( M \in \mathcal{M} \). Sample a dataset \( \mathcal{D} = \{(x_h^{(i)}, a_h^{(i)}, r_h^{(i)}, x_{h+1}^{(i)})_{i=1}^{N} \) with \( x_h^{(i)} \sim \pi_M, a_h^{(i)} \sim \pi_M, (r_h^{(i)}, x_{h+1}^{(i)}) \sim M_h^* \) of size \( N \). Then with probability at least \( 1 - \delta \), for any \( h \in [H] \), with probability at least \( 1 - \delta \), we have:

\[
\left| \mathcal{E}_B(M, M, h) - \hat{E}_B(M, M, h) \right| \leq \sqrt{\frac{\log(2H/\delta)}{2N}}.
\]

The result involves a standard application of Hoeffding’s inequality with a union bound over \( h \in [H] \), which can also be found in Jiang et al. (2017).
Lemma 6 (Terminate or Explore). Suppose that for any round $t$, $\hat{v}^{\pi^t}$ satisfies $|v^\pi^t - \hat{v}^{\pi^t}| \leq \epsilon/8$ and $M^*$ is never eliminated. Then in any round $t$, one of the following two statements must hold:

1. The algorithm does not terminate and there exists a $h \in [H]$ such that $\mathcal{E}_B(M^t, M^t, h) \geq \frac{3\epsilon}{8H}$;

2. The algorithm terminates and outputs a policy $\pi^t$ which satisfies $v^\pi^t \geq v^* - \epsilon$.

Proof. Let us first consider the situation where the algorithm does not terminate, i.e., $|\hat{v}^{\pi^t} - v_{M^t}| \geq \epsilon/2$. Via Lemma 2, we must have

$$\sum_{h=1}^{H} \mathcal{E}_B(M^t, M^t, h) \geq |v^{\pi^t} - v_{M^t}| = |v^{\pi^t} - \hat{v}^{\pi^t} + \hat{v}^{\pi^t} - v_{M^t}| \geq |\hat{v}^{\pi^t} - v_{M^t}| - |v^{\pi^t} - \hat{v}^{\pi^t}| \geq 3\epsilon/8.$$ 

By the pigeonhole principle, there must exist $h \in [H]$, such that

$$\mathcal{E}_B(M^t, M^t, h) \geq \frac{3\epsilon}{8H},$$

so we obtain the first claim. For the second claim, if the algorithm terminates at round $t$, we must have $|\hat{v}^{\pi^t} - v_{M^t}| \leq \epsilon/2$. Based on the assumption that $M^*$ is never eliminated, and $M^t$ is the optimistic model, we may deduce

$$v^{\pi^t} \geq \hat{v}^{\pi^t} - \frac{\epsilon}{8} \geq v_{M^t} - \frac{5\epsilon}{8} \geq v^* - \frac{5\epsilon}{8} \geq v^* - \epsilon.$$

Recall the definition of the witness rank (Definition 3):

$$W(\kappa, \beta, M, F, h) = \inf \{ \text{rank}(A) : \kappa \mathcal{E}_B(M, M^t, h) \leq A(M, M^t) \leq W(M, M^t, h), \forall M, M' \in M \}.$$

Let us denote $A^*_M$ as the matrix that achieves the witness rank $W(\kappa, \beta, M, F, h)$ at time step $h$. Denote the factorization by $A^*_M = (\zeta_h(M), \chi_h(M))$ with $\zeta_h, \chi_h \in \mathbb{R}^{W(\kappa, \beta, M, F, h)}$. Finally, recall that $\beta \geq \max_{M, M', h} \|\zeta_h(M)\|_2 \|\chi_h(M')\|_2$.

Lemma 7. Fix round $t$ and assume that $|\hat{E}_B(M^t, M^t, h) - \mathcal{E}_B(M^t, M^t, h)| \leq \frac{\epsilon}{8H}$ for all $h \in [H]$ and $|v^{\pi^t} - \hat{v}^{\pi^t}| \leq \epsilon/8$ hold. If Algorithm 1 does not terminate, then we must have $A^*_h(M^t, M^t) \geq \frac{\kappa \epsilon}{8H}$.

Proof. We first verify the existence of $h_t$ in the selection rule line 9 in Algorithm 1. From Lemma 6, we know that there exists $h \in [H]$ such that $\mathcal{E}_B(M^t, M^t, h) \geq \frac{3\epsilon}{8H}$, and for this $h$, we have

$$\hat{E}_B(M^t, M^t, h) \geq \frac{3\epsilon}{8H} - \frac{\epsilon}{8} = \frac{\epsilon}{4H}. \quad (10)$$

While this $h$ may not be the one selected in line 9, it verifies that $h_t$ exists, and further we do know that for $h_t$

$$\mathcal{E}_B(M^t, M^t, h_t) \geq \frac{2\epsilon}{8H} - \frac{\epsilon}{8H} = \frac{\epsilon}{8H}.$$

Now the constraints defining $A^*_h$ give $A^*_h(M^t, M^t) \geq \kappa \mathcal{E}_B(M^t, M^t, h_t)$, which proves the lemma. \qed

Recall the model elimination criteria at round $t$: $\mathcal{M}_t = \{M \in \mathcal{M}_{t-1} : \hat{W}(M^t, M, h_t) \leq \phi \}$.

Lemma 8. Suppose that $|\hat{W}(M^t, M, h_t) - W(M^t, M, h_t)| \leq \phi$ holds for all $t, h_t$, and $M \in \mathcal{M}$. Then
1. \( M^* \in \mathcal{M}_t \), for all \( t \).

2. Denote \( \tilde{\mathcal{M}}_t = \{ M \in \tilde{\mathcal{M}}_{t-1} : A^*_{\kappa,h_t}(M^t, M) \leq 2\phi \} \) with \( \tilde{\mathcal{M}}_0 = \mathcal{M} \). We have \( \mathcal{M}_t \subseteq \tilde{\mathcal{M}}_t \) for all \( t \).

Observe \( \tilde{\mathcal{M}}_t \) is defined via the matrix \( A^*_{\kappa,h_t} \).

**Proof.** Recall that we have \( \mathcal{W}(M^t, M^*, h_t) = 0 \). Assuming \( M^* \in \mathcal{M}_{t-1} \) and via the assumption in the statement, for every \( t \), we have
\[
\tilde{\mathcal{W}}(M^t, M^*, h_t) \leq \mathcal{W}(M^t, M^*, h_t) + \phi = \phi,
\]
so \( M^* \) will not be eliminated at round \( t \).

For the second result, we know that \( \tilde{\mathcal{M}}_0 = \mathcal{M} \). Assume inductively that, we have \( \mathcal{M}_{t-1} \subseteq \tilde{\mathcal{M}}_{t-1} \), and let us prove that \( \mathcal{M}_t \subseteq \tilde{\mathcal{M}}_t \). Towards a contradiction, let us assume that there exists \( M \in \mathcal{M}_t \) such that \( M \notin \tilde{\mathcal{M}}_t \). Since \( M \in \mathcal{M}_t \subset \mathcal{M}_{t-1} \subset \tilde{\mathcal{M}}_{t-1} \), the update rule for \( \tilde{\mathcal{M}}_t \) implies that
\[
A^*_{\kappa,h_t}(M^t, M) > 2\phi.
\]
But, using the deviation bound and the definition of \( A^*_{\kappa,h_t} \), we get
\[
\tilde{\mathcal{W}}(M^t, M, h_t) \geq \mathcal{W}(M^t, M, h_t) - \phi \geq A^*_{\kappa,h_t}(M^t, M) - \phi > \phi,
\]
which contradicts the fact that \( M \in \mathcal{M}_t \). Thus, by induction we obtain the result. \( \square \)

With our choice of \( \phi = \frac{\kappa\epsilon}{48H\sqrt{\mathcal{W}_n}} \), we may now quantify the number of rounds of Algorithm 1 using \( \tilde{\mathcal{M}}_t \).

**Lemma 9** (Iteration complexity). Suppose that
\[
\left| \tilde{\mathcal{W}}(M^t, M, h_t) - \mathcal{W}(M^t, M, h_t) \right| \leq \phi, \quad \left| \tilde{E}_B(M^t, M^t, h_t) - E_B(M^t, M^t, h_t) \right| \leq \frac{\epsilon}{8H},
\]
hold for all \( t, h_t, h \in [H] \), and \( M \in \mathcal{M} \), then the number of rounds of Algorithm 1 is at most \( HW_{\kappa} \log(\frac{3}{2\phi})/\log(5/3) \).

**Proof.** From Lemma 7, if the algorithm does not terminate at round \( t \), we find \( M^t \) and \( h_t \) such that
\[
A^*_{\kappa,h_t}(M^t, M^t) = \langle \zeta_{h_t}(M^t), \chi_{h_t}(M^t) \rangle \geq \frac{\kappa\epsilon}{8H} = 6\sqrt{\mathcal{W}_n}\phi,
\]
which uses the value of \( \phi = \frac{\kappa\epsilon}{48H\sqrt{\mathcal{W}_n}} \).

Recall the recursive definition of \( \tilde{\mathcal{M}}_t = \{ M \in \tilde{\mathcal{M}}_{t-1} : A^*_{\kappa,h_t}(M^t, M) \leq 2\phi \} \) from Lemma 8. For the analysis, we maintain and update \( H \) origin-centered ellipsoids where the \( h^\text{th} \) ellipsoid contains the set \( \{ \chi_{h_t}(M) : M \in \tilde{\mathcal{M}}_t \} \). Denote \( O^{h_t}_{t-1} \) as the origin-centered minimum volume enclosing ellipsoid (MVEE) of \( \{ \chi_{h_t}(M) : M \in \tilde{\mathcal{M}}_t \} \). At round \( t \), for \( \zeta_{h_t}(M^t) \), we just proved that there exists a vector \( \chi_{h_t}(M^t) \in O^{h_t}_{t-1} \) such that \( \langle \zeta_{h_t}(M^t), \chi_{h_t}(M^t) \rangle \geq 6\sqrt{\mathcal{W}_n}\phi \). Denote \( O^{h_t}_{t-1,+} \) as the origin-centered MVEE of \( \{ v \in O^{h_t}_{t-1} : \langle \zeta_{h_t}(M^t), v \rangle \leq 2\phi \} \). Based on Lemma 1, and the fact that \( O^{h_t}_{t-1} \subset O^{h_t}_{t-1,+} \), by the definition of \( \tilde{\mathcal{M}}_t \), we have:
\[
\frac{\text{vol}(O^{h_t}_{t-1})}{\text{vol}(O^{h_t}_{t-1,+})} \leq \frac{\text{vol}(O^{h_t}_{t-1,+})}{\text{vol}(O^{h_t}_{t-1})} \leq 3/5,
\]
which shows that if the algorithm does not terminate, then we shrink the volume of \( O^{h_t}_{t} \) by a constant factor. \( \square \)
Denote $\Phi \triangleq \sup_{M \in M, h} \|\zeta_h(M)\|_2$ and $\Psi \triangleq \sup_{M \in M, h} \|\chi_h(M)\|_2$. For $O^h_0$, we have $\text{vol}(O^h_0) \leq c_{\omega} \Psi^{W_\omega}$ where $c_{\omega}$ is the volume of the unit Euclidean ball in $W_\omega$-dimensions. For any $t$, we have

$$O^h_t \supseteq \{q \in \mathbb{R}^{W_\omega} : \max_{p : \|p\|_2 \leq \Phi} \langle q, p \rangle \leq 2\phi \} = \{q \in \mathbb{R}^{W_\omega} : \|q\|_2 \leq 2\phi/\Phi \}$$

Hence, we must have that at termination, $\text{vol}(O^h_T) \geq c_{\omega}(2\phi/\Phi)^{W_\omega}$. Using the volume of $O^h_0$ and the lower bound of the volume of $O^h_T$ and the fact that every round we shrink the volume of $O^h_T$ by a constant factor, we must have that for any $h \in [H]$, the number of rounds for which $h_t = h$ is at most:

$$W_\omega \log\left(\frac{\Phi \Psi}{2\phi}\right) / \log(5/3).$$

(11)

Using the definition $\beta \geq \Phi \Psi$, this gives an iteration complexity of $HW_\omega \log\left(\frac{\beta}{2\phi}\right) / \log(5/3)$. \hfill \qed

We are now ready to prove Theorem 2. Note that we are using $A^*_\omega$, rather than relying on $E_B$ or $W$.

**Proof of Theorem 2.** Below we condition on three events: (1) $\hat{\mathcal{W}}(M^t, M, h_t) - \mathcal{W}(M^t, M, h_t) \leq \phi$ for all $t$ and $M \in M$, (2) $\hat{\mathcal{E}}_B(M^t, M^t, h) - \mathcal{E}_B(M^t, M^t, h) \leq \frac{\epsilon}{\kappa H}$ for all $t$ and $h \in [H]$, and (3) $|\hat{v}^\pi_t - v^\pi_t| \leq \epsilon/8$ for all $t$.

Under the first and second condition, from the lemma above, we know that the algorithm must terminate in at most $T = W_\omega H \log(\beta/(2\phi))/\log(5/3)$ rounds. Once the algorithm terminates, based on Lemma 6, we know that we must have found a policy that is $\epsilon$-optimal.

Now, we show that with our choices for $n$, $n_e$, and $\phi$, the above conditions hold with probability at least $1 - \delta$. Based on value of $n_e = 32 H^2 \log(6HT/\delta) / \epsilon^2$, and Lemma 3, we can verify that the third condition $|\hat{v}^\pi_t - v^\pi_t| \leq \epsilon/8$ holds for all $t \in [T]$ with probability $1 - \delta/3$, and the condition $|\hat{\mathcal{E}}_B(M^t, M^t, h) - \mathcal{E}_B(M^t, M^t, h)| \leq \epsilon/(8H)$ holds for all $t \in [T]$ and $h \in [H]$ with probability at least $1 - \delta/3$. Based on the value of $n = 18432 H^2 KW_\omega \log(12T |M| |F|/\delta)//(\kappa \epsilon)^2$, the value of $\phi$, and the deviation bound from Lemma 4, we can verify that the condition $|\hat{\mathcal{W}}(M^t, M, h_t) - \mathcal{W}(M^t, M, h_t)| \leq \phi$ holds for all $t \in [T]$, $M \in M$ with probability at least $1 - \delta/3$. Together these ensure the algorithm terminates in $T$ iterations. The number trajectories is at most $(n_e + n) \cdot T$, and the result follows by substitute the value of $n_e$, $n$, and $T$. \hfill \qed

### B Proof of Theorem 3

**Algorithm 2** Extension to $\mathcal{F}$ with Unbounded Complexity. Arguments: $(\mathcal{M}, \mathcal{F}, \epsilon, \delta, \epsilon)$

1: Compute $\tilde{\mathcal{F}}$ from $\mathcal{F}$ and $\mathcal{M}$ via (12)
2: Set $\phi = \kappa \epsilon / (48H \sqrt{W_\omega})$ and $T = HW_\omega \log(\beta/(2\phi))/\log(5/3)$
3: Set $n_e = \Theta(H^2 \log(6HT/\delta)/\epsilon^2)$ and $n = \Theta(H^2 KW_\omega \log(12T |M| \tilde{\mathcal{F}}|/\delta)/(\kappa \epsilon^2))$
4: Run Algorithm 1 with inputs $(\mathcal{M}, \tilde{\mathcal{F}}, n_e, n, \epsilon, \delta, \phi)$ and return the found policy.

We are interested in generalizing Theorem 2 to accommodate a broader class of test functions $\mathcal{F}$, for example $\{f : \|f\|_\infty \leq 1\}$ that induces the total-variation distance. This class is not a Glivenko-Cantelli class, so it does not enable uniform convergence, and we cannot simply use empirical mean estimator as in (6).

The key is to define a much smaller function class $\tilde{\mathcal{F}} \subset \mathcal{F}$ that does enjoy uniform convergence, and at the same time is expressive enough such that the witnessed model misfit w.r.t. $\tilde{\mathcal{F}}$ is the same as that w.r.t. $\mathcal{F}$.
Moreover, we have that \( F \) maximizes the witness model misfit for \( f \) contains the functions in total variation (Devroye and Lugosi, 2012). As we have done here, the idea is to define a smaller function class containing just the potential maximizers. Importantly, this smaller function class is computed independently and so there is no risk of overfitting. The main innovation here is that we extend the Scheffé estimator to conditional distributions, and also to handle arbitrary classes of the data

To define \( \tilde{F} \), we need one new definition. For a model \( M \) and a policy \( \pi \), we use \( x_h \sim (\pi, M) \) to denote that \( x_h \) is sampled by executing \( \pi \) in the model \( M \), instead of the true environment, for \( h \) steps. With this notation, define \( f_{\pi,M_1,M_2,h} \) as:

\[
\arg\max_{f \in F} E \left[ \mathbb{E}_{(r,x_{h+1})} \sim M_2 \left[ f(x_h, a_h, r, x_{h+1}) \right] - \mathbb{E}_{(r,x_{h+1})} \sim M_1 \left[ f(x_h, a_h, r, x_{h+1}) \right] \mid x_h \sim (\pi, M_1), a_h \sim \pi_M \right].
\]

Then we define

\[
\tilde{F} \triangleq \left\{ \pm f_{\pi,M_1,M_2,h} : M_1, M_2, M_3 \in \mathcal{M}, h \in \mathcal{H} \right\}. \tag{12}
\]

This construction is based on the Scheffé estimator, which was originally developed for density estimation in total variation (Devroye and Lugosi, 2012). As we have done here, the idea is to define a smaller function class containing just the potential maximizers. Importantly, this smaller function class is computed independently of the data, so there is no risk of overfitting. The main innovation here is that we extend the Scheffé estimator to conditional distributions, and also to handle arbitrary classes \( F \).

**Lemma 10.** For any true model \( M^* \in \mathcal{M} \), policy \( \pi_M \), \( h \in \mathcal{H} \), and target model \( M' \), we have

\[
\mathcal{W}(M, M', h; \mathcal{F}) = \mathcal{W}(M, M', h; \tilde{F}).
\]

Moreover \( |\tilde{F}| \leq 2|\mathcal{M}|^3 \mathcal{H} \).

**Proof.** The bound on \( |\tilde{F}| \) is immediate. For the other claim, by the realizability assumption for \( \mathcal{M} \), \( \tilde{F} \) contains the functions \( f_{\pi,M,M^*,M',h} \) for each \( (M, M', h) \) pair. These are precisely the test functions that maximize the witness model misfit for \( \mathcal{F} \), and so the IPM induced by \( \tilde{F} \) achieves exactly the same values. \( \square \)

Replacing \( \tilde{W}(M, M', h) \) in (6), which uses \( \mathcal{F} \), to instead use \( \tilde{\mathcal{F}} \), we obtain Algorithm 2 and Theorem 3 as a corollary to Theorem 2. The key is that we have eliminated the dependence on \( |\mathcal{F}| \) in the bound.

**C Analysis using \( \mathcal{W}_U \)**

In this section we sketch the argument showing that the alternative definition of witness model misfit in (8) also suffices for polynomial sample complexity in terms of the witness model rank. Recall the definition

\[
\mathcal{W}_U(M, M', h) \triangleq E \left[ \| P'_{x_h,a_h} R_{x_h,a_h} - P^*_{x_h,a_h} R^*_{x_h,a_h} \|_{TV} \mid x_h \sim \pi_M, a_h \sim U(A) \right].
\]

For simplicity we are only considering the total variation class here.

The algorithm that uses \( \mathcal{W}_U \) is nearly identical to Algorithm 1, except we use a new estimator for the witness model misfit. First, we use Lemma 10 to reduce the total variation class \( \mathcal{F} = \{ f : \| f \|_\infty \leq 1 \} \) to a set \( \tilde{\mathcal{F}} \) of size \( |\tilde{\mathcal{F}}| \leq 2|\mathcal{M}|^3 \mathcal{H} \), defined in a slightly different way:

\[
\tilde{\mathcal{F}} \triangleq \left\{ \pm f_{\pi,M_1,M_2,h} : M_1, M_2, M_3 \in \mathcal{M}, h \in \mathcal{H} \right\},
\]

\[
f_{\pi,M_1,M_2,h} = \arg\max_{f \in \tilde{\mathcal{F}}} E \left[ \mathbb{E}_{(r,x_{h+1})} \sim M_2 \left[ f \right] - \mathbb{E}_{(r,x_{h+1})} \sim M_1 \left[ f \right] \mid x_h \sim (\pi, M_1), a_h \sim U(A) \right].
\]
Note that here \( a_h \sim U(A) \) when computing \( f_{\pi, M_1, M_2, h} \). Then, given a dataset \( D = \{(x_h^{(i)}, a_h^{(i)}, r_h^{(i)}, x_{h+1})\}_{i=1}^n \), with \( x_h^{(i)} \sim \pi_M, a_h^{(i)} \sim U(A), (r_h^{(i)}, x_{h+1}) \sim M_h^* \), we compute \( W_U(M, M', h) \) as

\[
\hat{W}_U(M, M', h) = \max_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^n \left( E_{(r, x') \sim M_h^*} [f(x_h^{(i)}, a_h^{(i)}, r, x')] - f(x_h^{(i)}, a_h^{(i)}, r_h^{(i)}, x_{h+1}) \right). \tag{13}
\]

We use this estimator instead of (6), but the rest of the algorithm is unchanged (see Algorithm 3). This modified algorithm enjoys a guarantee in terms of a different definition of witness rank \( W_{\kappa, U} \) where we instead search of matrices sandwiched between \( \kappa \mathcal{E}_B \) and \( \mathcal{W}_U \), entrywise.

**Theorem 5** (Sample Complexity using \( W_U \)). Under Assumption 1 and Assumption 2, for any \( \epsilon, \delta, \kappa \in (0, 1] \), set \( \phi = \frac{\kappa \epsilon}{48 H \sqrt{W_{\kappa, U}}} \), and denote \( T = H W_{\kappa, U} \log(\beta/2\phi)/\log(5/3) \), run Algorithm 3 with inputs \((\mathcal{M}, \mathcal{F}, n_e, n, \epsilon, \delta, \phi)\), where

\[
n_e = \Theta \left( \frac{H^2 \log(HT/\delta)}{\epsilon^2} \right), \quad n = \Theta \left( \frac{H^2 W_{\kappa, U} \log(|\mathcal{M}|/\delta)}{\kappa^2 \epsilon^2} \right),
\]

then with probability at least \( 1 - \delta \), the algorithm outputs a policy \( \pi \) such that \( v^\pi \geq v^* - \epsilon \), using at most

\[
\hat{O} \left( \frac{H^3 W_{\kappa, U}^2 \log(|\mathcal{M}|)}{\kappa^2 \epsilon^2} \right).
\]

Note that in comparison with Theorem 2, this result at face value looks better, since there is no explicit dependence on \( K \) in the final bound. However, in essentially all examples we are aware of, we must set \( \kappa = 1/K \) to account for mismatch between actions distributions in \( \mathcal{W}_U \) and \( \mathcal{E}_B \) to ensure that \( \mathcal{W}_U \geq \kappa \mathcal{E}_B \). As such, this bound is typically worse by a factor of \( K \).

**Proof Sketch.** The only difference is that we use \( \hat{W}_U \) as our estimator. By a standard uniform convergence argument, for fixed \( M \) and time point \( h \), for all \( M' \in \mathcal{M} \) with probability at least \( 1 - \delta \) we have

\[
\left| \hat{W}(M, M', h) - W(M, M', h) \right| \leq \sqrt{\frac{\log(8|\mathcal{M}|4H/\delta)}{2n}}.
\]

Note we are using Lemma 10 here as well. Following the proof of Theorem 2, condition on this event, with the right hand side equal to \( \phi \), as well as the other two events there (that we have \( \hat{O}(\epsilon) \) accurate Bellman error estimates and value estimates). Using these assumptions the algorithm must terminate in \( T = W_{\kappa, U} H \log(\beta/(2\phi))/\log(5/3) \) iterations, where \( W_{\kappa, U} \) is the witness model rank, defined using the \( \mathcal{W}_U \) formulation. As in the previous proof we still set \( \phi = \frac{\kappa \epsilon}{48 H \sqrt{W_{\kappa, U}}} \) which requires

\[
n = \Theta \left( \frac{H^2 W_{\kappa, U} \log(|\mathcal{M}|HT/\delta)}{\kappa^2 \epsilon^2} \right).
\]

The rest of the proof is unchanged. \( \square \)

## D Separation Results and Lower Bounds

### D.1 Proof of Proposition 1

To prove Proposition 1, we need the following lower bound for best-arm identification in stochastic multi-armed bandits.
Lemma 11 (Theorem 2 from Krishnamurthy et al. (2016)). For $K \geq 2$, $\epsilon < \sqrt{1/8}$, and any best-arm identification algorithm, there exists a multi-armed bandit problem for which the best arm $i^*$ is $\epsilon$ better than all others, but for which the estimate $\hat{i}$ of the best arm must have $\mathbb{P}[\hat{i} \neq i^*] \geq 1/3$ unless the number of samples collected is at least $K/(72\epsilon^2)$.

Proof of Proposition 1. Below we explicitly give the construction of $\mathcal{M}$. Every MDP in this family shares the same reward function, and actually also shares the same transition structure for all levels $h \in [H - 1]$. The models only differ in their transition at the last time step.

Fix $H$ and $K \geq 2$. Each MDP $M^{a^*} \in \mathcal{M}$ corresponds to an action sequence $a^* = \{a_1^*, a_2^*, \ldots, a_{H-1}^*\}$ where $a_k^* \in [K]$. Thus there are $K^{H-1}$ models. The reward function, which is shared by all models, is

$$R(x) \triangleq 1 \{x = x^*\}$$

where $x^*$ is a special state that only appears at level $H$. Let $x'$ denote another special state at level $H$.

For any model $M^{a^*}$, at any level $h < H - 1$, the state $x_h$ is simply the history of actions $x_h \triangleq \{a_1, a_2, \ldots, a_{h-1}\}$ applied so far, and taking $a \in \mathcal{A}$ at state $x_h$ deterministically transitions to $x_h \circ a \triangleq \{a_1, a_2, \ldots, a_{h-1}, a\}$. The transition at level $h = H - 1$ is defined as follows:

$$P^{a^*}(x_{H-1}, a_{H-1}) \triangleq \begin{cases} 0.5 + \epsilon 1 \{x_{H-1} \circ a_{H-1} = a^*\}, & x_H = x^* \\ 0.5 - \epsilon 1 \{x_{H-1} \circ a_{H-1} = a^*\}, & x_H = x'. \end{cases}$$

(15)

Thus, in each model $M^{a^*}$, each action sequence $\{a_1, a_2, \ldots, a_{H-1}\}$ can be regarded as an arm in MAB problem with $K^{H-1}$ arms, where all the arms yield $\text{Ber}(0.5)$ reward except for the optimal arm $a^*$ which yields $\text{Ber}(0.5 + \epsilon)$ reward. In fact, this construction is information-theoretically equivalent to the construction used in the standard MAB lower bound, which appears in the proof of Lemma 11. That lower bound directly applies and since we have $K^{H-1}$ arms here, the result follows.

D.2 Proof of Theorem 1

Theorem 1 has two claims: (1) There exists a family of MDPs in which any model-free algorithm will incur exponential sample complexity in the worst case, and (2) Algorithm 3 achieves polynomial sample complexity in this family. As we have discussed, the actual result is stronger in that the model class is a simple Factored MDP and the analysis for our algorithm applies to all Factored MDPs. In Appendix D.2.1 we prove the first claim by constructing a family of simple factored MDPs and showing that any model-free algorithm must incur $\Omega(2^H)$ sample complexity in the worst case. Then in Appendix D.2.2 we prove that Algorithm 3 achieves a sample complexity polynomial in $L$ (and all other parameters) for all Factored MDPs.

D.2.1 Sample Inefficiency of Model-free Algorithms

Proof of Theorem 1, Part 2. We prove the claim by constructing a family of Factored MDPs, defined by transition operators $\mathcal{P}$, and showing that any model-free algorithm—that is, any algorithm that always accesses state $x$ exclusively through $[Q(x, \cdot)]_{Q \in \mathcal{Q}}$—will incur exponential sample complexity when given $Q = \text{OP}(\mathcal{P})$ as input.

Model Class Construction. Fix $d > 2$ and set $H \triangleq d + 2$. The state variables take values in $\mathcal{O} = \{-1, 0, 1, 2\}$. The state space is $\mathcal{X} = [H] \times \mathcal{O}^d$ with the natural partition across time steps and the action space is $\mathcal{A} = \{-1, +1\}$. The initial state is fixed as $x = 1 \circ [0]^d$, where $[a]^d$ stands for a $d$-dimensional vector where every coordinate is $a$ and $\circ$ denotes concatenation. Our model class contains $2^d$ models, each of which is uniquely indexed by an action sequence (or a path) of length $d$, $\mathbf{p} = \{p_1, \ldots, p_d\}$ with $p_i \in \{-1, 1\}$.
Fixing \( \mathbf{p} \), we describe the transition dynamics for \( P^\mathbf{p} \) below. All models share the same reward function, which will be described afterwards.

In \( P^\mathbf{p} \), the parent of the \( i \)th factor is itself so that each factor evolves independently. Furthermore, all transitions are deterministic, so we abuse notation and let \( P^\mathbf{p}_h(\cdot,\cdot) \) denote the deterministic value of the \( i \)th factor at time step \( h + 1 \), as a function of its value at step \( h \) and action \( a \). That is, if at time step \( h \) we are in state \((h, x_1, \ldots, x_d)\), upon taking action \( a \) we will transition deterministically to \((h + 1, P^\mathbf{p}_h^{i,1}(x_1, a), \ldots, P^\mathbf{p}_h^{i,d}(x_d, a))\).

Levels 1 to \( H - 1 \) form a complete binary tree; see Figure 1 for an illustration. For any layer \( h \leq H - 2 \),

\[
\begin{align*}
P^\mathbf{p}_h(v, a) &= v, \quad \forall v \in \mathcal{V}, a \in \mathcal{A}, i \neq h; \\
P^\mathbf{p}_h(v, a) &= a, \quad \forall v \in \mathcal{V}, a \in \mathcal{A}, i = h.
\end{align*}
\]

In words, any internal state at level \( h \leq H - 1 \) simply encodes the sequence of actions that leads to it. These transitions do not depend on the planted path \( \mathbf{p} \) and are identical across all models. Note that it is not possible to have \( x_i = 2 \) for any \( i \in [d], h \leq H - 1 \).

Now we define the transition from level \( H - 1 \) to \( H \), where each state only has 1 action, say +1:

\[
P^\mathbf{p}_H(p_i, +1) = p_i, \quad \forall i \in [d], \quad \text{and} \quad P^\mathbf{p}_H(\bar{p_i}, +1) = 2, \quad i \in [d].
\]

Here \( \bar{p_i} \) is the negation of \( p_i \). In words, the state at level \( H \) simply copies the state at level \( H - 1 \), except that the \( i \)th factor will take value 2 if it disagrees with \( p_i \) (see Figure 1). Thus, the agent arrives at a state without the symbol “2” at level \( H \) only if it follows the action sequence \( \mathbf{p} \).

The reward function is shared across all models. Non-zero rewards are only available at level \( H \), where each state only has 1 action. The reward is 1 if \( x \) does not contain the symbol “2” and the reward is 0.
\[ R((h, x_1, \ldots, x_d)) \triangleq 1 \{ h = H \} \prod_{i=1}^{d} 1 \{ x_i \neq 2 \}. \] (16)

A coarse upper bound on \( L \) for these Factored MDPs is \( L \leq dH|\mathcal{A}||\mathcal{O}|^2 = O(H^2) \) since \(|\mathcal{PA}| = 1\) for all \( i \), \(|\mathcal{O}| = 4\), \(|\mathcal{A}| = 2\), and \( d = H - 2\).

**Sample Inefficiency of Model-free Algorithms.** To show that model-free algorithms cannot have polynomial sample complexity, we construct another class of non-factored models, such that (1) learning in this new class is intractable, and (2) the two families are indistinguishable to any model-free algorithm. The new model class is obtained by transforming each \( P^p \in \mathcal{P} \) into \( \tilde{P}^p \). \( \tilde{P}^p \) has the same state space and transitions as \( P^p \), except for the transition from level \( H - 1 \) to \( H \). This last transition is:

\[ \tilde{P}^p_h((H - 1, x_1, \ldots, x_d)) = \begin{cases} (H, x_1, \ldots, x_d) & \text{if } x_i = p_i \forall i \in [d] \\ H \circ [2]^d & \text{otherwise.} \end{cases} \]

The reward function is the same as in the original model class, given in (16). This construction is equivalent to a multi-armed bandit problem with one optimal arm among \( 2^{H-2} \) arms, so the sample complexity of any algorithm (not necessarily restricted to model-free ones) is \( \Omega(2^H) \).\(^9\) In fact this model class is almost identical to the one used in the proof of Proposition 1.

To prove that the two model families are indistinguishable for model-free algorithms (Definition 1), we show that the \( Q \)-projections in \( P^p \) are identical to those in \( \tilde{P}^p \). This implies that the behavior of a model-free algorithm is identical in \( P^p \) and \( \tilde{P}^p \), so that the sample complexity must be identical, and hence \( \Omega(2^H) \).

Let \( \mathcal{M} = \{ P^p \}_{p \in (-1,1]^d} \) and \( \tilde{\mathcal{M}} = \{ \tilde{P}^p \}_{p \in (-1,1]^d} \). Let \( Q \triangleq \text{OP}(\mathcal{M}) \) and \( \tilde{Q} \triangleq \text{OP}(\tilde{\mathcal{M}}) \). Since all MDPs of interest have fully deterministic dynamics, and non-zero rewards only occur at the last step, it suffices to show that for any deterministic sequence of actions, \( a \), (1) the final reward has the same distribution for \( P^p \) and \( \tilde{P}^p \), and (2) the \( Q \)-projections \( [Q(x_h, \cdot)]_{Q \in \mathcal{Q}} \) and \( [\tilde{Q}(x_h, \cdot)]_{\tilde{Q} \in \tilde{\mathcal{Q}}} \) are equivalent at all states generated by taking \( a \) in \( P^p \) and \( \tilde{P}^p \), respectively. The reward equivalence is obvious, so it remains to study the \( Q \)-projections.

In \( P^p \) and at level \( H \), since the reward function is shared, the \( Q \)-projection is \([1]_{|Q|}\) for the state without “2” and \([0]_{|Q|}\) otherwise. Thus, upon taking \( a = p \) we see the \( Q \)-projection \([1]_{|Q|}\) and otherwise we see \([0]_{|Q|}\). Similarly, in \( \tilde{P}^p \) the \( Q \)-projection is \([0]_{|\tilde{Q}|}\) if the state is \( H \circ [2]^d \) and it is \([1]_{|\tilde{Q}|}\) otherwise. The equivalence here is obvious as \(|Q| = |\tilde{Q}| = 2^d|\).

For level \( H - 1 \), no matter the true model path \( p \), the \( Q^p \) associated with path \( p' \) has value \( Q^p(a, +1) = 1 \{ a = p' \} \) at state \( a \). Hence the \( Q \)-projection at \( a \) can be represented as \( [1 \{ a = p' \}]_{p' \in \{-1,1\}^d} \), for both \( P^p \) and \( \tilde{P}^p \). Note that the \( Q \)-projection does not depend on the true model \( p \) because all models agree on the dynamics before the last step. Similarly, for \( h < H - 1 \) where each state has two actions \( \{-1, 1\} \), we have:

\[ Q^p(a_{1:h-1}, -1) = 1 \{ a_{1:h-1} \circ -1 = p'_{1:h} \}, Q^p(a_{1:h-1}, 1) = 1 \{ a_{1:h-1} \circ 1 = p'_{1:h} \}. \]

Hence, the \( Q \)-projection can be represented as:

\[ [1 \{ a_{1:h-1} \circ -1 = p'_{1:h} \}, 1 \{ a_{1:h-1} \circ 1 = p'_{1:h} \}]_{p' \in \{-1,1\}^d}. \]

again with no difference between \( P^p \) and \( \tilde{P}^p \). Thus, the model \( P^p \) and \( \tilde{P}^p \) induce exactly the same \( Q \)-projection for all paths, implying that any model-free algorithm (in the sense of Definition 1), must behave identically on both. Since the family \( \tilde{\mathcal{M}} = \{ \tilde{P}^p \}_p \) admits an information-theoretic sample complexity lower bound of \( \Omega(2^H) \), this same lower bound applies to \( \mathcal{M} = \{ P^p \}_p \) for model-free algorithms. \( \square \)

\(^9\)Note that the reward function is known and non-random, so we do not have any dependence on an accuracy parameter \( \epsilon \).
D.2.2 PAC bound for Factored MDP

Recall that we follow conventions and assume that the reward function is known and shared by all the models. Since the only difference between two models is their transitions, we use $\mathcal{P} = \{ P : (R^*, P) \in \mathcal{M} \}$ to represent the model class.

We first define a new witness model misfit definition $\mathcal{W}_F$ for any $P, P' \in \mathcal{P}$ as

$$
\mathcal{W}_F(P, P', h) \triangleq \mathbb{E} \left[ \sum_{i=1}^{d} \left\| P^i(i) : |x_h[p_a_i], a_h) - P^*(i) : |x_h[p_a_i], a_h) \right\|_{TV} |x_h \sim \pi_P, a_h \sim U(\mathcal{A}) \right] 
$$

(17)

This definition is related to the original fitness model misfit using total variation in (3), but differs in that $a_h$ is sampled uniformly from $\mathcal{A}$ and that the TV-distance between $P'$ and $P^*$ are factored. First, we show that the matrix $\mathcal{W}_F$ has rank at most $\sum_{i=1}^{d} K |O| |p_a(i)|$, which is less than total number of parameters in all CPTs used to specify the transition at $h$.

Claim 6. Denote $L_h \triangleq \sum_{i=1}^{d} K |O|^{1+|p_a(i)|}$, and assume $\mathcal{P}$ obeys the Factored MDP structure. There exists a witness function $\zeta_h : \mathcal{P} \rightarrow \mathbb{R}^{L_h/|O|}$ and $\chi_h: \mathcal{P} \rightarrow \mathbb{R}^{L_h/|O|}$, such that for any $P, P' \in \mathcal{M}$, and $h \in [H]$,

$$
\mathcal{W}_F(P, P', h) = \langle \zeta_h(P), \chi_h(P') \rangle,
$$

and $\|\zeta_h(P)\|_2 \cdot \|\chi_h(P')\|_2 \leq O(L_h/K)$.

Proof. Given any policy $\pi$, let us denote $d^\pi_h(x) \in \Delta(\mathcal{X}_h)$ as the state distribution resulting from $\pi$ at time step $h$. Then we can write $d^\pi_h(x) = d^\pi_h(x[u]d^\pi_d(x[d \setminus u]|x[u])$, where recall that for a subset $u \subseteq [d]$, we write $x[u]$ to denote the corresponding assignment of those state variables in $x$, and $d \setminus u = [d] \setminus u \subseteq [d]$ is just for shorthand. We use $d^\pi_h$ to denote the probability mass function and we use $P^\pi_h$ to denote the distribution.

For any $P, P' \in \mathcal{P}$, we can factorize $\mathcal{W}_F(P, P', h)$ as follows:

$$
\mathcal{W}_F(P, P', h) = \mathbb{E} \left[ \sum_{i=1}^{d} \left\| P^i(i) : |x_h[p_a_i], a_h) - P^*(i) : |x_h[p_a_i], a_h) \right\|_{TV} |x_h \sim \pi_P, a_h \sim U(\mathcal{A}) \right] 
$$

\begin{align*}
&= \frac{1}{K} \sum_{i=1}^{d} \sum_{x_h, a} d^\pi_h(x_h) \left\| P^i(i) : |x_h[p_a_i], a) - P^*(i) : |x_h[p_a_i], a) \right\|_{TV} \\
&= \frac{1}{K} \sum_{i=1}^{d} \sum_{x_h, a} d^\pi_h(x_h[p_a_i])d^\pi_d(x_h[d \setminus p_a_i]|x_h[p_a_i]) \left\| P^i(i) : |x_h[p_a_i], a) - P^*(i) : |x_h[p_a_i], a) \right\|_{TV} \\
&= \frac{1}{K} \sum_{i=1}^{d} \sum_{x_h, a} \sum_{u \in O^{p_a(i)}} \mathbb{P}^\pi_h [x_h[p_a_i] = u] \left\| P^i(i) : |u, a) - P^*(i) : |u, a) \right\|_{TV} \\
&= \langle \zeta_h(P), \chi_h(P') \rangle.
\end{align*}

Here $\zeta_h(P)$ is indexed by $(i, a, u)$ with $i \in [d], a \in \mathcal{A}, u \in O^{p_a(i)}$ with value $\zeta_h(i, a, u; P) \triangleq \mathbb{P}^\pi_h [x_h[p_a_i] = u]$. $\chi_h(P')$ is also indexed by $i, a, u$, with value $\chi_h(i, a, u; P') \triangleq \left\| P^*(i) : |u, a) - P^*(i) : |u, a) \right\|_{TV}$. Note that $\zeta_h$’s value only depends on $P$, while $\chi_h$’s values only depend on $P'$. Moreover the dimensions of $\zeta_h$ and $\chi_h$ are $\sum_{i=1}^{d} K |O|^{p_a(i)} = L_h/|O|$, each entry of $\zeta_h$ is bounded by $1/K$, and each entry of $\chi_h$ is at most 2. Hence, we must have $\beta = \sup_{\zeta, \chi} \|\zeta\|_2 \cdot \|\chi\|_2 \leq O(L/K)$. \(\square\)
We will require the following tensorization property for the total variation of product measures.

**Claim 7.** Let \( P_1, \ldots, P_n \) and \( Q_1, \ldots, Q_n \) be distributions where \( P_i \in \Delta(S_i) \) for finite sets \( S_i \). Define the product measures \( P^{(n)}, Q^{(n)} \) as \( P^{(n)}(s_1, \ldots, s_n) \equiv \prod_{i=1}^n P_i(s_i) \). Then

\[
\frac{1}{n} \sum_{i=1}^n \| P_i - Q_i \|_{TV} \leq \left\| P^{(n)} - Q^{(n)} \right\|_{TV} \leq \sum_{i=1}^n \| P_i - Q_i \|_{TV}.
\]

For completeness we provide the proof in Appendix D.2.3. Since \( P'(\cdot|x_h, a), P^*(\cdot|x_h, a) \) are both product measure over the individual state variables, by Claim 7, we can relate the witness model misfit defined using the uniform action distribution (8), to our alternative definition using the tensorized TV distance (17):

\[
\frac{1}{d} W_F(P, P', h) \leq W_U(P, P', h) \leq W_F(P, P', h).
\]

Further, since \( a_h \sim U(A) \), we can relate \( E_B \) to \( W_U \).

**Claim 8.** For any \( P, P' \in \mathcal{P} \) and \( h \in [H] \), we always have

\[
E_B(P, P', h) \leq K W_U(P, P', h).
\]

The proof is deferred to Appendix D.2.3. Combining the above results, we have:

\[
\frac{1}{Kd} E_B(P, P', h) \leq \frac{1}{d} W_U(P, P', h) \leq \frac{1}{d} W_F(P, P', h) \leq W_U(P, P', h).
\]

Thus, we have a matrix \( W_F/d \) that is entrywise between \((1/Kd)E_B\) and \( W_U \), which yields the following claim.

**Claim 9.** Recall the definition of witness rank in Definition 3, where \( W_U \) is defined in (8). Set \( \kappa = \frac{1}{Kd} \), we have \( W(1/Kd, \beta, \mathcal{P}, \mathcal{F}, h) \leq L_h / |O| \), for \( \beta \leq O(L/K) \).

Now, applying Theorem 5, we see that Algorithm 3 has sample complexity

\[
\tilde{O} \left( \frac{HL^2 K^2 d^2}{|O|^2 \epsilon^2} \log \left( \frac{|P|}{\delta} \right) \right),
\]

where we are omitting logarithmic dependence on \( H, L, K, d, \epsilon \) and poly-log dependence on \( \delta, |P| \). Note that since all transition models in \( \mathcal{P} \) obey the same factorization, the set \( \mathcal{P} \) has \( \ell_\infty \) log-covering number \( L \log(1/\epsilon) \) at scale \( \epsilon \). Since our arguments only require estimating expectations (i.e., linear functionals) with respect to \( P \in \mathcal{P} \), we may appeal to standard uniform convergence arguments to extend beyond finite classes.

We omit the details here, but this argument gives a final sample complexity of

\[
\tilde{O} \left( \frac{HL^3 K^2 d^2}{|O|^2 \epsilon^2} \log (1/(\epsilon \delta)) \right).
\]

Note that \( L > |O| \), so the error degrades when the set of values each state feature can take increases.
D.2.3 Missing Proofs from Appendix D.2.2

Proof of Claim 7. For the first claim, considering \( \|P_1 - Q_1\|_{TV} \), we have:

\[
\|P_1 - Q_1\|_{TV} = \sum_{s_1} |P_1(s_1) - Q_1(s_1)| = \sum_{s_1} \left| P_1(s_1) \sum_{s_{2:n}} P_{2:n}(s_{2:n}) - Q_1(s_1) \sum_{s_{2:n}} Q_{2:n}(s_{2:n}) \right|
\]

\[
\leq \sum_{s_1:n} |P_{1:n}(s_1:n) - Q_{1:n}(s_1:n)| = \|P(n) - Q(n)\|_{TV}.
\]

The same bound applies for all \( i \in [n] \) which proves the first result.

For the second part, define \( W_i \in \Delta(S_1 \times \cdots \times S_n) \) with \( W_i(s_1:n) = \prod_{j=i} P_j(s_j) \prod_{j=i+1} Q_j(s_j) \), with \( i \in \{0, \ldots, n\} \). This gives \( W_0 = Q^{(n)} \), and \( W_n = P^{(n)} \). Now, by telescoping, we have

\[
\|P^{(n)} - Q^{(n)}\|_{TV} = \|W_0 - W_n\|_{TV} \leq \sum_{i=0}^{n-1} \|W_i - W_{i+1}\|_{TV}.
\]

For \( \|W_i - W_{i+1}\|_{TV} \), we have

\[
\|W_i - W_{i+1}\|_{TV} = \left| \prod_{j=1}^{i} \frac{P_j}{P_j} \prod_{j=i+1}^{n} Q_j - \prod_{j=i+1}^{n} P_j \prod_{j=i+2}^{n} Q_j \right|_{TV} = \|Q_{i+1} - P_{i+1}\|_{TV}.
\]

Proof of Claim 8. Due to Fact 1, we have

\[
\mathcal{E}_B(P, P', h) = \mathbb{E} \left[ \mathbb{E}_{x_{h+1} \sim P'_{x_{h+1}, a_h}} [V_P(x_{h+1})] - \mathbb{E}_{x_{h+1} \sim P'_{x_{h+1}, a_h}} [V_P(x_{h+1})] \mid x_h \sim \pi_P, a_h \sim \pi_P^* \right]
\]

\[
\leq \mathbb{E} \left[ \sum_{a_h} \pi_P'(a_h|x_h) \left| \mathbb{E}_{x_{h+1} \sim P'_{x_{h+1}, a_h}} [V_P(x_{h+1})] - \mathbb{E}_{x_{h+1} \sim P^*_h, a_h} [V_P(x_{h+1})] \right| \mid x_h \sim \pi_P \right]
\]

\[
\leq \mathbb{E} \left[ \sum_{a_h} \pi_P'(a_h|x_h) \|P'_{x_h, a_h} - P^*_{x_h, a_h}\|_{TV} \mid x_h \sim \pi_P \right]
\]

\[
\leq K \mathbb{E} \left[ \mathbb{E}_{a_h \sim U(A)} \|P'_{x_h, a_h} - P^*_{x_h, a_h}\|_{TV} \mid x_h \sim \pi_P \right] = KW(P, P', h),
\]

where we use Holder’s inequality, the boundness assumption on \( V_P \), and the fact that \( \pi_P'(a|x) \leq 1 \).

E Q-projections in tabular settings

Here we show that the Q-projection yields no information loss in tabular environments. Thus from the perspective of Definition 1, model-based and model-free algorithms are information-theoretically equivalent.

In tabular settings, the state space \( \mathcal{X} \) and action space \( \mathcal{A} \) are both finite and discrete. It is also standard to use a fully expressive \( Q \)-function class, that is \( \mathcal{Q} = \{ Q : \mathcal{X} \times \mathcal{A} \to [0, 1] \} \), where the range here arises due to the bounded reward. For each state \( x \in \mathcal{X} \) define the function \( Q^x \) such that for all \( a \in \mathcal{A} \), \( Q^x(x', a) = 1 \{ x = x' \} \). Observe that since \( \mathcal{Q} \) is fully expressive, we are ensured that \( Q^x \in \mathcal{Q}, \forall x \in \mathcal{X} \).

At any state \( x' \in \mathcal{X} \), from the Q-projection \( \Phi_Q(x') \) we can always extract the values \( [Q^x(x', a)]_{x \in \mathcal{X}} \) for some fixed action \( a \). By construction of the \( Q^x \) functions, exactly one of these values will be one, while all others will be zero, and thus we can recover the state \( x' \) simply by examining a few values in \( \Phi_Q(x') \). In other words, the mapping \( x \mapsto \Phi_Q(x) \) is invertible in the tabular case, and so there is no information lost through the projection. Hence in tabular setting, one can run classic model-free algorithms such as Q-learning (Watkins and Dayan, 1992) under our definition.
Algorithm 4 Guessing $W_{\kappa^*}/\kappa^*$, Arguments: $(\mathcal{M}, \mathcal{F}, \epsilon, \delta)$

1: \textbf{for} epoch $i = 1, 2, \ldots$ \textbf{do}
2: \hspace{1em} Set $N_i = 2^{i-1}$ and $\delta_i = \delta/(i(i+1))$
3: \hspace{1em} \textbf{for} $j = 1, 2, \ldots$ \textbf{do}
4: \hspace{2em} Set $\kappa_{i,j} = (1/2)^{j-1}$, $\delta_{i,j} = \delta_i/(j(j+1))$, and $W_{i,j} = N_i \kappa_{i,j}^2$
5: \hspace{2em} if $W_{i,j} < 1$ then
6: \hspace{3em} Break
7: \hspace{1em} \textbf{end if}
8: \hspace{1em} Set $T_{i,j} = H W_{i,j} \log(\beta/(2\phi))/\log(5/3)$ and $\phi_{i,j} = \epsilon/(48H\sqrt{N_i})$
9: \hspace{1em} Set $n_{e_{i,j}} = \Theta\left(\frac{H^2 \log(6HT_{i,j})}{\epsilon^2}\right)$ and $n_{i,j} = \Theta\left(\frac{H^2 KN_i \log(|\mathcal{M}|F\delta_{i,j})}{\epsilon^2}\right)$
10: \hspace{1em} Run Algorithm 1 with $(\mathcal{M}, \mathcal{F}, n_{i,j}, n_{e_{i,j}}, \epsilon, \delta_{i,j}, \phi)$ for $T_{i,j}$ iterations
11: \hspace{1em} If Algorithm 1 returns a policy, then break and return the policy
12: \hspace{1em} \textbf{end for}
13: \hspace{1em} \textbf{end for}

F Extension to Unknown Witness Rank

Algorithm 1 and its analysis assumes that we know $\kappa$ and $W_\kappa$ (in fact any finite upper bound of $W_\kappa$), which could be a strong assumption in some cases. In this section, we show that we can apply a standard doubling trick to handle the situation where $\kappa$ and $W_\kappa$ are unknown.

Let us consider the quantity $W_\kappa/\kappa$. Let us denote $\kappa^* = \arg\min_{\kappa \in (0,1]} W_\kappa/\kappa$. Note that the sample complexity of Algorithm 1 is minimized at $\kappa^*$. Algorithm 4 applies the doubling trick to guess $W_{\kappa^*}$ and $\kappa^*$ jointly with Algorithm 1 as a subroutine. In the algorithm, $N_i$ in the other loop denotes a guess for $W/\kappa^2$ which we use to set the parameter $\phi$ and $n$. The following theorem characterizes the its sample complexity.

Theorem 10. For any $\epsilon, \delta \in (0,1)$, with $\mathcal{M}$ and $\mathcal{F}$ satisfying Assumption 1 and Assumption 2, with probability at least $1 - \delta$, Algorithm 4 terminates and outputs a policy $\pi$ with $v^\pi \geq v^* - \epsilon$, using at most

$$\tilde{O}\left(\frac{H^3 K W_{\kappa^*}^2 \log(|\mathcal{M}|/\delta)}{(\kappa^* \epsilon)^2}\right)$$

trajectories.

Proof. Consider the $j$th iteration in the $i$th epoch. Based on the value of $\phi_{i,j}$, $n_{e_{i,j}}$, $n_{i,j}$, using Lemma 4 and Lemma 3, with probability at least $1 - \delta_{i,j}$, for any $t \in [1, T_{i,j}]$ during the run of Algorithm 1, we have

$$|v^\pi_t - \hat{v}^\pi_t| \leq \epsilon/8, \tag{18}$$
$$|\hat{E}_B(M^t, M^t, h) - E_B(M^t, M^t, h)| \leq \epsilon/(8H), \forall h \in [H], \tag{19}$$
$$|\hat{W}(M^t, M^t, h_t) - W(M^t, M^t, h_t)| \leq \phi_{i,j}, \forall M^t \in \mathcal{M}. \tag{20}$$

The first condition above ensures that if Algorithm 1 terminates in the $j$th iteration and the $i$th epoch and outputs $\pi$, then $\pi$ must be near-optimal, based on Lemma 6. The third inequality above together with the elimination criteria in Algorithm 1 ensures that $M^*$ is never eliminated.

Denote $i_*$ as the epoch where $W_{\kappa^*}/(\kappa^*)^2 \leq N_{i_*} \leq 2W_{\kappa^*}/(\kappa^*)^2$, and $j_*$ as the iteration inside the $i_*$ epoch where $\kappa^* \leq \kappa_{i_*,j_*} \leq 2\kappa^*$. Since $W_{i_*,j_*} = N_{i_*} (\kappa_{i_*,j_*})^2$, we have:

$$W_{\kappa^*} \leq W_{i_*,j_*} \leq 8W_{\kappa^*}. \tag{21}$$

Below we condition on the event that $M^*$ is not eliminated during any epoch before $i_*$, and any iteration before $j_*$ in the $i_*$ epoch. We analyze the $j_*$ iteration in the $i_*$ epoch below. Since $N_{i_*} = 2^{i_*-1}$ and $N_{i_*} \leq 2W_{\kappa^*}/(\kappa^*)^2$, we must have $i_* \leq 1 + \log_2(2W_{\kappa^*}/(\kappa^*)^2)$. 

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Based on the value of $\phi_{i,i}$, $n_{i,i}$, $n_{i,e_{i,j}}$, and $T_{i,i}$, we know with probability at least $1 - \delta_{i,i}$, for any $t \in [1, T_{i,i}]$ in the execution of Algorithm 1, inequalities (18), (19), and (20) hold. Conditioned on this event, similar to the proof of Lemma 9, we can show that Algorithm 1 must terminate in at most $H W_n \log(\beta/2\phi) / \log(5/3)$ many rounds in this iteration.

From (21), we know that $W_{i,j} \geq W_e$, which implies that $T_{i,j} \geq H W_e \log(\beta/2\phi) / \log(5/3)$. In other words, in the $j^*$ iteration of the $i^*$ epoch, we run Algorithm 1 long enough to guarantee that it terminates and outputs a policy. We have already ensured that if it terminates, it must output a policy $\pi$ with $v^\pi \geq v^* - \epsilon$ (this is true for any $(i,j)$ pair).

Now we calculate the sample complexity. In the $i^*$ epoch, since we terminate when $W_{i,j} < 1$, the number of iterations is at most $\log_2 N_i < i$. Hence the number of trajectories collected in this epoch is at most

$$\sum_{j=1}^i (n_{i,j} + n_{i,j})T_{i,j} = \sum_{j=1}^i O(H^3KW_{i,j}^2 \log(T_{i,j}|M||F|/\delta_{i,j})/(\epsilon\kappa_{i,j})^2)$$

$$= O(iH^3KN_i^2 \log(T_{i,1}|M||F|/\delta_{i,i})/\epsilon^2),$$

where we used the fact that $N_i = W_{i,j} / (\kappa_{i,j})^2$, $T_{i,1} \geq T_{i,j}$, and $\delta_{i,i} \leq \delta_{i,j}$. Note that $\sum_{i=1}^{i^*} iN_i^2 = \sum_{i=1}^{i^*} i(2i-1)^2 \leq (i^* - 1)(2i^* - 1)^2/3 = O(i^* N_i^2)$. Hence the sample complexity in the $i^*$ epoch dominates the total sample complexity, which is

$$\tilde{O} \left((1 + \log_2(W_e / (\kappa^*))^2)H^3KW_e^2 \log(T_{i,0}|M||F|/\delta_{i,i})/\epsilon^2,\right)$$

where we used the fact that $i^* \leq 1 + \log_2(2W_e / (\kappa^*))^2$, and $N_i \leq 2W_e / (\kappa^*)^2$. Applying a union bound over $(i,j)$, with $i \leq i^*$, since we have $\sum_{i=1}^{i^*} \sum_{j=1}^{i} \delta_{i,j} \leq \sum_{i=1}^{i^*} \delta_{i,1} = \sum_{i=1}^{i^*} \delta / (i(i + 1)) \leq \delta$, the failure probability is at most $\delta$, which proves the theorem.

### G Details on Exponential Family Model Class

For any model $M \in \mathcal{M}$, conditioned on $(x, a) \in \mathcal{X} \times \mathcal{A}$, we assume $M_{x,a} \triangleq \exp(\langle \theta_{x,a}, T(r, x') \rangle) / Z(\theta_{x,a})$ with $\theta_{x,a} \in \Theta \subset \mathbb{R}^m$. Without loss of generality, we assume $\|\theta_{x,a}\| \leq 1$, and $\Theta = \{\theta : \|\theta\| \leq 1\}$. We design $\mathcal{G} = \{\mathcal{X} \times \mathcal{A} \rightarrow \Theta\}$, i.e., $\mathcal{G}$ contains all mappings from $(\mathcal{X} \times \mathcal{A})$ to $\Theta$. We design $\mathcal{F} = \{(x, a, r, x') \mapsto \langle g(x, a), T(r, x') \rangle : g \in \mathcal{G} \}$. Using Definition 2, we have:

$$\mathcal{W}(M, M', h) = \sup_{f \in \mathcal{F}} \mathbb{E}_{x \sim \pi_M, a \sim \pi_M} \left[ \mathbb{E}_{(r,x') \sim M_h} [f(x, a, r, x') - \mathbb{E}_{(r,x') \sim M_h} [f(x, a, r, x')]] \right]$$

$$= \mathbb{E}_{x \sim \pi_M, a \sim \pi_M} \left[ \sup_{\theta \in \Theta} \left( \mathbb{E}_{(r,x') \sim M_h} [\langle \theta, T(r, x') \rangle] - \mathbb{E}_{(r,x') \sim M_h} [\langle \theta, T(r, x') \rangle] \right) \right]$$

$$= \mathbb{E}_{x \sim \pi_M, a \sim \pi_M} \left[ \mathbb{E}_{(r,x') \sim M_h} [T(r, x')] - \mathbb{E}_{(r,x') \sim M_h} [T(r, x')] \right],$$

where the second equality uses the fact that $\mathcal{G}$ contains all possible mappings from $\mathcal{X} \times \mathcal{A} \rightarrow \Theta$.

We assume that for any $\theta \in \Theta$, the hessian of the log partition function $\nabla^2 \log(Z(\theta))$ is positive definite with eigenvalues bounded between $[\gamma, \beta]$ with $0 \leq \gamma \leq \beta$. Below, we show that under the above assumptions, Bellman Domination (Fact 2) still holds up to a constant, even without explicitly using Assumption 2.

**Claim 11** (Bellman Domination for Exponential Families). *In the exponential family setting, we have

$$\frac{\gamma}{\sqrt{2\beta}} \mathcal{E}_B(M, M', h) \leq \mathcal{W}(M, M', h).$$*
Proof. We leverage Theorem 3.2 from Gao et al. (2018), which implies that
\[ \frac{\gamma}{\sqrt{\beta}} \mathbb{E}_{x_h \sim \pi_M, a_h \sim \pi_{M'}} \sqrt{D_{KL}(M'_{x_h, a_h} || M^*_{x_h, a_h})} \leq W(M, M', h). \]

By Pinsker’s inequality, we have:
\[ \frac{\gamma}{\sqrt{2\beta}} \mathbb{E}_{x_h \sim \pi_M, a_h \sim \pi_{M'}} \left\| M'_{x_h, a_h} - M^*_{x_h, a_h} \right\|_{TV} \leq W(M, M', h), \]
where the LHS is the witness model misfit defined using total variation directly (3). Note that Bellman domination applies to the TV-based witness model misfit due to the regularity assumption on the total reward, which concludes the proof.

Note that the constant \( \frac{\gamma}{\sqrt{2\beta}} \) can be absorbed into \( \kappa \) in the definition of witness rank (Definition 3).