Model-free Representation Learning and Exploration in Low-rank MDPs

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Abstract

The low rank MDP has emerged as an important model for studying representation learning and exploration in reinforcement learning. With a known representation, several model-free exploration strategies exist. In contrast, all algorithms for the unknown representation setting are model-based, thereby requiring the ability to model the full dynamics. In this work, we present the first model-free representation learning algorithms for low rank MDPs. The key algorithmic contribution is a new minimax representation learning objective, for which we provide variants with differing tradeoffs in their statistical and computational properties. We interleave this representation learning step with an exploration strategy to cover the state space in a reward-free manner. The resulting algorithms are provably sample efficient and can accommodate general function approximation to scale to complex environments.

1 Introduction

A key driver of recent empirical successes in machine learning is the use of rich function classes for discovering transformations of complex data, a sub-task referred to as representation learning. For example when working with images or text, it is standard to train extremely large neural networks in a self-supervised fashion on large datasets, and then fine-tune the network on supervised tasks of interest. The representation learned in the first stage is essential for sample-efficient generalization on the supervised tasks. Can we endow Reinforcement Learning (RL) agents with a similar capability to discover representations that provably enable sample efficient learning in downstream tasks?

In the empirical RL literature, representation learning often occurs implicitly simply through the use of deep neural networks, for example in DQN (Mnih et al., 2015). Recent work has also considered more explicit representation learning via auxiliary losses like inverse dynamics (Pathak et al., 2017), the use of explicit latent state space models (Hafner et al., 2019; Sekar et al., 2020), and via bisimulation metrics (Gelada et al., 2019; Zhang et al., 2020). Crucially, these explicit representations are again often trained in a way that they can be reused across a variety of related tasks, such as domains sharing the same (latent state) dynamics but differing in reward functions.

While these works demonstrate the value of representation learning in RL, theoretical understanding of such approaches is limited. Indeed obtaining sample complexity guarantees is quite subtle as recent lower bounds demonstrate that various representations are not useful or not learnable (Modi et al., 2020; Du et al., 2019b; Van Roy and Dong, 2019; Lattimore and Szepesvari, 2020; Hao et al., 2020). Despite these lower bounds, some prior theoretical works do provide sample complexity guarantees for non-linear...
function approximation (Jiang et al., 2017; Sun et al., 2019; Osband and Roy, 2014; Wang et al., 2020b; Yang et al., 2020), but these approaches do not obviously enable generalization to related tasks. More direct representation learning approaches were recently studied in Du et al. (2019a); Misra et al. (2020); Agarwal et al. (2020b), who develop algorithms that provably enable sample efficient learning in any downstream task that shares the same dynamics.

Our work builds on the most general of the direct representation learning approaches, namely the FLAMBE algorithm of Agarwal et al. (2020b), that finds features under which the transition dynamics are nearly linear. The main limitation of FLAMBE is the assumption that the dynamics can be described in a parametric fashion. In contrast, we take a model-free approach to this problem, thereby accommodating much richer dynamics.

Concretely, we study the low rank MDP (also called linear MDP, factored linear MDP, etc.), in which the transition operator $T : (x, a) \to \Delta(\mathcal{X})$ admits a low rank factorization as $T(x' | x, a) = \langle \phi^*(x, a), \mu^*(x') \rangle$ for feature maps $\phi^*, \mu^*$. For model-free representation learning, we assume access to a function class $\Phi$ containing the underlying feature map $\hat{\phi}^*$. This is a much weaker inductive bias than prior work in the “known features” setting where $\phi^*$ is known in advance (Jin et al., 2020b; Yang and Wang, 2020; Agarwal et al., 2020a) and the model-based setting (Agarwal et al., 2020b) that assumes realizability for both $\mu^*$ and $\hat{\phi}^*$.

While our model-free setting captures richer MDP models, addressing the intertwined goals of representation learning and exploration is much more challenging. In particular, the forward and inverse dynamics prediction problems used in prior works are no longer admissible under our weak assumptions. Instead, we address these challenges with a new representation learning procedure based on the following insight: for any function $f : \mathcal{X} \to \mathbb{R}$, the Bellman backup of $f$ is a linear function in the feature map $\phi^*$. This leads to a natural minimax objective, where we search for a representation $\hat{\phi}$ that can linearly approximate the Bellman backup of all functions in some “discriminator” class $\mathcal{F}$. Importantly, the discriminator class $\mathcal{F}$ is induced directly by the class $\Phi$, so that no additional realizability assumptions are required. We also provide an incremental approach for expanding the discriminator set, which leads to a more computationally practical variant of our algorithm.

The two algorithms reduce to minimax optimization problems over non-linear function classes. While such problems can be solved empirically with modern deep learning libraries, they do not come with rigorous computational guarantees. To this end, we investigate the special case of finite feature classes ($|\Phi| < \infty$). We show that when $\Phi$ is efficiently enumerable, our optimization problems can be reduced to eigenvector computations, which leads to provable computational efficiency. To our knowledge, our results represent the first statistically and computationally efficient model-free algorithms for representation learning in RL.

2 Problem setting

We consider learning in an episodic MDP $\mathcal{M}$ with a state space $\mathcal{X}$, a finite action space $\mathcal{A} = \{1, \ldots, K\}$ and horizon $H$. In each episode, an agent generates a trajectory $\tau = (x_0, a_0, x_1, \ldots, x_{H-1}, a_{H-1}, x_H)$, where (i) $x_0$ is a starting state, (ii) $x_{h+1} \sim T_h(\cdot | x_h, a_h)$, and (iii) the actions are chosen by the agent according to some non-stationary policy $a_h \sim \pi(\cdot | x_h)$. Here, $T_h$ denotes the (possibly non-stationary) transition dynamics $T_h : \mathcal{X} \times \mathcal{A} \to \Delta(\mathcal{X})$ for each timestep. For notation, $\pi_h$ denotes $h$-step policy that chooses actions $a_0, \ldots, a_h$. We also use $\mathbb{E}_x[\cdot]$ and $\mathbb{E}_\tau[\cdot]$ to denote the expectations over states and actions and probability of an event respectively, when using policy $\pi$ in $\mathcal{M}$. Further, we use $[H]$ to denote $\{0, 1, \ldots, H - 1\}$. We consider learning in a low-rank MDP defined as:

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

$$\forall x, x', a \in \mathcal{X} : T(x' | x, a) = \langle \phi^*(x, a), \mu^*(x') \rangle.$$
and additionally $\|\phi^*(x, a)\|_2 \leq 1$ and for all $g : \mathcal{X} \to [0, 1]$, $\| \int g(x) \mu^*(x) dx \|_2 \leq \sqrt{d}$. We assume that $\mathcal{M}$ is low-rank with embedding dimension $d$, i.e., for each $h \in [H]$, the transition operator $T_h$ admits a rank-$d$ decomposition.

We will denote the embedding for $T_h$ by $\phi^*_h$ and $\mu^*_h$. In addition to the low-rank representation, we will also consider a latent variable representation of $\mathcal{M}$, as defined in Agarwal et al. (2020b), as follows:

**Definition 2.** The latent variable representation of a transition operator $T : \mathcal{X} \times \mathcal{A} \to \Delta(\mathcal{X})$ is a latent space $\mathcal{Z}$ along with functions $\psi : \mathcal{X} \times \mathcal{A} \to \Delta(\mathcal{Z})$ and $\nu : \mathcal{Z} \to \Delta(\mathcal{X})$, such that $T(\cdot|x, a) = \int \nu(\cdot|z) \psi(z|x, a) dz$. The latent variable dimension of $T$, denoted $d_{LV}$, is the cardinality of smallest latent space $\mathcal{Z}$ for which $T$ admits a latent variable representation. In other words, this representation gives a non-negative factorization of the transition operator $T$.

When state space $\mathcal{X}$ is finite, all transition operators $T_h(\cdot|x, a)$ admit a trivial latent variable representation. More generally, the latent variable representation enables us to augment the trajectory $\tau$ as: $\tau = \{x_0, a_0, z_1, x_1, \ldots, z_{H-1}, x_{H-1}, a_{H-1}, x_H\}$, where $z_{h+1} \sim \psi_h(\cdot|x_h, a_h)$ and $x_{h+1} \sim \nu_h(\cdot|z_{h+1})$. In general we neither assume access to nor do we learn this representation, and it is solely used to reason about the following reachability assumption:

**Assumption 1.** There exists a constant $\eta_{\text{min}} > 0$ such that

$$\forall h \in [H], z \in \mathcal{Z}_h : \max_{\pi} P_{\pi}[z_{h+1} = z] \geq \eta_{\text{min}}.$$  

Assumption 1 posits that in MDP $\mathcal{M}$, for each factor (latent variable) at any level $h$, there exists a policy which reaches it with a non-trivial probability. This generalizes the reachability of latent states assumption from prior block MDP results (Du et al., 2019a; Misra et al., 2020). Note that, exploring all latent states is still non-trivial, as a policy which chooses actions uniformly at random may hit these latent states with an exponentially small probability.

**Representation learning in low-rank MDPs** We consider MDPs where the state space $\mathcal{X}$ is large and the agent must employ function approximation to conduct effective learning. Given the low rank MDP assumption, we grant the agent access to a class of representation functions mapping a state-action pair $(x, a)$ to a $d$-dimensional embedding. Specifically, the feature class is $\Phi = \{ \Phi_h : h \in [H] \}$, where each mapping $\phi_h \in \Phi_h$ is a function $\phi_h : \mathcal{X} \times \mathcal{A} \to \mathbb{R}^d$. The feature class can now be used to learn $\phi^*$ and exploit the low-rank decomposition for efficient learning. We assume that our feature class $\Phi$ is rich enough:

**Assumption 2 (Realizability).** For each $h \in [H]$, we have $\phi^*_h \in \Phi_h$. Further, we assume that $\forall \phi_h \in \Phi_h, \forall (x, a) \in \mathcal{X} \times \mathcal{A}, \|\phi_h(x, a)\|_2 \leq 1$.

A key property of a low-rank MDPs, which we will use frequently in subsequent section, is the following lemma due to Jin et al. (2020b). We provide a proof in Appendix H.1 for completeness.

**Lemma 1 ((Jin et al., 2020b)).** For a low-rank MDP $\mathcal{M}$ with embedding dimension $d$, for any function $f : \mathcal{X} \to [0, 1]$, we have:

$$\mathbb{E}[f(x_{h+1})|x_h, a_h] = \langle \phi^*_h(x_h, a_h), \theta^*_f \rangle$$

where $\theta^*_f \in \mathbb{R}^d$ and we have $\|\theta^*_f\|_2 \leq \sqrt{d}$. \footnote{Sometimes we drop $h$ in the subscript for brevity.}
Learning goal  We focus on the problem of reward-free exploration (Jin et al., 2020a; Agarwal et al., 2020b) where the agent does not get an explicit reward signal and instead tries to learn good enough features that enable offline optimization of any given reward. In our model free case, we provide this reward-free learning guarantee for any reward function \( R \) in a bounded reward class \( \mathcal{R} \). Specifically, for such a bounded reward function \( R : \mathcal{X} \times \mathcal{A} \to [0, 1] \), the learned features \( \{ \phi_h \}_{h \in [H]} \) and the collected data should allow the agent to compute a near-optimal policy \( \pi_R \), such that \( v^*_R \geq v^* - \varepsilon \).\(^2\) We desire (w.p. \( \geq 1 - \delta \)) sample complexity bounds which are \( \text{poly}(d, H, K, 1/\eta_{\text{min}}, 1/\varepsilon, \log |\Phi|, \log(1/\delta)) \).

2.1 Related work

Much recent attention has been devoted to linear function approximation (c.f., Jin et al., 2020b; Yang and Wang, 2020). These results provide important building blocks for our work. In particular, the low rank MDP model we study is from Jin et al. (2020b) who assume that the feature map \( \phi^* \) is known in advance. However, as we are focused on nonlinear function approximation, it is more apt to compare to related nonlinear approaches, which can be categorized in terms of their dependence on the size of the function class:

**Polynomial in \( |\Phi| \) approaches** Many approaches, while not designed explicitly for our setting, can yield sample complexity scaling polynomially with \( |\Phi| \) in our setup. Note, however, that polynomial-in-\( |\Phi| \) scaling can be straightforwardly obtained by concatenating all of candidate feature maps and running the algorithm of Jin et al. (2020b). This is the only obvious way to apply Eluder dimension results here (Osbands and Roy, 2014; Wang et al., 2020b; Ayoub et al., 2020), and it also pertains to work on model selection (Pachchiano et al., 2020; Lee et al., 2020). Indeed, the key observation that enables a logarithmic-in-\( |\Phi| \) sample complexity is that all value function are in fact represented as sparse linear functions of this concatenated feature map.

However, exploiting sparsity in RL (and in contextual bandits) is quite subtle. In both settings, it is not possible to obtain results scaling logarithmically in both the ambient dimension and the number of actions (Lattimore and Szepesvári, 2020; Hao et al., 2020). That said, it is possible to obtain results scaling polynomially with the number of actions and logarithmically with the ambient dimension, as we do here.

**Logarithmic in \( |\Phi| \) approaches** For logarithmic-in-\( |\Phi| \) approaches, the assumptions and results vary considerably. Several results focus on the block MDP setting (Du et al., 2019a; Misra et al., 2020; Foster et al., 2020), where the dynamics are governed by a discrete latent state space, which is decodable from the observations. This setting is a special case of our low rank MDP setting. Additionally, these works make stronger function approximation assumptions than we do. As such our work can be seen as generalizing and relaxing assumptions, when compared with existing block MDP results.

Most closely related to our work are the OLIVE and FLAMBE algorithms (Jiang et al., 2017; Agarwal et al., 2020b). OLIVE is a model-free RL algorithm that can be instantiated to produce a logarithmic-in-\( |\Phi| \) sample complexity guarantee in precisely our setting (it also applies more generally). However it is not computationally efficient even in tabular settings (Dann et al., 2018). In contrast, our algorithm involves a more natural minimax optimization problem that we show is computationally tractable in the “abstraction selection” case, which is even more general than the “known feature” setting (Section 5).

FLAMBE is computationally efficient, but it is model-based, so the function approximation assumptions are stronger than ours. Thus the key advancement is our weaker model-free function approximation assumption which does not require modeling \( \mu^* \) whatsoever. On the other hand, FLAMBE does not require reachability assumptions as we do, and we leave eliminating reachability assumptions with a model-free approach as an important open problem.

**Related algorithmic approaches** Central to our approach is the idea of embedding plausible futures into a “discriminator” class and using this class to guide the learning process. Bellemare et al. (2019) also propose a min-max representation learning objective using a class of adversarial value functions, but their work only

\(^2\)Here, \( v^*_R = \mathbb{E}_x \left[ \sum_{h=0}^{H-1} R_h(x_h, a_h) \right] \) is the expected value of policy \( \pi \) and \( v^*_R = \max_\pi v^*_R \) is the optimal expected value.
empirically demonstrates its usefulness as an auxiliary task during learning and does not study exploration. Similar ideas of using a discriminator class have been deployed in model-based RL Farahmand et al. (2017); Sun et al. (2019); Modi et al. (2020); Ayoub et al. (2020), but the application to model-free representation learning and exploration is novel to our knowledge.

3 Algorithm and Analysis

Before turning to the algorithm description and intuition, we clarify useful notation for \( h \) step policies. An \( h \)-step policy \( \rho_h \) chooses actions \( a_0, \ldots, a_h \), consequently inducing a distribution over \( (x_h, a_h, x_{h+1}) \). We routinely append several random actions to such a policy, and we use \( \rho_h^{+i} \) to denote the policy that chooses \( a_{0:h} \) according to \( \rho_h \) and then takes actions uniformly at random for \( i \) steps, inducing a distribution over \( (x_{h+i}, a_{h+i}, x_{h+i+1}) \). As an edge case, for \( i \geq j \geq 0 \), \( \rho_{j}^{+i} \) takes actions \( a_0, \ldots, a_{i-j} \) uniformly. The mnemonic is that the last action taken by \( \rho_j \) is \( a_{i+j} \).

Our algorithm, Model Free Feature Learning and Exploration (MOFFLE) described in Algorithm 1, takes as input a feature set \( \Phi \), a reward class \( \mathcal{R} \), and some parameters. It outputs a feature map and a dataset such that FQI, using linear functions of the returned features, can be run with the returned dataset to obtain a near optimal policy for any reward function in \( \mathcal{R} \). The algorithm runs in two stages:

**Exploration** We use the EXPLORE sub-routine (Algorithm 2) in the main algorithm MOFFLE to compute exploratory policies \( \rho_{h-3}^{+3} \) for each timestep \( h \in \mathcal{H} \).

**Representation learning** We subsequently learn a feature \( \tilde{\phi}_h \) for each level using Algorithm 4, that allows us to use FQI to plan for any reward \( R_{0:H-1} \in \mathcal{R} \) afterwards.

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**Algorithm 1** MOFFLE \((\mathcal{R}, \Phi, \eta_{\min}, \varepsilon, \delta)\): Model-Free Feature Learning and Exploration

1: Set \( \mathcal{D} \leftarrow \emptyset, \varepsilon_{\text{apx}} \leftarrow \frac{\varepsilon^2}{\mathcal{S}^2 \mathcal{H}^2 \kappa^2 \mathcal{K}} \).
2: Compute exploratory policies
   \( \{\rho_{h-3}^{+3}\}_{h \in \mathcal{H}} \leftarrow \text{EXPLORE} \left( \Phi, \eta_{\min}, \frac{\delta}{2} \right) \).
3: for \( h \in \mathcal{H} \) do
4:   Learn representation \( \tilde{\phi}_h \) for timestep \( h \) by calling
   \( \text{LEARNREP} \left( \rho_{h-3}^{+3}, \Phi_h, \mathcal{G}_{h+1}, \mathcal{H}, \varepsilon_{\text{apx}}, \frac{\delta}{\mathcal{H}} \right) \).
5: Collect an exploratory dataset \( \mathcal{D}_h \) of \( (x_h, a_h, x_{h+1}) \) tuples using \( \rho_{h-3}^{+3} \).
6: Set \( \mathcal{D} \leftarrow \mathcal{D} \cup \{\mathcal{D}_h\} \).
7: end for
8: return \( \{\rho_{h-3}^{+3}\}_{h \in \mathcal{H}}, \mathcal{D}, \tilde{\phi}_{0:H-1} \).

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3.1 Computing exploratory policies

We first describe the exploration algorithm (pseudocode in Algorithm 2). Algorithm 2 uses a step-wise forward exploration scheme similar to FLAMBE Agarwal et al. (2020b), but without estimating a transition model. To understand the design choices in the algorithm, it is helpful to consider how we can discover a policy cover over the latent state space \( \mathcal{Z}_{h+1} \). If we knew the mapping to latent states, we could create the reward functions \( \mathbf{1}(z_{h+1} = z) \) for all \( z \in \mathcal{Z}_{h+1} \) and compute policies to optimize such rewards, but we do not have access to this mapping. Additionally, we do not have access to the features \( \phi^* \) to enable tractable planning even for the known rewards. Algorithm 2 tackles both of these challenges. For the first challenge, we note that by Definition 2 of the latent variables and Lemma 1, there always exists \( f \) such that

\[
\mathbb{E}[\mathbf{1}(z_{h+1} = z) | x_{h-1}, a_{h-1}] = \mathbb{E}[f(x_h, a_h) | x_{h-1}, a_{h-1}] = \langle \phi_{h-1}(x_{h-1}, a_{h-1}), \theta^*_j \rangle.
\]
Our algorithm will seek to discover features $\hat{\phi}_{h-2}$ so that for all appropriately bounded $\theta$, there is a $w$ such that

$$
\mathbb{E}[\langle \phi_{h-1}^*(x_{h-1}, a_{h-1}), \theta \rangle | x_{h-2}, a_{h-2}] \approx \langle \hat{\phi}_{h-2}(x_{h-2}, a_{h-2}), w \rangle.
$$

(1)

Given this property, we prove that coverage over $\mathcal{Z}_{h+1}$ can be ensured using coverage of all the reachable directions under $\hat{\phi}_{h-2}$ in the MDP followed by two uniform actions, and we provide planning algorithms that have this guarantee. Thus, we use a cover over $\mathcal{Z}_h$ to learn features $\hat{\phi}_h$ satisfying (1), and then plan in the previously learned features $\hat{\phi}_{h-2}$ to obtain a cover over $\mathcal{Z}_{h+1}$. This way, planning trails feature learning like FLAMBE, but with an additional step of lag due to differences between model-free and model-based reasoning. We now describe how this high-level intuition is realized through the steps of the algorithm, and the corresponding theoretical results.

### Algorithm 2: EXPLORE ($\Phi, \eta_{\min}, \delta_{\epsilon}$)

1. Set $\mathcal{D}_h = \emptyset$ for each $h \in [H]$.
2. for $h = 0, \ldots, H - 1$ do
3.     Set exploratory policy for timestep $h$ to $\rho_{h-3}^+$.
4.     Learn representation $\hat{\phi}_h$ for timestep $h$ by calling:

$$
\text{LEARNREP} (\rho_{h-3}^+, \Phi_h, \mathcal{F}_{h+1}, \eta_{reg}, \delta_e).$

5. Collect $n$ samples $(x_h, a_h, x_{h+1})$ using policy $\rho_{h-3}^+$ and add them to $\mathcal{D}_h$.
6. if $h \geq 2$ then
7.     Call planner (Algorithm 3) with features $\hat{\phi}_{h-2}$, dataset $\{\mathcal{D}_j\}_{j=0}^{h-2}$ and $\beta$ to obtain policy $\rho_{h-2}$.
8. end if
9. end for
10. return Exploratory policies $\{\rho_{h-3}^+\}_{h \in [H]}$.

The algorithm proceeds in stages where for each $h$, we first use an exploratory policy $\rho_{h-3}^+$ (line 4) to learn features $\hat{\phi}_h$ which allow us to approximate Bellman backups of bounded functions. For a formal statement, it is helpful to introduce the shorthand

$$
b_{\text{err}} (\pi_h, \hat{\phi}_h, f; B) = \min_{\|w\|_2 \leq B} \mathbb{E}_{\pi_h} \left[ (\langle \phi_h(x_h, a_h), w \rangle) - \mathbb{E} [f(x_{h+1}) | x_h, a_h] \right]^2
$$

(2)

for any policy $\pi_h$, feature $\phi_h$, function $f$ and constant $B$. This is the error in approximating the conditional expectation of $f(x_{h+1})$ using linear functions in the features $\phi_h(x_h, a_h)$. Note that Lemma 1 implies that $b_{\text{err}} (\pi_h, \hat{\phi}_h, f; B) = 0$ for all functions $f$, and hence we seek to learn features $\hat{\phi}_h$ (line 4) such that, for some fixed scalar $B$,

$$
\max_{f \in \mathcal{F}_{h+1}} b_{\text{err}} (\rho_{h-3}^+, \hat{\phi}_h, f; B) \leq \varepsilon_{reg}.
$$

(3)

Here, $\mathcal{F}_{h+1} \subset (\mathcal{X} \rightarrow [0, 1])$ is the discriminator class that contains all functions $f$ in the form of:

$$
f(x_{h+1}) = \text{clip}_{[0,1]} \left( \mathbb{E}_{\text{unif}(A)} \langle \phi_{h+1}(x_{h+1}, a), \theta \rangle \right)
$$

(4)

where $\phi_{h+1} \in \Phi_{h+1}$ and $\|\theta\|_2 \leq B$ for some $B \geq \sqrt{d}$, and the choice of this class is directly inspired by our desideratum in (1).

Having learned these features, we collect a dataset of $(x_h, a_h, x_{h+1})$ tuples using policy $\rho_{h-3}^+$ (line 5). Using the collected data, we call an offline planning sub-routine (line 7) which returns a policy $\rho_{h-2}$ and
induces a roll-in distribution over \((x_{h-2}, a_{h-2})\) (line 7). The reason for planning at \(h - 2\) is precisely based on our earlier intuition, formalizing which, we show that the policy \(\rho_{h-2}^{\pm 2} = \rho_{h-2} \circ \text{unif}(A) \circ \text{unif}(A)\) is exploratory and hits all latent states in \(z \in Z_{h+1}\):

\[
\max_{\pi} \mathbb{P}_\pi [z_{h+1} = z] \leq \kappa \mathbb{P}_{\rho_{h-2}^{\pm 2}} [z_{h+1} = z],
\]

where \(\kappa > 0\) is a constant we specify later. Taking the action \(a_{h+1}\) uniformly at random inductively returns an exploratory policy \(\rho_{h-2}^{\pm 3}\) for state-action pairs \((x_{h+1}, a_{h+1})\). Note that for the first step \(h = 0\), the null policy \(\rho_{h-3}^{\pm 3}\) satisfies the exploration guarantee in (5).

Apart from specifying \textsc{LearnRep}, the main missing piece is the offline planning sub-routine used to produce policy \(\rho_{h-2}\). For this, we incorporate techniques from batch RL Chen and Jiang (2019) and reward-free exploration in the known features setting Wang et al. (2020a); Zanette et al. (2020). In Algorithm 3, we repeatedly invoke a batch RL algorithm to learn near-optimal policies for a sequence of carefully designed reward functions. Inspired by techniques from reward-free exploration, we use reward functions that are quadratic in the learned features \(\hat{\phi}_{h-2}\). For batch RL, we use \text{Fitted Q Iteration} with function class comprising all linear functions of \(\phi \in \Phi\). The resulting policy \(\rho_{h-2}\) effectively covers all directions spanned by \(\phi_{h-2}\) which we can show also yields (5).

### Algorithm 3 FQI based Elliptical Planner

1: **Input:** Exploratory dataset \(\mathcal{D} := \{\mathcal{D}\}_{0:H}, \beta > 0\).
2: Initialize \(\Gamma_0 = I_{d \times d}\).
3: for \(t = 1, 2, \ldots\), do
   4: Using Algorithm 6, compute
      \[
      \pi_t = \text{FQI} \left( \mathcal{D}, R_H = \left\| \hat{\phi}_H (x, a) \right\|_2^{\frac{2}{\Gamma_{t-1}}} \right).
      \]
5: If the estimated objective is at most \(\frac{3\beta}{4}\), halt and output \(\rho := \text{unif}(\{\pi_t\}_{\tau<t})\).
6: Estimate feature covariance matrix as:
   \[
   \hat{\Sigma}_\pi = \frac{1}{n_{\text{plan}}} \sum_{i=1}^{n_{\text{plan}}} \hat{\phi}_H \left( x^{(i)}_H, a^{(i)}_H \right) \hat{\phi}_H \left( x^{(i)}_H, a^{(i)}_H \right)^\top.
   \]
7: Update \(\Gamma_t \leftarrow \Gamma_{t-1} + \hat{\Sigma}_\pi\).
8: end for

We provide the following guarantee for the policies returned by Algorithm 2 with a complete proof in Appendix A.

**Theorem 2.** Fix \(\delta \in (0, 1)\). Consider an MDP \(\mathcal{M}\) which admits a low rank factorization with dimension \(d\) in Definition 1 and satisfies Assumption 1. If the features \(\hat{\phi}_h\) learned in line 4 in Algorithm 2 satisfy the condition in (3) for \(B \geq \sqrt{d}\) and \(\varepsilon_{\text{reg}} = \hat{\Theta} \left( \frac{\eta_{\min}^{1/3}}{d^2 K^4 \log^4(1+8/\beta)} \right)\), then with probability at least \(1 - \delta\), the sub-routine \textsc{Explore} collects an exploratory mixture policy \(\rho_{h-3}^{\pm 3}\) for each level \(h\) such that:

\[
\forall \pi : \mathbb{E}_\pi[f(x_h, a_h)] \leq \kappa K \mathbb{E}_{\rho_{h-3}^{\pm 3}}[f(x_h, a_h)]
\]

for any \(f : \mathcal{X} \times \mathcal{A} \to \mathbb{R}^+\) and \(\kappa = \frac{64dK^4 \log(1+8/\beta)}{\eta_{\min}}\). The total number of episodes used in line 7 by Algorithm 2 is:

\[
\hat{O} \left( \frac{H^5 d^6 K^{13} B^4 \log(\Phi/\delta_e)}{\eta_{\min}} \right),
\]

7
with $\beta$ chosen to satisfy $\beta \log (1 + 8/\beta) \leq \eta_{\min}^2 \frac{1}{12dHK^2}$. 

The precise dependence on parameters $d$, $H$, $K$ and $\eta_{\min}$ is likely improvable. The exponent on $K$ arises from multiple importance sampling steps over the uniform action choice, while the dependence on other quantities can be improved when the features $\phi(x, a) \in \Delta(d)$ for all $x$, $a$ and $\phi \in \Phi$. Improving these dependencies further is an interesting avenue for future progress.

3.2 Representation learning for downstream tasks

As established, in the first phase, MOFFLE finds exploratory policies $\{\rho_{h-3}^+\}_{h[H]}$ satisfying the coverage guarantee in (6). In the second phase, we use these policies to learn a representation $\bar{\phi}_{0:H-1}$ that enables downstream policy optimization for the pre-specified reward class $\mathcal{R}$. We use FQI for downstream optimization which allows us to appeal to prior results (Chen and Jiang, 2019), provided we can establish three conditions: (1) (concentrability) we have adequate coverage over the state space, (2) (realizability) we can express $Q^*$ with our function class, and (3) (completeness) our class is closed under Bellman backups. The first condition is implied by Theorem 2.

Approximate realizability and completeness can be guaranteed by invoking the same LEARNREP subroutine we used to learn features in the exploration phase with slightly different parameters. Indeed, analogous to (3), we learn features $\bar{\phi}_{0:H-1} \in \Phi$ such that $\bar{\phi}_h$ satisfies

$$
\max_{g \in \mathcal{G}_h} \text{b_err} \left( \rho_{h-3}^+; \bar{\phi}_h, g; B \right) \leq \varepsilon_{\text{apx}},
$$

(7)

where $\mathcal{G}_h \subset (X \rightarrow [0, H])$ is the set of functions

$$
g(x') = \text{clip}_{[0,H]} \left( \max_a \left( R(x', a) + \langle \phi_{h+1}(x', a), \theta \rangle \right) \right),
$$

with $R \in \mathcal{R}$, $\phi_{h+1} \in \Phi_{h+1}$, $\|\theta\|_2 \leq B$ and $B \geq H \sqrt{d}$. The discriminator class $\mathcal{G}_h$ is similar to $\mathcal{F}_h$ in (3), where we clip $f$ in $[0, 1]$, set $R(x', a) = 0$ and take expectation with respect to $a \sim \text{unif}(A)$ instead of a maximum. The main conceptual difference over (3) is that the discriminator class $\mathcal{G}_h$ now incorporates reward information, which enables downstream planning.

With $\bar{\phi}_{0:H-1}$ and given any reward function $R \in \mathcal{R}$, we define the $Q$ function class $\mathcal{Q}_h(\bar{\phi}, R)$ as

$$
\left\{ \text{clip}_{[0,H]} \left( R_h(x, a) + \langle \bar{\phi}_h(x, a), w \rangle \right) : \|w\|_2 \leq B \right\}.
$$

Using (7) and the low rank MDP properties, we show that this function class satisfies approximate realizability and approximate completeness, so we can invoke results for FQI and obtain the following representation learning guarantee:

**Theorem 3.** If the features $\bar{\phi}_{0:H-1}$ learnt by MOFFLE satisfy the condition in (7) for all $h$ with $\varepsilon_{\text{apx}} = \tilde{O} \left( \frac{\varepsilon^2 \eta_{\min}}{dHK^2} \right)$, then for any reward function $R \in \mathcal{R}$, running FQI with the value function class $Q(\bar{\phi}, R)$ and an exploratory dataset $D$, returns a policy $\hat{\pi}$, which satisfies $v_R^* \geq v_R^* - \varepsilon$ with probability at least $1 - \delta$. The total number of episodes collected by MOFFLE in line 5 are:

$$
\tilde{O} \left( \frac{H^7d^2K^5 \log(|\Phi|\|\mathcal{R}\|B/\delta)}{\varepsilon^2 \eta_{\min}} \right).
$$
4 Min-max-min representation learning

In this section, we describe our novel representation learning objective used to learn \( \hat{\phi}_h \) and \( \bar{\phi}_h \). The key insight is that the low-rank property of the MDP \( \mathcal{M} \) can be used to learn a feature map \( \hat{\phi} \) which can approximate the Bellman backup of all linear functions under feature maps \( \phi \in \Phi \), and that approximating the backups of these functions enables subsequent near optimal planning.

**Algorithm 4** \textsc{LearnRep} \((\rho_{h-3}^{+3}, \Phi_h, \mathcal{V}, L, \varepsilon, \delta_v)\)

1: Collect dataset \( \mathcal{D} \) of tuples \((x_h, a_h, x_{h+1})\) using \( \rho_{h-3}^{+3} \).
2: \textbf{return} representation \( \hat{\phi}_h \) as the solution of

\[
\arg\min_{\phi \in \Phi_h} \max_{v \in \mathcal{V}} \left\{ \min_{\|w\|_2 \leq B} \mathcal{L}_D(\phi, w, v) - \min_{\phi \in \Phi_h, \|\tilde{w}\|_2 \leq L\sqrt{d}} \mathcal{L}_D(\tilde{\phi}, \tilde{w}, v) \right\}. \tag{8}
\]

We present the algorithm with an abstract discriminator class \( \mathcal{V} \subset (\mathcal{X} \to [0, L]) \) that is instantiated either with \( F_{h+1} \) or \( G_{h+1} \) defined previously. Recalling (3) and (7), we seek a feature map \( \hat{\phi}_h \) that approximately minimizes \( \max_{v \in \mathcal{V}} b_{\text{err}} \left( \rho_{h-3}^{+3}, \hat{\phi}_h, v; B \right) \). Unfortunately, the quantity \( b_{\text{err}}(\cdot) \) contains a conditional expectation inside the square loss, so we cannot estimate it from samples \((x_h, a_h, x_{h+1}) \sim \rho_{h-3}^{+3}\). This is an instance of the well-known double sampling issue Baird (1995); Antos et al. (2008). Instead, we introduce a correction term to obtain the final population objective:

\[
\mathcal{L}_{\rho_{h-3}^{+3}}(\phi_h, w, v) = \mathbb{E}_{\rho_{h-3}^{+3}} \left[ \langle \phi_h(x_h, a_h), w \rangle - v(x_{h+1}) \right] ^2,
\]

which is amenable to estimation from samples. However this loss function contains an undesirable conditional variance term, since via the bias-variance decomposition:

\[
\mathcal{L}_{\rho_{h-3}^{+3}}(\phi_h, w, v) = b_{\text{err}} \left( \rho_{h-3}^{+3}, \phi_h, v; B \right) + \mathbb{E}_{\rho_{h-3}^{+3}} \left[ \mathbb{E} \left[ v(x_{h+1}) \mid x_h, a_h \right] \right].
\]

This excess variance term can lead the agent to erroneously select a bad feature \( \hat{\phi}_h \), since discriminators \( v \in \mathcal{V} \) with low conditional variance will be ignored. However, via Lemma 1, we can rewrite the conditional variance as \( \mathcal{L}_{\rho_{h-3}^{+3}}(\phi_h, \theta^*_v, v) \) for some \( \|\theta^*_v\|_2 \leq L\sqrt{d} \), which suggests that we introduce a correction term to obtain the final population objective:

\[
\arg\min_{\phi \in \Phi_h} \max_{v \in \mathcal{V}} \left\{ \min_{\|w\|_2 \leq B} \mathcal{L}_{\rho_{h-3}^{+3}}(\phi, w, v) - \min_{\phi \in \Phi_h, \|\tilde{w}\|_2 \leq L\sqrt{d}} \mathcal{L}_{\rho_{h-3}^{+3}}(\tilde{\phi}, \tilde{w}, v) \right\}. \tag{9}
\]

Using dataset \( \mathcal{D} \), we let \( \mathcal{L}_D(\cdot) \) denote the empirical estimate of \( \mathcal{L}_{\rho_{h-3}^{+3}}(\cdot) \), and, in Algorithm 4, we simply optimize the empirical version of (9) to obtain feature map \( \hat{\phi}_h \).

4.1 Oracle representation learning

For the first feature learning guarantee, we assume access to a computational oracle for solving the min-max-min objective in (8). In Appendix C we show that solving this optimization problem with norm bound \( B = L\sqrt{d} \) produces a feature map that satisfies (3) and (7). For example, with \( n \) samples and function class \( F_{h+1} \) defined above, the learned feature \( \hat{\phi}_h \) satisfies

\[
\max_{f \in F_{h+1}} b_{\text{err}} \left( \rho_{h-3}^{+3}, \hat{\phi}_h, f; L\sqrt{d} \right) \leq \tilde{O} \left( \frac{L^2 d^2 \log \frac{|\Phi||\mathcal{V}|}{\varepsilon}}{n} \right).
\]

Using this along with Theorem 2 and Theorem 3, we show the following overall sample complexity result for MOFFLE with a complete proof in Appendix C:
Corollary 4. Fix $\delta \in (0, 1)$. If LEARNREP is implemented via Algorithm 4, then MOFFLE returns an exploratory dataset $\mathcal{D}$ such that for any $R \in \mathcal{R}$, running FQI with value function class $\mathcal{Q}(\hat{\phi}, R)$ returns an $\varepsilon$-optimal policy with probability at least $1 - \delta$. The total number of episodes used by the algorithm is:

$$
\tilde{O} \left( \frac{H^6 d^8 K^{13} \log \left( \frac{|\Phi|}{\varepsilon} \right)} {\eta_{\min}} + \frac{H^7 d^9 K^5 \log \left( \frac{|\Phi||R|}{\varepsilon} \right)} {\varepsilon^2 \eta_{\min}} \right).
$$

4.2 Iterative greedy representation learning

The min-max-min objective in the previous section in (8) is not provably computationally tractable for non-enumerable and non-linear function classes. In this section, we show that we can instead solve this problem with an iterative approach that alternates between a squared loss minimization problem and a max-min objective in each iteration. The resulting algorithm is empirically more viable than (8).

This iterative procedure is displayed in Algorithm 5. Given the discriminator class $\mathcal{V}$, the algorithm grows finite subsets $\mathcal{V}^1, \mathcal{V}^2, \ldots \subseteq \mathcal{V}$ in an incremental and greedy fashion with $\mathcal{V}^1 = \{v_1\}$ initialized arbitrarily. In the $t$th iteration, we have discriminator class $\mathcal{V}^t$ and we estimate a feature $\hat{\phi}_{t,h}$ which has low total squared loss with respect to all functions in $\mathcal{V}^t$ (line 6). Importantly the total square loss (sum) avoids the double sampling issue that arises with the worst case loss over class $\mathcal{V}$ (max), so no correction term is required.

Next, we try to certify that $\hat{\phi}_{t,h}$ is a good representation by searching for a witness function $v_{t+1} \in \mathcal{V}$ for which $\hat{\phi}_{t,h}$ has large excess square loss (line 7). The optimization problem in (11) does require a correction term to address double sampling, but since $\hat{\phi}_{t,h}$ is fixed, it can be written as a simpler max-min program, when compared with the oracle approach. If the objective value for this program is smaller than some threshold, then our certification successfully verifies that $\hat{\phi}_{t,h}$ can approximate the Bellman backup of all functions in $\mathcal{V}$, so we terminate and output $\hat{\phi}_{t,h}$. On the other hand, if the objective is large, we add the witness $v_{t+1}$ to our growing discriminator class and advance to the next iteration.

One technical point worth noting is that in (11) we relax the norm constraint on $w$ to allow it to grow with $\sqrt{t}$. This is required by our iteration complexity analysis which we summarize in the following lemma:

Lemma 5. (Informal) Fix $\delta_1 \in (0, 1)$. If the dataset $\mathcal{D}$ is sufficiently large, then with probability at least $1 - \delta_1$, Algorithm 5 terminates after $T = \frac{52L^2 d^2}{\varepsilon_{tol}}$ iterations and returns a feature $\hat{\phi}_h$ such that:

$$\max_{v \in \mathcal{V}} \mathbb{b}_{err}(\rho_{h-3}^{+1}, \hat{\phi}_h, v; \sqrt{\frac{13L^4 d^3}{\varepsilon_{tol}}}) \leq \varepsilon_{tol}.$$  

The size of $\mathcal{D}$ scales polynomially with the relevant parameters, e.g., for $\mathcal{V} = \mathcal{F}_{h+1}$, we set $n = \tilde{O} \left( \frac{d^3 \log \left( \frac{|\Phi|}{\varepsilon_{tol}} \right)} {\varepsilon_{tol}} \right)$.

Proof sketch. From Lemma 1, we know that for any $v \in \mathcal{V}$, $\mathbb{E}[v(\cdot)|x_h, a_h] = \langle \phi_h^*(x_h, a_h), \theta_{v}^* \rangle$. Our analysis uses this $d$-dimensional representation of functions in $\mathcal{V}$, i.e., $\phi_{v}^* := \phi_{v}^*$. For any iteration $t$, let $w_{t,i} = \arg\min_w \mathcal{L}_D(\hat{\phi}_{t,h}, w, v_i)$. Using Lemma 12 in Appendix D.2, we can show that for each non-terminal iteration $t$,

$$\sum_{i \leq t} \mathbb{E}_{\rho_{h-3}^{+1}} \left( \hat{\phi}_{t,h}(x_h, a_h)^\top w_{t,i} - \phi_h^*(x_h, a_h)^\top \theta_t^* \right)^2 \leq t \bar{\varepsilon}, \quad ||\Sigma_t^{-1} \theta_{t+1}||_2 \geq \sqrt{\frac{8d\bar{\varepsilon}_0}{(d^2 t \bar{\varepsilon}_0 + \lambda^2)}}.$$
Algorithm 5 Feature Selection via Greedy Improvement

1: **input:** Feature class $\Phi_h$, discriminator class $\mathcal{V}$, dataset $\mathcal{D} := \{x_{i,h}^t, a_{i,h}^t, x_{i,h}^{t+1}\}_{i=1}^n$ and tolerance $\varepsilon_{\text{tol}}$.
2: Set $\mathcal{V}^0 \leftarrow \emptyset$ and choose $v_1 \in \mathcal{V}$ arbitrarily.
3: Set $\varepsilon_0 \leftarrow \frac{\varepsilon_{\text{tol}}}{\sqrt{2d^2}}$, $t \leftarrow 1$ and $t \leftarrow \infty$.
4: **repeat**
5: Set $\mathcal{V}^t \leftarrow \mathcal{V}^{t-1} \cup \{v_t\}$.
6: **(Fit feature)** Compute $\hat{\phi}_{t,h}$ as:

$$
\hat{\phi}_{t,h}, W_t = \arg\min_{\phi \in \Phi_h, W \in \mathbb{R}^{d \times t}} \sum_{i=1}^t \mathcal{L}_D(\phi, W^i, v_i) \quad (10)
$$

7: **(Find witness)** Find greedy adversarial test function:

$$
f_{t+1} = \arg\max_{v \in \mathcal{V}} \max_{\tilde{\phi} \in \Phi_h} \left( \min_{\|\tilde{\phi}\|_2 \leq \sqrt{\frac{2d}{t}}} \mathcal{L}_D(\hat{\phi}_{t,h}, w, v) - \mathcal{L}_D(\tilde{\phi}, \tilde{w}, v) \right) \quad (11)
$$

8: Set test loss $l$ to the objective value in (11).
9: **until** $l < 24d^2 \varepsilon_0 + \varepsilon_0^2$.
10: **return** Feature $\hat{\phi}_{T,h}$ from last iteration $T$.

where $\tilde{\varepsilon}$ is an error term dependent on the size of $\mathcal{D}$, $\sum = \sum_{i \leq t} \theta_i^* \theta_i^* + \lambda I$ and $\varepsilon_0$ is a carefully chosen constant.

The relation intuitively says that the vector $\theta_{t+1}$ is not adequately spanned by the previous $\theta_i^*$ vectors. Using an elliptic potential argument (Carpentier et al., 2020), we show that this can only happen for a bounded number of iterations. In addition, for the last iteration $T$, the elliptic potential falls below a certain value and guarantees that:

$$
\max_{v \in \mathcal{V}} b_{\text{err}} \left( \rho_{h-3}^{\frac{1}{3}}, \hat{\phi}_{T,h}, v; \frac{\sqrt{T^2dT}}{2} \right) \leq 48d^2 \varepsilon_0 + 4\varepsilon_0^2.
$$

Therefore, $\varepsilon_0$ is chosen such that the upper bound is less than $\varepsilon_{\text{tol}}$. We provide a complete proof in Appendix D.1.

Notice that the norm bound in (12) scales with the accuracy parameter $\varepsilon_{\text{tol}}$. While this does degrade the overall sample complexity when compared with using the oracle approach, it can still be used in MOFFLE leading to a more computationally viable algorithm. We summarize the overall result in the following corollary.

**Corollary 6.** Fix $\delta \in (0, 1)$. If LEARNREP is implemented via Algorithm 5, MOFFLE returns an exploratory dataset $\mathcal{D}$ such that for any $R \in \mathcal{R}$, running FQI with value function class $Q(\hat{\phi}, R)$ returns an $\varepsilon$-optimal policy with probability at least $1 - \delta$. The total number of episodes used by the algorithm are:

$$
\hat{O}(\frac{H^6d^{16}K^{31}}{\eta_{\text{min}}^{11}} \log \left( \frac{\|\Phi_h\|_2}{\delta} \right) + \frac{H^{19}d^{10}K^{15}}{\varepsilon_{\text{tol}}^{6} \eta_{\text{min}}^{3}} \log \left( \frac{\|\Phi_h\|_2}{\delta} \right)).
$$
5 Enumerative feature class: A computationally tractable instance

The greedy feature selection method described in Section 4.2 improves over the min-max-min objective in (8) by breaking it into separate minimization and max-min problems. While there are heuristics which can be used for solving the max-min problem, these are not provably computationally efficient. In this section, we show that when $\Phi$ is a finite class and is efficiently enumerable, the min-max-min objective reduces to a tractable eigenvector problem. Note that the finite/enumerable feature class generalizes the problem of efficient abstraction selection (Jiang et al., 2015; Modi et al., 2020), in which each feature map $\phi$ is a state abstraction function.

For enumerable features, in Algorithm 2, we learn $\tilde{\phi}_h$ using a slightly different objective:

$$\min_{\phi \in \Phi_h} \max_{f \in F_{h+1}} \left\{ \min_{\|w\|_2 \leq B} \mathcal{L}_D(\phi, w, f) - \mathcal{L}_D(\tilde{\phi}, \tilde{w}, f) \right\}$$ (13)

where $F_{h+1}$ is now the discriminator class that contains all unclipped functions $f$ in form of:

$$f(x_{h+1}) = \mathbb{E}_{\text{unif}(A)} \left[ \langle \phi_{h+1}(x_{h+1}, a), \theta \rangle \right],$$ (14)

where $\phi_{h+1} \in \Phi_{h+1}$ and $\|\theta\|_2 \leq \sqrt{d}$.

Consider the min-max-min objective where we fix $\phi, \tilde{\phi} \in \Phi_h$. For this instance of the min-max-min objective, we show that (13) can be reduced to:

$$\max_{f \in F_{h+1}} f(D)^\top \left( A(\phi)^\top A(\phi) - A(\tilde{\phi})^\top A(\tilde{\phi}) \right) f(D)$$ (15)

where $A(\phi) = I_{d \times d} - X \left( \frac{1}{n} X^\top X + \lambda I_{d \times d} \right)^{-1} \left( \frac{1}{n} X^\top \right)$ for a parameter $\lambda$. Here, $X, \tilde{X} \in \mathbb{R}^{n \times d}$ are the sample covariate matrices for features $\phi, \tilde{\phi}$ respectively and $f(D) \in \mathbb{R}^n$. The objective in (15) is obtained by using a ridge regression solution for $w, \tilde{w}$ in (13) which also implies that $B = 1/\lambda$ in (13). Finally, for any fixed feature $\phi'$ in the definition of $f \in F_{h+1}$, we can rewrite (15) as:

$$\max_{\|\theta\|_2 \leq \sqrt{d}} \theta^\top X'^\top \left( A(\phi)^\top A(\phi) - A(\tilde{\phi})^\top A(\tilde{\phi}) \right) X' \theta$$

where $X' \in \mathbb{R}^{n \times d}$ is again a sample matrix defined using $\phi' \in \Phi_{h+1}$. Thus, for a fixed tuple of $(\phi, \tilde{\phi}, \phi')$, the max-min objective is a tractable eigenvector computation problem. As a result, we can efficiently solve the min-max-min objective in (13) by enumerating over each candidate feature in $(\phi, \tilde{\phi}, \phi')$ to solve

$$\min_{\phi \in \Phi_h} \max_{\phi' \in \Phi_{h+1}} \max_{\|\theta\|_2 \leq \sqrt{d}} \theta^\top X'^\top \left( A(\phi)^\top A(\phi) - A(\tilde{\phi})^\top A(\tilde{\phi}) \right) X' \theta.$$ (16)

While the analysis is more technical, (13) still allows us to plan using $\tilde{\phi}_h$ in Algorithm 2 to guarantee that the policies $\rho_{h-3}^{+3}$ are exploratory. Unfortunately, for learning the final representations $\tilde{\phi}_{0: H-1}$ in MOFFLE, using the unclipped discriminator class $F$ in (13) does not satisfy the completeness guarantee required by FQI. Thus, this variant of MOFFLE does not provide a representation learning guarantee, where a concise feature map can be used for several downstream tasks. However, we can still define a value function class $Q_h$ using all features $\phi_h \in \Phi_h$ and run FQI with the data collected by policies $\rho_{h-3}^{+3}$ to learn an $\epsilon$-optimal policy for any fixed reward function $R$. We summarize the overall result in the following corollary:
Theorem 7. Fix $\delta \in (0, 1)$. In Algorithm 2, if $\hat{\phi}_h$ is learned using the eigenvector formulation (16), then MOFFLE returns an exploratory dataset $D$ such that for any $R \in \mathcal{R}$, running FQI using the full representation class $\Phi$ returns an $\varepsilon$-optimal policy with probability at least $1 - \delta$. The total number of episodes used by the algorithm are $\text{poly}(d, H, K, 1/\eta_{\min}, 1/\varepsilon, \log |\Phi|, \log(1/\delta))$.

A detailed version of the corollary and the proof can be found in Appendix E.

6 Discussion

In this paper, we present, MOFFLE, a new model-free algorithm for representation learning and exploration in low rank MDPs. We develop several representation learning schemes that vary in their computational and statistical properties, each yielding a different instantiation of the overall algorithm. Importantly MOFFLE can leverage a general function class $\Phi$ for representation learning, which provides it with the expressiveness and flexibility to scale to rich observation environments in a provably sample-efficient manner.

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A Exploration and sample complexity results for Algorithm 2

A.1 Proof of Theorem 2

Theorem (Restatement of Theorem 2). Fix $\varepsilon \in (0, 1)$. Consider an MDP $\mathcal{M}$ which admits a low rank factorization with dimension $d$ in Definition 1 and satisfies Assumption 1. If the features $\hat{\phi}_h$ learnt in line 4 of Algorithm 2 satisfy the condition in (3) for $B = \sqrt{d}$ and $\varepsilon_{\text{reg}} = \tilde{O}\left(\frac{\eta_{\min}^{\beta} \kappa}{d^2 K^d \log^3(1+8/\beta)}\right)$, then with probability at least $1 - \delta$, the sub-routine EXPLORE collects an exploratory mixture policy $\rho_{h-3}^+$ for each level $h$ such that:

$$\forall \pi: \mathbb{E}_\pi[f(x_h, a_h)] \leq \kappa K \mathbb{E}_{\rho_{h-3}^+} [f(x_h, a_h)]$$

for any $f : \mathcal{X} \times \mathcal{A} \to \mathbb{R}^+$ and $\kappa = \frac{64d K^4 \log(1+8/\beta)}{\eta_{\min}}$. The total number of episodes used in line 7 by Algorithm 2 is:

$$\tilde{O}\left(\frac{H^5 d^5 K^{13} B^4 \log \left(\frac{\Phi}{\varepsilon}\right)}{\eta_{\min}^5}\right).$$

The value of $\beta$ is chosen such that $\beta \log (1 + 8/\beta) \leq \frac{\eta_{\min}^{\beta}}{128d K^4 B^2}$.

Proof. We will now prove the result assuming that the following condition from (3) is satisfied by $\hat{\phi}_h$ for all $h \in [H]$ with probability at least $1 - \delta/2$:

$$\max_{f \in \mathcal{F}_{h+1}} \min_{\|w\|_2 \leq B} \mathbb{E}_{\rho_{h-3}^+} \left[ \left( \langle \hat{\phi}_h(x_h, a_h), w \rangle - \mathbb{E}[f(x_{h+1})|x_h, a_h] \right)^2 \right] \leq \varepsilon_{\text{reg}}. \quad (18)$$

Now, let us turn to the inductive argument to show that the constructed policies $\rho_{h-3}^+$ are exploratory for every $h$. For our analysis, we will assume Lemma 15 stated in Section F. We will establish the following inductive statement for each timestep $h$:

$$\forall z \in \mathcal{Z}_{h+1} : \max_{\pi} \mathbb{P}_{\pi}[z_{h+1} = z] \leq \kappa \mathbb{P}_{\rho_{h-2}^+}[z_{h+1} = z]. \quad (19)$$

Assume that the exploration statement is true for all timesteps $h' \leq h$. We first show an error guarantee similar to (17) under distribution shift:

Lemma 8. If the inductive assumption in (19) is true for all $h' \leq h$, then for all $v : \mathcal{X} \times \mathcal{A} \to \mathbb{R}^+$ we have:

$$\forall \pi: \mathbb{E}_\pi[v(x_h, a_h)] \leq \kappa K \mathbb{E}_{\rho_{h-3}^+} [v(x_h, a_h)]$$

(20)

Proof. Consider any timestep $h$ and non-negative function $v$. Using the inductive assumption, we have:

$$\mathbb{E}_\pi[v(x_h, a_h)] = \sum_{z \in \mathcal{Z}_h} \mathbb{P}_\pi[z_h = z] \cdot \int \mathbb{E}_{\pi_h}[v(x_h, a_h)] \nu^*(x_h|z) \, d(x_h)$$

$$\leq \kappa \sum_{z \in \mathcal{Z}_h} \mathbb{P}_{\rho_{h-3}^+}[z_h = z] \cdot \int \mathbb{E}_{\pi_h}[v(x_h, a_h)] \nu^*(x_h|z) \, d(x_h)$$

$$= \kappa \mathbb{E}_{\rho_{h-3}^+} [\mathbb{E}_{\pi_h}[v(x_h, a_h)]]$$

$$\leq \kappa K \mathbb{E}_{\rho_{h-3}^+} [v(x_h, a_h)]$$

Therefore, the result holds for any policy $\pi$, timestep $h' \leq h$ and non-negative function $v$. \qed

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As a result of Lemma 8, we have the same guarantee for the following squared-loss term for pair \((x_h, a_h)\) for some \(f \in \mathcal{F}_{h+1}\):

\[
v(x_h, a_h) = \mathbb{E}_{\pi_h} \left[ \left( \langle \hat{\phi}_h(x_h, a_h), w \rangle - \mathbb{E} [f(x_{h+1}) | x_h, a_h] \right)^2 \right].
\]

Thus, using the feature learning guarantee in (18) along with (20), we have:

\[
\forall f \in \mathcal{F}_{h+1} : \min_{\|w\|_2 \leq B} \mathbb{E}_{\pi} \left[ \left( \langle \hat{\phi}_h(x_h, a_h), w \rangle - \mathbb{E} [f(x_{h+1}) | x_h, a_h] \right)^2 \right] \leq \kappa K \varepsilon_{\text{reg}}.
\]

We now outline our key argument to establish exploration: Fix a latent variable \(z \in \mathcal{Z}_{h+1}\) and let \(\pi := \pi_h\) be the policy which maximizes \(\mathbb{P}_\pi[z_{h+1} = z]\). Thus, with \(f(x_h, a_h) = \mathbb{P}[z_{h+1} = z | x_h, a_h]\) we have:

\[
\mathbb{E}_{\pi} [f(x_h, a_h)] \leq K^2 \mathbb{E}_{\pi_{h-2} \times \text{unif}(A) \times \text{unif}(A)} [f(x_h, a_h)]
\]

\[
= K^2 \mathbb{E}_{\pi_{h-2}} \left[ \mathbb{E}_{\text{unif}(A)} [g(x_{h-1}, a_{h-1}) | x_{h-2}, a_{h-2}] \right]
\]

\[
\leq K^2 \mathbb{E}_{\pi_{h-2}} \left[ \left( \langle \hat{\phi}_{h-2}(x_{h-2}, a_{h-2}), w_g \rangle \right)^2 \right] + \sqrt{\kappa K^5 \varepsilon_{\text{reg}}}. \tag{21}
\]

The first inequality follows by using importance weighting on timesteps \(h - 1\) and \(h\), where we choose actions uniformly at random among \(A\). In the next step, we define \(g(x_{h-1}, a_{h-1}) = \mathbb{E}_{\text{unif}(A)} [f(x_h, a_h) | x_{h-1}, a_{h-1}] = \langle \hat{\phi}_{h-1}(x_{h-1}, a_{h-1}), \theta_f \rangle\) with \(\|\theta_f\|_2 \leq \sqrt{d}\). For (21), we use the result from Lemma 8 that \(\hat{\phi}_{h-2}\) has small squared loss for the regression target specified by \(g(\cdot)\) for a vector \(w_g\) with \(\|w_g\|_2 \leq B\). We further use the weighted RMS-AM inequality in the same step to bound the mean absolute error using the squared error bound.

**Lemma 9.** If the FQI planner (Algorithm 3) is called with a sample of size \(\tilde{O} \left( \frac{H^4 d^k \log \left( \frac{d^k H}{\delta e} \right)}{\beta^2} \right)\), then for all \(h \in [H]\), we have:

\[
\mathbb{E}_{\pi_{h-2}} \left[ \left( \langle \hat{\phi}_{h-2}(x_{h-2}, a_{h-2}), w_g \rangle \right)^2 \right] \leq \frac{\alpha}{2} \mathbb{E}_{\rho_{h-2}} \left[ \left( \langle \hat{\phi}_{h-2}(x_{h-2}, a_{h-2}), w_g \rangle \right)^2 \right] + \frac{T \beta}{2 \alpha} + \frac{\alpha \|w_g\|_2^2}{2 T} + \frac{\alpha \beta \|w_g\|_2^2}{2}.
\]

**Proof.** Applying Cauchy-Schwarz inequality followed by AM-GM, for any matrix \(\hat{\Sigma}\), we have:

\[
\mathbb{E}_{\pi_{h-2}} \left[ \left( \langle \hat{\phi}_{h-2}(x_{h-2}, a_{h-2}), w_g \rangle \right)^2 \right] \leq \mathbb{E}_{\pi_{h-2}} \left[ \left\| \hat{\phi}_{h-2}(x_{h-2}, a_{h-2}) \right\|_{\hat{\Sigma}_{h-2}} \cdot \|w_g\|_{\hat{\Sigma}} \right]
\]

\[
\leq \frac{1}{2\alpha} \mathbb{E}_{\pi_{h-2}} \left[ \left\| \hat{\phi}_{h-2}(x_{h-2}, a_{h-2}) \right\|_{\hat{\Sigma}_{h-2}}^2 \right] + \frac{\alpha}{2} \mathbb{E}_{\rho_{h-1}} \left[ \|w_g\|_{\hat{\Sigma}}^2 \right]
\]

Here, we choose \(\hat{\Sigma}\) to be the (normalized) matrix returned by the elliptic planner in Algorithm 3. As can be seen in the algorithm pseudocode, \(\hat{\Sigma}\) is obtained by summing up a (normalized) identity matrix and the empirical estimates of the population covariance matrix \(\Sigma_{\pi} = \mathbb{E}_{\pi} \hat{\phi}_{h-2}(x_{h-2}, a_{h-2}) \phi_{h-2}(x_{h-2}, a_{h-2})^\top\) where \(\{\pi_\tau\}_{\tau \leq T}\) are the \(T\) policies computed by the planner. Noting that \(\rho_{h-2}\) is a mixture of these \(T\) policies, we consider the following empirical and population quantities:

\[
\Sigma_{\rho_{h-2}} = \frac{1}{T} \sum_{t=1}^{T} \Sigma_{\pi_t}, \quad \Sigma = \Sigma_{\rho_{h-2}} + \frac{1}{T} I_{d \times d}, \quad \hat{\Sigma} = \frac{1}{T} \Gamma T = \frac{1}{T} \sum_{i=1}^{T} \hat{\Sigma}_{\pi_i} + \frac{1}{T} I_{d \times d}.
\]
Now, we use the termination conditions satisfied by the elliptic planner (shown in Lemma 15) in the following steps:

\[
\mathbb{E}_{\pi_{h-2}} \left[ \left\langle \hat{\phi}_{h-2}(x, a), w_g \right\rangle \right] \leq \frac{1}{2\alpha} \mathbb{E}_{\pi_{h-2}} \left[ \left\| \hat{\phi}_{h-2}(x_{h-2}, a_{h-2}) \right\|_{\Sigma_{h-1}}^2 \right] + \frac{\alpha}{2} \left\| w_g \right\|_{\Sigma}^2 \tag{22}
\]

\[
\leq \frac{T\beta}{2\alpha} + \frac{\alpha}{2} \left\| w_g \right\|_{\Sigma}^2 \leq \frac{T\beta}{2\alpha} + \frac{\alpha}{2} \left\| w_g \right\|_{\Sigma}^2 + \frac{\alpha}{2} \beta \left\| w_g \right\|_{2}^2 \tag{23}
\]

\[
= \frac{T\beta}{2\alpha} + \frac{\alpha}{2} \mathbb{E}_{\rho_{h-2}} \left[ \left( \left\langle \hat{\phi}_{h-2}(x_{h-2}, a_{h-2}), w_g \right\rangle \right) \right] + \frac{\alpha}{2} \left\| w_g \right\|_{2}^2 + \frac{\alpha}{2} \beta \left\| w_g \right\|_{2}^2 .
\]

For the second inequality, note that \( \frac{1}{T} \left\| \hat{\phi}_{h-2}(x_{h-2}, a_{h-2}) \right\|_{\Sigma_{h-1}}^2 \) is the reward function optimized by the FQI planner in the last iteration. Let \( V_T(\pi) \) denote the expected value of a policy \( \pi \) for this reward function and MDP \( M \). From the termination condition and the results for the FQI planner in Lemma 15, we get:

\[
\max_{\pi} V_T(\pi) \leq V_T(\pi_T) + \beta/8 \leq \hat{V}_T(\pi_T) + \beta/4 \leq \beta.
\]

Therefore, the first term on the rhs in (22) can be bounded by \( T\beta/2\alpha \). In step (23), we use the estimation guarantee for \( \Sigma = \Gamma_T/T \) for the FQI planner shown in Lemma 15. Then, in the last equality step, we expand the norm of \( w_g \) using the definition of \( \Sigma \) to arrive at the desired result.

Putting everything together, we now compute the number of samples used during FQI planning for the required error tolerance. Lemma 19 states that for a sample of size \( n \), the computed policy is sub-optimal by a value difference of order upto \( \hat{O} \left( \sqrt{H^4d^3K\log \left( \frac{|\Phi|}{n} \right)} \right) \). Setting the failure probability of FQI planning to be \( \delta_e/2H \) for each level \( h \in [H] \), and setting the planning error to \( \beta/8 \), we conclude that the total number of episodes used by Algorithm 3 for each timestep \( h \) is \( \hat{O} \left( \frac{H^4d^3K\log \left( \frac{|\Phi|}{n} \right)}{\beta^2} \right) \).

Using Lemma 9 in (21), we get:

\[
\mathbb{E}_{\pi} \left[ f(x_h, a_h) \right] \leq \frac{\alpha K^2}{2} \mathbb{E}_{\rho_{h-2}} \left[ \left( \left\langle \phi_{h-2}^*(x_{h-2}, a_{h-2}), \theta_g^* \right\rangle \right) \right] + \alpha K^2 \left\| w_g \right\|_{2}^2 + \frac{\alpha \beta K^2 \left\| w_g \right\|_{2}^2}{2} + \sqrt{\kappa K^5 \varepsilon_{\text{reg}}} \tag{24}
\]

\[
\leq \alpha K^2 \mathbb{E}_{\rho_{h-2}} \left[ \left( \left\langle \phi_{h-2}^*(x_{h-2}, a_{h-2}), \theta_g^* \right\rangle \right) \right] + \alpha K^3 \varepsilon_{\text{reg}} + \frac{K^2 T \beta}{2\alpha} + \frac{\alpha K^2 \left\| w_g \right\|_{2}^2}{2T} + \frac{\alpha \beta K^2 \left\| w_g \right\|_{2}^2}{2} + \sqrt{\kappa K^5 \varepsilon_{\text{reg}}} . \tag{25}
\]

The next inequality in (25) again uses the approximation guarantee for features \( \hat{\phi} \) in (18) along with the inequality \( (a + b)^2 \leq 2a^2 + 2b^2 \). Finally, we note that the inner product inside the expectation is always bounded between \([0, 1]\) which allows use to use the fact that \( f(x)^2 \leq f(x) \) for \( f : X \rightarrow [0, 1] \). Substituting the upper bound for \( \left\| w_g \right\|_{2} \), we get:

\[
\mathbb{E}_{\pi} \left[ f(x_h, a_h) \right] \leq \alpha K^2 \mathbb{E}_{\rho_{h-2}} \left[ \left( \left\langle \phi_{h-2}^*(x_{h-2}, a_{h-2}), \theta_g^* \right\rangle \right) \right] + \alpha K^3 \varepsilon_{\text{reg}} + \sqrt{\kappa K^5 \varepsilon_{\text{reg}}} + \frac{\beta K^2 T}{2\alpha} + \frac{\alpha \beta K^2 B^2}{2} + \frac{\alpha K^2 B^2}{2T} , \tag{26}
\]
The equality step (26) follows by the definition of the function \( g(\cdot) \).

We now set \( \kappa \geq 2\alpha K^2 \) in (26). Therefore, if we set the parameters \( \alpha, \beta, \varepsilon_{\text{reg}} \) such that

\[
\max \left\{ \alpha \kappa K^3 \varepsilon_{\text{reg}} + \sqrt{\frac{\beta K^2 T}{2\alpha}}, \frac{\alpha \beta K^2 B^2}{2}, \frac{\alpha K^2 B^2}{2T} \right\} \leq \eta_{\text{min}}/8,
\]

(26) can be re-written as:

\[
\max_{\pi} \mathbb{P}_{\pi} [z_{h+1} = z] \leq \frac{K}{2} \mathbb{P}_{\rho_{h-2}} [z_{h+1} = z] + \frac{\eta_{\text{min}}}{2} \leq \frac{\kappa}{2} \mathbb{P}_{\rho_{h-2}} [z_{h+1} = z]
\]

where in the last step, we use Assumption 1. Hence, we prove the exploration guarantee in Theorem 2 by induction.

To find the feasible values for the constants, we first note that \( T \leq 8d \log (1 + 8/\beta) / \beta \) (Lemma 15). We start by setting \( \beta K^2 T = \eta_{\text{min}}/8 \) which gives \( \alpha/T = 4\beta K^2 / \eta_{\text{min}} \). Using the upper bound on \( T \), we get

\[
\alpha \leq \frac{32d K^2 \log(1+8/\beta)}{\eta_{\text{min}}}.
\]

Next, we set the term \( \alpha \kappa K^3 \varepsilon_{\text{reg}} + \sqrt{\kappa K^5 \varepsilon_{\text{reg}}} \leq \eta_{\text{min}}/8 \). Using the value of \( \kappa = 2\alpha K^2 \) we get:

\[
2\alpha^2 K^5 \varepsilon_{\text{reg}} + \sqrt{2\alpha K^7 \varepsilon_{\text{reg}}} \leq \eta_{\text{min}}/8,
\]

which is satisfied by \( \varepsilon_{\text{reg}} = \Theta \left( \frac{\eta_{\text{min}}^3}{d^3 K^3 \log(1+8/\beta)} \right) \).

Lastly, we will consider the term \( \frac{\alpha \beta K^2 B^2}{2} \) and by setting it less than \( \eta_{\text{min}}/8 \), we get:

\[
\beta \log (1 + 8/\beta) \leq \frac{\eta_{\text{min}}^2}{128d B^2 K^4}.
\]

One can verify that under this condition we also have \( \frac{\alpha K^2 B^2}{2T} \leq \eta_{\text{min}}/8 \) and setting \( \beta = \tilde{O} \left( \frac{\eta_{\text{min}}^2}{d B^2 K^4} \right) \) satisfies the feasibility constraint for \( \beta \). Here, we assume that \( B \) only has a poly log dependence on \( \beta \) and show later that this is true for all our feature selection methods. Notably, the only cases when \( B \) depends on \( \beta \) in our results is when \( B = O \left( \frac{1}{\varepsilon_{\text{reg}}} \right) \) for a constant \( c = \{1/2, 1\} \) which has a log\(^2\)\((1 + 8/\beta)\) term.

Substituting the value of \( \kappa \) and \( \beta \) in Lemma 9 with an additional factor of \( H \) to account for all \( h \) gives us the final sample complexity bound in Theorem 2. Finally, the change of measure guarantee follows from the result in Lemma 8.

### A.2 Improved sample complexity bound for simplex features

We can obtain more refined results when the agent instead has access to a latent variable feature class \( \{\Psi_h\}_{h \in [H]} \) with \( \psi_h : \mathcal{X} \times \mathcal{A} \rightarrow \Delta(\mathcal{d}_{LV}) \). We call this the simplex features setting and show the improved results in this section. In order to achieve this improved result, we make two modifications to EXPLORE: 1) We use a smaller discriminator function class \( \mathcal{F}_{h+1} := \{ f(x_{h+1}, a_{h+1}) = \phi_{h+1}(x_{h+1}, a_{h+1})[i] : \phi_{h+1} \in \Phi_{h+1}, i \in [d_{LV}] \} \) and 2) in EXPLORE, instead of calling the planner with learnt features \( \phi_h \) and taking three uniform actions, we plan for the features \( \hat{\phi}_{h-1} \) and add two uniform actions to collect data for feature learning in timestep \( h \). The key idea here is that instead of estimating the expectation of any bounded function \( f \), we only need to focus on the expectation of coordinates of \( \phi^* \) as included in class \( \mathcal{F}_{h+1} \). Further, since \( \phi^*_{h+1}[i] \) is already a linear function of the feature \( \phi^*_{h+1} \), we take only one action at random at timestep \( h \).

**Theorem 10** (Exploration with simplex features). Fix \( \delta \in (0, 1) \). Consider an MDP \( \mathcal{M} \) which admits a low rank factorization with dimension \( d \) in Definition 1 and satisfies Assumption 1. If the features \( \phi_h \) learnt in
Algorithm 2 is:

\[ \beta \]

The value of \( \beta \) is chosen such that \( \log (1 + 8/\beta) \leq \frac{\eta^{2}_{\text{min}}}{128dK^{2}B^{2}} \).

The proof of the theorem follows:

Proof: For simplex features, the key observation is that for any latent state \( z \in Z_{h+1} \), the function \( f(x_h) \) is already a member of the discriminator function class \( \mathcal{F}_h := \{ f(x_h) = \mathbb{E}_{\text{unif}(A)} [\phi_h(x_h, a_h[i]) : \phi_h \in \Phi_h, i \in [d_{LV}]] \} \). Thus, when we rewrite the term \( \mathbb{E}_{\pi}[f(x_h, a_h)] \) as a linear function, we only need to backtrack one timestep to use the feature selection guarantee:

\[
\mathbb{E}_{\pi}[f(x_h, a_h)] \leq K \mathbb{E}_{\pi_{h-1}\text{unif}(A)} [f(x_h, a_h)]
= K \mathbb{E}_{\pi_{h-1}} [g(x_{h-1}, a_{h-1})]
\leq K \mathbb{E}_{\pi_{h-1}} [\langle \phi_{h-1}(x, a), w_q \rangle] + \sqrt{K^{3} \varepsilon_{\text{reg}}},
\]

where we define \( g(x_{h-1}, a_{h-1}) = \mathbb{E}_{\text{unif}(A)}[f(x_h, a_h)|x_{h-1}, a_{h-1}] \). Therefore, the new value of \( \kappa \) becomes \( 2\alpha K \) and by shaving off this \( K \) factor in the chain of inequalities, we get the following constraint set for the parameters:

\[
\max \left\{ \alpha K^{2} \varepsilon_{\text{reg}} + \sqrt{K^{3} \varepsilon_{\text{reg}}}, \frac{\beta KT}{2\alpha}, \frac{\alpha \beta K B^{2}}{2}, \frac{\alpha K B^{2}}{2T} \right\} \leq \eta_{\text{min}}/8.
\]

Thus, the values of these parameters for the simplex features case are as follows:

\[
\alpha = \frac{4\beta K}{\eta_{\text{min}}}, \quad T = \frac{1}{\alpha} \leq \frac{32dK \log(1 + 8/\beta)}{\eta_{\text{min}}}, \quad \varepsilon_{\text{reg}} = \Theta \left( \frac{\eta^{3}_{\text{min}}}{(d^{2}K^{5}\log^{2}(1 + 8/\beta)} \right).
\]

Hence, the updated constraint for \( \beta \) is:

\[
\beta \log (1 + 8/\beta) \leq \frac{\eta^{2}_{\text{min}}}{64dB^{2}K^{2}}.
\]

Other than the values for these parameters, the algorithm remains the same. Therefore, substituting the new values of \( \kappa \) and \( \beta \) in the expression \( \tilde{O} \left( \frac{H^{4}d^{4}K^{2}\log \left( \frac{\Phi}{\varepsilon_{\text{reg}}} \right)}{\beta^{2}} \right) \) as before, we get the improved sample complexity result.
B Proof of Theorem 3

We show that after obtaining the exploratory policies $\rho_{h-3}^3$ for all $h \in [H]$ using MOFFLE, we can collect a dataset $\mathcal{D}$ to learn a feature $\tilde{\phi}_h \in \Phi_h$ for all levels and use FQI to plan for any reward function $R \in \mathcal{R}$. Specifically, we use the sub-routine LEARNREP to compute a feature $\tilde{\phi}_h \in \Phi_h$ such that:

$$\max_{g \in \mathcal{G}_{h+1}} \min_{\|w\|_2 \leq B} \mathbb{E}_{\rho_{h-3}^3} \left[ \left( \langle \tilde{\phi}_h(x_h, a_h), w \rangle - \mathbb{E}[g(x_{h+1})|x_h, a_h] \right)^2 \right] \leq \varepsilon_{\text{apx}}, \quad (31)$$

where $\mathcal{G}_{h+1} \subset (\mathcal{X} \to [0, H])$ is the set of functions

$$g(x') = \text{clip}_{[0,H]} \left( \max_a \left( R(x', a) + \langle \tilde{\phi}_{h+1}(x', a), \theta \rangle \right) \right),$$

with $R \in \mathcal{R}, \tilde{\phi}_{h+1} \in \Phi_{h+1}, \|\theta\|_2 \leq B$ and $B \geq H\sqrt{d}$. Using $\tilde{\phi}_{0:H-1}$, we define the value function class $Q = \{Q_h(\tilde{\phi}, R)\}_{h=0}^{H-1}$ for any given reward $R \in \mathcal{R}$. For a level $h \in [H]$, $Q_h(\cdot)$ is defined as the set of following functions:

$$Q_h(x, a) = \text{clip}_{[0,H]} \left( R_h(x, a) + \langle \tilde{\phi}_h(x, a), w \rangle \right)$$

The learnt feature serves two purposes as discussed in the main text:

- (realizability) The optimal value function for any timestep $h + 1$ and reward $R_{h+1} \in \mathcal{R}$, is defined as $V^*_h(x) = \max_a \left( R_{h+1}(x', a) + \mathbb{E}[Q^*_h(x')|x', a] \right) = \max_a \left( R_{h+1}(x', a) + \langle \tilde{\phi}^*_h, \theta^*_h \rangle \right)$. Thus, we have realizability as $V^*_h \in \mathcal{G}_{h+1}$, which in turn implies that $\exists f \in Q_h$, s.t. $f \approx R_h + \mathbb{E}[V^*_h(\cdot)]$.

- (completeness) For completeness, note that $\mathcal{G}_{h+1}$ contains the Bellman backup of all possible $Q_{h+1}(\cdot)$ value functions we may encounter while running FQI with $Q$ as defined above. Therefore, for any such $Q_{h+1}$, we have that $\exists f \in Q_h$, s.t. $f \approx \mathcal{T}Q_{h+1}$.

Thus, the final sample complexity result for offline planning using FQI with value function class $Q(\tilde{\phi}, R)$ is as follows:

**Theorem (Restatement of Theorem 3).** If the features $\tilde{\phi}_h$ learnt by MOFFLE satisfy the condition in (7) for all $h$ with $\varepsilon_{\text{apx}} = \tilde{O} \left( \varepsilon^{2\eta_{\text{min}}} / dH^{2}K \right)$, then for any reward function $R \in \mathcal{R}$, running FQI with the value function class $Q(\tilde{\phi}, R)$ and an exploratory dataset $\mathcal{D}$, returns a policy $\hat{\pi}$ which satisfies $v^*_R \geq v^*_R - \varepsilon$ with probability at least $1 - \delta$. The total number of episodes collected by MOFFLE in line 5 are:

$$\tilde{O} \left( \frac{H^7d^2K^5 \log \left( \frac{|\mathcal{R}|R|B}{d^2\varepsilon} \right)}{\varepsilon^{2\eta_{\text{min}}} / dH^{2}K} \right).$$

**Proof.** We run FQI with the learnt representation $\tilde{\phi}_h$ using the value function class $Q_h(\tilde{\phi}_h, R_h)$ defined for each $h \in [H]$. Lemma 21 shows that when (31) is satisfied with an error $\varepsilon_{\text{apx}}$, running FQI using a total of $n_h = \tilde{O} \left( \frac{H^6dK \log \left( \frac{|\mathcal{R}|R|B}{d^2\varepsilon} \right)}{\beta^2} \right)$ episodes collected from each exploratory policy $\rho_{h-3}^3$ returns a policy $\hat{\pi}$ which satisfies:

$$\mathbb{E}_R \left[ \sum_{h=0}^{H-1} R_h(x_h, a_h) \right] \geq \max_{\pi} \mathbb{E}_R \left[ \sum_{h=0}^{H-1} R_h(x_h, a_h) \right] - \beta - 2H^2K\varepsilon_{\text{apx}}$$
with probability at least $1 - \delta'$. Then union bounding over all possible $\tilde{\phi}$, and setting $\delta = \delta'/|\Phi|$, $\beta = \varepsilon/2$, $\varepsilon_{apx} = \frac{\varepsilon^2}{16H^2K}$, we get the final planning result with a value error of $\varepsilon$ and probability at least $1 - \delta$.

Substituting $\kappa = \tilde{O}\left(\frac{32dK^4}{\eta_{\text{min}}}\right)$, we get $n_h = \tilde{O}\left(\frac{H^6d^2K^5\log\left(\frac{|\Phi||R|}{\varepsilon}\right)}{\varepsilon^2\eta_{\text{min}}}\right)$. The final sample complexity is thus $n = \tilde{O}\left(\frac{H^7d^2K^5\log\left(\frac{|\Phi||R|}{\varepsilon}\right)}{\varepsilon^2\eta_{\text{min}}}\right)$ where we sum up the collected episodes across all levels. \qed

C Proofs for oracle representation learning

In this section, we present the sample complexity result for MOFFLE when a computational oracle FLO is available. Since we need to set $B \geq L\sqrt{d}$ in the min-max-min objective ((9) and (8)), we assume FLO solves (8) with $B = L\sqrt{d}$. The computational oracle is defined as follows:

**Definition 3** (Minimax optimization oracle). Given a feature class $\Phi_h$ and an abstract discriminator class $V \subset (X \rightarrow [0, L])$, we define the minimax Feature Learning Oracle (FLO) as a subroutine that takes a dataset $D$ of tuples $(x_h, a_h, x_{h+1})$ and returns a solution to the following objective:

$$\hat{\phi}_h = \arg\min_{\phi \in \Phi_h} \max_{v \in V} \min_{w \in \{0, L\}} \mathbb{E}_{\text{unif}(A)} [R(x_{h+1}, a_{h+1} + \langle \phi_{h+1}(x_{h+1}, a_{h+1}), \theta \rangle)]$$

where $\phi_{h+1} \in \Phi_{h+1}$, $||\theta||_2 \leq L\sqrt{d}$, $R \in \mathcal{R}$ for any policy $\pi_{h+1}$ over $x_{h+1}$. Note that, $\mathcal{F}_h$ in the main text uses a singleton reward class $R(x_{h+1}, a_{h+1}) = 0$ with $L = 1$ and $\pi_{h+1} = \text{unif}(A)$. Similarly, $\mathcal{G}_h$ uses $L = H$ with $\pi_{h+1}$ as the greedy arg-max policy.

**Lemma 11** (Deviation bound for FLO). If the min-max feature learning objective is solved by the FLO for a sample of size $n$, then for $V \subset (X \rightarrow [0, L]) := \{v(x_{h+1}) = \text{clip}_{[0, L]}(\mathbb{E}_{\pi_{h+1} \sim \pi_{h+1}(x_{h+1})}[R(x_{h+1}, a_{h+1}) + \langle \phi_{h+1}(x_{h+1}, a_{h+1}), \theta \rangle]) : \phi_{h+1} \in \Phi_{h+1}, ||\theta||_2 \leq L\sqrt{d}, R \in \mathcal{R}\}$, with probability at least $1 - \delta$, we have:

$$\max_{v \in V} b_{\text{err}}(\hat{\rho}_{h=3}^{\text{FLO}}, \hat{\phi}_h, v; L\sqrt{d}) \leq \frac{512L^2d^2\log\left(\frac{2n|\Phi_h||\Phi_{h+1}||\mathcal{R}|}{\delta}\right)}{n}.$$ 

**Proof.** Firstly, note the term $b_{\text{err}}(\hat{\rho}_{h=3}^{\text{FLO}}, \hat{\phi}_h, v; L\sqrt{d})$ is a shorthand for

$$\min_{||w||_2 \leq L\sqrt{d}} \mathcal{L}_{\hat{\rho}_{h=3}^{\text{FLO}}} (\hat{\phi}_h, w, v) - \mathcal{L}_{\hat{\rho}_{h=3}^{\text{FLO}}} (\phi^*_v, \theta^*_v, v)$$

where $\theta^*_v = \arg\min_{||\theta||_2 \leq L\sqrt{d}} \mathcal{L}_{\hat{\rho}_{h=3}^{\text{FLO}}} (\phi^*_v, \theta, v)$.

Now, using the result in Lemma 23 from Appendix H and denoting $\mathcal{L}_{\hat{\rho}_{h=3}^{\text{FLO}}} (\cdot)$ as $\mathcal{L}(\cdot)$, with probability at least $1 - \delta$, we have:

$$|\mathcal{L}(\phi, w, v) - \mathcal{L}(\phi^*_v, \theta^*_v, v) - (\mathcal{L}_D(\phi, w, v) - \mathcal{L}_D(\phi^*_v, \theta^*_v, v))|$$

$$\leq \frac{1}{2} (\mathcal{L}(\phi, w, v) - \mathcal{L}(\phi^*_v, \theta^*_v, v)) + \frac{128L^2d^2\log\left(\frac{2n|\Phi_h||\Phi_{h+1}||\mathcal{R}|}{\delta}\right)}{n}.$$ 

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for all \( \|w\|_2 \leq L\sqrt{d} (B = L\sqrt{d}), \phi \in \Phi_h \) and \( v \in V \).

By the definition of FLO, for any \( v \in V \), we know that there exists \( \theta_v^* \) such that \((\phi^*, \theta_v^*)\) is the population minimizer \( \arg\min_{\phi \in \Phi_h, \|w\|_2 \leq L\sqrt{d}} \mathcal{L}(\phi, \hat{w}, v) \). Using this and the concentration result, for all \( v \in V \), with \((\hat{\phi}_v, \hat{w}_v)\) as the solution of the innermost min in (32), we have:

\[
\mathcal{L}_D(\phi^*, \theta_v^*, v) - \mathcal{L}_D(\hat{\phi}_v, \hat{w}_v, v) \leq \frac{3}{2} \left( \mathcal{L}(\hat{\phi}_v, \hat{w}_v, v) - \mathcal{L}(\hat{\phi}_v, \hat{w}_v, v) \right) + \frac{128L^2d^2 \log \left( \frac{2n|\Phi_h||\Phi_h+1||\mathcal{R}|}{\delta} \right)}{n}
\]

Now, for the oracle solution \( \hat{\phi} \), for all \( v \in V \), we have:

\[
\mathcal{L}_D(\hat{\phi}, \hat{w}_v, v) - \mathcal{L}_D(\hat{\phi}, \hat{w}_v, v)
\]

\[
= \mathcal{L}_D(\hat{\phi}, \hat{w}_v, v) - \mathcal{L}_D(\hat{\phi}, \hat{w}_v, v) + \mathcal{L}_D(\phi^*, \theta_v^*, v) - \mathcal{L}_D(\hat{\phi}, \hat{w}_v, v)
\]

\[
\geq \frac{1}{2} \left( \mathcal{L}(\hat{\phi}, \hat{w}_v, v) - \mathcal{L}(\phi^*, \theta_v^*, v) \right) - \frac{128L^2d^2 \log \left( \frac{2n|\Phi_h||\Phi_h+1||\mathcal{R}|}{\delta} \right)}{n}
\]

Combining the two chains of inequalities, we get:

\[
\mathcal{L}(\hat{\phi}, \hat{w}_v, v) - \mathcal{L}(\phi^*, \theta_v^*, v) \leq 2 \left( \mathcal{L}_D(\hat{\phi}, \hat{w}_v, v) - \mathcal{L}_D(\hat{\phi}, \hat{w}_v, v) \right) + \frac{256L^2d^2 \log \left( \frac{2n|\Phi_h||\Phi_h+1||\mathcal{R}|}{\delta} \right)}{n}
\]

\[
\leq 2 \max_{g \in V} \left( \mathcal{L}_D(\hat{\phi}, \hat{w}_g, v) - \mathcal{L}_D(\hat{\phi}, \hat{w}_g, v) \right) + \frac{256L^2d^2 \log \left( \frac{2n|\Phi_h||\Phi_h+1||\mathcal{R}|}{\delta} \right)}{n}
\]

\[
\leq \frac{512L^2d^2 \log \left( \frac{2n|\Phi_h||\Phi_h+1||\mathcal{R}|}{\delta} \right)}{n}
\]

Hence, we have proved the desired result.

Here, we explicitly give a result for the discriminator function classes used by MOFFLE. However, a similar result can be easily derived for a general discriminator class \( V \) with the dependence \( \log N \) where \( N \) is either the cardinality or an appropriate complexity measure of \( V \).

### C.1 Proof of Corollary 4

**Corollary** (Restatement of Corollary 4). Fix \( \delta \in (0, 1) \). If the LEARNREP sub-routine to learn features \( \hat{\phi}_h \) in Algorithm 2 and \( \hat{\phi}_h \) in Algorithm 1 is implemented using the oracle FLO, MOFFLE returns an exploratory dataset \( D \) such that for any \( R \in \mathcal{R} \), running FQI with value function class \( Q(\hat{\phi}, R) \) returns an \( \varepsilon \)-optimal policy with probability at least \( 1 - \delta \). The total number of episodes used by the algorithm are:

\[
\tilde{O} \left( \frac{H^6d^8K^{13} \log \left( \frac{|\Phi|}{\delta} \right)}{\eta_{\min}^3} + \frac{H^7d^3K^5 \log \left( \frac{|\Phi|R}{\delta} \right)}{\varepsilon^2 \eta_{\min}} \right)
\]

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Proof. In MOFFLE, we call the sub-routine LEARNREP twice for discriminator classes \( \mathcal{F} \) and \( \mathcal{G} \) with \( L = 1 \) and \( L = H \) respectively. Similarly, the error threshold given as input to LEARNREP are \( \varepsilon_{\text{reg}} \) and \( \varepsilon_{\text{apx}} \).

Firstly, we consider learning \( \hat{\phi}_h \) that satisfies (3) so that we can collect an exploratory dataset. Let \( \mathcal{R} = \{0\} \) and \( L = 1 \) (i.e. consider \( V = \mathcal{F} \)), for any level \( h \), applying Lemma 11, we know that if

\[
n \geq \frac{512d^2 \log \left( \frac{2n|\Phi_h||\Phi_{h+1}||\mathcal{R}|}{\delta/(3H)} \right)}{\varepsilon_{\text{reg}}},
\]

then condition (3) holds with probability at least \( 1 - \delta/(3H) \). Setting \( n_{\text{explore}} = \tilde{O} \left( \frac{d^2 \log (|\Phi_h||\Phi_{h+1}||\mathcal{R}|)}{\varepsilon_{\text{reg}}} \right) = \tilde{O} \left( \frac{d^4K^2 \log (|\Phi|)}{\eta_{\min}} \right) \) we get:

\[
n_{\text{explore}} = \tilde{O} \left( \frac{d^2 \log (|\Phi_h||\Phi_{h+1}||\mathcal{R}|)}{\varepsilon_{\text{reg}}} \right) = \tilde{O} \left( \frac{d^4K^2 \log (|\Phi|)}{\eta_{\min}} \right).
\]

Substituting the value \( B = \sqrt{d} \) in Theorem 2, we get the sample complexity for the elliptic planner as:

\[
n_{\text{fqi}} = \tilde{O} \left( \frac{H^5d^6K^{-13}B^4 \log \left( \frac{|\Phi|}{\delta} \right)}{\eta_{\min}^2} \right) = \tilde{O} \left( \frac{H^5d^6K^{-13} \log \left( \frac{|\Phi|}{\delta} \right)}{\eta_{\min}^2} \right).
\]

Then we consider learning \( \hat{\phi}_h \) that satisfies (7). Let \( L = H \) and consider original \( \mathcal{R} \) (i.e. consider \( V = \mathcal{G} \)). Similarly, for any level \( h \), setting \( \varepsilon_{\text{apx}} = \tilde{O} \left( \frac{\varepsilon_2 \eta_{\min}}{dH^8K^8} \right) \) and applying Lemma 11, we know that if

\[
n_{\text{learnrep}} = \tilde{O} \left( \frac{H^6d^2K^5 \log \left( \frac{|\Phi||\mathcal{R}|}{\delta/(3H)} \right)}{\varepsilon^2\eta_{\min}} \right),
\]

then condition (7) is satisfied with probability at least \( 1 - \delta/3H \).

Notice that (7) holds and we collect an exploratory dataset by applying Theorem 2. Then Theorem 3 implies the required sample complexity for offline FQI planning with \( \hat{\phi}_{0:H-1} \) to guarantee \( \varepsilon \) error with probability at least \( 1 - \delta/(3H) \) is:

\[
n_{\text{fqi}} = \tilde{O} \left( \frac{H^7d^2K^5 \log \left( \frac{|\Phi||\mathcal{R}|}{\delta} \right)}{\varepsilon^2\eta_{\min}} \right).
\]

Finally, union bounding over \( h \in [H] \), the final sample complexity is \( H(n_{\text{explore}} + n_{\text{learnrep}}) + n_{\text{fqi}} \). Reorganizing these terms completes the proof.

\[\square\]

**D Proofs for greedy representation learning method**

We again start by showing a sample complexity result for the feature learning (line 6) and witness computation (line 7) steps in Algorithm 5 for a general discriminator class. We will later use the result to show a feature selection guarantee for Algorithm 5 in Lemma 5.

**Lemma 12** (Deviation bounds for Algorithm 5). Let \( \bar{\varepsilon} = \frac{64d(B + L \sqrt{d})^2 \log \left( \frac{2n|\Phi_h||\Phi_{h+1}||\mathcal{R}|}{\delta} \right)}{2n} \). If Algorithm 5 is called with a dataset \( \mathcal{D} \) of size \( n \) and termination loss cutoff \( 3\varepsilon_1/2 + \bar{\varepsilon} \), then with probability at least
1 − δ, for all \( v \in \mathcal{V} \subset (\mathcal{X} \to [0, L]) := \{v(x_{h+1}) = \text{clip}_{[0,L]}(E_{a_{h+1} \sim \pi_{h+1}(x_{h+1})}[R(x_{h+1}, a_{h+1}) + \langle \phi_{h+1}(x_{h+1}, a_{h+1}) \rangle]) : \phi_{h+1} \in \Phi_{h+1}, \|\theta\|_2 \leq L \sqrt{d}, R \in \mathcal{R} \} \) and \( t \leq T \), we have:

\[
\sum_{i \leq t} E_{\rho_{h-3}^{t+1}} \left[ \left( \hat{\phi}_{t,h}(x_h, a_h)^\top w_{t,i} - \phi^*_h(x_h, a_h)^\top \theta^*_t \right)^2 \right] \leq t \bar{\varepsilon},
\]

\[
E_{\rho_{h-3}^{t+1}} \left[ \left( \hat{\phi}_{t,h}(x_h, a_h)^\top w - \phi^*_h(x_h, a_h)^\top \theta^*_t \right)^2 \right] \geq \varepsilon_1
\]

for all \( \|w\|_2 \leq B_t \) where \( w_{t,i} = \arg\min_{\|\tilde{w}\|_2 \leq B_t} \mathcal{L}_D(\hat{\phi}_{t,h}, \tilde{w}, v_i) \) and \( \theta^*_t = \arg\min_{\|\tilde{\theta}\|_2 \leq L \sqrt{d}} \mathcal{L}_D(\phi^*_h, \tilde{w}, v_i) \)

where \( B_t = \frac{L \sqrt{d}}{2} \) in Algorithm 5.

Further, at termination, the learnt feature \( \hat{\phi}_{T,h} \) satisfies:

\[
\max_{v \in \mathcal{V}} b_{\text{err}} \left( \rho_{h-3}^{t+3}, \hat{\phi}_{T,h}, v; B \right) \leq 3\varepsilon_1 + 4\bar{\varepsilon}.
\]

**Proof.** We again denote \( \mathcal{L}_{\rho_{h-3}^{t+3}}(\cdot) \) as \( \mathcal{L}(\cdot) \) and set \( \bar{\varepsilon} = \frac{64d(B + L \sqrt{d})^2 \log\left( \frac{2n||\rho_h||_{\Phi_{h+1}}}{} \right)}{n} \). Further, we remove the subscript \( h \) for simplicity unless not clear by context. We begin by using the result in Lemma 23 such that, with probability at least \( 1 - \delta \), for all \( \|w\|_2 \leq B \) (\( B \geq L \sqrt{d} \)), \( \phi \in \Phi_h \) and \( v \in \mathcal{V} \), we have

\[
|\mathcal{L}(\phi, w, v) - \mathcal{L}(\phi^*, \theta^*_v, v) - (\mathcal{L}_D(\phi, w, v) - \mathcal{L}_D(\phi^*, \theta^*_v, v))| \leq \frac{1}{2} (\mathcal{L}(\phi, w, v) - \mathcal{L}(\phi^*, \theta^*_v, v)) + \bar{\varepsilon}/2.
\]

Thus, for the feature fitting step in (10) in iteration \( t \), with probability at least \( 1 - \delta \) we have:

\[
\sum_{v_i \in \mathcal{V}} E \left[ \left( \hat{\phi}_t^\top w_{t,i} - \phi^* \theta^*_t \right)^2 \right] = \sum_{v_i \in \mathcal{V}} \left( \mathcal{L}(\hat{\phi}_t, w_{t,i}, v_i) - \mathcal{L}(\phi^*, \theta^*_t, v_i) \right) \leq \sum_{v_i \in \mathcal{V}} 2 \left( \mathcal{L}_D(\hat{\phi}_t, w_{t,i}, v_i) - \mathcal{L}_D(\phi^*, \theta^*_t, v_i) \right) + |\mathcal{V}| \bar{\varepsilon} \leq t \bar{\varepsilon},
\]

which means the first inequality in the lemma statement holds.

For the adversarial test function at iteration \( t \) with \( B_t \leq B \), let \( \tilde{w} := \arg\min_{\|\tilde{w}\|_2 \leq B} \mathcal{L}_D(\hat{\phi}_t, w, v_{t+1}) \). Using the same sample size for the adversarial test function at each non-terminal iteration with loss cutoff \( c \), for any vector \( w \in \mathbb{R}^d \) with \( \|w\|_2 \leq B_t \) we get:

\[
E \left[ \left( \hat{\phi}_t^\top w - \phi^* \theta^*_{t+1} \right)^2 \right] = \mathcal{L}(\hat{\phi}_t, w, v_{t+1}) - \mathcal{L}(\phi^*, \theta^*_{t+1}, v_{t+1}) \geq \frac{2}{3} \left( \mathcal{L}_D(\hat{\phi}_t, w, v_{t+1}) - \mathcal{L}_D(\phi^*, \theta^*_{t+1}, v_{t+1}) \right) - \frac{\varepsilon}{3} \geq \frac{2}{3} \left( \mathcal{L}_D(\hat{\phi}_t, \tilde{w}, v_{t+1}) - \mathcal{L}_D(\phi^*, \theta^*_{t+1}, v_{t+1}) \right) - \frac{\varepsilon}{3} \geq \frac{2c}{3} + \frac{2}{3} \left( \min_{\hat{\phi} \in \Phi_h, \|\tilde{w}\|_2 \leq L \sqrt{d}} \mathcal{L}_D(\hat{\phi}, \tilde{w}, v_{t+1}) - \mathcal{L}_D(\phi^*, \theta^*_{t+1}, v_{t+1}) \right) - \frac{\varepsilon}{3} \geq \frac{2c}{3} + \frac{1}{3} \left( \mathcal{L}(\hat{\phi}_{t+1}, \tilde{w}_{t+1}, v_{t+1}) - \mathcal{L}(\phi^*, \theta^*_{t+1}, v_{t+1}) \right) - \frac{2\varepsilon}{3} \geq \frac{2c}{3} - \frac{2\varepsilon}{3}.
\]
In the first inequality, we invoke Lemma 23 to move to empirical losses. In the third inequality, we add and subtract the ERM loss over \((\phi, w)\) pairs along with the fact that the termination condition is not satisfied for \(v_{t+1}\). In the next step, we again use Lemma 23 for the ERM pair \((\tilde{\phi}_{t+1}, \tilde{w}_{t+1})\) for \(v_{t+1}\).

Thus, if we set the cutoff \(c\) for test loss to \(3\varepsilon_1/2 + \tilde{\varepsilon}\), for a non-terminal iteration \(t\), for any \(w \in \mathbb{R}^d\) with \(\|w\|_2 \leq B_t\), we have:

\[
E \left[ \left( \phi_t^\top w - \phi_{*,*}^\top \theta_{t+1}^* \right)^2 \right] \geq \varepsilon_1,
\]

(33)

which implies the second inequality in the lemma statement holds.

At the same time, for the last iteration, for all \(v \in \mathcal{V}\), the feature \(\tilde{\phi}_T\) satisfies:

\[
\min_{\|w\|_2 \leq B} E \left[ \left( \tilde{\phi}_T^\top w - \phi_{*,*}^\top \theta_{*}^* \right)^2 \right] \leq 2 \left( \mathcal{L}_D(\tilde{\phi}_T, \tilde{w}_v, v) - \mathcal{L}_D(\phi_{*}, \theta_{*}, v) \right) + \tilde{\varepsilon} \\
\leq 2 \left( \mathcal{L}_D(\tilde{\phi}_T, \tilde{w}_v, v) - \mathcal{L}_D(\phi_{*}, \theta_{*}, v) \right) \leq 2 \left( \mathcal{L}_D(\tilde{\phi}_T, \tilde{w}_v, v) - \mathcal{L}_D(\tilde{\phi}_v, \tilde{w}_v, v) - \mathcal{L}_D(\tilde{\phi}_{*}, \tilde{w}_v, v) \right) + \tilde{\varepsilon} \\
\leq 2 \left( \mathcal{L}_D(\tilde{\phi}_T, \tilde{w}_v, v) - \mathcal{L}_D(\tilde{\phi}_{*}, \tilde{w}_v, v) \right) \leq 3\varepsilon_1 + 4\tilde{\varepsilon}.
\]

This gives us the third inequality in the lemma, thus completes the proof. 

\[\square\]

D.1 Proof of Lemma 5

**Lemma** (Restatement of Lemma 5). Fix \(\delta_1 \in (0, 1)\). If the greedy feature selection algorithm (Algorithm 5) is run with a sample \(\mathcal{D}\) of size \(n = \tilde{O}\left(\frac{L^6d^7\log\left(\frac{\max_{(x,a)\in\mathcal{X}}d_{\max}(a)}{\varepsilon_{\text{tol}}}/\|\theta\|_2}{\delta_1}\right)}{\varepsilon_{\text{tol}}}\right)\), then with \(B = \sqrt{\frac{13L^4d^6}{\varepsilon_{\text{tol}}}}\), it terminates after \(T = \frac{52L^2d^2}{\varepsilon_{\text{tol}}}\) iterations and returns a feature \(\tilde{\phi}_h\) such that for \(\mathcal{V} \subset (\mathcal{X} \to [0, L]) := \{v(x_{h+1}) = \text{clip}_{[0,L]}(E_{a_{h+1} \sim \pi_{h+1}(x_{h+1})}[R(x_{h+1}, a_{h+1}) + \langle \phi_{h+1}(x_{h+1}, a_{h+1}), \theta \rangle]) : \phi_{h+1} \in \Phi_{h+1}, \|\theta\|_2 \leq L\sqrt{d}, R \in \mathcal{R}\}\), we have:

\[
\max_{v \in \mathcal{V}} \text{b.err} \left( \rho_{h-3}^3 \tilde{\phi}_h, v; B \right) \leq \varepsilon_{\text{tol}}.
\]

**Proof.** For ease of notation, we will not use the subscript \(\rho_{h-3}^3\) in the expectations below \((\mathcal{L}(\cdot) := \mathcal{L}_{\rho_{h-3}^3}(\cdot))\). Similarly, we will use \(\phi_t\) to denote feature \(\phi_{t,h}(x, a_h)\) of iteration \(t\) and \((x', a')\) for \((x_{h+1}, a_{h+1})\) unless required by context. Further, for any iteration \(t\), let \(W_t = [w_{t,1} | w_{t,2} | \ldots | w_{t,t}] \in \mathbb{R}^{d \times t}\) be the matrix with columns \(w_{t,i}\) as the linear parameter \(w_{t,i} = \arg\min_{\|w\|_2 \leq L\sqrt{d}} \mathcal{L}_D(\tilde{\phi}_{t,h}, w, v_i)\). Similarly, let \(A_t = [\theta_t^1 | \theta_t^2 | \ldots | \theta_t^*]\).

In the proof, we assume that the total number of iterations \(T\) does not exceed \(\frac{52L^2d^2}{\varepsilon_{\text{tol}}}\) and set parameters accordingly. We later verify that this assumption holds. Further, let \(\tilde{\varepsilon} = \frac{\varepsilon_{\text{tol}}^2}{2704d^2}\) and \(\varepsilon_0 = T_{\max} \cdot \tilde{\varepsilon} = \varepsilon_{\text{tol}}/52d^3\).

To begin, based on the deviation bound in Lemma 12, we note that if the sample \(\mathcal{D}\) in Algorithm 5 is of size \(n = \tilde{O}\left(\frac{L^6d^7\log\left(\frac{\max_{(x,a)\in\mathcal{X}}d_{\max}(a)}{\varepsilon_{\text{tol}}}/\|\theta\|_2}{\delta_1}\right)}{\varepsilon_{\text{tol}}}\right)\) and the termination loss cutoff set to \(3\varepsilon_1/2 + \tilde{\varepsilon}\) such that, with probability at least \(1 - \delta_1\), for all non-terminal iterations \(t\) we have:

\[
\sum_{v_i \in \mathcal{V}} E \left[ \left( \phi_t^\top W_t^i - \phi_{*,*}^\top A_t^i \right)^2 \right] \leq t\tilde{\varepsilon} \leq \varepsilon_0,
\]

(34)

\[
E \left[ \left( \phi_t^\top w - \phi_{*,*}^\top \theta_{t+1}^* \right)^2 \right] \geq \varepsilon_1
\]

(35)

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where $\tilde{\varepsilon}$ is an error term dependent on the size of $D$ and $w$ is any vector with $\|w\|_2 \leq B_1 \leq B$. Further, when the algorithm does terminate, we get the loss upper bound to be $3\varepsilon+4\tilde{\varepsilon}$.

Using (34) and (35), we will now show that the maximum iterations in Algorithm 5 is bounded. At round $t$, for functions $v_1, \ldots, v_t \in \mathcal{V}$ in Algorithm 5, let $\theta^*_i = \theta^*_{v_i}$ as before and further let $\Sigma_t = A_t A_t^\top + \lambda I_{d \times d}$. Using the linear parameter $\theta^*_t$ of the adversarial test function $v_{t+1}$, define $\hat{w}_t = W_t A_t^\top \Sigma_t^{-1} \theta^*_{t+1}$. For this $\hat{w}_t$, we can bound its norm as:

$$
\|W_t A_t^\top \Sigma_t^{-1} \theta^*_{t+1}\|_2 \leq \|W_t\|_2 \|A_t^\top \Sigma_t^{-1}\|_2 \|\theta^*_{t+1}\|_2 \leq L^2 d \sqrt{\frac{t}{4\lambda}}.
$$

Here, $\|W_t\|_2 \leq L \sqrt{dt}$, $\|\theta^*_{t+1}\|_2 \leq L \sqrt{d}$, and $\|A_t^\top \Sigma_t^{-1}\|_2$ can be shown to be less than $\sqrt{1/4\lambda}$. Setting $B_t = L^2 d \sqrt{\frac{t}{4\lambda}}$, from (35), we have

$$
\varepsilon_1 \leq \mathbb{E} \left[ (\hat{\phi}_t^\top \hat{w}_t - \phi^*_{v_t} \theta^*_{t+1})^2 \right] = \mathbb{E} \left[ (\hat{\phi}_t^\top W_t A_t^\top \Sigma_t^{-1} \theta^*_{t+1} - \phi^*_{v_t} \Sigma_t^{-1} \theta^*_{t+1})^2 \right]
$$

$$
\leq \|\Sigma_t^{-1} \theta^*_{t+1}\|_2^2 \cdot \mathbb{E} \left[ \|\hat{\phi}_t^\top W_t A_t^\top - \phi^*_{v_t} \Sigma_t\|_2^2 \right]
$$

$$
\leq 2 \|\Sigma_t^{-1} \theta^*_{t+1}\|_2^2 \cdot \mathbb{E} \left[ \|\hat{\phi}_t^\top W_t A_t^\top - \phi^*_{v_t} A_t^\top\|^2 + \lambda^2 \|\phi^*_{v_t}\|^2_2 \right]
$$

$$
\leq 2 \|\Sigma_t^{-1} \theta^*_{t+1}\|_2^2 \cdot \left( \sigma^2(A_t) \mathbb{E} \left[ \|\hat{\phi}_t^\top W_t - \phi^*_{v_t} A_t\|^2_2 \right] + \lambda^2 \right)
$$

$$
\leq 2 \|\Sigma_t^{-1} \theta^*_{t+1}\|_2^2 \cdot \left( L^2 dt \varepsilon_0 + \lambda^2 \right).
$$

The second inequality uses Cauchy-Schwarz. The last inequality applies the upper bound $\sigma_1(A_t) \leq L \sqrt{dt}$ and the guarantee from (34). Using the fact that $t \leq T$, this implies that

$$
\|\Sigma_t^{-1} \theta^*_{t+1}\|_2 \geq \sqrt{\frac{\varepsilon_1}{2(L^2 dt \varepsilon_0 + \lambda^2)}}.
$$

We now use the generalized elliptic potential lemma from Carpentier et al. (2020) to upper bound the total value of $\|\Sigma_t^{-1} \theta^*_{t+1}\|_2$. From Lemma 24 in Appendix H.3, if $\lambda \geq L^2 d$ and we do not terminate in $T$ rounds, then

$$
T \sqrt{\frac{\varepsilon_1}{2(L^2 dt \varepsilon_0 + \lambda^2)}} \leq \sum_{t=1}^{T} \|\Sigma_t^{-1} \theta^*_{t+1}\|_2 \leq 2 \sqrt{T \frac{d}{\lambda}}.
$$

From this chain of inequalities, we can deduce

$$
T \varepsilon_1 \leq 8(d/\lambda) \left( L^2 dt \varepsilon_0 + \lambda^2 \right),
$$

therefore

$$
T \leq \frac{8d\lambda}{\varepsilon_1 - 8L^2 d^2 \varepsilon_0 / \lambda}.
$$

Now, if we set $\varepsilon_1 = 16L^2 d^2 \varepsilon_0 / \lambda$ in the above inequality, we can deduce that

$$
T \leq \frac{\lambda^2}{L^2 d \varepsilon_0}.
$$

---

3Applying SVD decomposition and the property of matrix norm, $\|A_t^\top \Sigma_t^{-1}\|_2$ can be upper bounded by $\max_{i \leq d} \sqrt{\lambda_i} \leq \frac{\sqrt{\lambda}}{\sqrt{4\lambda}}$ where $\lambda_i$ are the eigenvalues of $A_t A_t^\top$ and the final inequality holds by AM-GM.
Putting everything together, for input parameter $\varepsilon_{\text{tol}}$, the termination threshold for the loss $l$ is set such that $\frac{48L^2d^2\varepsilon_0}{\lambda} + \frac{4L^2d\varepsilon_0^2}{\lambda^2} \leq \varepsilon_{\text{tol}}$ which is satisfied for $\varepsilon_0 = \frac{\lambda\varepsilon_{\text{tol}}}{52L^2d^2}$. In addition, with $\lambda = L^2d$, we set the constants for Algorithm 5 as follows:

$$T \leq \frac{52L^2d^2}{\varepsilon_{\text{tol}}}, \quad B_t := \sqrt{\frac{L^2dt}{4}}, \quad B := \sqrt{\frac{13L^4d^3}{\varepsilon_{\text{tol}}}}.$$ 

Further, for Lemma 12, we set $\tilde{\varepsilon}$ to $\varepsilon_0/T = O\left(\frac{\varepsilon_0}{L^2d^2}\right)$.

### D.2 Proof of Corollary 6

**Corollary** (Restatement of Corollary 6). Fix $\delta \in (0, 1)$. If the LEARNREP sub-routine to learn features $\hat{\phi}_h$ in Algorithm 2 and $\hat{\phi}_h$ in Algorithm 1 is implemented using the oracle FLO, MOFFLE returns an exploratory dataset $D$ such that for any $R \in \mathcal{R}$, running FQI with value function class $Q(\hat{\phi}, R)$ returns an $\varepsilon$-optimal policy with probability at least $1 - \delta$. The total number of episodes used by the algorithm are:

$$\tilde{O}\left(\frac{H^6d^{16}K^{31}\log\left(\frac{\Phi}{\delta}\right)}{\eta_{\min}^1} + \frac{H^{19}d^{10}K^{15}\log\left(\frac{\Phi||R||}{\delta}\right)}{\varepsilon^2\eta_{\min}^3}\right).$$

**Proof.** In MOFFLE, we call the sub-routine LEARNREP twice for discriminator classes $\mathcal{F}$ and $\mathcal{G}$ with $L = 1$ and $L = H$ respectively. Similarly, the error threshold given as input to LEARNREP are $\varepsilon_{\text{reg}}$ and $\varepsilon_{\text{apx}}$. Using the result in Lemma 5, we know that for an approximation error of $\varepsilon_{\text{tol}}$, we need to set the sample size in Algorithm 5 to $n = \tilde{O}\left(\frac{L^6d^7\log\left(\frac{\Phi||R||}{\delta}\right)}{\varepsilon_{\text{tol}}^2}\right)$.

Setting the values of the parameter $\varepsilon_{\text{tol}} = \varepsilon_{\text{reg}} = \tilde{O}\left(\frac{\eta_{\min}^1}{d^2K^9\log(1 + 8/\beta)}\right)$ from Theorem 2 with $|\mathcal{R}| = 1$ and $L = 1$, we get the number of episodes per $h \in [H]$ for learning $\phi_h$ that satisfies (3) as:

$$n_{\text{explore}} = \tilde{O}\left(\frac{L^6d^7\log\left(\frac{\Phi||R||}{\delta}\right)}{\varepsilon_{\text{reg}}^3}\right) = \tilde{O}\left(\frac{d^3K^{27}\log\left(\frac{\Phi}{\delta}\right)}{\eta_{\min}^5}\right).$$

Substituting the value $B = \sqrt{\frac{13L^4d}{\varepsilon_{\text{reg}}}}$ in Theorem 2, we get the sample complexity for the elliptic planner as:

$$n_{\text{fqi}_1} = \tilde{O}\left(\frac{H^5d^6K^{13}B^4\log\left(\frac{\Phi}{\delta}\right)}{\eta_{\min}^5}\right) = \tilde{O}\left(\frac{H^5d^{16}K^{31}\log\left(\frac{\Phi}{\delta}\right)}{\eta_{\min}^1}\right).$$

Similarly, for learning $\tilde{\phi}_h$ that satisfies (7), we set $\varepsilon_{\text{tol}} = \varepsilon_{\text{apx}} = \tilde{O}\left(\frac{\varepsilon_{\text{min}}^2}{d^{11}H^{14}K^7}\right)$. Then, applying Lemma 12 with $L = H$, we get the number of episodes per $h \in [H]$ for learning $\phi_h$ as:

$$n_{\text{learnrep}} = \tilde{O}\left(\frac{L^6d^7\log\left(\frac{\Phi||R||}{\delta}\right)}{\varepsilon_{\text{apx}}^3}\right) = \tilde{O}\left(\frac{H^{18}d^{10}K^{15}\log\left(\frac{\Phi||R||}{\delta}\right)}{\varepsilon^6\eta_{\min}^3}\right).$$

Notice that (7) holds and we collect an exploratory dataset by applying Theorem 2. Then Theorem 3 implies the required sample complexity for offline FQI planning with $\tilde{\phi}_{0:H-1}$ is

$$n_{\text{fqi}_2} = \tilde{O}\left(\frac{H^7d^2K^5\log\left(\frac{\Phi||R||}{\delta}\right)}{\varepsilon^2\eta_{\min}^3}\right).$$
The final result in the theorem statement is obtained by setting the bound to $H(n_{\text{explore}} + n_{\text{learnrep}}) + n_{\text{fqi}} + n_{\text{fqi}^2}$.

E Results for enumerable representation class

We first derive the ridge regression based reduction of the min-max-min objective to eigenvector computation problems. For the enumerable feature class, we solve the modified objective in (13) for Algorithm 2:

$$
\min_{\phi \in \Phi_h} \max_{f \in \mathcal{F}_{h+1}} \left\{ \min_{\tilde{\phi} \in \Phi_h} \mathcal{L}_D(\phi, w, f) - \mathcal{L}_D(\tilde{\phi}, \tilde{w}, f) \right\}
$$

where $\mathcal{F}_{h+1}$ is now the discriminator class that contains all unclipped functions $f$ in form of:

$$
f(x_{h+1}) = \mathbb{E}_{\text{unif}(A)}[\langle \phi_{h+1}(x_{h+1}, a), \theta \rangle], \text{ for } \phi_{h+1} \in \Phi_{h+1}, \|\theta\|_2 \leq \sqrt{d}.
$$

Consider the min-max-min objective where we fix $\phi, \tilde{\phi} \in \Phi_h$. Rewriting the objective for a sample of size $n$, we get the following updated objective:

$$
\max_{f \in \mathcal{F}_{h+1}} \min_{\|w\|_2 \leq \sqrt{d}} \|Xw - f(D)\|_2^2 - \min_{\|\tilde{w}\|_2 \leq \sqrt{d}} \|\tilde{X}\tilde{w} - f(D)\|_2^2
$$

where $X, \tilde{X} \in \mathbb{R}^{n \times d}$ are the covariate matrices for features $\phi$ and $\tilde{\phi}$ respectively. We overload the notation and use $f(D) \in \mathbb{R}^n$ to denote the value of any $f \in \mathcal{F}$ on the $n$ samples. Now, instead of solving the constrained least squares problem, we use a ridge regression solution with regularization parameter $\lambda$. Thus, for any target $f$ in the min-max objective, for feature $\phi$, we get:

$$
w_f = \left( \frac{1}{n} X^\top X + \lambda I_{d \times d} \right)^{-1} \left( \frac{1}{n} X^\top f(D) \right)
$$

$$
\|Xw - f(D)\|_2^2 = \|X \left( \frac{1}{n} X^\top X + \lambda I_{d \times d} \right)^{-1} \left( \frac{1}{n} X^\top f(D) \right) - f(D)\|_2^2 = \|A(\phi)f(D)\|_2^2
$$

where $A(\phi) = I_{d \times d} - X \left( \frac{1}{n} X^\top X + \lambda I_{d \times d} \right)^{-1} \left( \frac{1}{n} X^\top \right)$. In addition, any regression target $f$ can be rewritten as $f = X'\theta$ for a feature $\phi' \in \Phi_{h+1}$ and $\|\theta\|_2 \leq \sqrt{d}$. Thus, for a fixed $\phi'$, $\phi$ and $\tilde{\phi}$, the maximization problem for $\mathcal{F}_{h+1}$ is the same as:

$$
\max_{\|\theta\|_2 \leq \sqrt{d}} \theta^\top X'^\top \left( A(\phi)^\top A(\phi) - A(\phi)^\top A(\phi') \right) X'\theta.
$$

(36)

where $X' \in \mathbb{R}^{n \times d}$ is again the sample matrix defined using $\phi' \in \Phi_{h+1}$. For each tuple of $(\phi, \tilde{\phi}, \phi')$, the maximization problem reduces to an eigenvector computation. As a result, we can efficiently solve the min-max-min objective in (13) by enumerating over each candidate feature in $(\phi, \tilde{\phi}, \phi')$ to solve

$$
\min_{\phi \in \Phi_h} \max_{\tilde{\phi} \in \Phi_h} \max_{\phi' \in \Phi_{h+1}} \min_{\|\theta\|_2 \leq \sqrt{d}} \theta^\top X'^\top \left( A(\phi)^\top A(\phi) - A(\phi)^\top A(\phi') \right) X'\theta.
$$

We now show that using the ridge estimator for an enumerable feature class, discriminator class $\mathcal{F}_{h+1}$ and an appropriately set value of $\lambda$ still allows us to establish a feature approximation result similar to FLO and greedy feature selection:
Lemma 13. For the features selected via the ridge estimator, with \( \lambda = \hat{\Theta} \left( \frac{1}{n^{1/3}} \right) \) for any function \( f \in \mathcal{F}_{h+1} \), with probability at least \( 1 - \delta \), we have:

\[
\max_{f \in \mathcal{F}_{h+1}} \mathcal{L}^{\phi_{h-3}}_{\hat{\phi}_{h-3}} (\hat{\phi}, \hat{w}_f, f) - \mathcal{L}^{\phi_{h-3}}_{\phi_{h-3}} (\phi_h^*, \theta_f^*, f) \leq \hat{O} \left( d^2 \log \left( \frac{2n|\Phi_h||\Phi_{h+1}|}{\delta n^{1/3}} \right) \right)
\]

where the discriminator function class \( \mathcal{F}_{h+1} \) is defined in (14).

Proof. We again denote \( \mathcal{L}^{\phi_{h-3}}_{\hat{\phi}_{h-3}} (\cdot) \) as \( \mathcal{L}(\cdot) \), \( \mathcal{F}_{h+1} \) as \( \mathcal{F} \). Firstly, as the discriminator function class \( \mathcal{F} \) is defined without clipping, we now have: \( \mathbb{E}[f(x')|x, a] = \langle \phi^*(x, a), \theta_f^* \rangle \) with \( \|\theta_f^*\|_2 \leq d \). Also, the scale of the ridge estimator \( \hat{w}_f = (\frac{1}{n} X^\top X + \lambda I_{d \times d})^{-1} (\frac{1}{n} X^\top f) \) now scales as \( \frac{1}{\lambda} \). Now, similar to Lemma 23, for all \( \phi \in \Phi_h \), \( \|w\|_2 \leq 1/\lambda \) and \( f \in \mathcal{F} \), we have:

\[
|\mathcal{L}(\phi, w, f) - \mathcal{L}(\phi^*, \theta_f^*, f) - (\mathcal{L}_D(\phi, w, f) - \mathcal{L}_D(\phi^*, \theta_f^*, f))| \\
\leq \frac{1}{2} (\mathcal{L}(\phi, w, f) - \mathcal{L}(\phi^*, \theta_f^*, f)) + 32d(1/\lambda + d)^2 \log \left( \frac{2n|\Phi_h||\Phi_{h+1}|}{\delta n} \right) \frac{2|\Phi_h||\Phi_{h+1}|}{n}.
\]

Now, let \( w_f^* \) denote the population ridge regression estimator for target \( f \in \mathcal{F} \) for features \( \phi^* \). Assume \( \lambda \leq 1/d \), which upper bounds the second term in the rhs above as \( \gamma := \frac{128d \log \left( \frac{2n|\Phi_h||\Phi_{h+1}|}{\lambda n} \right)}{\lambda^2 n} \). For the selected feature \( \hat{\phi} \), we have:

\[
\mathcal{L}_D(\hat{\phi}, \hat{w}_f, f) - \mathcal{L}_D(\hat{\phi}_f, \hat{w}_f, f) = \mathcal{L}_D(\hat{\phi}, \hat{w}_f, f) - \mathcal{L}_D(\hat{\phi}_f, \hat{w}_f, f) \leq \mathcal{L}_D(\hat{\phi}_f, \hat{w}_f, f) \leq \mathcal{L}_D(\hat{\phi}_f, \hat{w}_f, f) - \gamma
\]

Thus, with the feature selection output, we have:

\[
\mathcal{L}(\hat{\phi}, \hat{w}_f, f) \leq \mathcal{L}(\phi^*, \theta_f^*, f) \leq 2 \left( \mathcal{L}_D(\hat{\phi}, \hat{w}_f, f) - \mathcal{L}_D(\hat{\phi}_f, \hat{w}_f, f) \right) + 2 \left( \mathcal{L}_D(\phi^*, w_f^*, f) - \mathcal{L}_D(\phi^*, \theta_f^*, f) \right) + 2\gamma
\]

The third inequality uses the fact that \( \hat{\phi} \) is the solution of the ridge-regression based feature selection objective. Further, in all steps, we repeatedly apply the deviation bound from Lemma 23 to move from \( \mathcal{L}_D(\cdot) \) to \( \mathcal{L}(\cdot) \).
Now, for ridge regression estimate \( w^*_g \), we can bound the bias term on the rhs as follows:

\[
\mathcal{L}(\phi^*, w^*_g, g) - \mathcal{L}(\phi^*, \theta^*_g, g) = \mathbb{E} \left[ \left( \langle \phi^*, w^*_g \rangle - \langle \phi^*, \theta^*_g \rangle \right)^2 \right]
\]

\[
= \|w^*_g - \theta^*_g\|^2 = \sum_{i=1}^{d} \lambda_i \left( \langle v_i, w^*_g - \theta^*_g \rangle \right)^2
\]

\[
= \sum_{i=1}^{d} \lambda_i \left( \frac{\lambda_i}{\lambda + \lambda_i} \langle v_i, \theta^*_g \rangle - \langle v_i, \theta^*_g \rangle \right)^2
\]

\[
= \sum_{i=1}^{d} \frac{\lambda_i \lambda^2 \langle v_i, \theta^*_g \rangle^2}{(\lambda_i + \lambda)^2} \leq \frac{\lambda}{4} \|\theta^*_g\|^2 \leq \lambda \frac{d^2}{4},
\]

where \((\lambda_i, v_i)\) denote the \(i\)-th eigenvalue-eigenvector pair of the population covariance matrix \(\Sigma^*\) for feature \(\phi^*\). In the derivation above, we use the fact that \(w^*_g = (\Sigma + \lambda I)^{-1}[\phi^* g] = \frac{\lambda}{\lambda + \lambda_i} \langle v_i, \theta^*_g \rangle\). Therefore, the final deviation bound for \(\hat{\phi}\) is:

\[
\mathcal{L}(\hat{\phi}, \hat{w}_f, f) - \mathcal{L}(\phi^*, \theta^*_f, f) \leq \frac{3 \lambda d^2}{2} + \frac{1024 \log \left( \frac{2 \|\phi_h\|_{\Phi_{k+1}}}{\delta} \right)}{\lambda^2 n}.
\]

Thus, setting \(\lambda = \tilde{O} \left( \frac{1}{n^{1/3}} \right)\) gives the final result. \(\square\)

### E.1 Sample complexity of MOFFLE for enumerable feature class

Now that we have a feature selection guarantee assumed by the analysis of MOFFLE in Appendix A, we show an overall sample complexity result for this version of MOFFLE as follows:

**Corollary 14.** Fix \(\delta \in (0, 1)\). In Algorithm 2, if \(\phi_h\) is learned using the eigenvector formulation (16), then MOFFLE returns an exploratory dataset \(D\) such that for any \(R \in \mathcal{R}\), running FQI using the full representation class \(\Phi\) returns an \(\epsilon\)-optimal policy with probability at least \(1 - \delta\). The total number of episodes used by the algorithm are

\[
O \left( \frac{H^6 d^{22} K^{49} \log^5 \left( \frac{\|\Phi\|}{\delta} \right)}{\eta_{\min}^{17}} + \frac{H^7 d^3 K^3 \log \left( \frac{\|\Phi\|}{\delta} \right)}{\epsilon^2 \eta_{\min}} \right).
\]

**Proof.** In MOFFLE, we now use the eigenvector formulation for discriminator class \(\mathcal{F}\) with the error threshold \(\epsilon_{\text{reg}}\). Setting the values of the parameter \(\epsilon_{\text{reg}} = \tilde{\Theta} \left( \frac{\eta_{\min}^9}{d^2 K^3 \log^2 (1 + 8/\beta)} \right)\) from Theorem 2 and the deviation bound in Lemma 13, we get the number of episodes per \(h \in [H]\) for learning \(\phi_h\) as:

\[
n_{\text{explore}} = \tilde{O} \left( \frac{d^6 \log^3 \left( \frac{\|\Phi_h\|_{\Phi_{k+1}}}{{\delta}} \right)}{\epsilon_{\text{reg}}^3} \right) = \tilde{O} \left( \frac{d^12 K^{27} \log^3 \left( \frac{\|\Phi\|}{{\delta}} \right)}{\eta_{\min}^9} \right).
\]

Now, substituting the value \(B = 1/\lambda = \tilde{\Theta} \left( n_{\text{explore}}^{1/3} \right)\) in Theorem 2, we get the sample complexity for the elliptic planner as:

\[
n_{\text{ell}} = \tilde{O} \left( \frac{H^5 d^6 K^{13} B^4 \log \left( \frac{\|\Phi\|}{{\delta}} \right)}{\eta_{\min}^{12}} \right) = \tilde{O} \left( \frac{H^5 d^{22} K^{49} \log^5 \left( \frac{\|\Phi\|}{{\delta}} \right)}{\eta_{\min}^{17}} \right).
\]

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Finally, using Corollary 17 from Appendix G.2, the number of episodes collected for running FQI with the full representation class $\Phi$ can be bounded by:

$$n_{fqi} = \tilde{O}\left( \frac{H^6d^2K \log \left( \frac{\|\mathcal{R}\|}{\delta} \right)}{\varepsilon^2} \right) = \tilde{O}\left( \frac{H^6d^2K^3 \log \left( \frac{\|\mathcal{R}\|}{\delta} \right)}{\varepsilon^2\eta_{\min}} \right).$$

The final result in the theorem statement is obtained by setting the bound to $H(n_{\text{explore}} + n_{\text{learnrep}}) + n_{fqi}$. □

## F The analysis of FQI based elliptical planner

In this section, we show the iteration complexity and the estimation guarantee for FQI based elliptical planner (Algorithm 3). The analysis follows the similar approach as Agarwal et al. (2020b), while major difference here is that we apply FQI for policy optimization step.

**Lemma 15** (Estimation and iteration guarantees for Algorithm 3). If Algorithm 3 is run with a dataset of size $O\left( \text{poly}\left( d, H, K, T, 1/\eta_{\min}, \log |\Phi|, 1/\beta, \log(1/\delta) \right) \right)$ for a fix $\beta > 0, \delta \in (0, 1)$, then upon termination, it outputs a matrix $\Gamma_T$ and a policy $\rho$ that with probability at least $1 - \delta$:

$$\forall \pi : \mathbb{E}_{\pi} \left[ \hat{\phi}_{\tilde{H}^{-1}}(x_{\tilde{H}^{-1}}, a_{\tilde{H}^{-1}})^\top (\Gamma_T)^{-1} \hat{\phi}_{\tilde{H}^{-1}}(x_{\tilde{H}^{-1}}, a_{\tilde{H}^{-1}}) \right] \leq O(\beta),$$

$$\left\| \frac{\Gamma_T}{T} - \left( \mathbb{E}_\rho \left[ \hat{\phi}_{\tilde{H}^{-1}}(x_{\tilde{H}^{-1}}, a_{\tilde{H}^{-1}}) \hat{\phi}_{\tilde{H}^{-1}}(x_{\tilde{H}^{-1}}, a_{\tilde{H}^{-1}})^\top \right] + \frac{I_{d \times d}}{T} \right) \right\|_{\text{op}} \leq O(\beta/d).$$

Further, the iteration complexity is also bounded $T \leq \frac{8d}{\beta} \log \left( 1 + \frac{8}{\beta} \right)$.

**Proof.** Since the policy optimization step (Algorithm 6) is performed via an application of Lemma 19, we can find an $\beta/8$-suboptimal policy $\pi_t$ for the reward function induced by $\Gamma_{t-1}$. Then we use the sampling subroutine to estimate the value of this policy, which we denote $\hat{V}_t(\pi_t)$. As before, we terminate if $\hat{V}_t(\pi_t) \leq 3\beta/4$. If we terminate in round $t$, we output $\rho = \text{unif}\left( \{\pi_i\}_{i=1}^{t-1} \right)$ and we also output $\Gamma_t$. 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 $\Gamma_{t-1}$. We also denote the (element-wise) expectation of matrix $\hat{\Sigma}_{\pi_t}$ as $\bar{\Sigma}_{\pi_t}$.

With $O\left( \text{poly}\left( d, H, K, T, 1/\eta_{\min}, \log |\Phi|, 1/\beta, \log(1/\delta) \right) \right)$ sample complexity, we can show that with probability at least $1 - \delta$

$$\max_{t \in [T]} \max \left\{ d \cdot \left\| \hat{\Sigma}_{\pi_t} - \bar{\Sigma}_{\pi_t} \right\|_{\text{op}}, \left| \hat{V}_t(\pi_t) - V_t(\pi_t) \right|, \max_{\pi} V_t(\pi) - V_t(\pi_t) \right\} \leq \beta/8. \quad (37)$$

The first two bounds are obtained via standard concentration argument. The third one is proved by applying Lemma 19.

The accuracy guarantee for the covariance matrix $\Gamma_T$ is straightforward, since each $\hat{\Sigma}_{\pi_t}$ is $\tilde{O}(\beta/d)$ accurate and $\frac{\Gamma_T}{T} - \frac{I_{d \times d}}{T}$ is the average of such matrices.

Then, we turn to the iteration complexity. Now, if we terminate in iteration $t$, we know that $\hat{V}_t(\pi_t) \leq 3\beta/4$. This implies

$$\max_{\pi} V_t(\pi) \leq V_t(\pi_t) + \beta/8 \leq \hat{V}_t(\pi_t) + \beta/4 \leq \beta.$$
Similarly to the above inequality, we have

\[
T \left(3\beta/4 - \beta/4\right) \leq \sum_{t=1}^{T} \hat{V}_t(\pi_t) - \beta/4 \leq \sum_{t=1}^{T} V_t(\pi_t) - \beta/8 \\
= \sum_{t=1}^{T} \mathbb{E} \left[ \hat{\phi}^T_t \Gamma_{t-1}^{-1} \hat{\phi}_t \mid \pi_t \right] - \beta/8 = \sum_{t=1}^{T} \text{tr}(\Sigma_{\pi_t} \Gamma_{t-1}^{-1}) - \beta/8 \\
\leq \sum_{t=1}^{T} \text{tr}(\Sigma_{\pi_t} \Gamma_{t-1}^{-1}) \leq 2d \log \left(1 + \frac{T}{d}\right).
\]

In the last step, we apply elliptical potential lemma (e.g. Lemma 26 of Agarwal et al. (2020b)). Reorganizing the equation yields

\[
T \leq \frac{4d}{\beta} \log \left(1 + \frac{T}{d}\right). \quad \text{Further, if } T \leq \frac{8d}{\beta} \log \left(1 + \frac{8}{\beta}\right), \text{ then we have}
\]

\[
T \leq \frac{4d}{\beta} \log \left(1 + \frac{T}{d}\right) \leq \frac{4d}{\beta} \log \left(1 + \frac{8 \log \left(1 + \frac{8}{\beta}\right)}{\beta}\right) \leq \frac{4d}{\beta} \log \left(1 + \left(\frac{8}{\beta}\right)^2\right) \leq \frac{8d}{\beta} \log \left(1 + \frac{8}{\beta}\right).
\]

Therefore, we obtain an upper bound on \( T \) by this set and guess approach.

\[\square\]

G FQI planning results

In this section, we provide various FQI (Fitted Q-iteration) planning results. In Appendix G.1, we provide the general framework of FQI algorithms. In Appendix G.2, we show the sample complexity of FQI-FULL-CLASS that handles the offline planning for a class of rewards. In Appendix G.3, we provide the sample complexity guarantee for planning for the elliptical reward class. In Appendix G.4, we discuss the sample complexity result of planning with the learnt feature \( \bar{\phi} \). We want to mention that we abuse some notations in this section. For example, \( \mathcal{F}_h, \mathcal{G}_h \) would have different meanings from the main text. However, they should be clear within the context.

G.1 FQI planning algorithm

In this part, we present a general framework of FQI planner. Algorithm 6 subsumes three different algorithms: FQI-FULL-CLASS, FQI-REPRESENTATION, and FQI-ELLIPTICAL. FQI-FULL-CLASS and FQI-REPRESENTATION will be used to plan for a finite deterministic reward class, while FQI-ELLIPTICAL is specialized in planning for the elliptical reward class. This leads to the different bounds of parameters in the Q-value function classes and different clipping thresholds of the state-value functions. In addition, for FQI-FULL-CLASS and FQI-ELLIPTICAL, we use all features in \( \Phi \) to construct the Q-value function classes, while in FQI-REPRESENTATION we only utilize the the learnt representation \( \bar{\phi} \). The details can be found below.
Algorithm 6 FQI (Fitted Q-Iteration)

input: (1) exploratory dataset \( \{ \mathcal{D} \}_{0:H-1} \) sampled from \( \rho_{h-2}^{3} \) (2) reward function \( R = R_{0:H-1} : \mathcal{X} \times \mathcal{A} \rightarrow [0, 1] \), (3) function class: (i) for FQI-FULL-CLASS, \( \mathcal{F}_{h}(R_{h}) := \{ R_{h} + \langle \phi_{h}, w_{h} \rangle : \| w_{h} \|_{2} \leq H \sqrt{d}, \phi_{h} \in \Phi_{h} \}, h \in [H] \); (ii) for FQI-REPRESENTATION, \( \mathcal{F}_{h}(R_{h}) := \{ R_{h} + \text{clip}[0,H](\langle \phi_{h}, w_{h} \rangle) : \| w_{h} \|_{2} \leq B \}, h \in [H] \); (iii) for FQI-ELLIPTICAL, \( \mathcal{F}_{h}(R_{h}) := \{ R_{h} + \langle \phi_{h}, w_{h} \rangle : \| w_{h} \|_{2} \leq \sqrt{d}, \phi_{h} \in \Phi_{h} \}, h \in [H] \).

Set \( \hat{V}_{h}(x) = 0 \).

for \( h = H - 1, \ldots, 0 \) do

Pick \( n \) samples \( \{ (x_{h}^{(i)}, a_{h}^{(i)}, x_{h+1}^{(i)}) \}_{i=1}^{n} \) from the exploratory dataset \( \mathcal{D}_{h} \).

Solve least squares problem:

\[
\hat{f}_{h,R_{h}} \leftarrow \arg \min_{f_{h} \in \mathcal{F}_{h}(R_{h})} \mathcal{L}_{\mathcal{D}_{h},R_{h}}(f_{h}, \hat{V}_{h+1}),
\]

where \( \mathcal{L}_{\mathcal{D}_{h},R_{h}}(f_{h}, \hat{V}_{h+1}) := \sum_{i=1}^{n} \left( f_{h}(x_{h}^{(i)}, a_{h}^{(i)}) - R_{h}(x_{h}^{(i)}, a_{h}^{(i)}) - \hat{V}_{h+1}(x_{h+1}^{(i)}) \right)^{2} \)

Define \( \hat{\pi}_{h}(x) = \arg \max_{a} \hat{f}_{h,R_{h}}(x, a) \).

Define \( \bar{V}_{h}(x) = \text{clip}[0,H] \left( \max_{a} \hat{f}_{h,R_{h}}(x, a) \right) \) for FQI-FULL-CLASS and FQI-REPRESENTATION,

while define \( \bar{V}_{h}(x) = \text{clip}[0,1] \left( \max_{a} \hat{f}_{h,R_{h}}(x, a) \right) \) for FQI-ELLIPTICAL.

end for

return \( \hat{\pi} = (\hat{\pi}_{0}, \ldots, \hat{\pi}_{H-1}) \).

Unlike the regression problem in the main text, the objective here includes an additional reward function component. Therefore, we define a new loss function \( \mathcal{L}_{\mathcal{D}_{h},R_{h}} \) and will use \( \mathcal{L}_{\rho_{h-2}^{3},R_{h}} \) to denote its population version. Notice that the function class \( \mathcal{F}_{h}(R_{h}) \) in Algorithm 6 also depends on the reward function \( R \). If we pull out the reward term from \( \hat{f}_{h,R_{h}} \), we can obtain an equivalent solution of the least squares problem (38) as below:

\[
\hat{f}_{h,R_{h}} = R_{h} + \arg \min_{f_{h} \in \mathcal{F}_{h}(0)} \mathcal{L}_{\mathcal{D}_{h}}(f_{h}, \hat{V}_{h+1}), \quad \mathcal{L}_{\mathcal{D}_{h}}(f_{h}, \hat{V}_{h+1}) := \sum_{i=1}^{n} \left( f_{h}(x_{h}^{(i)}, a_{h}^{(i)}) + \hat{V}_{h+1}(x_{h+1}^{(i)}) \right)^{2}.
\]

Intuitively, the reward function \( R_{h} \) only makes the current least squares solution offset the original (reward-independent) least squares solution by \( R_{h} \).

G.2 Planning for a reward class with full representation class

In this part, we first establish the sample complexity of planning for a deterministic reward function \( R \) in Lemma 16. We will choose FQI-FULL-CLASS as the planner, where the Q-value function class consists of linear function of all features in the feature class with reward appended. Specifically, we have \( \mathcal{F}_{h}(R_{h}) := \{ R_{h} + \langle \phi_{h}, w_{h} \rangle : \| w_{h} \|_{2} \leq H \sqrt{d}, \phi_{h} \in \Phi_{h} \}, h \in [H] \). Equipped with this lemma, we also provide the sample complexity of planning for a finite deterministic reward class \( \mathcal{R} \) in Corollary 17.

Lemma 16 (Planning for a known reward with full representation class). Assume that we have the exploratory dataset \( \{ \mathcal{D} \}_{0:H-1} \) collected from \( \rho_{h-2}^{3} \) and satisfies (6) for all \( h \in [H] \). For a known deterministic reward function \( R = R_{0:H-1} : \mathcal{X} \times \mathcal{A} \rightarrow [0, 1] \) and \( \delta \in (0, 1) \), if we set

\[
n \geq \frac{512H^{6}d^{2}\kappa K}{\beta^{2}} \log \left( \frac{256H^{6}d^{2}\kappa K}{\beta^{2}} \right) + \frac{512H^{6}d^{2}K}{\beta^{2}} \log \left( \frac{2\Phi[H]}{\delta} \right),
\]
then with probability at least $1 - \delta$, the policy $\tilde{\pi}$ returned by FQI-FULL-CLASS satisfies

$$\mathbb{E}_{\tilde{\pi}} \left[ \sum_{h=0}^{H-1} R_h(x_h, a_h) \right] \geq \max_{\pi} \mathbb{E}_{\pi} \left[ \sum_{h=0}^{H-1} R_h(x_h, a_h) \right] - \beta.$$  

**Proof.** For notation simplicity, we will drop the $R_h$ subscript of $\tilde{f}_h R_h$ throughout the proof. Note that, this conflicts with the notation in later lemma statements (e.g. Lemma 18 where we put back the subscript), and we reserve it for the reward-augmented function class for clarity in this proof. We first bound the difference in cumulative rewards between $\tilde{\pi} := \tilde{\pi}_{0,H-1}$ and the optimal policy $\pi^*$ for the given reward function. Recall that $\tilde{\pi}_0$ is greedy w.r.t. $\tilde{f}_0$, which implies that $\tilde{f}_0(x_0, \tilde{\pi}_0(x_0)) \geq \tilde{f}_0(x_0, \pi^*(x_0))$ for all $x_0$. Hence, we have

$$V^* - V^\tilde{\pi} = \mathbb{E}_{\pi^*} \left[ R_0(x_0, a_0) + V^*(x_1) \right] - \mathbb{E}_{\tilde{\pi}} \left[ R_0(x_0, a_0) + V^\tilde{\pi}(x_1) \right]$$

$$\leq \mathbb{E}_{\pi^*} \left[ R_0(x_0, a_0) + V^*(x_1) - \tilde{f}_0(x_0, a_0) \right] - \mathbb{E}_{\tilde{\pi}} \left[ R_0(x_0, a_0) + V^\tilde{\pi}(x_1) - \tilde{f}_0(x_0, a_0) \right]$$

$$= \mathbb{E}_{\pi^*} \left[ R_0(x_0, a_0) + V^*(x_1) - \tilde{f}_0(x_0, a_0) \right] - \mathbb{E}_{\tilde{\pi}} \left[ R_0(x_0, a_0) + V^*(x_1) - \tilde{f}_0(x_0, a_0) \right]$$

$$+ \mathbb{E}_{\tilde{\pi}} \left[ V^*(x_1) - V^\tilde{\pi}(x_1) \right]$$

$$= \mathbb{E}_{\pi^*} \left[ Q^*_0(x_0, a_0) - \tilde{f}_0(x_0, a_0) \right] - \mathbb{E}_{\tilde{\pi}} \left[ Q^*_0(x_0, a_0) - \tilde{f}_0(x_0, a_0) \right] + \mathbb{E}_{\tilde{\pi}} \left[ V^*(x_1) - V^\tilde{\pi}(x_1) \right].$$

Continuing unrolling to $h = H - 1$, we get

$$V^* - V^\tilde{\pi} \leq \sum_{h=0}^{H-1} \mathbb{E}_{\tilde{\pi}_{0,h-1} \circ \pi^*} \left[ Q^*_h(x_h, a_h) - \tilde{f}_h(x_h, a_h) \right] - \sum_{h=0}^{H-1} \mathbb{E}_{\tilde{\pi}_{0,h}} \left[ Q^*_h(x_h, a_h) - \tilde{f}_h(x_h, a_h) \right].$$

Now we bound each of these terms. The two terms only differ in the policies that generate the data and can be handled similarly. Therefore, in the following, we focus on just one of them. For any function $V_{h+1} : \mathcal{X} \rightarrow \mathbb{R}$, we introduce Bellman backup operator $(T_{h} V_{h+1})(x_h, a_h) := R_h(x_h, a_h) + \mathbb{E} [V_{h+1}(x_{h+1}) | x_h, a_h]$. Let’s call the roll-in policy $\pi$ and drop the dependence on $h$. This gives us

$$\mathbb{E}_{\pi} \left[ Q^*(x, a) - \tilde{f}(x, a) \right] = \mathbb{E}_{\pi} \left[ R(x, a) + \mathbb{E} [V^*(x') | x, a] - \tilde{f}(x, a) \right]$$

$$\leq \mathbb{E}_{\pi} \left[ R(x, a) + \mathbb{E} [V^*(x') | x, a] - \tilde{f}(x, a) \right]$$

$$\leq \mathbb{E}_{\pi} \left[ \mathbb{E} [V^*(x') | x, a] - \mathbb{E} [\tilde{V}(x') | x, a] + R(x, a) + \mathbb{E} [\tilde{V}(x') | x, a] - \tilde{f}(x, a) \right]$$

$$\leq \mathbb{E}_{\pi} \left[ V^*(x') - \tilde{V}(x') + (T \tilde{V})(x, a) - \tilde{f}(x, a) \right],$$

where the last inequality is Jensen’s inequality.

From the definition of $\tilde{V}(x')$, we have

$$\mathbb{E}_{\pi} \left[ V^*(x') - \tilde{V}(x') \right] \leq \mathbb{E}_{\pi} \left[ \max_a Q^*(x', a) - \max_{a'} \tilde{f}(x', a') \right] \leq \mathbb{E}_{\pi \circ \tilde{\pi}} \left[ Q^*(x', a') - \tilde{f}(x', a') \right].$$

In the last inequality, we define $\tilde{\pi}$ to be the greedy one between two actions, that is we set $\tilde{\pi}(x') = \arg\max_{a'} \max_a \{Q^*(x', a'), \tilde{f}(x', a')\}$. This expression has the same form as the initial one, while at the next
timestep. Keep unrolling yields

\[
\mathbb{E}_\pi \left[ Q^*(x_h, a_h) - \hat{f}_h(x_h, a_h) \right] \leq \sum_{\tau = h}^{H-1} \max_{\pi_\tau} \mathbb{E}_{\pi_\tau} \left[ (T_\tau \hat{V}_{\tau+1})(x_\tau, a_\tau) - \hat{f}_\tau(x_\tau, a_\tau) \right]
\]

\[
\leq \sum_{\tau = h}^{H-1} \max_{\pi_\tau} \sqrt{\mathbb{E}_{\pi_\tau} \left[ (T_\tau \hat{V}_{\tau+1})(x_\tau, a_\tau) - \hat{f}_\tau(x_\tau, a_\tau) \right]^2}
\]

\[
\leq \sum_{\tau = h}^{H-1} \kappa K \mathbb{E}_{\rho_{\tau-3}^+} \left[ (T_\tau \hat{V}_{\tau+1})(x_\tau, a_\tau) - \hat{f}_\tau(x_\tau, a_\tau) \right]^2,
\]

where the last inequality is due to condition (6).

Further, we have that with probability at least \(1 - \delta\),

\[
\mathbb{E}_{\rho_{\tau-3}^+} \left[ (T_\tau \hat{V}_{\tau+1})(x_\tau, a_\tau) - \hat{f}_\tau(x_\tau, a_\tau) \right]^2 = \mathbb{E}_{\rho_{\tau-3}^+} \left[ (R_\tau(x_\tau, a_\tau) + \hat{V}_{\tau+1}(x_{\tau+1}) - \hat{f}_\tau(x_\tau, a_\tau))^2\right]
\]

\[
= E \left[ L_{D_\tau, R_\tau}(\hat{f}_\tau, \hat{V}_{\tau+1}) \right] - E \left[ L_{D_\tau, R_\tau}(T_\tau \hat{V}_{\tau+1}, \hat{V}_{\tau+1}) \right]
\]

\[
\leq \frac{256H^2d^2\log \frac{2n|\Phi|H}{\delta}}{n}. \tag{Step (*), Lemma 18}
\]

Plugging this back into the overall value performance difference, the bound is

\[
V^* - V^\hat{\pi} \leq H^2 \sqrt{\kappa K \frac{256H^2d^2\log \frac{2n|\Phi|H}{\delta}}{n}}.
\]

Setting RHS to be less than \(\beta\) and reorganize, we get

\[
n \geq \frac{256H^6d^2\kappa K}{\beta^2} \log \left( \frac{2n|\Phi|H}{\delta} \right).
\]

A sufficient condition for the inequality above is

\[
n \geq \frac{512H^6d^2\kappa K}{\beta^2} \log \left( \frac{256H^6d^2\kappa K}{\beta^2} \right) + \frac{512H^6d^2\kappa K}{\beta^2} \log \left( \frac{2|\Phi|H}{\delta} \right),
\]

which completes the proof. \(\square\)

**Corollary 17** (Planning for a reward class with full representation class). Assume that we have the exploratory dataset \(D\) for all \(h \in [H]\), and we are given a finite deterministic reward class \(R \subset (X \times A \to [0,1])\). For \(\delta \in (0,1)\) and any reward function \(\bar{R} \in R\), if we set

\[
n \geq \frac{512H^6d^2\kappa K}{\beta^2} \log \left( \frac{256H^6d^2\kappa K}{\beta^2} \right) + \frac{512H^6d^2\kappa K}{\beta^2} \log \left( \frac{2|\Phi|\bar{R}}{\delta} \right),
\]

then with probability at least \(1 - \delta\), the policy \(\hat{\pi}\) returned by FQI-FULL-CLASS satisfies

\[
\mathbb{E}_{\hat{\pi}} \left[ \sum_{h=0}^{H-1} R_h(x_h, a_h) \right] \geq \max_{\pi} \mathbb{E}_{\pi} \left[ \sum_{h=0}^{H-1} R_h(x_h, a_h) \right] - \beta.
\]
Proof. For any fixed reward $R \in \mathcal{R}$, we apply Lemma 16 and get that with probability $1 - \delta'$,

$$
\mathbb{E}_h \left[ \sum_{h=0}^{H-1} R_h(x_h,a_h) \right] \geq \max_{\pi} \mathbb{E}_\pi \left[ \sum_{h=0}^{H-1} R_h(x_h,a_h) \right] - \beta,
$$

if we set

$$
n \geq \frac{512H^6d^2\kappa K}{\beta^2} \log \left( \frac{256H^6d^2\kappa K}{\beta^2} \right) + \frac{512H^6d^2\kappa K}{\beta^2} \log \left( \frac{2\Phi|H|}{\delta} \right).
$$

Union bounding over $R \in \mathcal{R}$ and setting $\delta = \delta'/|\mathcal{R}|$ gives us the desired result. \hfill \Box

Lemma 18 (Deviation bound for Lemma 16). Given a deterministic reward function $R(\cdot) = R_{0:H-1} : \mathcal{X} \times \mathcal{A} \to [0,1]$ and a dataset $\mathcal{D}_h := \{x_h^{(i)}, a_h^{(i)}, x_h+1^{(i)}\}_{i=1}^n$ collected from $\rho_{h+3}^{+3}$, $h \in [H]$. With probability at least $1 - \delta$, $\forall h \in [H]$, $V_{h+1} \in V_{h+1}(R_{h+1})$, we have

$$
\mathbb{E} \left[ \mathcal{L}_{\mathcal{D}_h,R_h}( \hat{f}_{h,R_h} + \hat{f}_h, V_{h+1}) \right] - \mathbb{E} \left[ \mathcal{L}_{\mathcal{D}_h,R_h}(T_{h}V_{h+1}, V_{h+1}) \right] \leq \frac{256H^6d^2 \log \frac{2\Phi|H|}{\delta}}{n}.
$$

Here, $V_{h+1}(R_{h+1}) := \{\text{clip}_{[0,H]}(\max_a f_{h+1}(x_{h+1},a)) : f_{h+1} \in \mathcal{F}_{h+1}(R_{h+1})\}$ for $h \in [H-1]$ and $V_H = \{0\}$ is the clipped state-value function class, and $\mathcal{F}_h(R_h) := \{R_h + \langle \phi_h, w_h \rangle : \|w_h\|_2 \leq H\sqrt{d}, \phi_h \in \Phi_h\}$ for $h \in [H-1]$ is the Q-value function class.

Recall the definition, we get $\hat{f}_{h,R_h} = R_h + \hat{f}_h$, where $\hat{f}_h = \arg\min_{f_h \in \mathcal{F}_h(0)} \mathcal{L}_{\mathcal{D}_h}(f_h,V_{h+1})$, $\mathcal{F}_h(0) := \{\langle \phi_h, w_h \rangle : \|w_h\|_2 \leq H\sqrt{d}, \phi_h \in \Phi_h\}$, and $\mathcal{L}_{\mathcal{D}_h}(f_h,V_{h+1}) := \sum_{i=1}^n \left( f_h(x_h^{(i)}, a_h^{(i)}) - V_{h+1}(x_{h+1}^{(i)}) \right)^2$.

Therefore we have the following: $\mathcal{L}_{\mathcal{D}_h,R_h}(\hat{f}_{h,R_h}, V_{h+1}) = \mathcal{L}_{\mathcal{D}_h}(\hat{f}_h, V_{h+1})$ and $\mathcal{L}_{\mathcal{D}_h,R_h}(T_{h}V_{h+1}, V_{h+1}) = \mathcal{L}_{\mathcal{D}_h}(\langle \phi_h^*, \theta_{V_{h+1}}^* \rangle, V_{h+1})$.

Proof. Firstly, we fix $h \in [H]$. Noticing the structure of $\mathcal{F}_h(0)$, we can associate any $f_h \in \mathcal{F}_h(0)$ with $\phi_h \in \Phi_h$ and $w_h$ that satisfies $\|w_h\|_2 \leq H\sqrt{d}$. Therefore, we can equivalently write $\mathcal{L}_{\mathcal{D}_h}(f_h,V_{h+1}) = \mathcal{L}_{\mathcal{D}_h}(\phi_h,w_h,V_{h+1})$. Also noticing the structure of $V_{h+1}(R_{h+1})$, we can directly apply Lemma 23 with $\rho = \rho_{h+3}^{+3}$, $\rho' = \Phi_h$, $\Phi'' = \Phi_h$, $B = H\sqrt{d}$, $L = H$, $\mathcal{R} = \{R\}$, and $\pi'$ to be the greedy policy $\pi'(x_{h+1}) = \arg\max_{a'} (R(x_{h+1},a') + \langle \phi_h(x_{h+1},a'), 0 \rangle)$.

This implies that for all $\|w_h\|_2 \leq H\sqrt{d}, \phi_h \in \Phi_h$, and $V_{h+1} \in V_{h+1}(R_{h+1})$, with probability at least $1 - \delta'$, we have

$$
\mathcal{L}_{\rho_{h+3}^{+3}}(\phi_h,w_h,V_{h+1}) - \mathcal{L}_{\rho_{h+3}^{+3}}(\phi_h^*,\theta_{V_{h+1}}^*,V_{h+1}) \leq 2 \mathcal{L}_{\mathcal{D}_h}(\phi_h,w_h,V_{h+1}) - \mathcal{L}_{\mathcal{D}_h}(\phi_h^*,\theta_{V_{h+1}}^*,V_{h+1}) + \frac{128H^2d \log \frac{2\Phi}{\delta}}{n}.
$$

From the definition, we have $\hat{f}_h = \arg\min_{f_h \in \mathcal{F}_h(0)} \mathcal{L}_{\mathcal{D}_h}(f_h,V_{h+1})$. Noticing the structure of $\mathcal{F}_h(0)$, we can write $\hat{f}_h = \langle \hat{\phi}_h, \hat{w}_h \rangle$, where $\hat{\phi}_h, \hat{w}_h$ is the argmax that is the learned Q-function. Here we abuse the notation of $\hat{\phi}_h$, which is reserved for the learned feature.

Since $\phi_h^* \in \Phi_h$ and $\|\theta_{V_{h+1}}^*\|_2 \leq H\sqrt{d}$ from Lemma 1, we get

$$
\mathcal{L}_{\rho_{h+3}^{+3}}(\hat{\phi}_h,\hat{w}_h,V_{h+1}) - \mathcal{L}_{\rho_{h+3}^{+3}}(\phi_h^*,\theta_{V_{h+1}}^*,V_{h+1}) \leq \frac{128H^2d \log \frac{2}{\delta}}{n}.
$$

Perform the same union bound as Lemma 23, and additionally union bound over $h \in [H]$, and set $\delta = \delta'/\left(\Phi^2\|W_h\|H\right)$, with probability at least $1 - \delta$, we have

$$
\mathcal{L}_{\rho_{h+3}^{+3}}(\hat{\phi}_h,\hat{w}_h,V_{h+1}) - \mathcal{L}_{\rho_{h+3}^{+3}}(\phi_h^*,\theta_{V_{h+1}}^*,V_{h+1}) \leq \frac{128H^2d \log \frac{2\Phi^2H(2n)^d}{\delta}}{n}.
$$
Finally, relaxing the rhs in the inequality above and noticing by definition $\mathbb{E} \left[ \mathcal{L}_{\mathcal{D}_n}(\hat{f}_h, V_{h+1}) \right] = \mathcal{L}_{\rho^{+3}_h}(\hat{\phi}_h, \hat{w}_h, V_{h+1})$ and $\mathbb{E} \left[ \mathcal{L}_{\mathcal{D}_n, R_h}(T_h V_{h+1}, V_{h+1}) \right] = \mathcal{L}_{\rho^{+3}_h}(\phi^*_{V_{h+1}}, V_{h+1})$, we complete the proof. 

\section*{G.3 Elliptical planner}

In this part, we show the sample complexity of elliptical planner (FQI-ELLIPICAL), which is specialized in planning for the elliptical reward class defined in Lemma 19. The Q-value function class consists of linear function of all features in the feature class with reward appended. Specifically, we have $\mathcal{F}_h(R_h) := \{R_h + \langle \phi_h, w_h \rangle : \|w_h\|_2 \leq \sqrt{d}, \phi_h \in \Phi_h \}$, $h \in [H]$. We still use the full representation class, but with a different bound on the norm of the parameters when compared with FQI-FULL-CLASS.

\textbf{Lemma 19 (Elliptical planner).} Assume that we have the exploratory dataset $\{\mathcal{D}\}_{0:H-1}$ (collected from $\rho^{+3}_h$ and satisfies (6) for all $h \in [H]$). For $\delta \in (0, 1)$ and any deterministic elliptical reward function $R \in \mathcal{R}$, where $\mathcal{R} := \{R_{0:H-1} : R_{0:H-2} = 0, R_{H-1} \in \{\phi_{H-1}^{-1} \phi_{H-1} : \phi_{H-1} \in \Phi_{H-1}, \Gamma \in \mathbb{R}^{d \times d}, \lambda_{\min}(\Gamma) \geq 1\}\}$, if we set

$$n \geq \frac{584H^4d^3\kappa K}{\beta^2} \log \left( \frac{292H^4d^3\kappa K}{\beta^2} \right) + \frac{584H^4d^3\kappa K}{\beta^2} \log \left( \frac{2\Phi|H|}{\delta} \right),$$

then with probability at least $1 - \delta$, the policy $\hat{\pi}$ returned by FQI-ELLIPICAL satisfies

$$\mathbb{E}_{\hat{\pi}} \left[ \sum_{h=0}^{H-1} R_h(x_h, a_h) \right] \geq \max_{\pi} \mathbb{E}_{\pi} \left[ \sum_{h=0}^{H-1} R_h(x_h, a_h) \right] - \beta.$$

Remark: notice that the elliptical reward function only has non-zero value at timestep $H - 1$.

\textbf{Proof.} The proof follows the same steps in Lemma 16. Since we consider a deterministic elliptical reward function class here, we apply Lemma 20 instead of Lemma 18 in Step (*). Then following similar calculation gives us the result immediately. 

\textbf{Lemma 20 (Deviation bound for Lemma 19).} Consider the deterministic elliptical reward function classes $\mathcal{R} := \{R_{0:H-1} : R_{0:H-2} = 0, R_{H-1} \in \mathcal{R}_{H-1} := \{\phi_{H-1}^{-1} \phi_{H-1} : \phi_{H-1} \in \Phi_{H-1}, \Gamma \in \mathbb{R}^{d \times d}, \lambda_{\min}(\Gamma) \geq 1\}\}$, an exploratory dataset $\mathcal{D}_n := \{(x^{(i)}_h, a^{(i)}_h, x^{(i)}_{h+1})\}_{i=1}^n$ collected from $\rho^{+3}_h$, $h \in [H]$. With probability at least $1 - \delta$, $\forall R \in \mathcal{R}$, $h \in [H - 1], V_{h+1} \in V_{h+1}(R_{h+1})$, we have

$$\left| \mathbb{E} \left[ \mathcal{L}_{\mathcal{D}_n, R_h}(f_h, R_{h+1}, V_{h+1}) \right] - \mathbb{E} \left[ \mathcal{L}_{\mathcal{D}_n, R_h}(T_h V_{h+1}, V_{h+1}) \right] \right| \leq \frac{292d^3 \log \frac{2n\Phi|H|}{\delta}}{n^2}.$$

Here, $V_{h+1}(R_{h+1}) := \{\text{clip}_{[0,1]}(\max_a f_{h+1}(x_{h+1}, a)) : f_{h+1} \in \mathcal{F}_{h+1}(R_{h+1})\}$ for $h \in [H - 1]$ and $V_H = \{0\}$ is the clipped state-value function class, and $\mathcal{F}_h(R_h) := \{R_h + \langle \phi_h, w_h \rangle : \|w_h\|_2 \leq \sqrt{d}, \phi_h \in \Phi_h\}$ for $h \in [H - 1]$ is the reward dependent Q-value function class.

\textbf{Proof.} First, from Lemma 25, we know that there exists a $\gamma$-cover $\mathcal{C}_{\mathcal{R}_{H-1}}$ for the reward class $\mathcal{R}_{H-1}$. From the definition of $\mathcal{R}$, we know that $\mathcal{C}_R := \{R_{0:H-1} : R_{0:H-2} = 0, R_{H-1} \in \mathcal{C}_{\mathcal{R}_{H-1}}\}$ is a $\gamma$-cover of reward class $\mathcal{R}$ and $|\mathcal{C}_R| = |\mathcal{C}_{\mathcal{R}_{H-1}}|$. For any fixed $\tilde{R} \in \mathcal{C}_R$, we can follow the same steps in Lemma 18 to get a concentration result like (39). The only differences are that the norm of $w_h$ is now bounded by $\sqrt{d}$ instead of $H\sqrt{d}$ and we clip to $[0, 1]$. Therefore, for this fixed $\tilde{R}$, with probability at least $1 - \delta'$, we have that $\forall h \in [H - 1], \tilde{V}_{h+1} \in V_{h+1}(\tilde{R}_{h+1})$,

$$\left| \mathbb{E} \left[ \mathcal{L}_{\mathcal{D}_n, \tilde{R}_h}(\hat{f}_h, \tilde{R}_h, \tilde{V}_{h+1}) \right] - \mathbb{E} \left[ \mathcal{L}_{\mathcal{D}_n, \tilde{R}_h}(T_h V_{h+1}, V_{h+1}) \right] \right| \leq \frac{128 \log \frac{\|\phi\|^2(2n)^d|H|}{\delta}}{n^2}.$$
Union bounding over all $\tilde{R} \in \mathcal{C}_R$ and set $\delta = \delta' / |\mathcal{C}_R|$, with probability at least $1 - \delta$, we have

$$
|\mathbb{E} \left[ \mathcal{L}_{D_{h, \tilde{R}_h}}(\tilde{f}_{h, \tilde{R}_h}, V_{h+1}) \right] - \mathbb{E} \left[ \mathcal{L}_{D_{h, \tilde{R}_h}}(T_h \tilde{V}_{h+1}, \tilde{V}_{h+1}) \right] | \leq \frac{128d \log |\Phi|^2 (2n)^d |\mathcal{C}_R| H}{n \delta}.
$$

Notice that $\mathcal{C}_R$ is a $\gamma$-cover of $\mathcal{R}$, for any $R \in \mathcal{R}$, there exists $\tilde{R} \in \mathcal{C}_R$, so that $\|R - \tilde{R}\|_{\infty} \leq \gamma$. Therefore $\forall f_h \in \mathcal{F}_h(R_h)$ and $V_h \in \mathcal{V}_h(R_h)$, there exists some $\tilde{f}_h \in \mathcal{F}(\tilde{R}_h)$ and $\tilde{V}_h \in \mathcal{V}(\tilde{R}_h)$ that satisfies $\|\tilde{f}_h - f_h\|_{\infty} \leq \gamma$ and $\|\tilde{V}_h - V_h\|_{\infty} \leq \gamma$. Hence, for any $R \in \mathcal{R}$, with probability at least $1 - \delta$,

$$
\left| \mathbb{E} \left[ \mathcal{L}_{D_{h, R_h}}(\tilde{f}_{h, R_h}, V_{h+1}) \right] - \mathbb{E} \left[ \mathcal{L}_{D_{h, R_h}}(T_h \tilde{V}_{h+1}, V_{h+1}) \right] \right| \leq 128d \log \frac{|\Phi|^2 (2n)^d |\mathcal{C}_R| H}{\delta} + 36\sqrt{d} \gamma
$$

$$
\leq \frac{292d^3 \log \frac{2n|\Phi|H}{\delta}}{n} + 36\sqrt{d} \gamma.
$$

The last inequality is obtained by choosing $\gamma = \frac{\sqrt{d}}{n}$ and noticing $|\mathcal{C}_R| = |\Phi|_{H-1}(2\sqrt{d}/\gamma)^d \leq |\Phi|(2n)^d$. This completes the proof.

**G.4 Planning for a reward class with learnt representation function**

In this part, we will show that the learnt feature $\tilde{\phi}$ enables the downstream policy optimization for a finite deterministic reward class $\mathcal{R}$. The sample complexity is shown in Lemma 21. We will choose FQI-REPRESENTATION as the planner, where the Q-value function class only consists of linear function of learnt feature $\tilde{\phi}$ with reward appended. Specifically, we have $\mathcal{F}_h(R_h) := \{ \tilde{R}_h + \text{clip}_{[0,H]} (\tilde{\phi}_h, w_h) : \|w_h\|_2 \leq B \}$, $h \in [H]$. In addition to constructing the function class with learnt feature itself, we also perform clipping in $\mathcal{F}_h(R_h)$. This clipping variant helps us avoid the poly($B$) dependence in the sample complexity bound. Notice that clipped Q-value function classes also work for FQI-FULL-CLASS and FQI-Elliptical, and would save $d$ factor. We only introduce this variant here because $B$ is much larger than $H\sqrt{d}$ or $d$.

**Lemma 21 (Planning for a reward class with a learnt representation function).** Assume that we have the exploratory dataset $\{D\}_{0:H-1}$ (collected from $p_{h-3}^{+}$ and satisfies (6) for all $h \in [H]$), a learned feature $\tilde{\phi}_h$ that satisfies the condition in (7), and a finite deterministic reward class $\mathcal{R} \subset (\mathcal{X} \times \mathcal{A} \rightarrow [0, 1])$. For $\delta \in (0, 1)$ and any reward function $R \in \mathcal{R}$, if we set

$$
n \geq \frac{200H^6 d\kappa K}{\beta^2} \left( \log \left( \frac{100H^6 d\kappa K}{\beta^2} \right) + \frac{200H^6 d\kappa K}{\beta^2} \log \left( \frac{2|\mathcal{R}|B}{\delta} \right) \right),
$$

then with probability at least $1 - \delta$, the policy $\hat{\pi}$ returned by FQI-REPRESENTATION satisfies

$$
\mathbb{E}_{\hat{\pi}} \left[ \sum_{h=0}^{H-1} R_h(x_h, a_h) \right] \geq \max_{\pi} \mathbb{E}_{\pi} \left[ \sum_{h=0}^{H-1} R_h(x_h, a_h) \right] - \beta - 2H^2 \sqrt{\kappa K \varepsilon_{\text{apx}}}.
$$

**Proof.** Following similar steps in the proof of Lemma 16 and replacing Lemma 18 with Lemma 22 in Step(*), with probability at least $1 - \delta$, we have

$$
V^* - V_{\hat{\pi}} \leq H^2 \sqrt{\kappa K} \left( \sqrt{\frac{100H^2 d \log \frac{2n|\mathcal{R}|B}{\delta}}{n}} + 3\varepsilon_{\text{apx}} \right) \leq H^2 \sqrt{\kappa K} \left( \sqrt{\frac{100H^2 d \log \frac{2n|\mathcal{R}|B}{\delta}}{n}} + 2H^2 \sqrt{\kappa K \varepsilon_{\text{apx}}} \right).
$$

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Setting rhs to be less than $\beta + 2H^2\sqrt{nK\varepsilon_{\text{apx}}}$ and reorganize, we get the condition

$$n \geq \frac{100H^6dK\log\left(\frac{2n|\mathcal{R}|B}{\delta}\right)}{\beta^2}.$$  

A sufficient condition for the inequality above is

$$n \geq \frac{200H^6dK}{\beta^2} \log\left(\frac{100H^6dK}{\beta^2}\right) + \frac{200H^6dK}{\beta^2} \log\left(\frac{2|\mathcal{R}|B}{\delta}\right),$$

which completes the proof. \qed

**Lemma 22** (Deviation bound for Lemma 21). Assume that we have an exploratory dataset $\mathcal{D}_h := \{(x_h^{(i)}, a_h^{(i)}, x_{h+1}^{(i)})\}_{i=1}^n$ collected from $\rho_{h-3}^+, h \in [H]$, a learned feature $\hat{\phi}_h$ that satisfies the condition in (7), and a finite deterministic reward class $\mathcal{R} \subset (\mathcal{X} \times \mathcal{A} \rightarrow [0, 1])$. Then, with probability at least $1 - \delta, \forall R \in \mathcal{R}, h \in [H], V_{h+1} \in \mathcal{V}_{h+1}(R_{h+1})$, we have

$$\left| \mathbb{E}\left[ \mathcal{L}_{\mathcal{D}_h,R_h}(\hat{f}_{h,R_h}, V_{h+1}) \right] - \mathbb{E}\left[ \mathcal{L}_{\mathcal{D}_h,R_h}(\hat{T}_h, V_{h+1}) \right] \right| \leq \frac{100H^2d^2\log\left(\frac{2n|\mathcal{R}|B}{\delta}\right)}{n} + 3\varepsilon_{\text{apx}}.$$

*Here* $V_{h+1}(R_{h+1}) := \{\text{clip}_{[0,H]}(\max_a f_{h+1}(x_{h+1}, a)) : f_{h+1} \in \mathcal{F}_{h+1}(R_{h+1})\}$ for $h \in [H - 1]$, and $V_{H} = \{0\}$ is the clipped state-value function class and $\mathcal{F}_{h}(R_{h}) := \{R_h + \text{clip}_{[0,H]}(\langle \hat{\phi}_h, w_h \rangle) : \|w_h\|_2 \leq B\}$ for $h \in [H - 1]$ is the reward dependent Q-value function class.

**Proof.** First, we show that condition (7) implies following condition for all $h \in [H]$:

$$V_{h+1} \in \left\{\text{clip}_{[0,H]}(\max_a \left(R_{h+1}(x_{h+1}, a) + \text{clip}_{[0,H]}(\langle \phi_{h+1}(x_{h+1}, a), \theta \rangle)\right)) : \phi_{h+1} \in \Phi_{h+1}, \|\theta\|_2 \leq B, R \in \mathcal{R}\right\},$$

let $\bar{w}_{V_{h+1}} = \text{argmin}_{\|w_h\|_2 \leq B} \mathcal{L}_{\mathcal{D}_h}(\hat{\phi}_h, w_h, V_{h+1})$ with $B \geq H\sqrt{d}$, we have

$$\mathbb{E}_{\rho_{h-3}}\left[\left(\langle \hat{\phi}_h(x_h, a_h), \bar{w}_{V_{h+1}} \rangle - \mathbb{E}[V_{h+1}(x_{h+1})|x_h, a_h]\right)^2 \right] \leq \varepsilon_{\text{apx}}.$$  

This is due to the order of taking max and clipping doesn’t matter:

$$\text{clip}_{[0,H]}\left(\max_a \left(R_{h+1}(x_{h+1}, a) + \text{clip}_{[0,H]}(\langle \phi_{h+1}(x_{h+1}, a), \theta \rangle)\right)\right)$$

$$= \text{clip}_{[0,H]}\left(\max_a \left(R_{h+1}(x_{h+1}, a) + \langle \phi_{h+1}(x_{h+1}, a), \theta \rangle\right)\right).$$

Then we follow the similar structure as Lemma 23. We fix $R \in \mathcal{R}, h \in [H], \|w_h\|_2 \leq B$, and $V_{h+1} \in V_{h+1}(R_{h+1})$ (equivalently $w_{V_{h+1}}$). We also fix $\hat{\theta}_{V_{h+1}}$, where $\hat{\theta}_{V_{h+1}}$ satisfies $\|\hat{\theta}_{V_{h+1}}\|_2 \leq B$ and for all $(x_h, a_h), \langle \phi_{h}^*(x_h, a_h), \hat{\theta}_{V_{h+1}} \rangle - \mathbb{E}[V(x_{h+1})|x_h, a_h] = \langle \phi_{h}^*(x_h, a_h), \hat{\theta}_{V_{h+1}} - \theta_{V_{h+1}}^* \rangle \leq \gamma.$

Then we show a high probability bound on the following deviation term:

$$\left| \mathcal{L}_{\rho_{h-3}}(\hat{\phi}_h, w_h, V_{h+1}) - \mathcal{L}_{\rho_{h-3}}(\phi_{h}^*, \hat{\theta}_{V_{h+1}}, V_{h+1}) - \left(\mathcal{L}_{\hat{\mathcal{D}}_h}(\hat{\phi}_h, w_h, V_{h+1}) - \mathcal{L}_{\hat{\mathcal{D}}_h}(\phi_{h}^*, \hat{\theta}_{V_{h+1}}, V_{h+1})\right) \right|. $$

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Since we have clipping here, we define \( \mathcal{L}_{\rho_{h-3}}^c (\phi_h, w_h, V_{h+1}) := \mathbb{E}_{\rho_{h-3}} \left[ \left( \text{clip}_{[0,H]}(\langle \phi_h, w_h \rangle) - V_{h+1} \right)^2 \right] \) and \( \mathcal{L}_{\hat{V}_{h+1}}^c \) as its empirical version.

Let \( g_h(x_h, a_h) = \text{clip}_{[0,H]}(\langle \tilde{\phi}_h(x_h, a_h), w_h \rangle) \) and \( \tilde{g}_h(x_h, a_h) = \text{clip}_{[0,H]}(\langle \phi_h^*, (x_h, a_h), \tilde{\theta}_{V_{h+1}} \rangle) \). For random variable variable \( Y := (g_h(x_h, a_h) - V_{h+1}(x_h+1))^2 - (\tilde{g}_h(x_h, a_h) - V_{h+1}(x_h+1))^2 \), we have:

\[
\mathbb{E}[Y] = \mathbb{E} \left[ (g_h(x_h, a_h) - V_{h+1}(x_h+1))^2 - (\tilde{g}_h(x_h, a_h) - V_{h+1}(x_h+1))^2 \right] 
= \mathbb{E} \left[ (g_h(x_h, a_h) + \tilde{g}_h(x_h, a_h) - 2V_{h+1}(x_h+1))(g_h(x_h, a_h) - \tilde{g}_h(x_h, a_h)) \right] 
= \mathbb{E} \left[ (g_h(x_h, a_h) - \tilde{g}_h(x_h, a_h))^2 \right] - 2\mathbb{E} \left[ (\mathbb{E}[V_{h+1}(x_h+1)|x_h, a_h]) - \tilde{g}_h(x_h, a_h) \right] (g_h(x_h, a_h) - \tilde{g}_h(x_h, a_h)) .
\]

Here the expectation is taken over \( \rho_{h-3}^+ \).

Noticing the approximation assumption of \( \tilde{\theta}_{V_{h+1}} \), and \( g_h(x_h, a_h) \) and \( \tilde{g}_h(x_h, a_h) \) are bounded by \( [0, H] \), we have

\[
\left| \mathbb{E}[Y] - \mathbb{E}\left[(g_h(x_h, a_h) - \tilde{g}_h(x_h, a_h))^2\right] \right| \leq 2 \left| \mathbb{E}[V_{h+1}(x_h+1)|x_h, a_h] - \tilde{g}_h(x_h, a_h) \right| \|g_h - \tilde{g}_h\|_\infty 
\leq 2H \left\| \langle \phi_h^*, \tilde{\theta}_{V_{h+1}} \rangle - \langle \phi_h^*, \tilde{\theta}_{V_{h+1}} \rangle \right\|_\infty \leq 2H \gamma .
\]

Next, for the variance of the random variable, notice that \( g_h(x_h, a_h) \) and \( \tilde{g}_h(x_h, a_h) \) are bounded by \( [0, H] \), we have:

\[
\mathbb{V}[Y] \leq \mathbb{E}[Y^2] = \mathbb{E}\left[(g_h(x_h, a_h) + \tilde{g}_h(x_h, a_h) - 2V_{h+1}(x_h+1))^2 (g_h(x_h, a_h) - \tilde{g}_h(x_h, a_h))^2 \right] 
\leq 4H^2 \mathbb{E}\left[(g_h(x_h, a_h) - \tilde{g}_h(x_h, a_h))^2 \right] 
\leq 4H^2 (\mathbb{E}[Y] + 2H \gamma ) .
\]

Noticing \( Y \in [-4H^2, 4H^2] \) and applying Bernstein’s inequality, with probability at least \( 1 - \delta' \), we can bound the deviation term above as:

\[
\left| \mathcal{L}_{\rho_{h-3}}^c (\tilde{\phi}_h, w_h, V_{h+1}) - \mathcal{L}_{\rho_{h-3}}^c (\phi_h^*, \tilde{\theta}_{V_{h+1}}, V_{h+1}) - \left( \mathcal{L}_{\tilde{V}_{h+1}}^c (\phi_h^*, w_h, V_{h+1}) - \mathcal{L}_{\tilde{V}_{h+1}}^c (\phi_h^*, \tilde{\theta}_{V_{h+1}}, V_{h+1}) \right) \right| 
\leq \sqrt{\frac{2\mathbb{V}[Y] \log \frac{2}{\delta'}}{n}} + \frac{4H^2 \log \frac{2}{\delta'}}{3n} 
\leq \sqrt{\left( \frac{8H^2 \mathbb{E}[Y]}{n} + \frac{16H^3 \gamma}{n} \right) \log \frac{2}{\delta'}} + \frac{4H^2 \log \frac{2}{\delta'}}{3n} 
\leq \sqrt{\frac{8H^2 \mathbb{E}[Y]}{n} \log \frac{2}{\delta'}} + \sqrt{\frac{16H^3 \gamma}{n} \log \frac{2}{\delta'}} + \frac{4H^2 \log \frac{2}{\delta'}}{3n} 
\leq \frac{1}{2} \mathbb{E}[Y] + \frac{4H^2 \log \frac{2}{\delta'}}{n} + \frac{4H^2 \log \frac{2}{\delta'}}{3n} ,
\]

where we set \( \gamma = \frac{H}{n} \).

Substituting the definition of \( Y \) into this equation and reorganize, we obtain

\[
\left| \mathcal{L}_{\rho_{h-3}}^c (\tilde{\phi}_h, w_h, V_{h+1}) - \mathcal{L}_{\rho_{h-3}}^c (\phi_h^*, \tilde{\theta}_{V_{h+1}}, V_{h+1}) - \left( \mathcal{L}_{\tilde{V}_{h+1}}^c (\phi_h^*, w_h, V_{h+1}) - \mathcal{L}_{\tilde{V}_{h+1}}^c (\phi_h^*, \tilde{\theta}_{V_{h+1}}, V_{h+1}) \right) \right| 
\leq \frac{1}{2} \left( \mathcal{L}_{\rho_{h-3}}^c (\tilde{\phi}_h, w_h, V_{h+1}) - \mathcal{L}_{\rho_{h-3}}^c (\phi_h^*, \tilde{\theta}_{V_{h+1}}, V_{h+1}) \right) + \frac{10H^2 \log \frac{2}{\delta'}}{n} .
\]
Further, consider a finite point-wise cover of the function class $\mathcal{G}_h := \{g_h(x, a_h) = \langle \phi_h(x, a_h), w \rangle : \|w\|_2 \leq B \}$. Note that, with an $\ell_2$-cover $\overline{W}_h$ of $\mathcal{V}_h = \{|w|_2 \leq B\}$ at scale $\gamma$, we have for all $(x_h, a_h)$, there exists $\bar{w}_h \in \overline{W}_h, \|\langle \bar{\phi}_h, w - \bar{w}_h \rangle\|_\infty \leq \gamma$. Similarly, for any $V_{h+1} \in V_{h+1}(R_{h+1})$, we know that $\mathbb{E}[V_{h+1}(x_h + 1)|x_h, a_h] = \langle \phi_h^*(x, a_h), \theta_h^* \rangle_{x_h + 1}$ for some $\|\theta_h^*\|_2 \leq B$. Thus, we choose $\overline{W}_{h+1}$ as an $\ell_2$-cover of the set $\{w_{h+1} \in \mathbb{R}^d : \|w_{h+1}\|_2 \leq B\}$ at scale $\gamma$. For all $V_{h+1}(\cdot) = \text{clip}_{[0, H]}(\max_a \langle R_{h+1}(\cdot, a) + \langle \phi_{h+1}(\cdot, a), w_{h+1} \rangle \rangle) \in V_{h+1}(R_{h+1})$, there exists $\bar{w}_{h+1} \in \overline{W}_{h+1}$ such that $\|\bar{w}_{h+1} - w_{h+1}\|_2 \leq \gamma$. This implies that $\overline{V}_{h+1}(\cdot) = \text{clip}_{[0, H]}(\max_a \langle R_{h+1}(\cdot, a) + \langle \phi_{h+1}(\cdot, a), \bar{w}_{h+1} \rangle \rangle)$, we have $\|V_{h+1} - \overline{V}_{h+1}\|_\infty \leq \gamma$. Therefore, for $\theta_{V_{h+1}} = \theta_h^*_{V_{h+1}}$, we have $\langle \phi_h^*(x, a_h), \overline{\theta}_{V_{h+1}} \rangle - \mathbb{E}[V(x_{h}+1)|x_h, a_h] = \|\mathbb{E}[\overline{V}(x_{h}+1)|x_h, a_h] - \mathbb{E}[V(x_{h}+1)|x_h, a_h]\|$, which implies $\|\overline{W}_{h+1}\| \leq \left(\frac{2BH}{\gamma}\right)^d$ and $\|\overline{W}_h\| \leq \left(\frac{2B}{\gamma}\right)^d$.

Thus, applying a union bound over elements in $\overline{W}_h$, $\overline{W}_{h+1}$, with probability $1 - \|\overline{W}_h\|/\|\overline{W}_{h+1}\|$, for all $w_h \in \overline{W}_h$ and $V_{h+1} \in V_{h+1}(R_{h+1})$, we have:

$$
\begin{align*}
\mathcal{L}^c_{\rho_{h-3}}(\bar{\phi}_h, w_h, V_{h+1}) - \mathcal{L}^c_{\rho_{h-3}}(\phi^*_h, \theta^*_{V_{h+1}}, V_{h+1}) & \leq \mathcal{L}^c_{\rho_{h-3}}(\bar{\phi}_h, w_h, V_{h+1}) - \mathcal{L}^c_{\rho_{h-3}}(\phi^*_h, \theta^*_{V_{h+1}}, V_{h+1}) \\
& \leq \mathcal{L}^c_{\rho_{h-3}}(\phi^*_h, \bar{\theta}_{V_{h+1}}, V_{h+1}) - \mathcal{L}^c_{\rho_{h-3}}(\phi^*_h, \theta^*_{V_{h+1}}, V_{h+1}) \\
& \quad + \mathcal{L}^c_{\rho_{h-3}}(\phi^*_h, \bar{\theta}_{V_{h+1}}, V_{h+1}) - \mathcal{L}^c_{\rho_{h-3}}(\phi^*_h, \theta^*_{V_{h+1}}, V_{h+1}) \\
& \leq 2H\gamma + 2 \left(\mathcal{L}^c_{\bar{\Delta}_h}(\bar{\phi}_h, \bar{w}_h, V_{h+1}) - \mathcal{L}^c_{\bar{\Delta}_h}(\phi^*_h, \bar{\theta}_{V_{h+1}}, V_{h+1})\right) + \frac{10H^2 \log \frac{2}{\gamma}}{n} + 2H\gamma \\
& \leq 4H\gamma + \frac{10H^2 \log \frac{2}{\gamma}}{n} + 2 \left(\mathcal{L}^c_{\bar{\Delta}_h}(\phi_h, w_h, V_{h+1}) - \mathcal{L}^c_{\bar{\Delta}_h}(\phi^*_h, \bar{\theta}_{V_{h+1}}, V_{h+1})\right) + 4H\gamma \\
& = 8H\gamma + \frac{20H^2 \log \frac{2}{\gamma}}{n} + 2 \left(\mathcal{L}^c_{\bar{\Delta}_h}(\phi_h, w_h, V_{h+1}) - \mathcal{L}^c_{\bar{\Delta}_h}(\phi^*_h, \bar{w}_{V_{h+1}}, V_{h+1})\right) \\
& \quad + 2 \left(\mathcal{L}^c_{\bar{\Delta}_h}(\phi_h, \bar{w}_{V_{h+1}}, V_{h+1}) - \mathcal{L}^c_{\bar{\Delta}_h}(\phi^*_h, \bar{w}_{V_{h+1}}, V_{h+1})\right) \\
& \leq 8H\gamma + \frac{20H^2 \log \frac{2}{\gamma}}{n} + 2 \left(\mathcal{L}^c_{\bar{\Delta}_h}(\phi_h, w_h, V_{h+1}) - \mathcal{L}^c_{\bar{\Delta}_h}(\phi_h, \bar{w}_{V_{h+1}}, V_{h+1})\right) \\
& \quad + 3 \left(\mathcal{L}^c_{\rho_{h-3}}(\phi_h, \bar{w}_{V_{h+1}}, V_{h+1}) - \mathcal{L}^c_{\rho_{h-3}}(\phi^*_h, \bar{\theta}_{V_{h+1}}, V_{h+1})\right) + \frac{20H^2 \log \frac{2}{\gamma}}{n} \\
& \leq 8H\gamma + \frac{20H^2 \log \frac{2}{\gamma}}{n} + 2 \left(\mathcal{L}^c_{\bar{\Delta}_h}(\phi_h, w_h, V_{h+1}) - \mathcal{L}^c_{\bar{\Delta}_h}(\phi_h, \bar{w}_{V_{h+1}}, V_{h+1})\right) \\
& \quad + 3 \left(\mathcal{L}^c_{\rho_{h-3}}(\phi_h, w_h, V_{h+1}) - \mathcal{L}^c_{\rho_{h-3}}(\phi^*_h, \theta^*_{V_{h+1}}, V_{h+1})\right) \\
& \quad + 3 \left(\mathcal{L}^c_{\rho_{h-3}}(\phi_h, w_h, V_{h+1}) - \mathcal{L}^c_{\rho_{h-3}}(\phi^*_h, \theta^*_{V_{h+1}}, V_{h+1})\right) \\
& \leq 8H\gamma + \frac{20H^2 \log \frac{2}{\gamma}}{n} + 2 \left(\mathcal{L}^c_{\bar{\Delta}_h}(\phi_h, w_h, V_{h+1}) - \mathcal{L}^c_{\bar{\Delta}_h}(\phi^*_h, \bar{w}_{V_{h+1}}, V_{h+1})\right) \\
& \quad + 6H\gamma + 3 \left(\mathcal{L}^c_{\rho_{h-3}}(\phi_h, \bar{w}_{V_{h+1}}, V_{h+1}) - \mathcal{L}^c_{\rho_{h-3}}(\phi^*_h, \theta^*_{V_{h+1}}, V_{h+1})\right) + 6H\gamma \\
& \leq 20H\gamma + \frac{20H^2 \log \frac{2}{\gamma}}{n} + 2 \left(\mathcal{L}^c_{\bar{\Delta}_h}(\phi_h, w_h, V_{h+1}) - \mathcal{L}^c_{\bar{\Delta}_h}(\phi_h, \bar{w}_{V_{h+1}}, V_{h+1})\right) + 3\varepsilon_{apx}.
\end{align*}

In the second last inequality, the construction of $\overline{W}_h$ tells us that there exists $\bar{w}_{V_{h+1}} \in \overline{W}_h$ satisfies
\[ \| \tilde{w}_{h+1} - \bar{w}_{h+1} \|_2 \leq \gamma. \] In the last inequality, we notice that

\[
E_{\rho_h^{-3}} \left[ \left( \frac{\phi_h(x_h, a_h), \tilde{w}_{h+1}}{D_{\rho_h^{-3}}} \right) - E \left[ V_{h+1}(x_{h+1} | x_h, a_h) \right] \right]^2 \leq \varepsilon_{apx}
\]

From the definition, we have \( \hat{f}_h = \text{argmin}_{f_h \in F_h(0)} \mathcal{L}_{D_h}^c (f_h, V_{h+1}) \). Noticing the structure of \( \mathcal{F}_h(0) \), we can write \( \hat{f}_h = \text{clip}_{[0, H]} \left( \phi_h \right) \), where \( \hat{w}_h = \text{argmin}_{\|w_h\|_2 \leq \theta} \mathcal{L}_{D_h}^c (\phi_h, w_h, V_{h+1}) \). This implies \( \mathcal{L}_{D_h}^c (\hat{f}_h, \hat{w}_h, V_{h+1}) \leq \mathcal{L}_{D_h}^c (\phi_h, \hat{w}_h, V_{h+1}) \leq 0 \).

Union bounding over \( h \in [H] \) and \( R \in \mathcal{R} \), and set \( \delta = \delta' / (\|\hat{W}_h\| \|\bar{W}_{h+1}\| \|\mathcal{R}\| H) \), we get that with probability at least \( 1 - \delta \),

\[
\left| \mathcal{L}_{D_h}^c (\hat{f}_h, \hat{w}_h, V_{h+1}) - \mathcal{L}_{D_h}^c (\phi_s^*, \theta_s^*, V_{h+1}) \right| \leq \frac{100H^2d \log \frac{2nB \mathcal{R}}{\delta}}{n} + 3\varepsilon_{apx}.
\]

Finally, noticing the property that \( E \left[ \mathcal{L}_{D_h}^c (\hat{f}_h, V_{h+1}) \right] = \mathcal{L}_{D_h}^c (\phi_s^*, \theta_s^*, V_{h+1}) \) and \( E \left[ \mathcal{L}_{D_h, \mathcal{R}_h} (\mathcal{T}_h V_{h+1}, V_{h+1}) \right] = \mathcal{L}_{D_h}^c (\phi_s^*, \theta_s^*, V_{h+1}) \), we complete the proof. \qed

## H Auxiliary lemmas

### H.1 Proof of Lemma 1

In this part, we provide the proof of Lemma 1 for completeness. This result is widely used throughout the paper.

**Lemma** (Restatement of Lemma 1). For a low-rank MDP \( M \) with embedding dimension \( d \), for any function \( f : \mathcal{X} \rightarrow [0, 1] \), we have:

\[
E \left[ f(x_h+1) | x_h, a_h \right] = \left\langle \phi_h^*(x_h, a_h), \theta_f^* \right\rangle,
\]

where \( \theta_f^* \in \mathbb{R}^d \) and we have \( \|\theta_f^*\|_2 \leq \sqrt{d} \). A similar linear representation is true for \( E_{a \sim \pi_{h+1}} \left[ f(x_{h+1}, a) | x_h, a_h \right] \) where \( f : \mathcal{X} \times \mathcal{A} \rightarrow [0, 1] \) and a policy \( \pi_{h+1} : \mathcal{X} \rightarrow \Delta(\mathcal{A}) \).

**Proof.** For state-value function \( f \), we have

\[
E \left[ f(x_{h+1}) | x_h, a_h \right] = \int f(x_{h+1}) T_h(x_{h+1} | x_h, a_h) d(x_{h+1})
\]

\[
= \int f(x_{h+1}) \left\langle \phi_h^*(x_h, a_h), \mu_h^*(x_{h+1}) \right\rangle d(x_{h+1})
\]

\[
= \left\langle \phi_h^*(x_h, a_h), \int f(x_{h+1}) \mu_h^*(x_{h+1}) d(x_{h+1}) \right\rangle
\]

\[
= \left\langle \phi_h^*(x_h, a_h), \theta_f^* \right\rangle,
\]

where \( \theta_f^* := \int f(x_{h+1}) \mu_h^*(x_{h+1}) d(x_{h+1}) \) is a function of \( f \). Additionally, we obtain \( \|\theta_f^*\| \leq \sqrt{d} \) from Definition 1.

For Q-value function \( f \), we similarly have

\[
E_{a \sim \pi_{h+1}} \left[ f(x_{h+1}, a) | x_h, a_h \right] = \left\langle \phi_h^*(x_h, a_h), \theta_f^* \right\rangle,
\]

where \( \theta_f^* := \int f(x_{h+1}, a_{h+1}) \pi(a_{h+1} | x_{h+1}) \mu_h^*(x_{h+1}) d(x_{h+1}) d(a_{h+1}) \) and \( \|\theta_f^*\| \leq \sqrt{d} \). \qed
H.2 Deviation bound for regression with squared loss

In this section, we derive a generalization error bound for squared loss for a class \( \mathcal{F} \) which subsumes the discriminator classes \( \mathcal{F}_h \) and \( \mathcal{G}_h \) in the main text. When we apply Lemma 23, \((x^{(i)}, a^{(i)}, x^{(i)})\) tuples usually stands for \((x^{(i)}_h, a^{(i)}_h, x^{(i)}_{h+1})\) tuples, and function classes \( \Phi \) and \( \Phi' \) usually refers to \( \Phi_h \) and \( \Phi_{h+1} \). In the proof of Lemma 23, we abuse the notation of \( \mathcal{F}, \mathcal{G}, \Phi \) and \( \Phi' \), and they are different from \( \mathcal{F}_h, \mathcal{G}_h, \Phi_h \) and \( \Phi \) in the main text.

**Lemma 23.** For a dataset \( \mathcal{D} := \{(x^{(i)}, a^{(i)}, x^{(i)})\}_{i=1}^n \sim \rho \), finite feature classes \( \Phi \) and \( \Phi' \) and finite reward function class \( \mathcal{R} : \mathcal{X} \times \mathcal{A} \to [0, 1] \), we can show that, with probability at least \( 1 - \delta \):

\[
\left| \mathcal{L}_\rho(\phi, w, f) - \mathcal{L}_\rho(\phi^*, \theta^*_f, f) - \left( \mathcal{L}_\mathcal{D}(\phi, w, f) - \mathcal{L}_\mathcal{D}(\phi^*, \theta^*_f, f) \right) \right| \\
\leq \frac{1}{2} \left( \mathcal{L}_\rho(\phi, w, f) - \mathcal{L}_\rho(\phi^*, \theta^*_f, f) \right) + \frac{32d(B + L \sqrt{d})^2 \log \frac{2n|\Phi||\Phi'||\mathcal{R}|}{\delta}}{n}
\]

for all \( \phi \in \Phi, \|w\|_2 \leq B \) and function \( f : \mathcal{X} \to [0, 1] \) in class \( \mathcal{F} := \{ f(x') = \text{clip}([0, L], \mathbb{E}_{a \sim \pi}(x') [R(x', a') + \langle \phi'(x', a'), \theta \rangle]) : \phi' \in \Phi', \|\theta\|_2 \leq B, R \in \mathcal{R} \} \) for any policy \( \pi' \) over \( x' \).

**Proof.** Consider a function \( f' \in \mathcal{F} \) such that \( f(x') = \text{clip}([0, L], \mathbb{E}[R(x', a) + \langle \phi'(x', a), \theta \rangle]) \). Applying Lemma 1, we know that for every such \( f' \), there exists some \( \theta^*_f \), s.t. \( \mathbb{E}[f'(x)|x,a] = \langle \phi^*(x,a), \theta^*_f \rangle \) and \( \|\theta^*_f\| \leq L \sqrt{d} \).

To begin, we introduce notation for the discriminator class with a single reward function \( R \) as \( \mathcal{F}(R) := \{ f(x') = \text{clip}([0, L], \mathbb{E}_{a \sim \pi}(x') [R(x', a') + \langle \phi'(x', a'), \theta \rangle]) : \phi' \in \Phi', \|\theta\|_2 \leq B, R \in \mathcal{R} \} \).

We first give a high probability bound on the following deviation term:

\[
\left| \mathcal{L}_\rho(\phi, w, f) - \mathcal{L}_\rho(\phi^*, \theta^*_f, f) - \left( \mathcal{L}_\mathcal{D}(\phi, w, f) - \mathcal{L}_\mathcal{D}(\phi^*, \theta^*_f, f) \right) \right| .
\]

Let \( g(x,a) = \langle \phi(x,a), w \rangle \) and \( \tilde{g}(x,a) = \langle \phi^*(x,a), \tilde{\theta}_f \rangle \). For the random variable \( Y := (g(x,a) - f(x',a'))^2 - (\tilde{g}(x,a) - f(x',a'))^2 \), we have:

\[
\mathbb{E}[Y] = \mathbb{E} \left[ (g(x,a) - f(x',a'))^2 - (\tilde{g}(x,a) - f(x',a'))^2 \right] \\
= \mathbb{E} \left[ (g(x,a) + \tilde{g}(x,a) - 2 f(x',a')) (g(x,a) - \tilde{g}(x,a)) \right] \\
= \mathbb{E} \left[ (g(x,a) + \tilde{g}(x,a) - 2 \langle \phi^*, \theta^*_f \rangle - \tilde{g}(x,a) + \text{noise}(x,a,x',a')) (g(x,a) - \tilde{g}(x,a)) \right] \\
= \mathbb{E} \left[ (g(x,a) - \tilde{g}(x,a))^2 - 2 \langle \phi^*, \theta^*_f \rangle - \tilde{g}(x,a) \rangle (g(x,a) - \tilde{g}(x,a)) \right].
\]

Here the expectation is taken according to the distribution \( \rho \). In the second last equality, for sample \( (x,a,x',a') \), we denote \( f(x',a') = \mathbb{E}[f(x',a' | x,a)] \) as noise\( (x,a,x',a') \). The last equality is due to the fact that

\[
\mathbb{E}[	ext{noise}(x,a,x',a') (g(x,a) - \tilde{g}(x,a))] = \mathbb{E}_{x,a} \mathbb{E}_{x',a' | x,a} [	ext{noise}(x,a,x',a')(g(x,a) - \tilde{g}(x,a))] = 0.
\]

Noticing the approximation assumption of \( \tilde{\theta}_f \), and \( g(x,a) \) and \( \tilde{g}(x,a) \) is bounded by \([B, B]\) and \([-L \sqrt{d}, L \sqrt{d}]\) respectively, we have

\[
\left| \mathbb{E}[Y] - \mathbb{E} \left[ (g(x,a) - \tilde{g}(x,a))^2 \right] \right| \leq 2 \|g - \tilde{g}\|_\infty \|\langle \phi^*, \theta^*_f \rangle - \tilde{\theta}_f \|_\infty \leq 2 (B + L \sqrt{d}) \gamma.
\]
Next, for the variance of the random variable, we have:

\[
\mathbb{V}[Y] \leq \mathbb{E}[Y^2] = \mathbb{E}\left[(g(x, a) + \tilde{g}(x, a) - 2f(x', a'))^2 (g(x, a) - \tilde{g}(x, a))^2\right]
\]

\[
\leq 4(B + L \sqrt{d})^2 \mathbb{E}\left[(g(x, a) - \tilde{g}(x, a))^2\right]
\]

\[
\leq 4(B + L \sqrt{d})^2 \mathbb{E}[Y] + 8(B + L \sqrt{d})^3 \gamma.
\]

Noticing \(Y \in [-(B + L \sqrt{d})^2, (B + L \sqrt{d})^2]\) and applying Bernstein’s inequality, with probability at least 1 - \(\delta'/2\), we can bound the deviation term above as:

\[
\mathbb{E}(\mathbb{V}[Y] \log \frac{2}{\delta}) + \frac{4(B + L \sqrt{d})^2 \log \frac{2}{\delta}}{3n}
\]

\[
\leq \frac{8(B + L \sqrt{d})^2 \mathbb{E}[Y] \log \frac{2}{\delta}}{n} + \left(16(B + L \sqrt{d})^3 \gamma\right) \log \frac{2}{\delta} + \frac{4(B + L \sqrt{d})^2 \log \frac{2}{\delta}}{3n}
\]

\[
\frac{8(B + L \sqrt{d})^2 \mathbb{E}[Y] \log \frac{2}{\delta}}{n} + \left(16(B + L \sqrt{d})^3 \gamma\right) \log \frac{2}{\delta} + \frac{4(B + L \sqrt{d})^2 \log \frac{2}{\delta}}{3n}
\]

\[
\frac{8(B + L \sqrt{d})^2 \mathbb{E}[Y] \log \frac{2}{\delta}}{n} + \left(16(B + L \sqrt{d})^3 \gamma\right) \log \frac{2}{\delta} + \frac{4(B + L \sqrt{d})^2 \log \frac{2}{\delta}}{3n}
\]

where in the last inequality is obtained by choosing \(\gamma = \frac{(B + L \sqrt{d})}{n}\).

Further, consider a finite point-wise cover of the function class \(G := \{g(x, a) = \langle \phi(x, a), w \rangle : \phi \in \Phi, \|w\|_2 \leq B\}\). Note that, with a \(\ell_2\)-cover \(\mathcal{W}\) of \(\mathcal{W} = \{\|w\|_2 \leq B\}\) at scale \(\gamma\), we have for all \((x, a)\) and \(\phi \in \Phi\), there exists \(\tilde{w} \in \mathcal{W}, \|\langle \phi(x, a), w - \tilde{w} \rangle\| \leq \gamma\). Similarly, for any \(f \in \mathcal{F}(R)\), we cover the linear term in \(\mathcal{F}(R)\). We again choose \(\Theta\) as an \(\ell_2\)-cover of the set \(\{\theta \in \mathbb{R}^d : \|\theta\|_2 \leq B\}\) at scale \(\gamma\). For all \(f \in \mathcal{F}(R)\), we know that there exists some \(\phi'\) so that \(f(\cdot) = \text{clip}_{[0, L]}(\mathbb{E}_{a' \sim a'}[R(\cdot, a') + \langle \phi'(\cdot, a'), \theta \rangle]) \in \mathcal{F}(R)\). Since there exists \(\tilde{\theta} \in \Theta\) such that \(\|\tilde{\theta} - \theta\|_2 \leq \gamma\), we know that we can pick \(\tilde{f} = \text{clip}_{[0, L]}(\mathbb{E}_{a' \sim a'}[R(\cdot, a') + \langle \phi'(\cdot, a'), \tilde{\theta} \rangle])\) (which is in our covering set) and get \(\left|\langle \phi(x, a), \tilde{\theta}_f - \theta_{f}^* \rangle\right| = \left|\mathbb{E}\left[f(x'|x, a)\right] - \mathbb{E}[\tilde{f}(x'|x, a)]\right| \leq \|\tilde{f} - f\|_\infty \leq \gamma\) (here, we use \(\tilde{\theta}_f = \theta_{f}^*\)). Via standard argument, we can set \(|\Theta| = \left(\frac{2B}{\gamma}\right)^d\) and \(|\mathcal{W}| = \left(\frac{2B}{\gamma}\right)^d\), which implies \(|\Theta| \leq (2n)^d\) and \(|\mathcal{W}| \leq (2n)^d\).

Thus, applying a union bound over elements in \(\mathcal{W}, \Theta, \Phi, \Phi'\) and \(\mathcal{R}\), with probability 1 - \(\Phi'\|\mathcal{W}\|\Theta\|\mathcal{R}\|\delta'\),
For any sequence of vectors \( \phi, \phi^* \in \Phi \) and \( f \in \mathcal{F} \), we have:

\[
|L_\rho(\phi, w) - L_\rho(\phi^*, \theta^*_f, f) - (L_\mathcal{D}(\phi, w) - L_\mathcal{D}(\phi^*, \theta^*_f, f))| \\
\leq \sqrt{8(B + \sqrt{d})^2 \mathbb{E}[Y_w]} \log \frac{2}{\delta} + \frac{4B + L \sqrt{d}}{n} + \frac{4B + L \sqrt{d}}{n} \log \frac{2}{\delta} + \frac{4B + L \sqrt{d}}{n} \sqrt{\log \frac{2}{\delta}}
\]

where we add subscript to \( Y \) to distinguish \( Y_w := (\langle \phi(x, a), \bar{w} \rangle - f(x', a') - (\bar{g}(x, a) - f(x', a'))^2 \) from \( Y_w := (\langle \phi(x, a), \bar{w} \rangle - f(x', a') - (\bar{g}(x, a) - f(x', a'))^2 \).

Finally, setting \( \delta = \delta'/(\|\phi(\|\mathcal{F}(\|\mathcal{W})\|\|\mathcal{R})\| \), we get \( \frac{2}{\delta} \leq \log \frac{2(2n)^2d|\phi(\|\mathcal{F}(\|\mathcal{W})\|\|\mathcal{R})|}{\delta} \leq 2d \log \frac{2n|\phi(\|\mathcal{F}(\|\mathcal{W})\|\|\mathcal{R})|}{\delta}. \)

This completes the proof.

### H.3 Generalized elliptic potential lemma

**Lemma 24** (Generalized elliptic potential lemma, adapted from Proposition 1 of Carpentier et al. (2020)).

For any sequence of vectors \( \theta_1^*, \theta_2^*, \ldots, \theta_T^* \in \mathbb{R}^{d \times T} \) where \( \|\theta_T^*\| \leq \sqrt{d} \), for \( \lambda \geq L^2d \), we have:

\[
\sum_{t=1}^{T} \|\Sigma_{t-1}^{-1}\theta_t^*\|_2 \leq 2\sqrt{\frac{dT}{\lambda}}.
\]

**Proof.** Proposition 1 from Carpentier et al. (2020) shows that for any bounded sequence of vectors \( \theta_1^*, \theta_2^*, \ldots, \theta_T^* \in \mathbb{R}^{d \times T} \), we have:

\[
\sum_{t=1}^{T} \|\Sigma_{t-1}^{-1}\theta_t^*\|_2 \leq \sqrt{\frac{dT}{\lambda}}.
\]

Now, we have:

\[
\Sigma_t = \Sigma_{t-1} + \theta_t^*\theta_t^* \preceq \Sigma_{t-1} + \lambda I_{d \times d} \preceq 2\Sigma_{t-1}
\]

where we use the fact that \( \|\theta_t^*\theta_t^*\|_2 \leq L^2d \leq \lambda \). Using this relation, we can show the property that for any vector \( x \in \mathbb{R}^d \), \( 4x^\top \Sigma_{t-1}^{-1}x \geq x^\top \Sigma_{t-1}^{-2}x \).

First noticing the above p.s.d. dominance inequality, we have \( I_{d \times d}/2 \preceq \Sigma_t^{-1/2}\Sigma_t^{-1/2} \preceq \Sigma_t^{-1/2} \). Therefore, all the eigenvalues of \( \Sigma_t^{-1/2}\Sigma_t^{-1/2} \) (thus \( \Sigma_t^{-1/2} \)) are no less than 1/2. Applying SVD decomposition, we can get all eigenvalues of matrix \( \Sigma_{t-1}^{-1}2\Sigma_{t-1}^{-1} = (\Sigma_{t-1}^{-1})^\top (\Sigma_{t-1}^{-1}) \) are no less than 1/4. Then consider any vector \( y \in \mathbb{R}^d \), we have \( 4y^\top \Sigma_{t-1}^{-2}y \geq y^\top y \). Let \( x = \Sigma_{y-1}^{-1}y \), we get this property.

Applying the above result, we finally have the following:

\[
\sum_{t=1}^{T} \|\Sigma_t^{-1}\theta_{t+1}^*\|_2 \leq 2\sum_{t=1}^{T} \|\Sigma_t^{-1}\theta_t^*\|_2 \leq 2\sqrt{\frac{dT}{\lambda}}. \]

\[\square\]
H.4 Covering lemma for the elliptical reward class

In this part, we provide the statistical complexity of the elliptical reward class. The result is used when we analyze the elliptical planner.

Lemma 25 (Covering lemma for the elliptical reward class). For the elliptical reward class \( R_h := \{ \phi_h^\top \Gamma^{-1} \phi_h : \phi_h \in \Phi_h, \Gamma \in \mathbb{R}^{d \times d}, \lambda_{\min}(\Gamma) \geq 1 \} \), where \( h \in [H] \), there exists a \( \gamma \)-cover \( C_{R_h} \) of size \( |\Phi_h|(2\sqrt{d}/\gamma)^d \).

Proof. Firstly, for any \( \Gamma \in \mathbb{R}^{d \times d} \) with \( \lambda_{\min}(\Gamma) \geq 1 \), applying matrix norm inequality yields \( \|\Gamma\|_F \geq \sqrt{d} \). Further, we have

Next, consider the matrix class \( \bar{A} := \{ A \in \mathbb{R}^{d \times d} : \|A\|_F \leq \sqrt{d} \} \). From the definition of the Frobenius norm, for any \( A \in \bar{A} \) and any \((i, j)\)-th element, we have \( |A_{ij}| \leq \sqrt{d} \). Applying the standard covering argument for each of the \( d^2 \) elements, there exists a \( \gamma \)-cover of \( \bar{A} \), whose size is upper bounded by \((2\sqrt{d}/\gamma)^d \). Denote this \( \gamma \)-cover as \( \bar{A}_\gamma \). For any \( \Gamma \in \mathbb{R}^{d \times d} \) with \( \lambda_{\min}(\Gamma) \geq 1 \), we can pick some \( A \in \bar{A}_\gamma \) so that \( \|\Gamma^{-1} - A\Gamma\|_F \leq \gamma \).

Then for any \( \phi_h \in \Phi_h \), we have

This implies that \( C_{R_h} := \{ \phi_h^\top A \phi_h : \phi_h \in \Phi_h, A \in \bar{A}_\gamma \} \) is a \( \gamma \)-cover of \( R_h \), which completes the proof. \( \square \)