FLAMBE: Structural Complexity and Representation Learning of Low Rank MDPs

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Abstract

In order to deal with the curse of dimensionality in reinforcement learning (RL), it is common practice to make parametric assumptions where values or policies are functions of some low dimensional feature space. This work focuses on the representation learning question: how can we learn such features? Under the assumption that the underlying (unknown) dynamics correspond to a low rank transition matrix, we show how the representation learning question is related to a particular non-linear matrix decomposition problem. Structurally, we make precise connections between these low rank MDPs and latent variable models, showing how they significantly generalize prior formulations for representation learning in RL. Algorithmically, we develop FLAMBE, which engages in exploration and representation learning for provably efficient RL in low rank transition models.

1 Introduction

The ability to learn effective transformations of complex data sources, sometimes called representation learning, is an essential primitive in modern machine learning, leading to remarkable achievements in language modeling, vision, and serving as a partial explanation for the success of deep learning more broadly (Bengio et al., 2013). In Reinforcement Learning (RL), several works have shown empirically that learning succinct representations of perceptual inputs can accelerate the search for decision-making policies (Pathak et al., 2017; Tang et al., 2017; Oord et al., 2018; Srinivas et al., 2020). However, representation learning for RL is far more subtle than it is for supervised learning (Du et al., 2019a; Van Roy and Dong, 2019; Lattimore and Szepesvari, 2019), and the theoretical foundations of representation learning for RL are nascent.

The first question that arises in this context is: what is a good representation? Intuitively, a good representation should help us achieve greater sample efficiency on downstream tasks. For supervised learning, several theoretical works adopt the perspective that a good representation should permit simple models to achieve high accuracy on tasks of interest (Baxter, 2000; Maurer et al., 2016; Arora et al., 2019; Tosh et al., 2020). Lifting this perspective to reinforcement learning, it is natural to ask that we can express value functions and policies as simple functions of our representation. This may allow us to leverage recent work on sample efficient RL with parametric function approximation.

The second question is: how do we learn such a representation when it is not provided in advance? This question is particularly challenging because representation learning is intimately tied to exploration. We cannot learn a good representation without a comprehensive dataset of experience from the environment, but a good representation may be critical for efficient exploration.

This work considers these questions in the context of low rank MDPs (Jiang et al., 2017) (also known as factorizing MDPs (Rendle et al., 2010) and linear MDPs (Jin et al., 2019; Yang and Wang, 2019b)), which
**Algorithm** | **Setting** | **Sample Complexity** | **Computation**
--- | --- | --- | ---
PCID (Du et al., 2019b) | block MDP | $d^4 H^2 K^4 \left( \frac{1}{\eta^2 \gamma^2} + \frac{1}{\varepsilon^2} \right)$ | Oracle efficient
HOMER (Misra et al., 2019) | block MDP | $d^8 H^4 K^4 \left( \frac{1}{\eta^4} + \frac{1}{\varepsilon^2} \right)$ | Oracle efficient
OLIVE (Jiang et al., 2017) | low Bellman rank | $\frac{d^4 H^2 K}{\varepsilon^2}$ | Inefficient
Sun et al. (2019) | low Witness rank | $\frac{d^4 H^2 K}{\varepsilon^2}$ | Inefficient
FLAMBE (this paper) | low rank MDP | $d^3 H^3 K^2 \left( \frac{1}{\eta^5} + \frac{1}{\eta^2 \varepsilon^2} \right)$ | Oracle efficient

Table 1: Comparison of methods for representation learning in RL. Settings from least to most general are: block MDP, low rank MDP, low Bellman rank, low Witness rank. In all cases $d$ is the embedding dimension, $H$ is the horizon, $K$ is the number of actions, $\eta$ and $\gamma$ parameterize reachability and margin assumptions, and $\varepsilon$ is the accuracy. Dependence on function classes and logarithmic factors are suppressed. Block MDP algorithms discover a one-hot representation to discrete latent states. Bellman/Witness rank approaches can take a class $\Phi$ of embedding functions and search over simple policies or value functions composed with $\Phi$ (see Section 4 and Appendix A.3 for details).

we argue provide a natural framework for studying representation learning in RL. Concretely, these models assume there exists low dimensional embedding functions $\phi(x, a), \mu(x')$ such that the transition operator $T$ satisfies $T(x' | x, a) = \langle \phi(x, a), \mu(x') \rangle$, where $T(x' | x, a)$ specifies the probability of the next state $x'$ given the previous state $x$ and action $a$. Low rank MDPs address the first issue above (on what constitutes a good representation) in that if the features $\phi$ are known to the learner, then sample efficient learning is possible (Jin et al., 2019; Yang and Wang, 2019b).

**Our contributions.** We address the question of learning the representation $\phi$ in a low rank MDP. To this end our contributions are both structural and algorithmic.

1. **Expressiveness of low rank MDPs.** Our algorithmic development leverages a re-formulation of the low rank dynamics in terms of an equally expressive, but more interpretable latent variable model. We provide several structural results for low rank MDPs, relating it to other models studied in prior work on representation learning for RL. In particular, we show that low rank MDPs are significantly more expressive than the block MDP model (Du et al., 2019b; Misra et al., 2019).

2. **Feature learning.** We develop a new algorithm, called FLAMBE for “Feature learning and model based exploration”, that learns a representation for low rank MDPs. We prove that under realizability and reachability assumptions, FLAMBE learns a uniformly accurate model of the environment as well as a feature map that enables the use of linear methods for RL, in a statistically and computationally efficient manner. These guarantees enable downstream reward maximization, for any reward function, with no additional data collection. Our analysis of FLAMBE crucially leverages the latent variable representation as we describe in Section 5.

Our results and techniques provide new insights on representation learning for RL and also significantly increase the scope for provably efficient RL with rich observations (see Table 1).

## 2 Low Rank MDPs

We consider an episodic Markov decision process $\mathcal{M}$ with episode length $H \in \mathbb{N}$, state space $\mathcal{X}$, and a finite action space $\mathcal{A} = \{1, \ldots, K\}$. In each episode, a trajectory $\tau = (x_0, a_0, x_1, a_1, \ldots, x_{H-1}, a_{H-1}, x_H)$ is generated, where (a) $x_0$ is a starting state, and (b) $x_{h+1} \sim T_h(\cdot | x_h, a_h)$, and (c) all actions $a_{0:H-1}$ are chosen by the agent. We assume the starting state is fixed and that there is only one available action at time $h$.
The operators $T_h : \mathcal{X} \times \mathcal{A} \to \Delta(\mathcal{X})$ denote the (non-stationary) transition dynamics for each time step.

As is standard in the literature, a policy $\pi : \mathcal{X} \to \Delta(\mathcal{A})$ is a (randomized) mapping from states to actions. We use the notation $\mathbb{E} [\cdot | \pi, \mathcal{M}]$ to denote expectations over states and actions observed when executing policy $\pi$ in MDP $\mathcal{M}$. We abuse notation slightly and use $[H]$ to denote $\{0, \ldots, H - 1\}$.

**Definition 1.** An operator $T : \mathcal{X} \times \mathcal{A} \to \Delta(\mathcal{X})$ admits a low rank decomposition with dimension $d \in \mathbb{N}$ if there exists two embedding functions $\phi^* : \mathcal{X} \times \mathcal{A} \to \mathbb{R}^d$ and $\mu^* : \mathcal{X} \to \mathbb{R}^d$ such that

$$\forall x, x' \in \mathcal{X}, a \in \mathcal{A} : T(x') = \langle \phi^*(x, a), \mu^*(x') \rangle.$$  

For normalization, we assume that $\|\phi^*(x, a)\|_2 \leq 1$ for all $x, a$ and for any function $g : \mathcal{X} \to [0, 1]$, $\| \int \mu^*(x) g(x) dx \|_2 \leq \sqrt{d}$. An MDP $\mathcal{M}$ is a low rank MDP if for each $h \in [H]$, $T_h$ admits a low rank decomposition with dimension $d$. We use $\phi^*_h, \mu^*_h$ to denote the embeddings for $T_h$.

Throughout we assume that $\mathcal{M}$ is a low rank MDP with dimension $d$. Note that the condition on $\mu^*$ ensures that the Bellman backup operator is well-behaved.

**Function approximation for representation learning.** We consider state spaces $\mathcal{X}$ that are arbitrarily large, so that some form of function approximation is necessary to generalize across states. For representation learning, it is natural to grant the agent access to two function classes $\Phi \subset \mathcal{X} \times \mathcal{A} \to \mathbb{R}^d$ and $\Upsilon \subset \mathcal{X} \to \mathbb{R}^d$ of candidate embeddings, which we can use to identify the true embeddings $(\phi^*, \mu^*)$. To facilitate this model selection task, we posit a realizability assumption.

**Assumption 1** (Realizability). We assume that for each $h \in [H]$: $\phi^*_h \in \Phi$ and $\mu^*_h \in \Upsilon$.

We desire sample complexity bounds that scale logarithmically with the cardinality of the classes $\Phi$ and $\Upsilon$, which we assume to be finite. Extensions that permit infinite classes with bounded statistical complexity (e.g., VC-classes) are not difficult.

In Appendix A, we show that the low rank assumption alone, without Assumption 1, is not sufficient for obtaining performance guarantees that are independent of the size of the state space. Hence, additional modeling assumptions are required, and we encode these in $\Phi, \Upsilon$.

**Learning goal.** We focus on the problem of reward-free exploration (Hazan et al., 2019; Jin et al., 2020), where the agent interacts with the environment with no reward signal. When considering model-based algorithms, a natural reward-free goal is system identification: given function classes $\Phi, \Upsilon$, the algorithm should learn a model $\hat{\mathcal{M}} := (\hat{\phi}_{0:H-1}, \hat{\mu}_{0:H-1})$ that uniformly approximates the environment $\mathcal{M}$. We formalize this with the following performance criteria:

$$\forall \pi, h \in [H] : \mathbb{E} \left[ \left\| \hat{\phi}_h(x_h, a_h) \hat{\mu}_h(\cdot) - T_h(\cdot | x_h, a_h) \right\|_{\text{TV}} | \pi, \mathcal{M} \right] \leq \varepsilon. \quad (1)$$

Here, we ask that our model accurately approximates the one-step dynamics from the state-action distribution induced by following any policy $\pi$ for $h$ steps in the real environment.

System identification also implies a quantitative guarantee on the learned representation $\hat{\phi}_{0:H-1}$: we can approximate the Bellman backup of any value function on any data-distribution.

**Lemma 1.** If $\hat{\mathcal{M}} = (\hat{\phi}_{0:H-1}, \hat{\mu}_{0:H-1})$ satisfies (1), then

$$\forall h \in [H], V : \mathcal{X} \to [0, 1], \exists \theta_h : \max_\pi \mathbb{E} \left[ \left\| \langle \theta_h, \hat{\phi}_h(x_h, a_h) \rangle - \mathbb{E} [V(x_{h+1}) | x_h, a_h] \right\| | \pi, \mathcal{M} \right] \leq \varepsilon.$$

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1. This easily accommodates the standard formulation with a non-degenerate initial distribution by defining $T_0(\cdot | x_0, a_0)$ to be the initial distribution. This setup is notationally more convenient, since we do not need special notation for the starting distribution.

2. See the proof of Lemma B.1 in Jin et al. (2019) for this form of the normalization assumption.
Thus, linear function approximation using our learned features suffices to fit the $Q$ function associated with any policy and explicitly given reward. The guarantee also enables dynamic programming techniques for policy optimization. In other words, (1) verifies that we have found a good representation, in a quantitative sense, and enables tractable reward maximization for any known reward function.

3 Related work

Low rank models are prevalent in dynamics and controls (Thon and Jaeger, 2015; Littman and Sutton, 2002; Singh et al., 2004). The low rank MDP in particular has been studied in several works in the context of planning (Barreto et al., 2011; Barreto and Fragoso, 2011), estimation (Duan et al., 2020), and in the generative model setting (Yang and Wang, 2019a). Regarding nomenclature, to our knowledge the name low rank MDP appears first in Jiang et al. (2017), although Rendle et al. (2010) refer to it as factorizing MDP and Barreto et al. (2011) refer to a similar model as stochastic factorization. More recently, it has been called the linear MDP by Jin et al. (2019). We use low rank MDP because it highlights the key structural property of the dynamics, and because we study the setting where the embeddings are unknown, which necessitates non-linear function approximation.

Turning to reinforcement learning with function approximation and exploration, a large body of effort focuses on (essentially) linear methods (Yang and Wang, 2019b; Jin et al., 2019; Cai et al., 2019; Modi et al., 2020; Du et al., 2019c; Wang et al., 2019). Closest to our work are the results of Jin et al. (2019) and Yang and Wang (2019b), who consider low rank MDPs with known feature maps $\phi_{0:H-1}^*$ (Yang and Wang (2019b) also assumes that $\mu_{0:H-1}^*$ is known up to a linear map). These results are encouraging and motivate our representation learning formulation, but, on their own, these methods cannot leverage the inductive biases provided by neural networks to scale to rich state spaces.

There are methods for more general, non-linear, function approximation, but these works either (a) require strong environment assumptions such as determinism (Wen and Van Roy, 2013; Du et al., 2020), (b) require strong function class assumptions such as bounded Eluder dimension (Russo and Van Roy, 2013; Osend and Van Roy, 2014), (c) have sample complexity scaling linearly with the function class size (Lattimore et al., 2013; Ortner et al., 2014) or (d) are computationally intractable (Jiang et al., 2017; Sun et al., 2019; Dong et al., 2019). Note that Ortner et al. (2014); Jiang et al. (2015) consider a form of representation learning, abstraction selection, but the former scales linearly with the number of candidate abstractions, while the latter does not address exploration.

Bellman/Witness rank. We briefly expand on this final category of computationally inefficient methods. For model-free reinforcement learning, Jiang et al. (2017) give an algebraic condition, in terms of a notion called the Bellman rank, on the environment and a given function approximation class, under which sample efficient reinforcement learning is always possible. Sun et al. (2019) extend the definition to model-based approaches, with the notion of Witness rank. As we will see in the next section, the low rank MDP with a function class derived from $\Phi$ (and $\Upsilon$) admits low Bellman (resp., Witness) rank, and so these results imply that our setting is statistically tractable.

Block MDPs. Finally, we turn to theoretical works on representation learning for RL. Du et al. (2019b) introduce the block MDP model, in which there is a finite latent state space $\hat{S}$ that governs the transition dynamics, and each “observation” $x \in \mathcal{X}$ is associated with a latent state $s \in \hat{S}$, so the state is decodable. The natural representation learning goal is to recover the latent states, and Du et al. (2019b); Misra et al. (2019) show that this can be done, in concert with exploration, in a statistically and computationally efficient manner. Since the block MDP can be easily expressed as a low rank MDP, our results can be specialized to this setting, where they yield comparable guarantees. On the other hand, we will see that the low rank MDP is significantly more expressive, and so our results greatly expand the scope for provably efficient representation learning and reinforcement learning.

\footnote{Formally, we append the immediate reward to the features.}
Therefore, a block MDP is a low rank MDP with rank $\nu$ have disjoint supports in their respective emissions and, as we will see in the next section, yields insights that facilitate algorithm design. We now examine additional requires that $\psi$ take $\Delta(\mathcal{X})$ is endowed with additional structure, the latent variable dimension $d_{LV}$ is the cardinality of smallest latent space $\mathcal{Z}$ for which $T$ admits a latent variable representation.

See Figure 1. In this representation, (1) each $(x, a)$ pair induces a “posterior” distribution $\psi(x, a) \in \Delta(\mathcal{Z})$ over $z$, (2) we sample $z \sim \psi(x, a)$, and (3) then sample $x' \sim \nu(\cdot | z)$, where $\nu$ specifies the “emission” distributions. As notation, we typically write $\nu(x) \in \mathbb{R}^\mathcal{Z}$ with coordinates $\nu(x)[z] = \nu(x | z)$ and we call $\psi, \nu$ the simplex features, following the example described by Jin et al. (2019). When considering $H$-step MDPs, this representation allows us to augment the trajectory $\tau$ with the latent variables $\tau = (x_0, a_0, z_1, x_1, \ldots, x_{H-1}, a_{H-1}, x_H)$. Here note that $z_h$ is the latent variable that generates $x_h$.

Note that all transition operators admit a trivial latent variable representation, as we may always take $\psi(x, a) = T(\cdot | x, a)$. However, when $T$ is endowed with additional structure, the latent variable representations are more interesting. For example, this viewpoint already certifies a factorization $T(x' | x, a) = \langle \psi(x, a), \nu(x') \rangle$ with embedding dimension $|\mathcal{Z}|$, and so $d_{LV}$ (if it is finite) is an upper bound on the rank of the transition operator. On the other hand, compared with Definition 1, this factorization additionally requires that $\psi(x, a)$ and $\nu(\cdot | z)$ are probability distributions. Since the factorization is non-negative, $d_{LV}$ is the non-negative rank of the transition operator.

The latent variable representation enables a natural comparison of the expressiveness of various models, and, as we will see in the next section, yields insights that facilitate algorithm design. We now examine models that have been introduced in prior works and their properties relative to Definition 1.

**Block MDPs.** A block MDP (Du et al., 2019b; Misra et al., 2019) is clearly a latent variable model with $\mathcal{Z}$ corresponding to the latent state space $\mathcal{S}$ and the additional restriction that two latent variables $z$ and $z'$ have disjoint supports in their respective emissions $\nu(\cdot | z)$ and $\nu(\cdot | z')$ (see the left panel of Figure 2). Therefore, a block MDP is a low rank MDP with rank $d \leq |\mathcal{S}|$, but the next result shows that a low rank MDP is significantly more expressive.

**Proposition 1.** For any $d \geq 2$ and any $M \in \mathbb{N}$ there exists an environment on $|\mathcal{X}| = M$ states, that can be expressed as a low rank MDP with embedding dimension $d$, but for which any block MDP representation...
must have $M$ latent states.

In fact, the MDP that we construct for the proof, admits a latent variable representation with $|Z| = d$, but does not admit a non-trivial block MDP representation. This separation exploits the decodability restriction of block MDPs, which is indeed quite limiting in terms of expressiveness.

**Simplex features.** Given the latent variable representation and the fact that it certifies a rank of at most $d_{LV}$, it is natural to ask if this representation is canonical for all low rank MDPs. In other words, for any transition operator with rank $d$, can we express it as a latent variable model with $|Z| = d$, or equivalently with simplex features of dimension $d$?

As discussed above, this model is indeed more expressive than the block MDP. However, the next result answers the above question in the negative. The latent variable representation is exponentially weaker than the general low rank representation in the following sense:

**Proposition 2.** For any even $n \in \mathbb{N}$, there exists an MDP that can be cast as a low rank MDP with embedding dimension $O(n^2)$, but which has $d_{LV} \geq 2^{\Omega(n)}$.

See the center and right panels of Figure 2. The result is proved by recalling that the latent variable dimension determines the non-negative rank of $T$, which can be much larger than its rank (Rothvoß, 2017; Yannakakis, 1991). It showcases how low rank MDPs are quite different from latent variable models of comparable dimension and demonstrates how embedding functions with negative values can provide significant expressiveness.

**Bellman and Witness rank.** As our last concrete connection, we remark here that the low rank MDP with a function class derived from $\Phi$ (and $\Upsilon$) admits low Bellman (resp., Witness) rank.

**Proposition 3 (Informal).** The low rank MDP model always has Bellman rank at most $d$. Additionally, given $\Phi$ and assuming $\phi^*_{0,H-1} \in \Phi$, we can construct a function classes $(\mathcal{G}, \Pi)$, so that OLIVE when run with $(\mathcal{G}, \Pi)$ has sample complexity $\tilde{O}(\text{poly}(d, H, K, \log |\Phi|, \epsilon^{-1}))$.

See Proposition 6 for a more precise statement. An analogous result hold for the Witness rank notion of Sun et al. (2019) (see Proposition 7 in the appendix). Unfortunately both OLIVE, and the algorithm of Sun et al. (2019) are not computationally tractable, as they involve enumeration of the employed function class. We turn to the development of computationally tractable algorithms in the next section.

5 Main results

We now turn to the design of algorithms for representation learning and exploration in low rank MDPs. As a computational abstraction, we consider the following optimization and sampling oracles.

**Definition 3 (Computational oracles).** Define the following oracles for the classes $\Phi$, $\Upsilon$:  

1. The maximum likelihood oracle, MLE, takes a dataset $D$ of $(x, a, x')$ triples, and returns  
   \[
   \text{MLE}(D) := \arg\max_{\phi \in \Phi} \sum_{(x,a,x') \in D} \log(\langle \phi(x,a), \mu(x') \rangle).
   \]

2. The sampling oracle, SAMP, is a subroutine which, for any $(\phi, \mu) \in \Phi \times \Upsilon$ and any $(x, a)$, returns a sample $x' \sim \langle \phi(x,a), \mu(\cdot) \rangle$. Multiple calls to the procedure result in independent samples.
We assume access to both oracles as a means towards practical algorithms that avoid explicitly enumerating over all functions in \( \Phi \) and \( \Upsilon \). Note that related assumptions are quite common in the literature (Misra et al., 2019; Du et al., 2019b; Agarwal et al., 2014), and in practice, both oracles can be reasonably approximated whenever optimizing over \( \Phi, \Upsilon \) is feasible (e.g., neural networks). Regarding MLE, other optimization oracles are possible, and in the appendix (Remark 13) we sketch how our proof can accommodate a generative adversarial oracle as a replacement (Goodfellow et al., 2014; Arora et al., 2017). While the sampling oracle is less standard, one might implement SAMP via optimization methods like the Langevin dynamics (Welling and Teh, 2011) or through reparameterization techniques such as the Gumbel-softmax trick (Jang et al., 2017; Figurnov et al., 2018).\(^4\) In addition, the sampling oracle can be avoided at the cost of additional real world experience, an approach we describe formally in Theorem 4 below.

5.1 Algorithm description

The algorithm is called FLAMBE, for “Feature Learning And Model-Based Exploration.” Pseudocode is displayed in Algorithm 1. FLAMBE proceeds in stages, where in stage \( h \), we use a certain exploratory policy \( \rho_h \) to collect a dataset of transitions that we pass to the MLE oracle. The optimization oracle returns embedding functions \( (\hat{\phi}_h, \hat{\mu}_h) \) which define the learned transition operator \( \hat{T}_h \). Then FLAMBE calls a planning sub-routine to compute the exploratory policy \( \rho_{h+1} \) for the next time. After all \( H \) stages, we have estimates \( \hat{T}_{0:H-1} \), which comprise the learned model \( \hat{M} \).

For the planning step, intuitively we seek an exploratory policy \( \rho \) that induces good coverage over the state space when executed in the model. We do this in Algorithm 2 using a technique inspired by elliptical potential arguments from linear bandits (Dani et al., 2008). Using the \( h \)-step model \( T_{0:h-1} \), we iteratively maximize certain quadratic forms of our learned features \( \hat{\phi}_{h-1} \) to find new directions not covered by the previously discovered policies, and we update the exploratory policy to include the maximizer. The algorithm terminates when no policy can achieve large quadratic form, which implies that we have found all reachable directions in \( \hat{\phi}_{h-1} \). This yields a mixture policy \( \rho_h \) that is executed by sampling one of the mixture components and executing that policy for the entire episode. The component policies are linear in the learned features \( \hat{\phi}_{1:h-1} \).

The challenge in our analysis is to relate this coverage in the model to that in the true environment as we discuss in the next section.

Algorithm 2 is a model-based planner, so it requires no interaction with the environment. The main computational step is the optimization problem (2). This can be solved efficiently with access to the sampling oracle, essentially by running the algorithm of Jin et al. (2019) (See Lemma 6 in the appendix). Note that we are optimizing over all policies, which is possible because the Bellman backups in a low rank MDP are linear functions of the features (c.f., Lemma 1). The sampling oracle can also be used to approximate all expectations, and, with sufficient accuracy, this has no bearing on the final results. Our proofs do account for the sampling errors.

5.2 Theoretical Results

For the analysis, we require one additional assumption. Recall the latent variable representation of Definition 2 and the fact that we can augment the trajectories with the latent variables, and let \( Z_h \) denote the latent state space for \( T_h \), i.e., the values that \( z_{h+1} \) can take. Our reachability assumption posits that for the MDP \( M \), the latent variables can be reached with non-trivial probability.

\(^4\)We do not explicitly consider approximate oracles, but additive approximations can be accommodated in our proof. In particular, if SAMP returns a sample from a distribution that is \( \epsilon_{\text{samp}} \) close in total variation to the target distribution in \( \text{poly}(1/\epsilon_{\text{samp}}) \) time, then we retain computational efficiency.
Algorithm 1 FLAMBE: Feature Learning And Model-Based Exploration

Input: Environment $\mathcal{M}$, function classes $\Phi$, $\Upsilon$, subroutines MLE and SAMP, parameters $\beta$, $n$.
Set $\rho_0$ to be the null policy, which takes no actions.

for $h = 0, \ldots, H - 1$ do
  Set $\rho_h^{\text{train}} \leftarrow \rho_h \circ \text{unif}(A)$. \{Uniform over available actions.\}
  Collect $n$ triples $D_h \leftarrow \{(x_h^{(i)}, a_h^{(i)}, x_{h+1}^{(i)})\}_{i=1}^{n}$ by executing $\rho_h^{\text{train}}$ in $\mathcal{M}$.
  Solve maximum likelihood problem: $(\phi_h, \mu_h) \leftarrow \text{MLE}(D_h)$.
  Set $\hat{T}_h(x_{h+1} \mid x_h, a_h) = \left(\hat{\phi}_h(x_h, a_h), \hat{\mu}_h(x_{h+1})\right)$.
  Call planner (Algorithm 2) with $h$ step model $\hat{T}_{0:h-1}$ and $\beta$ to obtain $\rho_h^{\text{pre}}$.
  Set $\rho_{h+1} = \rho_h^{\text{pre}} \circ \text{unif}(A)$.
end for

Algorithm 2 Elliptical planner

Input: MDP $\hat{\mathcal{M}} = (\phi_{0:h}, \mu_{0:h})$, subroutine SAMP, parameter $\beta > 0$. Initialize $\Sigma_0 = I_{d \times d}$.

for $t = 1, 2, \ldots,$ do
  Compute (see text for details)
  \[
  \pi_t = \arg\max_{\pi} \mathbb{E} \left[ \phi_h(x_h, a_h)^\top \Sigma_t^{-1} \phi_h(x_h, a_h) \mid \pi, \hat{\mathcal{M}} \right].
  \] (2)
  If the objective is at most $\beta$, halt and output $\rho = \text{unif}(\{\pi_t\}_{t < \ell})$.
  Compute $\Sigma_{\pi_t} = \mathbb{E} \left[ \phi_h(x_h, a_h)^\top \phi_h(x_h, a_h) \mid \pi, \hat{\mathcal{M}} \right]$. Update $\Sigma_t \leftarrow \Sigma_{t-1} + \Sigma_{\pi_t}$.
end for

Assumption 2 (Reachability). There exists a constant $\eta_{\text{min}} > 0$ such that
\[
\forall h \in \{0, \ldots, H - 1\}, z \in \mathcal{Z}_h : \max_{\pi} \mathbb{P}[z_{h+1} = z \mid \pi, \mathcal{M}] \geq \eta_{\text{min}}.
\]

The assumption generalizes prior reachability assumptions in block MDPs (Du et al., 2019b; Misra et al., 2019), where the latent variables are referred to as “latent states.” Note that reachability does not eliminate the exploration problem, as a random walk may still visit a latent variable with exponentially small probability. However, reachability is a limitation that unfortunately imposes an upper bound on the latent variable dimension $d_{LV}$, as formalized in the next proposition.

Proposition 4. If MDP $\mathcal{M}$ has rank $d$ and satisfies Assumption 2, then for each $h$, the latent variable dimension of $T_h$ satisfies $d_{LV} \leq dK^2/\eta_{\text{min}}^2$.

Thus, removing the reachability assumption is an important direction for future work. Unfortunately, reachability is currently required by existing algorithms even for the simpler block MDP setting, except under very strong oracle assumptions (Feng et al., 2020). As such, even progress in the context of block MDPs would be quite encouraging.

We now state the main guarantee.

Theorem 2. Fix $\delta \in (0, 1)$. If $\mathcal{M}$ is a low rank MDP with dimension $d$ and horizon $H$ and Assumption 1 holds, then FLAMBE with subroutine Algorithm 2, $\beta = \tilde{O}(\eta_{\text{min}}^2/d)$, and
\[
n = \Omega \left( \max \left\{ \frac{d^2 H^2 \log^2(1 + d/\eta_{\text{min}})}{\eta_{\text{min}}^2}, \frac{1}{\varepsilon^2 \eta_{\text{min}}} \right\} \cdot dK^2 \log(1 + d/\eta_{\text{min}}) \log(H \Phi \| \Upsilon \| / \delta) \right),
\]
computes a model $\hat{\mathcal{M}}$ such that (1) holds with probability at least $1 - \delta$. The total number of trajectories collected is $nH$ and the algorithm runs in polynomial time with polynomially many calls to MLE and SAMP (Definition 3).
Thus, FLAMBE provably learns low rank MDP models in a statistically and computationally efficient manner, under Assumption 1 and Assumption 2. While the result is comparable to prior work in the dependencies on $d, H,$ and $\varepsilon$, we instead highlight the more conceptual advances over prior work.

- The key advancement over the block MDP algorithms (Du et al., 2019b; Misra et al., 2019) is that FLAMBE applies to a significantly richer class of models with comparable assumptions.

- Over Jin et al. (2019); Yang and Wang (2019b), the key advancement is that we address the representation learning setting where the embeddings $\phi^{0}_{0:H-1}$ are not known a priori. On the other hand, our bound scales with the minimum visitation probability $\eta_{\min}$ and the number of actions $K$. We believe that additional structural assumptions on $\Phi$ are required to avoid the dependence on $K$ in our setting.

- Over Jiang et al. (2017); Sun et al. (2019), the key advancement is computational efficiency. However, the low rank MDP is less general than what is covered by their theory, our sample complexity is slightly worse, and we require Assumption 2.

As remarked earlier, the logarithmic dependence on the sizes of $\Phi, \Upsilon$ can be relaxed to alternative notions of capacity for continuous classes.

We also state a sharper bound for a version of FLAMBE that operates directly on the simplex factorization.

The main difference is that we use a conceptually simpler planner (See Algorithm 3 in the appendix) and the sample complexity bound scales with $d_{LV}$.

**Theorem 3.** Fix $\delta \in (0, 1)$. If $M$ admits a simplex factorization with embedding dimension $d_{LV}$, Assumption 1 holds, and all $\phi \in \Phi$ satisfy $\phi(x, a) \in \Delta([d_{LV}])$, then FLAMBE with Algorithm 3 as the subroutine and appropriate setting $^5$ of $n$ computes a model $\hat{M}$ such that (1) holds with probability at least $1 - \delta$. The total number of trajectories collected is

$$O \left( \max \left\{ \frac{d_{LV}^2 H^2}{\eta_{\min}^2}, \frac{1}{\varepsilon^2} \right\} \cdot d_{LV}HK^2 \log(H||\Phi||\Upsilon||/\delta) \right).$$

The algorithm runs in polynomial time with polynomially many calls to MLE and SAMP (Definition 3).

The bound agrees with Theorem 2 in its dependence on $H, K, \varepsilon$, and the function class complexity. If $d_{LV} \approx dK^2/\eta_{\min}^2$, which is the largest $d_{LV}$ can be under Assumption 2, then Theorem 2 yields a better guarantee. On the other hand, if $d_{LV} \approx d$, which holds in the block MDP, then Theorem 3 is preferable. However, Theorem 3 requires that we encode simplex constraints into our function class $\Phi$, for example using the softmax. When $d_{LV}$ is small, this may be a practically useful design choice.

As our final result, we consider replacing the model-based planning subroutine with a subroutine that collects trajectories from the environment. In Appendix D we prove the following theorem.

**Theorem 4.** Fix $\delta \in (0, 1)$. In the setup of Theorem 3, FLAMBE (with the planner described in Appendix D) computes a model $\hat{M}$ such that (1) holds with probability $1 - \delta$. The algorithm collects $\text{poly}(d_{LV}, H, K, 1/\eta_{\min}, 1/\varepsilon, \log(||\Phi||\Upsilon||/\delta))$ trajectories and runs in polynomial time with $H$ calls to MLE.

Importantly, this instantiation of FLAMBE does not require that the function classes support efficient sampling, i.e., we do not use SAMP. On the other hand, the sample complexity degrades in comparison with our results using model-based planners. We also note that the result considers simplex representations as in Theorem 3 because (a) the calculations are considerably simpler, and (b) in light of Proposition 4 handling general representations under Assumption 2 only incurs a polynomial overhead. We believe that extending the result to accommodate general representations directly is possible.

$^5$This version does not require the parameter $\beta$. 

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Challenges in the analysis. The key challenge is to ensure that $\rho_{h+1}$ induces good coverage over the state space at time $h + 1$ when executed in the environment. For this, a natural approach is to measure coverage in terms of directions in the learned features $\hat{\phi}_h$, which suggests running Algorithm 2 on the $\hat{T}_{0:h}$ (rather than $\hat{T}_{0:h-1}$ as we do). However, coverage w.r.t. $\hat{\phi}_h$ does not imply coverage measured w.r.t., $\phi_\star^h$, since even if the model is accurate, the features may not be. As we may miss directions in $\phi_\star^h$, this approach, as well as many others, can lead to exponential error amplification.

Instead, we leverage the latent variable representation and measure coverage via the density ratio on the latent variables: we want that for each $z$, $\mathbb{P}[z_{h+1} = z \mid \rho_{h+1}, \mathcal{M}]$ is large relative to any other policy. We obtain $\rho_{h+1}$ by covering directions in the learned feature map $\hat{\phi}_{h-1}$ at the previous time and composing with a random action. As the model is accurate, we can show that $\rho_{h+1}$ will visit all latent variables $z_{h+1}$, and crucially, we can do this without requiring $\hat{\phi}_h$ to be close to $\phi_\star^h$ (which it will not be in general). Then, since $z_{h+1}$ is the latent variable that generates $x_{h+1}$, we ensure good coverage over all states at time $h + 1$ which enables model learning in the next iteration.

6 Discussion

This paper studies representation learning and exploration for low rank MDPs. We provide an intuitive interpretation of these models in terms of a latent variable representation, and we prove a number of structural results certifying that low rank MDPs are significantly more expressive than models studied in prior work. We also develop FLAMBE, a computationally and statistically efficient model based algorithm for system identification in low rank MDPs. Policy optimization follows as a corollary.

Our results raise a number of promising directions for future work. On the theoretical side, can we eliminate the reachability assumption for computationally tractable algorithms leveraging non-linear function approximation? This question is intimately tied to the roll of optimism in reinforcement learning, as the optimism principle is challenging to implement with non-linear models. Can we develop tractable model-free algorithms for representation learning in the low rank MDP? Finally, on the empirical side, can we leverage the algorithmic insights of FLAMBE to develop practically effective representation learning algorithms for complex reinforcement learning tasks? We look forward to answering these questions in future work.

A Proofs for the structural results

In this appendix we provide proofs for the structural results in the paper. We first provide the proof of Lemma 1. In Appendix A.2 we focus on results relating to realizability and reachability. Then in Appendix A.3 we turn to the separation results of Proposition 1 and Proposition 2. Finally in Appendix A.4 we provide details about the connection to the Bellman and Witness rank.

A.1 Proof of Lemma 1

Proof of Lemma 1. Fix $h$ and $V : \mathcal{X} \to [0, 1]$. We drop the dependence on $h$ from the notation, with $x, a$ always corresponding to states and actions at time $h$ and $x'$ corresponding to an action at time $h + 1$. Observe that as $\mathcal{M}$ is a low rank MDP, we have

$$\forall x, a : \mathbb{E} \left[ V(x') \mid x, a, \hat{\mathcal{M}} \right] = \left\langle \hat{\phi}(x, a), \int \hat{\mu}(x') V(x') \right\rangle =: \left\langle \hat{\phi}(x, a), \theta \right\rangle$$
Combining with (1), we have that for any policy $\pi$:

$$E\left[\left\langle \hat{\phi}(x, a), \theta \right\rangle - E\left[ V(x') \mid x, a, M \right] \mid \pi, M \right]$$

$$= E\left[ E\left[ V(x') \mid x, a, M' \right] - E\left[ V(x') \mid x, a, M \right] \right]$$

$$\leq E\left[ \left\| \left\langle \hat{\phi}(x, a), \hat{\mu}(\cdot) \right\rangle - T(\cdot \mid x, a) \right\|_{TV} \mid \pi, M \right] \leq \varepsilon. \quad \Box$$

### A.2 On realizability and reachability

**Proposition 5.** Fix $M \in \mathbb{N}$, $n \leq M/2$, and any algorithm. There exists a low rank MDP over $M$ states with rank 2 and horizon 2 such that, if the algorithm collects $n$ trajectories and outputs a policy $\hat{\pi}$, then with probability at least $1/8$, $\hat{\pi}$ is at least $1/8$-suboptimal for the MDP.

The result shows that if the low rank MDP has $M$ states, then we require $n = \Omega(M)$ samples to find a near-optimal policy with moderate probability. Thus low rank structure alone is not sufficient to obtain sample complexity guarantees that are independent of the number of states.

**Proof of Proposition 5.** The result is obtained by embedding a binary classification problem into a low rank MDP and appealing to a standard binary classification lower bound argument. We construct a family of one-step transition operators, all of which have rank 2. The state space at the current time is of size $M$ and there are two actions $\mathcal{A} := \{0, 1\}$. From each $(x, a)$ pair we transition deterministically either to $x_g$ or $x_b$, and we receive reward 1 from $x_g$ and reward 0 from $x_b$.

Formally, we denote the states as $\{x_1, \ldots, x_M\}$ and index each instance by a binary vector $v \in \{0, 1\}^M$, which specifies the good action for each state. The transition operator is

$$T_v(\cdot \mid x, a) = \begin{cases} x_g & \text{if } a = v_j \\ x_b & \text{if } a \neq v_j \end{cases}$$

There are therefore $2^M$ instances. Note that as there are only two states at the next time, we trivially see that that transition operator of each instance is rank 2 and the linear MDP representation is:

$$\phi_v^*(x, a) = (1 \{a = v_j\}, 1 \{a \neq v_j\}) \quad \text{and} \quad \mu_v^*(x') = (1 \{x' = x_g\}, 1 \{x' = x_b\})$$

The starting distribution is uniform over $[M]$, so that in $n$ episodes, the agent collects a dataset $\{(x^{(i)}, a^{(i)}, y^{(i)})\}_{i=1}^n$ where $x^{(i)} \sim \text{unif}(x_1, \ldots, x_M)$, $a^{(i)}$ is chosen by the agent and $y^{(i)}$ denotes whether the agent transitions to $x_g$ or $x_b$. Information theoretically, this is equivalent to obtaining $n$ samples from the following data generating process: sample $j \sim \text{Unif}([M])$ and reveal $v_j$.

In this latter process, we can apply a standard binary classification lower bound argument. Let $P_v$ denote the data distribution where indices $j$ are sampled uniformly at random and labeled by $v_j$. Let $P_v^{(n)}$ denote the product measure where $n$ samples are generated iid from $P_v$. By randomizing the instance, for any example that does not appear in the sample, the probability of error is $1/2$. Therefore the probability of error for any classifier is

$$\max_v E_{S \sim P_v^{(n)}} P_j [\hat{f}(j) \neq v_j] \geq E_{v \sim \text{Unif}([0,1]^M)} E_{S \sim P_v^{(n)}} P_j [\hat{f}(j) \neq v_j]$$

$$= \frac{1}{M} \sum_{j=1}^M E_v E_{S \sim P_v^{(n)}} 1 \{\hat{f}(j) \neq v_j\} \geq \frac{1}{M} \sum_{j=1}^M \frac{1}{2} P_S [j \notin S]$$

$$= \frac{1}{2} \left(1 - \frac{1}{M}\right)^n \geq \frac{1}{2} (1 - n/M).$$
The second inequality uses the fact that if $j$ does not appear in the sample then $v_j \sim \text{Ber}(1/2)$. Equivalently, we can first sample $n$ unlabeled indices, then commit to the label just on these indices, so that the label for any index not in the sample remains random. Thus for any classifier, there exists some instance for which on average over the sample, the probability of error is at least $1/4$ as long as $n \leq M/2$. This also implies that with constant probability over the sample the error rate is at least $1/s$, since for any random variable $Z$ taking values in $[0, 1]$, we have

$$
\mathbb{E}[Z] \leq 1/s (1 - \mathbb{P}[Z > 1/s]) + \mathbb{P}[Z \geq 1/s] \leq 1/s + \mathbb{P}[Z \geq 1/s].
$$

Taking $Z = \mathbb{P}_j[\hat{f}(j) \neq v_j]$, we have

$$
\mathbb{P}_{S \sim p_0(n)}[\mathbb{P}_j[\hat{f}_j \neq v_j] \geq 1/s] \geq \frac{1}{2} (1 - n/M) - 1/8 \geq 1/s,
$$

where the last inequality holds with $n \leq M/2$.

Now, notice that we can identify any predictor with a policy in the obvious way and also that the suboptimality for a policy is precisely the classification error for the predictor. With this correspondence, we obtain the result.

**Proof of Proposition 4.** Fix stage $h$. Assume that $X := |\mathcal{X}|, d_{LV} := |Z_h|$ are finite, where $Z_h$ is the latent state space associated with transition operator $T_h$. Recall that $\psi_h(x, a) \in \Delta(Z)$ maps each state action pair to a distribution over latent states. As $X, |\mathcal{A}|, d_{LV}$ are all finite, we may collect these vectors as a matrix $\Psi \in \mathbb{R}^{XK \times d_{LV}}$ with rows corresponding to $\psi_h(x, a)$. A policy $\pi$ induces a distribution over $(x, a)$ pairs, which we call $p_{\pi, h} \in \Delta(\mathcal{X} \times \mathcal{A})$. The corresponding distribution over latent variables at stage $h$ is therefore $p_{\pi, h}^{\top} \Psi$.

We re-express $p_{\pi, h}$ in two steps. First, we can write $p_{\pi, h} = A_{\pi, h} \times \tilde{p}_{\pi, h}$ where $A_{\pi, h} \in \mathbb{R}^{XK \times X}$ is a matrix where the $x^\text{th}$ column describes the distribution $\pi(\cdot \mid x) \in \Delta(\mathcal{A})$, and $\tilde{p}_{\pi, h} \in \Delta(\mathcal{X})$ is the distribution over $x_h$ induced by policy $\pi$. Note that $A_{\pi, h}$ is column stochastic (it is non-negative with each column summing to 1). In fact it has additional structure, since in column $x$, on the rows corresponding to $(x, \cdot)$ are non-zero, but this will not be essential for our arguments. As $A_{\pi, h}^{\top}$ is therefore row-stochastic and the product of two row-stochastic matrices is also row-stochastic, we have that $A_{\pi, h}^{\top} \Psi \in \mathbb{R}^{XK \times d_{LV}}$ is also row-stochastic.

Next, we use the dynamics at stage $h - 1$ to re-write $\tilde{p}_{\pi, h}$, which is the state distribution induced by policy $\pi$ at stage $h$. As $T_{h-1}$ is also rank $d$, we can write $T(x_h \mid x_{h-1}, a_{h-1}) = (\phi_{h-1}(x_{h-1}, a_{h-1}), \mu_{h-1}(x_h))$, and can collect the embeddings $\mu_{h-1}(x_h)$ as columns of a $d \times X$ matrix $U_{h-1}$. With these definitions, we have that

$$
\tilde{p}_{\pi, h} = \mathbb{E} \left[ U_{h-1}^{\top} \phi_{h-1}(x_{h-1}, a_{h-1}) \mid \pi, \mathcal{M} \right] = U_{h-1}^{\top} v_{\pi, h-1}.
$$

Here $\mathcal{M}$ is the MDP in consideration. In summary, for any policy $\pi$, the distribution over latent variable $z_{h+1}$ (which generates $x_{h+1}$) induced by policy $\pi$ can be written as

$$
\mathbb{P} [z_{h+1} = \cdot \mid \pi, \mathcal{M}] = v_{\pi, h-1}^{\top} U_{h-1} A_{\pi, h}^{\top} \Psi \in \mathbb{R}^Z.
$$

Now, let us use our linear-algebraic re-writing to express the reachability condition. If a latent variable $z \in Z_h$ is reachable, then there exists some policy $\pi_z$ such that $\mathbb{P}[z_{h+1} = z \mid \pi_z, \mathcal{M}] \geq \eta_{\text{min}}$. First of all, by importance weighting on the last action $a_h$, we have:

$$
\mathbb{P}[z_{h+1} = z \mid a_0, \ldots, a_{h-1} \sim \pi_z, a_h \sim \text{unif}(\mathcal{A}), \mathcal{M}] \geq \eta_{\text{min}} / K.
$$

The normalization condition on $\phi_{h-1}$ leads to the upper bound

$$
\frac{\eta_{\text{min}}}{K} \leq \left| v_{\pi_z, h-1}^{\top} U_{h-1} A_{h}^{\top} \Psi e_z \right| \leq \max_{v : \|v\|_2 \leq 1} \left| v^{\top} U_{h-1} A_{h} \Psi e_z \right| = \|U_{h-1} A_{h} \Psi e_z\|_2.
$$
where we use \( A_h \) to denote the action-selection matrix induced by the uniform policy.

Next, consider some \( \ell_\infty \)-bounded vector \( w \in \mathbb{R}^Z \) with \( \|w\|_\infty \leq 1 \). The fact that \( A_h^\top \Psi \) is row-stochastic implies that
\[
\forall \pi : \left\| A_h^\top \Psi w \right\|_\infty \leq \max_{x,a} \left| \psi(x, a)^\top w \right| \leq \|w\|_\infty.
\]

Therefore, using the normalization condition on \( U_{h-1} \) we have
\[
\max_{w: \|w\|_\infty \leq 1} \left\| U_{h-1} A_h^\top \Psi w \right\|_2^2 \leq \max_{w: \|w\|_\infty \leq 1} \left\| U_{h-1} w \right\|_2^2 \leq d.
\]

We will select a vector \( w \in \{\pm 1\}^{d_{LV}} \), for which we know this upper bound holds. We select the vector iteratively, peeling off latent variables that are reachable. For brevity, define \( B := U_{h-1} A_h^\top \Psi \) and observe that
\[
\|Bw\|_2^2 = \|Be_{z_1} w[z_1]\|_2^2 + \sum_{z \neq z_1} \sum_{z_1} Be_{z} w[z] + \sum_{z \notin \{z_1\}} Be_{z} w[z]\|_2^2.
\]

If \( z_1 \) is \( \eta_{\min} \) reachable, then the first term is at least \((\eta_{\min}/\kappa)^2\) by the above calculation and the fact that we take \( w[z_1] \in \{\pm 1\} \). Then we ensure that the cross-term is non-negative by setting \( w[z_1] \) appropriately. Note that \( w[z_1] \) is formally a function of the remaining coordinates of \( w \), but we have not introduced any constraint on these remaining coordinates. Therefore, for \( z_1 \) is \( \eta_{\min} \) reachable, we get (for this partially specified \( w \))
\[
\|Bw\|_2^2 \geq (\eta_{\min}/\kappa)^2 + \sum_{z \neq z_1} \sum_{z_1} Be_{z} w[z]\|_2^2.
\]

Continuing in this way, we iteratively peel off latent variables that are \( \eta_{\min} \) reachable, and for each we gain \((\eta_{\min}/\kappa)^2\) in the lower bound. Therefore, if all \( d_{LV} \) latent variables are reachable, there exists some \( w \in \{\pm 1\}^{d_{LV}} \) such that
\[
d_{LV} \cdot (\eta_{\min}/\kappa)^2 \leq \left\| U_{h-1} A_h^\top \Psi w \right\|_2^2 \leq d,
\]
which implies that we must have \( d_{LV} \leq d \kappa^2/\eta_{\min}^2 \).

\[\square\]

### A.3 Separation results

**Proof of Proposition 1.** Fix \( N \) and consider a MDP with horizon 2, where at stage 1 there is only one state \( x \) and two actions \( a_1, a_2 \). At stage 2 there are \( N \) possible states, so that \( T(\cdot \mid x, a_i) \in \Delta([N]) \) for each \( i \in \{1, 2\} \). We define the transition operator for stage 1, called \( T \) for brevity, explicitly in terms of its factorization. Let \( \phi(x, a_1) = e_1 \) and \( \phi(x, a_2) = e_2 \) where \( e_1, e_2 \in \mathbb{R}^2 \) denotes the two standard basis elements in two dimensions. We define \( \mu_1(i) = 1/N, \mu_2(i) = i/(\sum_{j=1}^N j) \) and \( \mu(i) = (\mu_1(i), \mu_2(i)) \in \mathbb{R}^2 \). Thus \( T(x' = \hat{i} \mid x, a) = (\phi(x, a), \mu(i)) \), which can be easily verified to be a valid transition operator. By construction \( T \) has rank 2.

For clarity we express \( T \) as the \( 2 \times N \) matrix.
\[
T := \begin{pmatrix} 1/N & 1/N & \cdots & 1/N \\ 1/(\sum_{j=1}^N j) & 2/(\sum_{j=1}^N j) & \cdots & N/(\sum_{j=1}^N j) \end{pmatrix}.
\]

We now show that the block MDP representation must have \( N \) latent states. Suppose the block MDP representation is \( T(x' = \hat{i} \mid x, a) = \langle \phi_B(x, a), \mu_B(i) \rangle \). The block MDP representation requires that for each
index \(i\) the vector \(\mu_B(i)\) is one-sparse. From this, we deduce a constraint that arises when two states belong to the same block. If \(i, j\) belong to the same block, say block \(b\), then for each \((x, a) \in \mathcal{X} \times \mathcal{A}\), we have

\[
T(x' = i \mid x, a) = \phi_B(x, a)[b] \mu_B(i)[b] = \frac{\mu_B(i)[b]}{\mu_B(j)[b]} \cdot \phi_B(x, a)[b] \mu_B(j)[b]
\]

\[
= \frac{\mu_B(i)[b]}{\mu_B(j)[b]} \cdot T(x' = j \mid x, a)
\]

In words, if states \(i, j\) at stage 2 belong to the same block, then the vectors \(T(x' = i \mid \cdot), T(x' = j \mid \cdot)\) must be pairwise linearly dependent.\(^6\) Based on our construction, \(T(x' = i \mid \cdot) = \mu(i)\), which is just the \(i^{th}\) column of the matrix \(T\). By inspection, all \(N\) vectors are pairwise linearly independent, and so we can conclude that the block MDP representation must have \(N\) latent states.

\(\square\)

**Proof of Proposition 2.** We consider a one step transition operator \(T\) that we instantiate to be the slack matrix describing a certain polyhedral set. Let \(n\) be even and let \(K_n\) be the complete graph on \(n\) vertices. To set up the notation we will work with vectors \(x \in \mathbb{R}_{\geq 0}^{\binom{n}{2}}\) that associate a weight to each edge. We index the vectors as \(x_{u,v}\) where \(u \neq v \in [n]\) correspond to vertices.

A result of Edmonds (1965) states that the perfect matching polytope, which is the convex hull of all edge-indicator vectors corresponding to perfect matchings, can be explicitly written in terms of “odd-cut” constraints:

\[
\mathcal{P}_n := \text{conv}\left\{ 1_M \in \mathbb{R}_{\geq 0}^{\binom{n}{2}} \mid M \text{ is a perfect matching in } K_n \right\}
\]

\[
= \left\{ x \in \mathbb{R}_{\geq 0}^{\binom{n}{2}} : x \geq 0, \forall v : \sum_{u} x_{u,v} = 1, \forall U \subseteq [n], |U| \text{ odd } \sum_{v \notin U} \sum_{u \in U} x_{u,v} \geq 1 \right\}.
\]

This polytope has exponentially many vertices and exponentially many constraints. Formally, there are \(V := \frac{n!}{2^{n/2}(n/2)!}\) vertices, corresponding to perfect matchings in \(K_n\), and the number of constraints is \(C := 2^{\Omega(n)}\) corresponding to the number of odd-sized subsets of \([n]\). By adding one dimension to account for the offsets in the inequality constraints, we can enumerate the vertices \(v_1, \ldots, v_V \in \mathbb{R}_{\geq 0}^{\binom{n}{2} + 1}\) and the constraints \(c_1, \ldots, c_C \in \mathbb{R}_{\geq 0}^{\binom{n}{2} + 1}\), such that \(\langle c_i, v_j \rangle \geq 0\) for all \(i, j\). Then, we define the slack matrix for this polytope to be \(Z \in \mathbb{R}_{\geq 0}^{V \times V}\) with entries \(Z_{i,j} = \langle c_i, v_j \rangle\).

This slack matrix clearly has rank \(\binom{n}{2} + 1 = O(n^2)\). On the other hand, we claim that the non-negative rank is at least \(2^{\Omega(n)}\). This follows from (a) the fact that \(\mathcal{P}_n\) has extension complexity \(2^{\Omega(n)}\) (Rothvoß, 2017), (b) the extension complexity of a polytope is exactly the non-negative rank of its slack matrix (Yannakakis, 1991; Fiorini et al., 2013).

Next, we define the transition operator \(T\). We associate each \((x, a)\) pair with a constraint \(c_i\) and each \(x'\) with a vertex \(v_j\). Then we define

\[
T(x' \mid x, a) = \frac{\langle c_i, v_j \rangle}{\sum_{k=1}^{V} \langle c_i, v_k \rangle}
\]

This is easily seen to be a distribution for each \((x, a)\) pair. We can represent \(T\) as a \(C \times V\) matrix \(T = DZ\) where \(D\) is a diagonal matrix (with strictly positive diagonal) and \(Z\) is the slack matrix defined above.

We conclude the proof with two facts from Cohen and Rothblum (1993). First, the non-negative rank is preserved under positive diagonal rescaling, and so the non-negative rank of \(T\) is also \(2^{\Omega(n)}\). Second, for a row-stochastic matrix \(P\), the non-negative rank is equal to the smallest number of factors we can use to

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\(^6\)Note that this is equivalent to the notion of backward kinematic inseparability (Misra et al., 2019).
write $P = RS$ where both $R$ and $S$ are row-stochastic (here factors refers to the internal dimension). It is immediate that the simplex features representation corresponds to such a row-stochastic factorization, and so we see that any simplex features representation of $T$ must have embedding dimension at least $2^{Ω(n)}$. 

A.4 On Bellman and Witness rank

We now state the formal version of Proposition 3. We consider the value-function/policy decomposition studied by Jiang et al. (2017) where we approximate the value functions with a class $\mathcal{G} : \mathcal{X} \rightarrow [0, H]$ and the policies with a class $\Pi : \mathcal{X} \rightarrow \mathcal{A}$. Given an explicit reward function $R$ with range $[0, 1]$ and the function class $\Phi$ of candidate embeddings, we define these two classes as:

$$\Pi(\Phi) := \left\{ \pi : x_h \mapsto \arg\max_{a \in A} \langle \phi_h(x_h, a), \theta_h \rangle + R(x_h, a_h) : \theta_{0:H-1} \in B_d(H \sqrt{d}), \phi_{0:H-1} \in \Phi \right\},$$

$$\mathcal{G}(\Pi) := \left\{ g : x_h \mapsto \max_a \langle \phi_h(x_h, a), \theta_h \rangle + R(x_h, a_h) : \theta_{0:H-1} \in B_d(H \sqrt{d}), \phi_{0:H-1} \in \Phi \right\}.$$

Here $B_d(\cdot)$ is the Euclidean ball in $d$ dimensions with the specified radius. We have the following proposition:

**Proposition 6.** The low rank MDP model with any function classes $\mathcal{G} \subset \mathcal{X} \rightarrow [0, B]$ and $\Pi \subset \mathcal{X} \rightarrow \Delta(\mathcal{A})$ has bellman rank at most $d$ with normalization parameter $O(B \sqrt{d})$. Additionally, for any known reward function $R$ with range $[0, 1]$ and assuming $\phi_{0:H-1} \in \Phi$, the optimal policy and value function lie in $(\mathcal{G}(\Phi), \Pi(\Phi))$, and so OLIVE has sample complexity $O\left(\text{poly}(d, H, K, \log |\Phi|, \epsilon^{-1})\right)$.

**Proof of Proposition 6.** The result is essentially Proposition 9 in Jiang et al. (2017), who address the simplex representation case. We address the general case and also verify the realizability assumption.

Consider any explicitly specified reward function $R : \mathcal{X} \times \mathcal{A} \times \{0, \ldots, H-1\} \rightarrow [0, 1]$ and any low rank MDP with embedding functions $\phi_{0:H-1}^\ast, \mu_{0:H-1}^\ast$ and embedding dimension $d$. For any policy $\pi, \pi'$ and any value function $g : \mathcal{X} \rightarrow \mathbb{R}$ we define the average Bellman error (Jiang et al., 2017) as

$$E(\pi, (g, \pi'), h) := \mathbb{E} \left[ g(x_h) - R_h(x_h, a_h) - g(x_{h+1}) \mid a_{0:h-1} \sim \pi, a_h = \pi'(x_h), \mathcal{M} \right],$$

We also introduce the shorthand

$$\Delta((g, \pi'), x_h) := \mathbb{E} \left[ g(x_h) - R_h(x_h, a_h) - g(x_{h+1}) \mid x_h, a_h = \pi'(x_h) \right].$$

Then, in the low rank MDP, the average Bellman error admits a factorization as follows

$$E(\pi, (g, \pi'), h) = \mathbb{E} \left[ \Delta((g, \pi'), x_h) \mid x_h \sim \pi \right]$$

$$= \left\langle \mathbb{E} \left[ \phi_{h-1}^\ast(x_{h-1}, a_{h-1}) \mid \pi \right], \int \mu_{h-1}^\ast(x_h) \Delta((g, \pi'), x_h) d(x_h) \right\rangle$$

$$=: \langle \nu_h(\pi), \xi_h((g, \pi')) \rangle$$

We also have the normalization $\|\nu_h(\pi)\|_2 \leq 1$ and $\|\xi_h((g, \pi))\|_2 \leq (2B + 1) \sqrt{d}$. This final calculation is based on the triangle inequality, the bounds on $g$ and $R$ and the normalization condition on $\mu_{h-1}^\ast$. Thus for any low rank MDP and any (bounded) function class $\mathcal{G}, \Pi$, the Bellman rank is at most $d$ with norm parameter $O(B \sqrt{d})$.

To prove that OLIVE has low sample complexity, we need to verify that the optimal policy and optimal value function lie in $\Pi(\Phi)$ and $\mathcal{G}(\Pi)$ respectively. Then we must calculate the statistical complexity of these
two classes. Observe that we can express the Bellman backup of any function $V : \mathcal{X} \to \mathbb{R}$ as a linear function in the optimal embedding $\phi^*$:

$$(T_h V)(x, a) := \mathbb{E}[R_h(x, a) + V(x') \mid x, a, h] = R_h(x, a) + \langle \phi^*_h(x, a), \int \mu^*_h(x') V(x') d(x') \rangle$$

$$= R_h(x, a) + \langle \phi^*_h(x, a), w \rangle.$$  

for some vector $w$. Moreover, if $V : \mathcal{X} \to [0, H]$, we know that $\|w\| \leq H \sqrt{d}$. In particular, this implies that the optimal $Q$ function is a linear function in the true embedding functions $\phi^*_{0:H-1}$, and so realizability holds for $\mathcal{G}(\Phi), \Pi(\Phi)$. These function classes have range $B = O(H \sqrt{d})$ so the normalization parameter in the Bellman rank definition is $O(Hd)$.

Finally, we must calculate the statistical complexity of these two classes. For $\Pi(\Phi)$ the Natarajan dimension is at most $\tilde{O}(H(d + \log |\Phi|))$, since for each $h$, we choose $\phi_h$ and a $d$-dimensional linear classifier. Analogously the pseudo-dimension of $\mathcal{G}(\Phi)$ is $\tilde{O}(H(d + \log |\Phi|))$. Formally, we give a crude upper bound on the growth function, focusing on $\Pi(\Phi)$. Fix $h$, let $S$ be a sample of $n$ pairs $(x, a)$, and let $h_1, h_2 : S \to \{0, 1\}$ such that $h_1(x, a) \neq h_2(x, a)$ for all points in the sample. Since once we fix $\phi \in \Phi$, we have a linear class, we can vary $h_1, h_2$ on at most $(n + 1)^d$ subsets $T \subset S$. Then by varying $\phi \in \Phi$ we can match $h_1, h_2$ in total on $|\Phi|(n + 1)^d \leq n^{O(d + \log |\Phi|)}$ subsets. If $S$ is shattered, this means that the Natarajan dimension is $O((d + \log |\Phi|) \log(d + \log |\Phi|))$. This calculation is for a fixed $h$, but the same argument yields the bound of $O(H(d + \log |\Phi|))$. Instantiating, we obtain the sample complexity bound for OLIVE.

For the model-based version using the witness rank, the arguments are more straightforward.

**Proposition 7.** The low rank MDP model with any candidate model class $\mathcal{P}$ has witness rank at most $d$, with norm parameter $O(\sqrt{d})$. Additionally, for any explicitly specified reward function $R$ with range $[0, 1]$ and under Assumption 1, the algorithm of Sun et al. (2019) (with witness class of all bounded functions) has sample complexity $\tilde{O}\left(\text{poly}(d, K, H, \log |\Phi|, \gamma, \epsilon^{-1})\right)$.

**Proof.** Given a model $M$ and an explicit reward function $R$, we use $\pi_M$ to denote the optimal policy for $R$ with transitions governed by $M$. Then, for two models $M_1, M_2$ and a time step $h$ the witness model misfit, when instantiated with the test function class as all bounded functions, is defined as

$$W(M_1, M_2, h) := \mathbb{E}\left[\|M_2(\cdot \mid x_h, a_h) - \mathcal{M}(\cdot \mid x_h, a_h)\|_{TV} \mid a_{0:h-1} \sim \pi_{M_1}, a_h = \pi_{M_2}, \mathcal{M}\right].$$

Here we use the notation $\mathcal{M}(\cdot \mid x_h, a_h)$ to denote the transition operator implied by $M$ at stage $h$. Recall that $\mathcal{M}$ is the true MDP. In words, the witness model misfit is the one-step total variation error between candidate model $M_2$ and the true environment $\mathcal{M}$ on the data distribution induced by executing policy $\pi_{M_2}$ in the world for $h$ steps.

Using the backing up argument from the proof of Proposition 6, it is easy to see that the witness model misfit admits a factorization as

$$W(M_1, M_2, h) = \mathbb{E}\left[\phi^*_{h-1}(x_{h-1}, a_{h-1}) \mid \pi_{M_1}, \mathcal{M}\right], \int \nu^*_{h-1}(x_h) \Delta(x_h, M_2)$$

where $\Delta(x_h, M_2)$ is the expected total variation distance between $M_2$ and $\mathcal{M}$ on $(x_h, \pi_{M_2}(x_h))$. Based on this calculation, the witness rank is at most $d$ and the normalization parameter is at most $O(\sqrt{d})$. It is more straightforward to see that realizability holds here, and so the algorithm of Sun et al. (2019) has the stated sample complexity.
B Analysis of FLAMBE

As a reminder, FLAMBE interacts with a low rank MDP $\mathcal{M}$, with time horizon $H$ and with non-stationary dynamics $T_h(x_{h+1} \mid x_h, a_h) = \langle \phi_h^\ast(x_h, a_h), \mu_h^\ast(x_{h+1}) \rangle$. We assume that for each $h$ the operators $\phi_h^\ast, \mu_h^\ast$ embed in $\mathbb{R}^d$. As we have mentioned $T_h$ also admits an alternative non-negative factorization $T_h(x_{h+1} \mid x_h, a_h) = (\psi_h^\ast(x_h, a_h), \nu_h^\ast(x_{h+1}))$, where $\psi_h^\ast(x_h, a_h) \in \Delta([d_{LV}])$ and where $\nu_h^\ast(\cdot) \in \Delta(\mathcal{X})$. We assume that for all $h$ the operators in the non-negative factorization embed to $d_{LV} > d$ dimensions, although $d_{LV}$ only appears in the final results for Theorem 3 and Theorem 4. Recall also that we augment each trajectory with the latent variables $\{z_h\}_{h=1}^H$ and where $z_h \in \mathcal{Z}_h$ generates $x_h$.

The analysis of FLAMBE proceeds by induction. In iteration $h$, we construct an estimate $\hat{T}_h$ for the transition model $T_h$, and we also build an exploratory policy $\rho_{h+1}$ that we use in the next iteration. Thus at the beginning of the $h$th iteration, we have an $h-1$ step dynamics model $\hat{T}_{0:h-1}$ and an exploratory policy $\rho_h$. The inductive hypothesis for the $h$th iteration is in terms of these two quantities.

$$\forall h' < h, \forall \pi : \mathbb{E}\left[\left\|\hat{T}_{h'}(\cdot \mid x_{h'}, a_{h'}) - T_{h'}(\cdot \mid x_{h'}, a_{h'})\right\|_{TV}^2 \mid \pi, \mathcal{M}\right] \leq \varepsilon_{TV}$$

$$\forall z \in \mathcal{Z}_h : \max_{\pi} \mathbb{P}[z_h = z \mid \pi, \mathcal{M}] \leq \kappa \cdot \mathbb{P}[z_h = z \mid \rho_h, \mathcal{M}]$$

(3) (4)

Here $\kappa, \varepsilon_{TV} > 0$ are constants that we will set towards the end of the proof.

As a mnemonic device, we index $h$-step policies with $h$. So $\rho_h$ is a policy that takes $h$ actions and induces a distribution over $x_h$. We also use the shorthand $\mathbb{E}_\pi[\cdot] = \mathbb{E}[\cdot \mid \pi, \mathcal{M}]$ to denote expectations when policy $\pi$ interacts with the real MDP $\mathcal{M}$ and $\mathbb{E}_\pi[\cdot] = \mathbb{E}[\cdot \mid \pi, \hat{\mathcal{M}}]$ for expectations when the policy interacts with the estimated MDP $\hat{\mathcal{M}}$, which has dynamics $\hat{T}_{0:h-1}$ in the $h$th epoch.

Before proceeding with the inductive analysis, let us first establish a simulation lemma granted by (3).

**Lemma 5** (Simulation lemma). Assume (3) holds. Then for any $f : \mathcal{X} \to [0, 1]$ and any $\pi$:

$$\left|\mathbb{E}_\pi[f(x_h)] - \hat{\mathbb{E}}_\pi[f(x_h)]\right| \leq h \sqrt{\varepsilon_{TV}}.$$  

The exact same conclusion applies if $f : \mathcal{X} \times \mathcal{A} \to [0, 1]$.

**Proof.** We introduce the bellman backup operators:

$$\hat{T}_{h+1}^\pi f : x_{h'} \mapsto \int T(x_{h'+1} \mid x_{h'}, a_{h'})\pi(a_{h'} \mid x_{h'})f(x_{h'+1})d(x_{h'+1}, a_{h'}) .$$

With $\hat{T}_{h+1}^\pi$ defined analogously. Expanding the expectations, we obtain

$$\mathbb{E}_\pi[f(x_h)] - \hat{\mathbb{E}}_\pi[f(x_h)] = \mathbb{E}_\pi\left[T_{h-1}(x_h \mid x_{h-1}, a_{h-1})f(x_h) - \hat{T}_{h-1}(x_h \mid x_{h-1}, a_{h-1})f(x_h)\right]dx_h$$

$$= \mathbb{E}_\pi(\hat{T}_{h-1}^\pi f(x_{h-1})) - \hat{\mathbb{E}}_\pi(\hat{T}_{h-1}^\pi f(x_{h-1}))$$

The first term is bounded via Hölder’s inequality

$$\mathbb{E}_\pi(\hat{T}_{h-1}^\pi f - \hat{T}_{h-1}^\pi f)(x_{h-1})$$

$$\leq \sup_{x_h} |f(x_h)| \mathbb{E}_\pi \left\|T_{h-1}(\cdot \mid x_{h-1}, a_{h-1}) - \hat{T}_{h-1}(\cdot \mid x_{h-1}, a_{h-1})\right\|_{TV} \leq 1 \cdot \sqrt{\varepsilon_{TV}},$$
where the last inequality follows from the assumptions on \( f \) and (3). For the second term, note that since \( \hat{T}^{\pi}_{h-1} \) is an expectation operator, the function \( \hat{T}^{\pi}_{h-1} f \) also has range \([0, 1]\). Hence we can apply the above argument \( h - 1 \) more times to obtain the result.

Let us now turn to the induction. Recall that \( \rho_h \) is our exploratory policy that induces a distribution over \( x_h \). We augment \( \rho_h \) with an action taken uniformly at random to obtain the “training policy” \( \rho^\text{train}_h \). Via an application of Theorem 12 (using Assumption 1), we know that with probability at least \( 1 - \delta \) we learn \( \hat{\phi}_h, \hat{\mu}_h \) such that (with \( \hat{T} = \langle \hat{\phi}_h, \hat{\mu}_h \rangle \))

\[
\mathbb{E}_{(x_h, a_h) \sim \rho^\text{train}_h} \left| \hat{T}_h(\cdot \mid x_h, a_h) - T_h(\cdot \mid x_h, a_h) \right|^2_{\text{TV}} \leq \frac{2 \log((\Phi) \| \Upsilon \| / \delta)}{n} =: \varepsilon_{\text{sup}}. \tag{5}
\]

This is the only step where we use the optimization oracle, MLE, and similar guarantee can also be obtained by other means. As one example, in Remark 13, we discuss a generative adversarial approach.

We now use this bound and (4) to establish (3) for time \( h \). Considering any policy \( \pi \), we define the “error function” \( \text{err}_x(x_h) := \int \pi(a_h \mid x_h) \left| \hat{T}_h(\cdot \mid x_h, a_h) - T_h(\cdot \mid x_h, a_h) \right|^2_{\text{TV}} \).

\[
\mathbb{E}_\pi \left| \hat{T}_h(\cdot \mid x_h, a_h) - T_h(\cdot \mid x_h, a_h) \right|^2_{\text{TV}} = \mathbb{E}_\pi [\text{err}_x(x_h)]
= \sum_{z \in \mathcal{Z}_h} \mathbb{P}[z_h = z \mid \pi, \mathcal{M}] \cdot \int \text{err}_x(x_h) \nu^*_h(x \mid z) d(x_h)
\leq \kappa \cdot \sum_{z \in \mathcal{Z}_h} \mathbb{P}[z_h = z \mid \rho_h, \mathcal{M}] \cdot \int \text{err}_x(x_h) \nu^*_h(x \mid z) d(x_h)
= \kappa \cdot \mathbb{E}_{\rho_h} [\text{err}_x(x_h)]
\leq \kappa \cdot \mathbb{E}_{\rho^\text{train}_h} \left[ \left| \hat{T}_h(\cdot \mid x_h, a_h) - T_h(\cdot \mid x_h, a_h) \right|^2_{\text{TV}} \right] \cdot \sup_{x_h, a_h} \left| \pi(a_h \mid x_h) \right|
\leq \kappa \cdot \varepsilon_{\text{sup}} =: \varepsilon_{\text{TV}}.
\]

The first inequality is (4), which allows us to transfer from the distribution induced by \( \pi \) to the distribution induced by \( \rho_h \). It is crucial that the pre-multiplier term involving \( \nu^*_h \) and \( \text{err}_x \) is non-negative which follows from the fact that \( \text{err}_x \) is non-negative and \( \nu^*_h(\cdot | i) \) is a (positive) measure. The final two inequalities are based on importance weighting for the action at time \( h \), using the fact that \( \rho^\text{train}_h(\cdot | x_h) = \text{unif}(\mathcal{A}) \). This final expression is our choice of \( \varepsilon_{\text{TV}} \), which establishes (3) for time \( h \).

For time \( h = 0 \), (3) follows immediately from (5), since \((x_0, a_0)\) are fixed. In particular all policies induce the same distribution over \((x_0, a_0)\) so transferring from \( \pi \) to \( \rho^\text{train}_0 \) is trivial. As \( K, \kappa \geq 1 \), this gives the base case.

Now, we turn to establishing (4). First consider any function \( f : \mathcal{X} \to [0, 1] \) and any policy \( \pi \), and apply Lemma 5:

\[
\mathbb{E}_\pi f(x_h) \leq \mathbb{E}_\pi f(x_h) + h \sqrt{\varepsilon_{\text{TV}}}
= \mathbb{E}_\pi \left\langle \hat{\phi}_{h-1}(x_h, a_{h-1}), \int \hat{\mu}_{h-1}(x_h) f(x_h) d(x_h) \right\rangle + h \sqrt{\varepsilon_{\text{TV}}}
\leq \mathbb{E}_\pi \left\| \hat{\phi}_{h-1}(x_h, a_{h-1}) \right\|_{\Sigma^{-1}} \cdot \left\| \int \hat{\mu}_{h-1}(x_h) f(x_h) d(x_h) \right\|_{\Sigma} + h \sqrt{\varepsilon_{\text{TV}}}
\leq \frac{1}{2a} \left( \mathbb{E}_\pi \left\| \hat{\phi}_{h-1}(x_h, a_{h-1}) \right\|_{\Sigma^{-1}} \right)^2 + \frac{a}{2} \left\| \int \hat{\mu}_{h-1}(x_h) f(x_h) d(x_h) \right\|_{\Sigma}^2 + h \sqrt{\varepsilon_{\text{TV}}}.
\]
Here the first inequality is Lemma 5, since by induction we have (3) for all \( h' < h \). Then we expand \( \hat{T}_{h-1} \) in terms of its low rank representation with embedding dimension \( d \). The second inequality is an application of the Cauchy-Schwarz inequality, which holds for any positive definite \( d \times d \) matrix \( \Sigma \). Finally we use the AM-GM inequality in the last step; this step holds for any \( \alpha > 0 \).

We instantiate \( \Sigma \) to be the covariance matrix induced by the exploratory policy \( \rho_{h+1} \) that is output from Algorithm 2. First, for any policy \( \pi \) we define the \( h-1 \) step model covariance as \( \Sigma_\pi := \mathbb{E}_\pi \hat{\phi}_{h-1}(x_{h-1}, a_{h-1}) \hat{\phi}_{h-1}(x_{h-1}, a_{h-1})^\top \), where the dependence on \( h-1 \) is suppressed in the notation. Note that both the expectation and the embedding are taken with respect to the model \( \hat{\mathcal{M}} \). Then, the output of Algorithm 2 is a \( h \)-step policy \( \rho_{h+1}^{\text{pre}} \) that is defined as a mixture over \( T \) policies \( \pi_1, \ldots, \pi_T \). Using these policies, we define \( \Sigma \) as follows:

\[
\Sigma = \sum \rho_{h+1}^{\text{pre}} + \frac{I_{d \times d}}{T} = \frac{1}{T} \sum_{t=1}^{T} \sum_{\pi_t} + \frac{I_{d \times d}}{T}
\]

As we run Algorithm 2 using \( \hat{T}_{0:h-1} \) we can apply Lemma 8 on the \( h \) step MDP \( \hat{T}_{0:h-1} \). In other words, in Lemma 8, we set \( H \leftarrow h \) and \( \mathcal{M} \leftarrow \hat{\mathcal{M}} \). The conclusion is that \( T \leq 4d \log(1 + 4/\beta) / \beta \), where \( \beta \) is the parameter to the subroutine, and we can also bound the first term above:

\[
\left( \mathbb{E}_\pi \left\| \hat{\phi}_{h-1}(x_{h-1}, a_{h-1}) \right\|^2 \right) \leq \left( \mathbb{E}_\pi \left\| \hat{\phi}_{h-1}(x_{h-1}, a_{h-1}) \right\|^2 \right)^{\Sigma_{h-1}}
\]

\[
= \mathbb{E}_\pi \hat{\phi}_{h-1}(x_{h-1}, a_{h-1})^\top \left( \sum_{\rho_{h+1}^{\text{pre}}} + \frac{I_{d \times d}}{T} \right)^{-1} \hat{\phi}_{h-1}(x_{h-1}, a_{h-1}) \leq r \beta.
\]

This bound holds for all policies.

Next, we turn to the second term. Expanding the definition of \( \Sigma \), we have

\[
\left\| \int \hat{\mu}_{h-1}(x_{h}) f(x_{h}) d(x_{h}) \right\|^2
\]

As we run Algorithm 2 using \( \hat{T}_{0:h-1} \) we can apply Lemma 8 on the \( h \) step MDP \( \hat{T}_{0:h-1} \). In other words, in Lemma 8, we set \( H \leftarrow h \) and \( \mathcal{M} \leftarrow \hat{\mathcal{M}} \). The conclusion is that \( T \leq 4d \log(1 + 4/\beta) / \beta \), where \( \beta \) is the parameter to the subroutine, and we can also bound the first term above:

\[
\left( \mathbb{E}_\pi \left\| \hat{\phi}_{h-1}(x_{h-1}, a_{h-1}) \right\|^2 \right) \leq \left( \mathbb{E}_\pi \left\| \hat{\phi}_{h-1}(x_{h-1}, a_{h-1}) \right\|^2 \right)^{\Sigma_{h-1}}
\]

\[
= \mathbb{E}_\pi \hat{\phi}_{h-1}(x_{h-1}, a_{h-1})^\top \left( \sum_{\rho_{h+1}^{\text{pre}}} + \frac{I_{d \times d}}{T} \right)^{-1} \hat{\phi}_{h-1}(x_{h-1}, a_{h-1}) \leq r \beta.
\]

The first inequality is Jensen’s inequality along with the fact that \( f(x_{h})^2 \leq f(x_{h}) \) since \( f : \mathcal{X} \rightarrow [0, 1] \). The second inequality is based on our normalization assumptions on \( \mu_{h-1} \), which we also impose on \( \hat{\mu}_{h-1} \).

Finally, collecting all the terms and using Lemma 5 once again, we obtain the bound

\[
\mathbb{E}_\pi f(x_{h}) \leq \frac{T \beta}{2 \alpha} + \frac{\alpha}{2} \mathbb{E}_\rho_{h+1} f(x_{h}) + \frac{\alpha d}{2T} + (1 + \alpha/2) h \sqrt{\varepsilon_{\text{TV}}}.
\]

This bound holds for all policies \( \pi \) and all functions \( f : \mathcal{X} \rightarrow [0, 1] \), assuming (3) holds up through (but not including) time \( h \).

Now, consider some latent variable \( z \in \mathcal{Z}_h \) and let \( \pi_z^* := \arg\max_\pi \mathbb{P}[z_{h+1} = z \mid \pi, \mathcal{M}] \) (again the dependence on \( h \) is suppressed). Instantiate the above bound with the function \( f(x_{h}) = \int \pi_z^*(a_{h} \mid x_{h}) \mathbb{P}[z_{h+1} = z \mid x_{h}, a_{h}] \), which is clearly bounded in \([0, 1]\). Via another importance weighting step (since \( \rho_{h+1} := \rho_{h+1}^{\text{pre}} \circ \text{unif}(\mathcal{A}) \)), we obtain

\[
\mathbb{P}[z_{h+1} = z \mid \pi_z^*, \mathcal{M}] \leq \frac{T \beta}{2 \alpha} + \frac{\alpha K}{2} \mathbb{P}[z_{h+1} = z \mid \rho_{h+1}, \mathcal{M}] + \frac{\alpha d}{2T} + (1 + \alpha/2) h \sqrt{\varepsilon_{\text{TV}}}.
\]
By the reachability condition (Assumption 2), the left hand side is at least $\eta_{\min}$. Therefore, if we set the parameters $\alpha, \beta, \varepsilon_{\sup}$ (the latter of which is implicit in $\varepsilon_{TV}$) such that

$$\max \left\{ \frac{T\beta}{2\alpha}, \frac{\alpha d}{2T}, \left(1 + \alpha/2\right)h\sqrt{\varepsilon_{TV}} \right\} \leq \frac{\eta_{\min}}{6},$$

we obtain

$$\mathbb{P}\left[z_{h+1} = z \mid \pi_{\ast}^*, \mathcal{M}\right] \leq \frac{\alpha K}{2}\mathbb{P}\left[z_{h+1} = z \mid \rho_{h+1}, \mathcal{M}\right] + \frac{\eta_{\min}}{2}$$

Re-arranging, we see that (4) holds for any $\kappa \geq \alpha K$.

With the sampling oracle, the argument is very similar. We call Lemma 9 to obtain $\hat{\Sigma}$ and $\rho$, and we do the Cauchy-Schwarz step using $\hat{\Sigma}$. By Lemma 9 the first term is still $O(T\beta)$ and for the second term we pay an additive $O(\beta)$ to translate from $\hat{\Sigma}$ to $\Sigma$ (since the spectral norm error is $O(\beta/d)$ and Euclidean norm of the term involving $\mu_{h-1}$ is at most $d$). This we have an additional $O(\alpha \beta)$ term in the bound. Thus in this case, the condition is

$$\max \left\{ \frac{T\beta}{\alpha}, \frac{\alpha d}{T}, \alpha \beta, \alpha h\sqrt{\varepsilon_{TV}} \right\} \leq O(\eta_{\min}).$$

Note that via Lemma 9, we have $T \leq O(d \log(1 + 1/\beta)/\beta)$, the new condition (the third one) subsumes the second one, but only incurs a logarithmic overhead.

**Final steps.** To finish the proof of Theorem 2, we set the parameters to verify (6), calculate the total sample complexity, and derive the performance guarantee using (4) and (3).

Let us first set the parameters. Recall that $T$ is the number of iterations employed by Algorithm 2 and we know that $T \leq 4d \log(1 + 4/\beta)/\beta$. We start by setting $\alpha/T = \eta_{\min}/(3d)$, which clearly verifies the second constraint in (6). Substituting into the first constraint, we set $\beta = \eta_{\min}^2/(9d)$. This gives a final bound on $\alpha$:

$$\alpha = \frac{\eta_{\min}T}{3d} \leq \frac{4\eta_{\min} \log(1 + 4/\beta)}{3\beta} = \frac{12d \log(1 + 36d/\eta_{\min}^2)}{\eta_{\min}}.$$

We take $\kappa$ to be $K$ times the right hand side here. Next we turn to the last constraint in (6), expanding the definitions, the requirement is

$$\varepsilon_{\sup} \leq \frac{\eta_{\min}^2}{36\alpha^4 H^2 K^2},$$

which, via our upper bound on $\alpha$, is implied by

$$\varepsilon_{\sup} \leq \frac{\eta_{\min}^5}{36 \cdot 12^3 d^3 H^2 K^2 \log^3(1 + 36d/\eta_{\min}^2)}.$$

Before computing the sample complexity, we obtain another constraint on $\varepsilon_{\sup}$ based on the desired system identification guarantee. At the end of the execution of the algorithm, we have a model $T_{0,H-1}$ and we desire the system identification guarantee in (1). This holds by our induction hypothesis, provided that $\sqrt{\varepsilon_{TV}} \leq \varepsilon$. Therefore, this imposes the constraint

$$\varepsilon_{\sup} \leq \frac{\varepsilon^2}{K^2 \alpha} \leq \frac{\varepsilon^2 \eta_{\min}}{12d K^2 \log(1 + 36d/\eta_{\min}^2)}.$$
Using the definition of $\varepsilon_{\text{sup}}$, which is derived from Theorem 12, the number of samples we need per stage is (also applying a union bound over each of the $H$ stages)

$$
n = O \left( \max \left\{ d^2 H^2 \log^2 \left( 1 + \frac{d}{\eta_{\min}} \right), \frac{1}{\varepsilon^2 \eta_{\min}} \right\} \cdot dK^2 \log(1 + \frac{d}{\eta_{\min}}) \log(H|\Phi||\Psi|/\delta) \right).
$$

The final sample complexity is $nH$.

With the sampling oracle, the argument is very similar. As we have discussed, the constraint $\alpha d/T \leq O(\eta_{\min})$ is subsumed by the constraint $\alpha \beta \leq O(\eta_{\min})$. Thus we set $\alpha = \Theta(\eta_{\min}/\beta)$, which yields $\beta \log(1 + 1/\beta) \leq O(\eta_{\min}^2/d)$ when applied to the first constraint. This yields the choice $\beta = \Theta(\eta_{\min}^2/d \log^{-1}(1 + d/\eta_{\min}))$, which actually gives the same scaling for $\alpha$ as we had before. Thus the rest of the calculation is unchanged, and the number of calls to the sampling oracle is $\text{poly}(d, H, 1/\beta, \log(1/\delta)) = \text{poly}(d, H, 1/\eta_{\min}, \log(1/\delta))$.

### B.1 Refined analysis for simplex representations.

Here we prove Theorem 3 by considering a different instantiation of the planning algorithm that directly attempts to visit each latent state. In particular, we instantiate Algorithm 1 with the planning routine presented in Algorithm 3. Note that this planner does not require the parameter $\beta$, but it does assume that $\phi(x, a) \in \Delta([d_{LV}])$ for each $(x, a)$.

For the proof, we employ the same induction hypothesis and the same argument for establishing (3). For (4) we use a simpler argument. Instead of computing $\rho_{h+1}$ via a call to Algorithm 2, we use the simpler planning routine in Algorithm 3. This yields the policy $\rho_{h}^{\text{pre}}$ with the guarantee in Lemma 7.

For any function $f : X \rightarrow [0, 1]$ and any policy $\pi$ we obtain

$$
\mathbb{E}_{\pi} f(x_h) \leq \mathbb{E}_{\pi} f(x_h) + h\sqrt{\varepsilon_{TV}}
= \mathbb{E} \left( \hat{\phi}_{h-1}(x_{h-1}, a_{h-1}), \int \mu_{h-1}(x_h)f(x_h)d(x_h) \right) + h\sqrt{\varepsilon_{TV}}
= \sum_{i=1}^{d_{LV}} \left( \int \mu_{h-1}(x_h)[i] f(x_h)d(x_h) \right) \cdot \mathbb{E}_{\pi} \hat{\phi}_{h-1}(x_{h-1}, a_{h-1})[i] + h\sqrt{\varepsilon_{TV}}
\leq d_{LV} \cdot \sum_{i=1}^{d_{LV}} \left( \int \mu_{h-1}(x_h)[i] f(x_h)d(x_h) \right) \cdot \mathbb{E}_{\rho_{h}^{\text{pre}}} \hat{\phi}_{h-1}(x_{h-1}, a_{h-1})[i] + h\sqrt{\varepsilon_{TV}}
= d_{LV} \mathbb{E}_{\rho_{h}^{\text{pre}}} f(x_h) + h\sqrt{\varepsilon_{TV}} \leq d_{LV} \mathbb{E}_{\rho_{h}^{\text{pre}}} f(x_h) + (1 + d_{LV})h\sqrt{\varepsilon_{TV}}.
$$

Define $\pi^*_i := \arg\max_x \mathbb{E}_{\pi} \hat{\phi}^*_h(x_h, a_h)[i]$. Via the same importance weighting argument we have

$$
\mathbb{E}_{\pi^*_i} \hat{\phi}^*_h(x_h, a_h)[i] \leq d_{LV} K \mathbb{E}_{\rho_{h+1}} \hat{\phi}^*_h(x_h, a_h)[i] + (1 + d_{LV})h\sqrt{\varepsilon_{TV}}.
$$

(7)

And so here, we have the constraint

$$
(1 + d_{LV})h\sqrt{\varepsilon_{TV}} \leq \eta_{\min}/2,
$$

which allows us to take $\kappa = 2d_{LV} K$.

In this setting, the constraints on $\varepsilon_{\text{sup}}$ are

$$
\varepsilon_{\text{sup}} \leq \min \left\{ \frac{\eta_{\min}^2}{32d_{LV}^3 H^2 K^2}, \frac{\varepsilon^2}{2d_{LV} R^2} \right\},
$$

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where the latter constraint comes from the optimality guarantee in (1). Therefore, we may take
\[ n = O \left( \max \left\{ \frac{d_{LV}H^2}{\eta_{\min}^2}, \frac{1}{\epsilon^2} \right\} \cdot d_{LV}K^2 \log \left( H \left| \Phi \right| \left| \Upsilon \right| / \delta \right) \right). \]

As above, the final sample complexity is \( nH \).

If we can sample efficiently from any model \((\phi, \mu)\), the same calculation applies, except via Lemma 7, we have an additive \(d_{LV}\varepsilon_{opt}\) on the right hand side of (7). If we set \(\varepsilon_{opt} = O(\eta_{\min}/d_{LV})\), the remaining calculations are affected only in constant factors. Hence, whenever \((\phi, \mu)\) admit efficiently sampling, we can run the algorithm in polynomial time with \(\text{poly}(d_{LV}, H, 1/\eta_{\min})\) calls to the sampling subroutine.

C Planning Algorithms

In this section, we present exploratory planning algorithms for low rank models, assuming that the dynamics are known. Formally, we consider an \( H \) step low rank MDP \( \mathcal{M} \) with deterministic start state \( x_0 \), fixed action \( a_0 \), and transition matrices \( T_0, \ldots, T_{H-1} \). Each transition operator \( T_h \) factorizes as \( T_h(x_{h+1} \mid x_h, a_h) = \langle \phi_h(x_h, a_h), \mu_h(x_{h+1}) \rangle \) and we assume \( \phi_{0:H-1}, \mu_{0:H-1} \) are known. To compartmentalize the results, we focus on exploratory planning at time \( H \), but we will invoke these subroutines with MDP models that have horizon \( h \leq H \). This simply requires rebinding variables.

We present two types of results. One style assumes that all expectations are computed exactly. As we are focusing purely on planning with known dynamics and rewards, this imposes a computational burden, but not a statistical one, while leading to a more transparent proof. To address the computational burden, we also consider algorithms that approximate all expectations with samples. For this, we assume that we can obtain sample transitions from the MDP model \( \mathcal{M} \) in a computationally efficient manner. Formally, the sampling oracle allows us to sample \( x' \sim T_h(\cdot \mid x, a) \) for any \( x, a \).

C.1 Planning with a sampling oracle

For the computational style of result, it will be helpful to first show how to optimize a given reward function whenever the model admits a sampling oracle. As notation, we always consider an explicitly specified non-stationary reward function \( R : \mathcal{X} \times \mathcal{A} \times \{0, \ldots, H-1\} \rightarrow [0, 1] \). Then, we define
\[ V(\pi, R) = \mathbb{E} \left[ \sum_{h=0}^{H-1} R(x_h, a_h, h) \mid \pi, \tilde{\mathcal{M}} \right]. \]

The next lemma is a simple application of the result of Jin et al. (2019).

**Lemma 6.** Suppose that the reward function \( R : \mathcal{X} \times \mathcal{A} \times \{0, \ldots, H-1\} \rightarrow [0, 1] \) is explicitly given and that \( T_{0:H-1} \) is a known low rank MDP that enables efficient sampling. Then for any \( \epsilon > 0 \) there is an algorithm for finding a policy \( \hat{\pi} \) such that with probability at least \( 1 - \delta \), \( V(\hat{\pi}, R) \geq \max_{\pi} V(\pi, R) - \epsilon \) in polynomial time with \( \text{poly}(d, H, 1/\epsilon, \log(1/\delta)) \) calls to the sampling routine.

**Proof.** As we have sampling access to the MDP, we can execute the LSVI-UCB of Jin et al. (2019). For any \( n \), if we execute the algorithm for \( n \) episodes, it produces \( n \) policies \( \pi_1, \ldots, \pi_n \) and guarantees
\[ \max_{\pi} V(\pi, R) - \frac{1}{n} \sum_{i=1}^{n} V(\pi_i, R) \leq c \sqrt{\frac{d^3 H^3 \log (ndH/\delta)}{n}} \]
with probability at least \( 1 - \delta \) where \( c > 0 \) is a universal constant. We are assured that one of the policies \( \pi_1, \ldots, \pi_n \) is at most \( \epsilon/2 \)-suboptimal by taking \( n = O \left( d^3 H^3 \log (dH/(\epsilon \delta))/\epsilon^2 \right) \).
We first consider a simpler planning algorithm that is adapted to the simplex features representation. Given a sampling oracle

Algorithm 3 Exploratory planner for simplex representations

| Input: MDP $\tilde{\mathcal{M}} = (\Phi_{0,H-1}, \mu_{0,H-1})$ with $\phi_h(x_h, a_h) \in \Delta([d_{LV}])$, $\mu_{h,i} \in \Delta(\mathcal{X})$. |
| for $i = 1, \ldots, d_{LV}$ do |
| Compute $\pi_i = \arg\max_x \mathbb{E}[\phi_{H-1}(x_{H-1}, a_{H-1})[i] | \tilde{\mathcal{M}}, \pi]$ |
| end for |
| Output policy mixture $\rho := \text{unif}(\{\pi_i\}_{i=1}^{d_{LV}})$ |

We find this policy via a simple policy evaluation step. For each policy $\pi_i$, we collect $O(H^2 \log(n/\delta)/\epsilon^2)$ roll-outs using the generative model, where we take actions according to $\pi_i$. Via a union bound, this guarantees that for each $i$ we have $\tilde{V}_i$ such that with probability at least $1 - \delta$

$$\max_i \left| \tilde{V}_i - V(\pi_i, R) \right| \leq \frac{\epsilon}{4}$$

Therefore, if we take $i = \arg\max_{i \in [n]} \tilde{V}_i$ we are assured that $V(\pi_i, R) \geq \max_i V(\pi, R) - \epsilon$ with probability at least $1 - 2\delta$.

The total number of samples required from the model are

$$nH \left( 1 + \frac{H^2 \log(n/\delta)}{\epsilon^2} \right) = \tilde{O} \left( \frac{d^3 H^6 \log(1/\delta)}{\epsilon^4} \right).$$

\[\square\]

C.2 Planning with simplex features

We first consider a simpler planning algorithm that is adapted to the simplex features representation. The pseudocode is displayed in Algorithm 3. The planner computes a mixture policy $\rho$, where component $\pi_i$ of the mixture focuses on activating coordinate $i$ of the feature map $\phi_{H-1}(x_{H-1}, a_{H-1})$. Each mixture component can be computed in a straightforward manner using a dynamic programming approach, such as LSVI. The basic guarantee for this algorithm is the following lemma.

Lemma 7 (Guarantee for Algorithm 3). If $\tilde{\mathcal{M}}$ is an $H$-step low rank MDP with simplex features of dimension $d_{LV}$, then the output of Algorithm 3, $\rho$, satisfies

$$\forall \pi, i, \mathbb{E} \left[ \phi_{H-1}(x_{H-1}, a_{H-1})[i] | \tilde{\mathcal{M}}, \pi \right] \leq d_{LV} \mathbb{E} \left[ \phi_{H-1}(x_{H-1}, a_{H-1})[i] | \tilde{\mathcal{M}}, \rho \right].$$

Given a sampling oracle $\text{SAMP}$ for $\tilde{\mathcal{M}}$, the algorithm runs in polynomial time with $\text{poly}(d_{LV}, H, 1/\epsilon_{\text{opt}}, \log(1/\delta))$ calls to $\text{SAMP}$, and with probability at least $1 - \delta$, $\rho$ satisfies

$$\forall \pi, i, \mathbb{E} \left[ \phi_{H-1}(x_{H-1}, a_{H-1})[i] | \tilde{\mathcal{M}}, \pi \right] \leq d_{LV} \mathbb{E} \left[ \phi_{H-1}(x_{H-1}, a_{H-1})[i] | \tilde{\mathcal{M}}, \rho \right] + \epsilon_{\text{opt}}.$$

Proof. The first result follows immediately from the non-negativity of $\phi_{H-1}(x_{H-1}, a_{H-1})[i]$, the optimality property of $\pi_i$, and the definition of $\rho$.

For the second result, by Lemma 6 we can optimize any explicitly specified reward function using a polynomial number of samples. If we call this sampling-based planner for each of the $d$ reward functions, with high probability (via a union bound) the policies $\pi_i$ are near-optimal for their corresponding reward functions. By appropriately re-scaling the accuracy parameter in Lemma 6 we obtain the desired guarantee. \[\square\]
C.3 Elliptical planner

The next planning algorithm applies to general low rank MDP, and it is more sophisticated. It proceeds in iterations, where in iteration \( t \) we maintain a covariance matrix \( \Sigma_{t-1} \) and, in (2), we search for a policy that maximizes quadratic forms with the inverse covariance \( \Sigma_{t-1}^{-1} \). With a sampling oracle this optimization can be done via a call to Lemma 6. If this maximizing policy \( \pi_t \) cannot achieve large quadratic forms against \( \Sigma_{t-1}^{-1} \), then we halt and output the mixture of all previous policies. Otherwise, we mix \( \pi_t \) into our candidate solution, update the covariance matrix accordingly, and advance to the next iteration. The performance guarantee for this algorithm is as follows.

Lemma 8 (Guarantee for Algorithm 2). If \( \tilde{M} \) is an \( H \)-step low rank MDP with embedding dimension \( d \) then for any \( \beta > 0 \), Algorithm 2 terminates after at most \( T + 1 \) iterations where \( T \leq 4d \log(1 + 4/\beta)/\beta \). Upon termination, \( \rho \) guarantees

\[
\forall \pi : \mathbb{E} \left[ \phi_{H-1}(x_{H-1}, a_{H-1})^\top (\Sigma_{\rho} + I/T)^{-1} \phi_{H-1}(x_{H-1}, a_{H-1}) \mid \tilde{M}, \pi \right] \leq T \beta.
\]

where \( \Sigma_{\rho} = \frac{1}{T} \sum_{t=1}^{T} \Sigma_{\pi_t} \).

Proof. The performance guarantee is immediate from the termination condition, using the fact that \( \Sigma_{T} = T \cdot (\Sigma_{\rho} + I/T) \).

For the iteration complexity bound, we condense the notation and omit the dependence on \( H - 1, x_{H-1}, a_{H-1} \) in all terms. We have

\[
\beta T \leq \sum_{t=1}^{T} \mathbb{E} \left[ \phi_{H-1}^\top (\Sigma_{t-1}^{-1} \phi) \mid \tilde{M}, \pi_t \right] = \sum_{t=1}^{T} \text{tr}(\Sigma_{\pi_t} \Sigma_{t-1}^{-1}) \leq 2d \log(1 + T/d)
\]

where the first inequality is based on the fact that we did not terminate at each iteration \( t \in [T] \) and the last inequality follows from a standard elliptical potential argument (e.g., Lemma 11 in (Dani et al., 2008); see Lemma 17 for a precise statement and proof). This gives an upper bound on \( T \) that is slightly stronger than the bound in the lemma statement. To see why, if \( T \leq 4d \log(1 + 4/\beta)/\beta \) then a weakening of the established condition is

\[
T \leq \frac{2d \log(1 + T/d)}{\beta} \leq \frac{2d}{\beta} \log(1 + 4 \log(1 + 4/\beta)/\beta) \leq \frac{4d}{\beta} \log(1 + 4/\beta). \tag*{\Box}
\]

With the sampling oracle, we modify the algorithm slightly and obtain a qualitatively similar guarantee. The modifications are discussed in the proof.

Lemma 9. The sample-based version of Algorithm 2 has the following guarantee. Assume \( \tilde{M} \) is an \( H \)-step low rank MDP with embedding dimension \( d \) and fix \( \beta > 0 \), \( \delta \in (0, 1) \). Then the algorithm terminates after at most \( T + 1 \) iterations, where \( T \leq O(d \log(1 + 1/\beta)/\beta \). Upon termination, it outputs a matrix \( \Sigma \) and a policy \( \rho \) such that with probability at least \( 1 - \delta \):

\[
\forall \pi : \mathbb{E} \left[ \phi_{H-1}(x_{H-1}, a_{H-1})^\top \left( \Sigma + I/T \right)^{-1} \phi_{H-1}(x_{H-1}, a_{H-1}) \mid \tilde{M}, \pi \right] \leq O(T \beta),
\]

\[
\left\| \Sigma - \left( \mathbb{E} \left[ \phi_{H-1}(x_{H-1}, a_{H-1}) \phi_{H-1}(x_{H-1}, a_{H-1})^\top \mid \rho, \tilde{M} \right] + I/T \right) \right\|_{op} \leq O(\beta/d).
\]

The algorithm runs in polynomial time with \( \text{poly}(d, H, 1/\beta, \log(1/\delta)) \) calls to the sampling oracle.
Proof. The algorithm is modified as follows. We replace all covariances with empirical approximations, obtained by calls to the sampling subroutine. We call the empirical versions \( \hat{\Sigma}_t, \hat{\Sigma}_{\pi_t} \), etc. Then, the policy optimization step (2) is performed via an application of Lemma 6 and so we find an \( \varepsilon_{\text{opt}} \)-suboptimal policy \( \hat{\pi}_t \) for the reward function induced by \( \hat{\Sigma}_t \). Then we use the sampling subroutine to estimate the value of this policy, which we denote \( \hat{V}_t(\hat{\pi}_t) \). As before, we terminate if \( \hat{V}_t(\hat{\pi}_t) \leq \beta \). If we terminate in round \( t \), we output \( \rho = \text{unif}\{\{\pi_t\}_{t=1}^{t-1}\} \) and we also output \( \hat{\Sigma} = \sum_{i=1}^{t-1} \hat{\Sigma}_{\pi_i} \). As notation, we use \( \hat{V}_t(\pi) \) to denote the value for policy \( \pi \) on the reward function used in iteration \( t \), which is induced by \( \hat{\Sigma}_t \).

With \( \text{poly}(d, H, T, 1/\varepsilon_{\text{opt}}, \log(1/\delta)) \) calls to the sampling subroutine and assuming the total number of iterations of the algorithm \( T \) is polynomial, we can verify that with probability \( 1 - \delta \)

\[
\max_{t \in [T]} \max \left\{ d \cdot \left\| \hat{\Sigma}_{\pi_t} - \Sigma_{\pi_t} \right\|_{\text{op}}, \left| \hat{V}_t(\hat{\Sigma}_{\pi_t}) - V_t(\pi_t) \right|, \max_{\pi} V_t(\pi) - V_t(\hat{\pi}_t) \right\} \leq \varepsilon_{\text{opt}}.
\]

The first two bounds follow from standard concentration of measure arguments. The final one is based on an application of Lemma 6.

Now, if we terminate in iteration \( t \), we know that \( \hat{V}_t(\hat{\pi}_t) \leq \beta \). This implies

\[
\max_{\pi} V_t(\pi) \leq V_t(\hat{\pi}_t) + \varepsilon_{\text{opt}} \leq \hat{V}_t(\hat{\pi}_t) + 2\varepsilon_{\text{opt}} \leq \beta + 2\varepsilon_{\text{opt}}.
\]

As we are interested in the reward function induced by \( \hat{\Sigma}_{t-1} \), this verifies the quality guarantee, provided \( \varepsilon_{\text{opt}} = O(\beta) \).

Finally, we turn to the iteration complexity. Similarly to above, we have

\[
T (\beta - 2\varepsilon_{\text{opt}}) \leq \sum_{t=1}^{T} \hat{V}_t(\hat{\pi}_t) - 2\varepsilon_{\text{opt}} \leq \sum_{t=1}^{T} V_t(\pi_t) - \varepsilon_{\text{opt}}
\]

\[
= \sum_{t=1}^{T} \mathbb{E} \left[ \phi^\top \hat{\Sigma}_{t-1}^{-1} \phi | \tilde{M}_t, \pi_t \right] - \varepsilon_{\text{opt}} = \sum_{t=1}^{T} \text{tr}(\Sigma_{\pi_t}^{-1} \hat{\Sigma}_{t-1}^{-1}) - \varepsilon_{\text{opt}}
\]

\[
\leq \sum_{t=1}^{T} \text{tr}(\Sigma_{\pi_t}^{-1} \hat{\Sigma}_{t-1}^{-1}) \leq 2d \log(1 + T/d)
\]

In other words, if we set \( \varepsilon_{\text{opt}} = O(\beta) \) then both the iteration complexity and the performance guarantee are unchanged. The accuracy guarantee for the covariance matrix \( \hat{\Sigma}_{t-1} \) is straightforward, since each \( \hat{\Sigma}_{\pi_t} \) is \( \varepsilon_{\text{opt}} \) accurate, and \( \hat{\Sigma} \) is the average of such matrices. \qed

### D Planning in the environment

It is also possible to plan in the environment leveraging our coverage and estimation guarantees. The advantage of this approach is that we do not need the sampling oracle, SAMP, but the downside is that we collect many more samples from the environment. To demonstrate that this is possible, we focus on the simplex representation, as in Theorem 3. While planning in the environment with general representations is possible, the arguments and calculations are much simpler in the simplex case. Additionally, recall that under Assumption 2, \( d_{LV} \leq dK^2 / \rho_{\text{min}} \), and so general representations (with reachability) can be accommodated with polynomial overhead in sample and computational complexity.

The argument is broken down into two parts. We first focus on optimizing a fixed given reward function by collecting experience from the environment, analogously to the sampling approach in Lemma 6. In the next subsection we choose the reward functions carefully to establish the guarantees required by FLAMBE. Since we are considering simplex representations, this second part is very similar to Algorithm 3.
Algorithm 4 Planning in the environment with simplex features

**input:** Exploratory policies $\hat{\rho}_{0:H-1}$, feature maps $\hat{\phi}_{0:H-1}$ with $\hat{\phi}_h(x, a) \in \Delta([d_L])$.

**for** $i = 1, \ldots, d_L$ **do**

- Compute $\hat{\pi}_i = $ LINEAR-FQI($n, \rho_{0:H-1}, \hat{\phi}_{0:H-1}$, $R_{H-1} := \hat{\phi}_{H-1}(x, a)[i])$ \{ $R_{0:H-2} \equiv 0$ \}

**end for**

**return** policy mixture $\rho := \text{unif}(\{\hat{\pi}_i\}_{i=1}^{d_L})$.

**function** LINEAR-FQI($n, \rho_{0:H-1}, \hat{\phi}_{0:H-1}$, $R_{0:H-1}$)

**input:** Sample size $n$, policies $\rho_{0:H-1}$, feature maps $\hat{\phi}_{0:H-1}$, rewards $R_{0:H-1} : \mathcal{X} \times \mathcal{A} \to [0, 1]$.

Set $\hat{V}_H(x) = 0$

**for** $h = H-1, \ldots, 0$ **do**

- Collect $n$ samples ${\{(x_h^{(i)}, \hat{\phi}_h^{(i)}, x_{h+1}^{(i)})\}_{i=1}^n}$ by following $\rho_h \circ \text{unif}(A)$ in $\mathcal{M}$.
- Solve least squares problem:
  $$\hat{\theta}_h \leftarrow \arg\min_{\theta \in \mathbb{R}^d : \|\theta\|_2 \leq \sqrt{H} \alpha} \sum_{i=1}^n \left( \left\langle \theta, \hat{\phi}_h(x_h^{(i)}, a_h^{(i)}) \right\rangle - \hat{V}_{h+1}(x_{h+1}^{(i)}) \right)^2.$$  

- Define $\hat{Q}_h(x, a) = R_h(x, a) + \left\langle \hat{\theta}_h, \hat{\phi}_h(x, a) \right\rangle$.

- Define $\hat{\pi}_h(x) = \arg\max_a \hat{Q}_h(x, a), \hat{V}_h(x) = \min\{\max_a \hat{Q}_h(x, a), H\}$.

**end for**

**return** $\hat{\pi} = (\hat{\pi}_0, \ldots, \hat{\pi}_{H-1})$.

### D.1 Optimizing a fixed reward function

To optimize a fixed reward function, the high level idea is that, via Lemma 1, we can approximate any Bellman backup using our features $\hat{\phi}$, and via (4), we can collect a dataset with good coverage. Using these two properties the planning algorithm, LINEAR-FQI, displayed as a subroutine in Algorithm 4 is quite natural. The algorithm is a least squares dynamic programming algorithm (FQI stands for “Fitted Q Iteration”). For each $h$, working from $H-1$ down to 0, we collect a dataset of $n$ samples by following $\rho_h$. Then, we solve a least squares regression problem to approximate the Bellman backup of the value function estimate $\hat{V}_{h+1}$ for the next time. We use this to define the value function and the policy for the current time in the obvious way.

Note that we index policies in two different ways: $\rho_h$ is the exploratory policy that induces a distribution over $x_h$, while $\hat{\pi}_h$ is the one-step policy that we acts on $x_h$. As with the other planning lemmas, we apply the next lemma with a value of $H$ that is not necessarily the real horizon in the environment. In particular, we will use this lemma in the $h^{\text{th}}$ iteration of FLAMBE, with planning horizon $h-1$ and with reward functions specified in the next subsection. By induction, we can assume that (3) and (4) hold.

**Lemma 10.** Assume that (3) and (4) hold for all $h \in [H]$. Then for any reward functions $R_{0:H-1} : \mathcal{X} \times \mathcal{A} \to [0, 1]$ and any $\delta \in (0, 1)$, if we set

$$n \geq \frac{2304d^2}{\varepsilon_{TV}^2} \log \left( \frac{1152d^3}{\varepsilon_{TV}^2} + \frac{2304d^2}{\varepsilon_{TV}^2} \right) \log(2H/\delta),$$

then the policy $\hat{\pi}_{0:H-1}$ returned by LINEAR-FQI satisfies

$$\mathbb{E} \left[ \sum_{h=0}^{H-1} r_h \mid \hat{\pi}_{0:H-1}, \mathcal{M} \right] \geq \max_\pi \mathbb{E} \left[ \sum_{h=0}^{H-1} r_h \mid \pi, \mathcal{M} \right] - 2H^3 \sqrt{2K\kappa \varepsilon_{TV}}.$$
Proof: The analysis is similar to that of Chen and Jiang (2019), who study a similar algorithm in the infinite-horizon discounted setting. Let $\mathbb{E}_1$ denote expectation induced by the distribution over $(x_h, a_h, x_{h+1})$ obtained by following $\rho_h \circ \text{unif}(A)$. For any function $f : \mathcal{X} \to \mathbb{R}$, let $\mathcal{B}_h f(x, a) := \mathbb{E}[f(x_{h+1}) \mid x_h, a_h]$ denote the Bellman backup operator for time $h$ without the immediate reward. Let $\hat{\mathcal{B}}_h$ denote the Bellman backup operator induced by the learned model at time $h$, again without the immediate reward. We omit the dependence on $x, a$ in these operators when it is clear from context. Note that by the normalization assumptions, we always have $\hat{V}_{h+1}(x_h+1) \in [0, H]$. Moreover, $\hat{\mathcal{B}}_h \hat{V}_{h+1}$ is a linear function in $\hat{\phi}$ where the coefficient vector has $\ell_2$ norm at most $H \sqrt{d}$.

We apply Lemma 11 with $B := H \sqrt{d}$, and we take a union bound over all $h \in [H]$. Defining $\Delta_n := 24H^2d\sqrt{2(d \log n + \log(2H/\delta))/n}$, we have that with probability at least $1 - \delta$, for all $h \in [H]$:

$$
\mathbb{E}_h \left[ \left( \langle \hat{\theta}_h, \hat{\phi}_h(x_h, a_h) \rangle - B_h \hat{V}_{h+1} \right)^2 \right] \leq \min_{\theta : \|\theta\|_2 \leq B} \mathbb{E}_h \left[ \left( \langle \theta, \hat{\phi}_h(x_h, a_h) \rangle - B_h \hat{V}_{h+1} \right)^2 \right] + \Delta_n
$$

$$
\leq \mathbb{E}_h \left[ \left( \hat{\mathcal{B}}_h \hat{V}_{h+1} - B_h \hat{V}_{h+1} \right)^2 \right] + \Delta_n
$$

$$
\leq H^2 \cdot \mathbb{E}_h \left\| \hat{T}_h(\cdot | x_h, a_h) - T_h(\cdot | x_h, a_h) \right\|_{TV}^2 + \Delta_n.
$$

The first inequality here is the least squares generalization analysis, additionally using that $\mathcal{B}_h \hat{V}_{h+1}$ is the Bayes optimal predictor. The second uses the fact that the Bellman backups in the model are linear functions in $\phi$ (with bounded coefficient vector). Precisely, we have

$$
\hat{\mathcal{B}}_h \hat{V}_{h+1}(x_h, a_h) = \left\langle \hat{\phi}_h(x_h, a_h), \int \hat{\mu}_h(x_{h+1}) \hat{V}_{h+1}(x_{h+1}) d(x_{h+1}) \right\rangle.
$$

Setting $\theta$ to be the second term, we obtain the second inequality. Finally, we apply Holder’s inequality and use the fact that $\hat{V}_{h+1}$ is bounded in $[0, H]$ by construction. Appealing to (3) we have

$$
\mathbb{E}_h \left[ \left( \langle \hat{\theta}_h, \hat{\phi}_h(x_h, a_h) \rangle - \mathcal{B}_h \hat{V}_{h+1} \right)^2 \right] \leq H^2 \varepsilon_{TV} + \Delta_n.
$$

Now applying (4), we transfer this squared error to the distribution induced by any other policy. This calculation is exactly the same as in the main induction argument, and it yields

$$
\mathbb{E}_\pi \left[ \left( \langle \hat{\theta}_h, \hat{\phi}_h(x_h, a_h) \rangle - \mathcal{B}_h \hat{V}_{h+1} \right)^2 \right] \leq \kappa K (H^2 \varepsilon_{TV} + \Delta_n).
$$

Next, we bound the difference in cumulative rewards between $\hat{\pi} := \hat{\pi}_{0:H-1}$ and the optimal policy $\pi^*$ for the reward function. For this, recall that we define $\hat{Q}_0(x, a) = R_0(x, a) + \langle \hat{\theta}_0, \hat{\phi}_0(x, a) \rangle$ and also that $\hat{\pi}_0$ is greedy with respect to this Q function, which implies that $\hat{Q}_0(x, \hat{\pi}_0(x)) \geq \hat{Q}_0(x, \pi^*(x))$ for all $x$. Therefore,

$$
V^* - V^\hat{\pi} = \mathbb{E} \left[ R(x_0, a_0) + V^*(x_1) \mid \pi^* \right] - \mathbb{E} \left[ R(x_0, a_0) + V^\hat{\pi}(x_1) \mid \hat{\pi} \right]
$$

$$
\leq \mathbb{E} \left[ R(x_0, a_0) + V^*(x_1) - \hat{Q}_0(x_0, a_0) \mid \pi^* \right] - \mathbb{E} \left[ R(x_0, a_0) + V^\hat{\pi}(x_1) - \hat{Q}_0(x_0, a_0) \mid \hat{\pi} \right]
$$

$$
= \mathbb{E} \left[ V^*(x_1) - \left\langle \hat{\theta}_0, \hat{\phi}_0(x_0, a_0) \right\rangle \mid \pi^* \right] - \mathbb{E} \left[ V^\hat{\pi}(x_1) - \left\langle \hat{\theta}_0, \hat{\phi}_0(x_0, a_0) \right\rangle \mid \hat{\pi} \right]
$$

$$
= \mathbb{E} \left[ V^*(x_1) - \left\langle \hat{\theta}_0, \hat{\phi}_0(x_0, a_0) \right\rangle \mid \pi^* \right] - \mathbb{E} \left[ V^\hat{\pi}(x_1) - \left\langle \hat{\theta}_0, \hat{\phi}_0(x_0, a_0) \right\rangle \mid \hat{\pi} \right]
$$

$$
+ \mathbb{E} \left[ V^*(x_1) - V^\hat{\pi}(x_1) \mid \hat{\pi} \right].
$$

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Continuing, we find

\[ V^* - V^\# \leq \sum_{h=0}^{H-1} \mathbb{E} \left[ V^*(x_{h+1}) - \left\langle \hat{\theta}_h, \hat{\phi}_h(x_h, a_h) \right\rangle | \hat{\pi}_{0:h-1} \circ \pi^* \right] - \sum_{h=0}^{H-1} \mathbb{E} \left[ V^*(x_{h+1}) - \left\langle \hat{\theta}_h, \hat{\phi}_h(x_h, a_h) \right\rangle | \tilde{\pi}_{0:h} \right]. \]

Next, we bound each of these terms. Let us focus on just one of them, call the roll-in policy \( \pi \) and drop the dependence on \( h \). Then,

\[ \mathbb{E}_\pi \left[ \mathbb{E} \left[ V^*(x') | x, a \right] - \left\langle \hat{\theta}, \hat{\phi}(x, a) \right\rangle \right] \leq \mathbb{E}_\pi \left[ |BV^*(x, a) - B\hat{V}(x, a)| + |B\hat{V}(x, a) - \left\langle \hat{\theta}, \hat{\phi}(x, a) \right\rangle| \right] \leq \mathbb{E}_\pi \left[ |V^*(x') - \hat{V}(x')| + |B\hat{V}(x, a) - \left\langle \hat{\theta}, \hat{\phi}(x, a) \right\rangle| \right], \]

where the second inequality is Jensen’s inequality. By definition

\[ \mathbb{E}_\pi \left[ V^*(x') - \hat{V}(x') \right] = \mathbb{E}_\pi \left[ \max_a Q^*(x', a) - \min_{a'} \left\{ H, \max R(x', a') + \left\langle \hat{\phi}(x', a'), \hat{\theta} \right\rangle \right\} \right] \leq \mathbb{E}_\pi \left[ \max_a Q^*(x', a) - \max_{a'} R(x', a') + \left\langle \hat{\phi}(x', a'), \hat{\theta} \right\rangle \right] \leq \mathbb{E}_{\pi \circ \tilde{\pi}} \left[ |BV^*(x', a') - \left\langle \hat{\phi}(x', a'), \hat{\theta} \right\rangle| \right]. \]

Here in the last inequality, we define \( \tilde{\pi} \) to choose the larger of the two actions, that is we set \( \tilde{\pi}(x') = \arg\max_a \max\{Q^*(x', a), R(x', a) + \left\langle \hat{\theta}, \hat{\phi}(x', a) \right\rangle \}. \) This expression has the same form as the initial one, but at the next time point, so unrolling, we get

\[ \mathbb{E} \left[ BV^*(x_h, a_h) - \left\langle \hat{\theta}_h, \hat{\phi}_h(x_h, a_h) \right\rangle \right] \leq \sum_{\tau=h}^{H-1} \max_{\pi_\tau} \mathbb{E}_{\pi_\tau} \left[ |B\hat{V}_{\tau+1}(x_\tau, a_\tau) - \left\langle \hat{\theta}_\tau, \hat{\phi}_\tau(x_\tau, a_\tau) \right\rangle| \right] \]

\[ \leq H \sqrt{\kappa K (H^2 \varepsilon_{TV} + \Delta_n)}. \]

Plugging this into the overall value difference, the final bound is

\[ V^* - V^\# \leq 2H^2 \sqrt{\kappa K (H^2 \varepsilon_{TV} + \Delta_n)}. \]

To wrap up, we want the term involving \( \Delta_n \) to be at most \( H^2 \varepsilon_{TV} \), so the term involving \( \Delta_n \) is of the same order as the term involving \( \varepsilon_{TV} \). By our definition of \( \Delta_n \), this requires

\[ n \geq \frac{24^2 d^2}{\varepsilon_{TV}^2} \cdot 2 \left( d \log n + \log(2H/\delta) \right). \]

A sufficient condition here is

\[ n \geq \frac{2304 d^3}{\varepsilon_{TV}^2} \log \left( \frac{1152 d^3}{\varepsilon_{TV}^2} \right) + \frac{2304 d^2}{\varepsilon_{TV}^2} \log(2H/\delta), \]

which yields the result.

\[ \square \]

**Lemma 11.** Let \( \{\phi_i, y_i\}_{i=1}^n \) be \( n \) samples drawn iid from some distribution where \( \phi \in \mathbb{R}^d \) satisfies \( \|\phi\|_2 \leq 1 \) and \( y \in [0, H] \) almost surely. Let \( \tilde{\theta} \in \mathbb{R}^d \) denote the constrained square loss minimizer, constrained so that \( \|\tilde{\theta}\|_2 \leq B \), where \( B \geq H \). Then for any \( \delta \in (0, 1) \), with probability at least \( 1 - \delta \) we have

\[ \mathbb{E} \left[ \|\left\langle \tilde{\theta}, \phi \right\rangle - y \|^2 \right] \leq \min_{\theta : \|\theta\|_2 \leq B} \mathbb{E} \left[ \|\left\langle \theta, \phi \right\rangle - y \|^2 \right] + 24B^2 \sqrt{\frac{2}{n} \left( d \log(n) + \log(2/\delta) \right)}. \]
Proof. Fix \( \theta \) with \( \| \theta \|_2 \leq B \). We will apply Hoeffding’s inequality on this \( \theta \) and then use a covering argument for uniform convergence. Let \( R(\theta) \) denote the expected square loss, with \( \hat{R}(\theta) \) as the empirical counterpart. Using the bounds on all quantities, the square loss has range \((B + H)^2 \leq 4B^2\), and so Hoeffding’s inequality yields that with probability at least \( 1 - \delta \)

\[
\left| R(\theta) - \hat{R}(\theta) \right| \leq 4B^2 \sqrt{\frac{2}{n} \log(2/\delta)}.
\]

Let \( V_\gamma \) denote a covering of \( \{ \theta : \| \theta \|_2 \leq B \} \) in the \( \ell_2 \) norm at scale \( \gamma \), which has \( \log | V_\gamma | \leq d \log(2B/\gamma) \) via standard arguments. Taking a union bound, the above inequality holds for all \( \theta \in V_\gamma \) with probability \( 1 - |V_\gamma|\delta \). By direct calculation, we see that \( \hat{R}(\theta) \) and \( R(\theta) \) are both \( 2(B + H) \)-Lipschitz. Therefore, we have that with probability \( 1 - |V_\gamma|\delta \), for all \( \theta \) with \( \| \theta \|_2 \leq B \)

\[
\left| R(\theta) - \hat{R}(\theta) \right| \leq 4B \gamma + 4B^2 \sqrt{\frac{2}{n} \log(2/\delta)}.
\]

Taking \( \gamma = 2B/\sqrt{n} \) we can rebind \( \delta \) and absorb the first term into the second. Thus, with probability at least \( 1 - \delta \), for all \( \theta \), we have

\[
\left| R(\theta) - \hat{R}(\theta) \right| \leq 12B^2 \sqrt{\frac{2}{n} (d \log(n) + \log(2/\delta))}.
\]

Now by the standard ERM analysis, we have

\[
R(\hat{\theta}) \leq \hat{R}(\theta) + 12B^2 \sqrt{\frac{2}{n} (d \log(n) + \log(2/\delta))} \leq \min_{\theta} \hat{R}(\theta) + 12B^2 \sqrt{\frac{2}{n} (d \log(n) + \log(2/\delta))}.
\]

\[
\leq \min_{\theta} R(\theta) + 24B^2 \sqrt{\frac{2}{n} (d \log(n) + \log(2/\delta))}.
\]

\( \square \)

D.2 Instantiating the reward functions.

We now use Algorithm 4 in FLAMBE. Assume that \( \hat{\phi}_h(x, a) \in \Delta([d_{LV}]) \) for all \( x, a, h \), analogous to in Theorem 3. The planning algorithm in Algorithm 4 is analogous to Algorithm 3, except that we perform the optimization in the environment using LINEAR-FQI, with parameter \( n \) that we will set subsequently.

At iteration \( h \) of FLAMBE, this yields \( d_{LV} \) policies \( \pi_1, \ldots, \pi_{d_{LV}} \) where \( \pi_i \) approximately maximizes the probability of reaching the \( i \)th coordinate of \( \hat{\phi}_{h-1} \) when executed in the real world.

Defining \( \varepsilon_{stat} \) to be the sub-optimality guaranteed by Lemma 10 (additionally taking a union bound over all \( H d_{LV} \) invocations), we have that at iteration \( h \) of FLAMBE

\[
\mathbb{E} \left[ \hat{\phi}_{h-1}(x_{h-1}, a_{h-1})[i] \mid \hat{\pi}_i, \mathcal{M} \right] \geq \max_{\pi} \mathbb{E} \left[ \hat{\phi}_{h-1}(x_{h-1}, a_{h-1})[i] \mid \pi, \mathcal{M} \right] - \varepsilon_{stat}.
\]

We define \( \rho^\text{pre}_h \) to be the uniform distribution over the \( \hat{\pi}_i \) policies, which induce a distribution over \( x_h \).
Now for any function \( f : \mathcal{X} \to [0, 1] \), appealing to (3) at time \( h \) we have
\[
\mathbb{E}_\pi f(x_h) \leq \mathbb{E}_\pi \left( \hat{\phi}_{h-1}(x_{h-1}, a_{h-1}) \right) + \int \hat{\mu}_{h-1}(x_h) f(x_h) + \sqrt{\varepsilon_{TV}}
\]
\[
= \sum_{i=1}^{d_{LV}} \left( \int \hat{\mu}_{h-1}(x_h)[i] f(x_h) \right) \cdot \mathbb{E}_\pi \hat{\phi}_{h-1}(x_{h-1}, a_{h-1})[i] + \sqrt{\varepsilon_{TV}}
\]
\[
\leq \sum_{i=1}^{d_{LV}} \left( \int \hat{\mu}_{h-1}(x_h)[i] f(x_h) \right) \cdot \left( \mathbb{E}_h \hat{\phi}_{h-1}(x_{h-1}, a_{h-1})[i] + \varepsilon_{stat} \right) + \sqrt{\varepsilon_{TV}}
\]
\[
\leq \sum_{i=1}^{d_{LV}} \left( \int \hat{\mu}_{h-1}(x_h)[i] f(x_h) \right) \cdot \left( d_{LV\epsilon} \mathbb{E}_{\rho_h^\epsilon} \hat{\phi}_{h-1}(x_{h-1}, a_{h-1})[i] + \varepsilon_{stat} \right) + \sqrt{\varepsilon_{TV}}
\]
\[
\leq d_{LV\epsilon} \mathbb{E}_{\rho_h^\epsilon} \hat{\phi}_{h-1}(x_{h-1}, a_{h-1}) \int \hat{\mu}_{h-1}(x_h)[i] f(x_h) + d_{LV\epsilon} \varepsilon_{stat} + \sqrt{\varepsilon_{TV}}
\]
\[
\leq d_{LV\epsilon} \mathbb{E}_{\rho_h^\epsilon} f(x_h) + d_{LV\epsilon} \varepsilon_{stat} + (1 + d_{LV}) \sqrt{\varepsilon_{TV}}.
\]

The first and last inequalities here use (3) on \( \hat{T}_{h-1} \), which holds by induction. The second inequality is the optimality guarantee for \( \pi_i \), and the third is based on the definition of \( \rho_h^\epsilon \). For the fourth inequality, we collect terms, and additionally use that \( f \) is \( \ell_\infty \) bounded and \( \hat{\mu}_{h-1}[i] \) is a measure, so \( \int \hat{\mu}_{h-1}(x_h)[i] f(x_h) \leq 1 \).

Via importance weighting, we have that for any latent variable \( z \in Z_{h+1} \)
\[
\max \mathbb{P}[z_{h+1} = z] \leq d_{LV} K \cdot \mathbb{P}_{\rho_h^\epsilon} [z_{h+1} = z] + d_{LV} \varepsilon_{stat} + (1 + d_{LV}) \sqrt{\varepsilon_{TV}}.
\]

As before, we must set the additive error to be at most \( \eta_{\min}/2 \), and unpacking the definition of \( \varepsilon_{stat} \) and \( \kappa = 2d_{LV} K \) in the simplex features case this gives the constraint
\[
2H^3 \sqrt{4d_{LV} K^2 \varepsilon_{TV}} + (1 + d_{LV}) \sqrt{\varepsilon_{TV}} \leq \eta_{\min}/2.
\]

Therefore, we set
\[
\varepsilon_{TV} \leq O \left( \frac{\eta_{\min}^2}{H^6 d_{LV}^2 K^2} \right).
\]

With this choice we establish the same induction as in the proof of Theorem 3, so we are just left to calculate the sample complexity. For the calls to MLE, we have that \( \varepsilon_{TV} = 2d_{LV} K^2 \varepsilon_{sup} \) which yields the constraint
\[
\varepsilon_{sup} \leq O \left( \min \left\{ \frac{\eta_{\min}^2}{H^6 d_{LV}^2 K^4}, \frac{\varepsilon^2}{d_{LV} K^2} \right\} \right).
\]

This means that for the calls to MLE we may set \( n \) as
\[
n = O \left( \max \left\{ \frac{d_{LV}^2 K^2 H^6}{\eta_{\min}^2}, \frac{1}{\varepsilon^2} \right\} \cdot d_{LV} K^2 \log(H|\Phi||\Upsilon|/\delta) \right),
\]
which is slightly worse than before. The calls to MLE incur a total sample complexity of \( nH \).

We also have to collect trajectories to invoke LINEAR-FQI. For this, we must set \( n \) as\n\[
n = \tilde{O} \left( \frac{d_{LV}^3 K^4 H^{12}}{\varepsilon_{TV}^2} \log(1/\delta) \right) = \tilde{O} \left( \frac{d_{LV}^3 K^4 H^{12}}{\eta_{\min}^4} \log(1/\delta) \right),
\]
and the calls to LINEAR-FQI require \( nHd_{LV} \) samples in total. Therefore, the total sample complexity is
\[
\tilde{O} \left( \max \left\{ \frac{d_{LV}^2 K^2 H^6}{\eta_{\min}^2}, \frac{1}{\varepsilon^2} \right\} \cdot Hd_{LV} K^2 \log(|\Phi||\Upsilon|/\delta) + \frac{d_{LV}^3 K^4 H^{13}}{\eta_{\min}^4} \log(1/\delta) \right).
\]
**E Maximum Likelihood Estimation**

In this section we adapt classical results for maximum likelihood estimation in general parametric models. We consider a conditional probability estimation setting where there is a joint distribution \( \mathcal{D} \) over \((\mathcal{X} \times \mathcal{Y})\) and we denote the density \( p(y \mid x) = f^*(x, y) \). We are given a function class \( \mathcal{F} : (\mathcal{X} \times \mathcal{Y}) \to \mathbb{R} \) with which to model the condition distribution \( f^* \), and we assume that \( f^* \in \mathcal{F} \), so that the problem is well-specified or realizable. Given a dataset \( D := \{(x_i, y_i)\}_{i=1}^n \sim \mathcal{D} \), we optimize the maximum likelihood objective

\[
\hat{f} := \arg\max_{f \in \mathcal{F}} \sum_{i=1}^n \log f(x_i, y_i). \tag{8}
\]

The following result is classical (c.f., Van de Geer, 2000, Chapter 7), but under-utilized in machine learning and reinforcement learning in particular. Our adaptation is inspired by Zhang (2006).

**Theorem 12.** Fix \( \delta \in (0, 1) \), assume \( |\mathcal{F}| < \infty \) and \( f^* \in \mathcal{F} \). Then with probability at least \( 1 - \delta \)

\[
E_{x \sim \mathcal{D}} \left\| \hat{f}(x, \cdot) - f^*(x, \cdot) \right\|_{TV}^2 \leq \frac{2 \log(|\mathcal{F}|/\delta)}{n}.
\]

**Remark 13.** Given a class of discriminators \( \mathcal{G} : (\mathcal{X}, \mathcal{Y}) \to [-1, 1] \), an alternative is to consider the following (conditional) “generative adversarial” objective:

\[
\hat{f} = \arg\min_{f \in \mathcal{F}} \max_{g \in \mathcal{G}} \frac{1}{n} \sum_{i=1}^n \left( g(x_i, y_i) - \mathbb{E}[g(x_i, y) \mid y \sim f(x, \cdot)] \right).
\]

This is the natural objective associated with the distance function induced by \( \mathcal{G} \) (Arora et al., 2017), and is also related to other GAN-style approaches. Owing to the realizability assumption, \( f^* \) will always have low objective value, scaling with the complexity of \( \mathcal{G} \). Additionally, if \( \mathcal{G} \) is expressive enough, one can establish a guarantee similar to **Theorem 12**, which can then be used in the analysis of FLAMBE. Formally, a sufficient condition is that \( \mathcal{G} \) contains the indicators of the Scheffe sets for all pairs \( f, f' \in \mathcal{F} \), in which case the total variation guarantee can be obtained by standard uniform convergence arguments. See Devroye and Lugosi (2012); Sun et al. (2019) for more details.

**Remark 14.** We also remark that the proof of **Theorem 12** actually establishes convergence in the squared Hellinger distance. We obtain the total variation guarantee simply by observing that the squared Hellinger distance dominates the squared total variation distance.

We prove **Theorem 12** in this section. We begin with a decoupling inequality.

**Lemma 15.** Let \( D, D' \) be independent random variables. Let \( L(f, D) \) be any function, and let \( \hat{f}(D) \) be any estimator taking as input random variable \( D \) and with range \( \mathcal{F} \). Then

\[
\mathbb{E}_D \left[ \exp \left( L(\hat{f}(D), D) - \log \mathbb{E}_{D'} \exp(L(\hat{f}(D), D')) - \log |\mathcal{F}| \right) \right] \leq 1
\]

Observe that in the second term, the “loss function” takes as input \( D' \), but the estimator takes as input \( D \). As such, the above inequality decouples the estimator from the loss.

**Proof.** Let \( \pi \) be the uniform distribution over \( \mathcal{F} \) and let \( g : \mathcal{F} \to \mathbb{R} \) be any function. Define \( \mu(f) := \frac{\exp(g(f))}{\sum_f \exp(g(f))} \), which is clearly a probability distribution. Now consider any other probability distribution \( \hat{\pi} \)
We instantiate this bound with \( \hat{\pi} \) where the final inequality uses that the squared Hellinger distance is non-negative. Next, note that we can write

\[
E \text{ (squared) Hellinger distance, which for densities } E \text{ to } F
\]

Here the inequality follows from the fact that

\[
\text{Lemma 2.3 in Tsybakov (2008) asserts that for any two conditional probability densities } f_1, f_2 \text{ we have}
\]

\[
\mathbb{E}_{x \sim D} \left[ H^2(q||p) \right] = \int \left( \sqrt{p(z)} - \sqrt{q(z)} \right)^2 dz
\]

Lemma 2.3 in Tsybakov (2008) asserts that

\[
\|p(\cdot) - q(\cdot)\|_{TV}^2 \leq H^2(q||p) \cdot \left( 1 - \frac{H^2(q||p)}{4} \right) \leq H^2(q||p),
\]

where the final inequality uses that the squared Hellinger distance is non-negative. Next, note that we can also write

\[
H^2(q||p) = \int p(z) + q(z) - 2\sqrt{p(z)q(z)}dz = 2 \cdot \mathbb{E}_{z \sim q} \left[ 1 - \sqrt{p(z)/q(z)} \right]
\]

Here the inequality follows from the fact that \( 1 - x \leq -\log(x) \). The result follows by applying this argument to \( \mathbb{E}_{x \sim D} \|f_1(x, \cdot) - f_2(x, \cdot)\|_{TV}^2 \).

\[\square\]
Proof of Theorem 12. First note that Lemma 15 can be combined with the Chernoff method to obtain an exponential tail bound: with probability $1 - \delta$ we have
\[-\log \mathbb{E}_{D'} \exp (L(\hat{f}(D), D')) \leq -L(\hat{f}(D), D) + \log |F| + \log(1/\delta).
\]
Now we set $L(f, D) = \sum_{i=1}^{n} -1/2 \cdot \log(f^*(x_i, y_i)/f(x_i, y_i))$ where $D$ is a dataset $\{(x_i, y_i)\}_{i=1}^{n}$ (and $D' = \{(x'_i, y'_i)\}_{i=1}^{n}$ is identically distributed). With this choice, the right hand side is
\[
\sum_{i=1}^{n} \frac{1}{2} \log(f^*(x_i, y_i)/\hat{f}(x_i, y_i)) + \log |F| + \log(1/\delta) \leq \log |F| + \log(1/\delta),
\]
since $\hat{f}$ is the empirical maximum likelihood estimator and we are in the well-specified setting. On the other hand, the left hand side is
\[- \log \mathbb{E}_{D'} \exp \left( \sum_{i=1}^{n} -1/2 \log \left( \frac{f^*(x'_i, y'_i)}{\hat{f}(x'_i, y'_i)} \right) \right) = -n \log \mathbb{E}_{x, y \sim D} \exp \left( -1/2 \log \left( \frac{f^*(x, y)}{\hat{f}(x, y)} \right) \right)
\geq \frac{n}{2} \cdot \mathbb{E}_{x \sim D} \left\| \hat{f}(x, \cdot) - f^*(x, \cdot) \right\|_{TV}^2.
\]
Here the first identity uses the independence of the terms, which holds because $\hat{f}$ is independent of the dataset $D'$. The second inequality is Lemma 16. This yields the theorem. \qed

F Auxillary Lemmas

Lemma 17 (Elliptical Potential Lemma). Consider a sequence of $d \times d$ positive semidefinite matrices $X_1, \ldots, X_T$ with $\max_t \text{tr}(X_t) \leq 1$ and define $M_0 = I_{d \times d}, \ldots, M_t = M_{t-1} + X_t$. Then
\[
\sum_{t=1}^{T} \text{tr}(X_t M_{t-1}^{-1}) \leq 2d \log(1 + T/d).
\]

Proof. Observe that by concavity of the log det(·) function, we have
\[
\log(\text{det}(M_{t-1})) \leq \log(\text{det}(M_t)) + \text{tr}(M_t^{-1}(M_{t-1} - M_t)).
\]
Re-arranging and summing across all rounds $t$ yields
\[
\sum_{t=1}^{T} \text{tr}(X_t M_{t-1}^{-1}) \leq \sum_{t=1}^{T} \log(\text{det}(M_t)) - \log(\text{det}(M_{t-1})) = \log(\text{det}(M_T)) - d.
\]
By the spectral version of the AM-GM inequality and linearity of trace, we upper bound the last term:
\[
\text{det}(M_T)^{1/d} \leq \text{tr}(M_T)/d \leq 1 + T/d.
\]
Now, we must convert from $M_t^{-1}$ to $M_{t-1}^{-1}$ on the left hand side. Fix a round $t$ and let us write $X_t = VV^T$, which is always possible as $X_t$ is positive semidefinite. Then by the Woodbury identity
\[
\text{tr}(X_t M_{t-1}^{-1}) = \text{tr} \left( V^T (M_{t-1} + VV^T)^{-1} V \right)
= \text{tr}(V^T M_{t-1}^{-1} V) - \text{tr}(V^T M_{t-1}^{-1} V (I + V^T M_{t-1}^{-1} V)^{-1} V^T M_{t-1}^{-1} V).
\]
All matrices are simultaneously diagonalizable, so we may pass to a common eigendecomposition. In particular, with the eigendecomposition $V^T M_{t-1}^{-1} V = \sum_{i=1}^d \lambda_i u_i u_i^T$, we obtain

$$\text{tr}(X_t M_{t}^{-1}) = \sum_{i=1}^d \lambda_i - \frac{\lambda_i^2}{1 + \lambda_i} = \sum_{i=1}^d \frac{\lambda_i}{1 + \lambda_i} \geq \frac{1}{2} \sum_{i=1}^d \lambda_i = \frac{1}{2} \text{tr}(X_t M_{t-1}^{-1}).$$

The inequality follows from the fact that $\lambda_i \leq \|V^T M_{t-1}^{-1} V\|_2 \leq 1$ due to our initial conditions on $M_0$ and the normalization for $X_t$. 

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