
Provably Efficient Q -learning with Function Approximation via Distribution Shift Error Checking Oracle

Simon S. Du

Institute for Advanced Study
ssdu@ias.edu

Yuping Luo

Princeton University
yupingl@cs.princeton.edu

Ruosong Wang

Carnegie Mellon University
ruosongw@andrew.cmu.edu

Hanrui Zhang

Duke University
hrzhang@cs.duke.edu

Abstract

Q -learning with function approximation is one of the most popular methods in reinforcement learning. Though the idea of using function approximation was proposed at least 60 years ago [27], even in the simplest setup, i.e., approximating Q -functions with linear functions, it is still an open problem how to design a provably efficient algorithm that learns a near-optimal policy. The key challenges are how to efficiently explore the state space and how to decide when to stop exploring *in conjunction with* the function approximation scheme.

The current paper presents a provably efficient algorithm for Q -learning with linear function approximation. Under certain regularity assumptions, our algorithm, **Difference Maximization Q -learning (DMQ)**, combined with linear function approximation, returns a near-optimal policy using polynomial number of trajectories. Our algorithm introduces a new notion, the **Distribution Shift Error Checking (DSEC) oracle**. This oracle tests whether there exists a function in the function class that predicts well on a distribution \mathcal{D}_1 , but predicts poorly on another distribution \mathcal{D}_2 , where \mathcal{D}_1 and \mathcal{D}_2 are distributions over states induced by two different exploration policies. For the linear function class, this oracle is equivalent to solving a top eigenvalue problem. We believe our algorithmic insights, especially the DSEC oracle, are also useful in designing and analyzing reinforcement learning algorithms with general function approximation.

1 Introduction

Q -learning is a foundational method in reinforcement learning [35] and has been successfully applied in various domains. Q -learning aims at learning the optimal state-action value function (Q -function). Once we have learned the Q -function, at every state, we can just greedily choose the action with the largest Q value, which is guaranteed to be an optimal policy.

Although being a fundamental method, theoretically, we only have a good understanding of Q -learning in the tabular setting. Strehl et al. [30] and Jin et al. [18] showed with proper exploration techniques, one can obtain a near-optimal Q -function (and so a near-optimal policy) using polynomial number of trajectories, in terms of number of states, actions and planning horizon. While these analyses provide valuable insights, they are of limited practical importance because the number of states in most applications is enormous. Even worse, it has been proved that in the tabular setting, the

number of trajectories needed to learn a near-optimal policy scales at least linearly with the number of states [16].

To resolve this problem, we need reinforcement learning methods that generalize, which, for Q -learning methods, is to constrain Q -function to a pre-specified function class, e.g., linear functions or neural networks. The basic assumption of this function approximation scheme is that the true Q -function lies in the function class. A natural problem is:

Can we design provably efficient Q -learning algorithms with function approximation?

Indeed, this is one of the major open problems in reinforcement learning [32]. The idea of using function approximation was proposed at least 60 years ago [27], where linear functions are used to approximate the value functions in playing checkers. However, even in the most basic setting, Q -learning with linear function approximation, there is no provably efficient algorithm in the general stochastic setting.

The key challenges are how to 1) efficiently explore the state space to learn a good predictor that generalizes across states and 2) decide when to stop exploring. In order to deal with these challenges, we need to exploit the fact that the true Q -function belongs to a pre-specified function class.

Our Contributions Our main theoretical contribution is a provably efficient algorithm for Q -learning with linear function approximation in the episodic Markov decision process (MDP) setting.

Theorem 1.1 (Main Theorem (informal)). *Suppose the Q -function is linear. Then under certain regularity assumptions, Algorithm 1, **Difference Maximization Q -learning (DMQ)** returns an ϵ -suboptimal policy π using $\text{poly}(1/\epsilon)$ number of trajectories.*

Our algorithm works for episodic MDPs with general stochastic transitions. In contrast, previous algorithms only work for deterministic systems, or rely on strong assumptions, e.g., a sufficiently good exploration policy is given. See Section 2 for more discussion. Our main assumption is that the Q -function is linear. Note this is somehow a necessary assumption because otherwise one should not use linear function approximation in the first place.

Before getting into details, we first give an overview of our main techniques. As we have discussed, the main technical challenge is to design an efficient exploration algorithm, and decide when to stop exploring. Our main algorithmic contribution is to introduce a new notion, the Distribution Shift Error Checking (DSEC) oracle (cf. Oracle 4.1 and Oracle 4.2). Given two distributions \mathcal{D}_1 and \mathcal{D}_2 , this oracle returns True if there exists a function in the pre-specified function class which predicts well on \mathcal{D}_1 but predicts poorly on \mathcal{D}_2 . We will show that this is an extremely useful notion. If the oracle returns False, then our learned predictor performs well on both distributions. If the oracle returns True, we know \mathcal{D}_2 contains information that we can explore, which implies the policy that generates \mathcal{D}_2 is a valuable exploration policy. We will discuss the DSEC oracle in more detail in Section 4.

With this oracle at hand, a natural question is how many times this oracle will return True, as we will not stop exploring if it always returns True. A technical contribution of this paper is to show for the linear function class, this oracle will only return True at most polynomial number of times. At a high level, whenever the oracle returns True, it means we will learn something new from \mathcal{D}_2 . However, since the complexity of the function class is bounded, we cannot learn new things too many times. Formally, we use a potential function argument to make this intuition rigorous (cf. Lemma A.5).

1.1 Organization

This paper is organized as follows. In Section 2, we review related work. In Section 3, we introduce necessary notations, definitions and assumptions. In Section 4, we describe the DSEC oracle in detail. In Section 5, we present our general algorithm for Q -learning with function approximation. In Section 6, we instantiate the general algorithm to the linear function approximation case, and present our main theorem. We conclude and discuss future works in Section 7. All technical proofs are deferred to the supplementary material.

2 Related Work

Classical theoretical reinforcement learning literature studies asymptotic behavior of concrete algorithms. The most related work is [24], which studies an online Q -learning algorithm with a fixed exploration policy. They showed that the estimated Q -function converges to the true Q -function asymptotically. Recently, Zou et al. [39] derived finite sample bounds for the same setting. The major drawback of these works is that they put strong assumptions on the fixed exploration policy. For example, Zou et al. [39] require that the covariance matrix induced by the exploration policy has lower bounded least eigenvalue. In general, it is hard to verify whether a policy has such benign properties.

While it is challenging to design efficient algorithms for Q -learning with function approximation, in the tabular setting, exploration becomes much easier, as one can first estimate the transition probabilities and then design exploration policies accordingly. There is a substantial body of work on tabular reinforcement learning [2, 16, 19, 5, 21, 10]. For Q -learning, Strehl et al. [30] introduced the delayed Q -learning algorithm which has $O(T^{4/5})$ regret bound. A recent work by Jin et al. [18] gave a UCB-based algorithm which enjoys $O(\sqrt{T})$ regret bound. More recent papers provided refined analyses that exploit benign properties of the MDP, e.g., the gap between the optimal action and the rest [28, 38], which our algorithm also utilizes. However, it is hard to generalize the exploration techniques in these previous works, since they all rely on the fact that the total number of states is finite.

Recently, exploration algorithms are proposed for Q -learning with function approximation. Osband et al. [25] proposed a Thompson-sampling based method for the linear function class. Later works further generalized sampling-based algorithms to Q -functions with neural network parameterization [6, 23, 13]. However, none of these works have polynomial sample complexity guarantees. Pazis and Parr [26] gave a nearest-neighbor-based algorithm for exploration in continuous state space. However, in general this type of algorithms has exponential dependence on the state dimension.

The seminal work by Wen and Van Roy [36] proposed an algorithm, optimistic constraint propagation (OCP), which enjoys polynomial sample complexity bounds for a family of Q -function classes, including the linear function class as a special case. However, their algorithm can only deal with deterministic systems, i.e., both transition dynamics and rewards are deterministic. A line of recent papers study Q -learning in the general state-action metric space [37, 29]. However, due to the generality, the sample complexity has exponential dependence on the dimension.

Finally, a recent series of work introduced *contextual decision processes* (CDPs) [22, 17, 9, 31, 11] and developed algorithms with polynomial sample complexity guarantees. Our paper is not directly comparable with these results, since they can deal with general function classes. In some cases, the function approximation is even not for the Q -function, but for modeling the map from the observed state to hidden states [11]. The result in [17] also applies to our setting. However, their bound depends on both the function class complexity and a quantity called the Bellman rank. Conceptually, since our bound does not depend on the Bellman rank, our result thus demonstrates that the function class complexity alone is enough for efficient learning.

3 Preliminaries

Notations We begin by introducing necessary notations. We write $[h]$ to denote the set $\{1, \dots, h\}$. For any finite set S , we write $\text{unif}(S)$ to denote the uniform distribution over S and $\triangle(S)$ to denote the probability simplex. Let $\|\cdot\|_2$ denote the Euclidean norm of a finite-dimensional vector in \mathbb{R}^d . For a symmetric matrix A , let $\|A\|_{\text{op}}$ denote its operator norm and $\lambda_i(A)$ denote its i -th eigenvalue. Throughout the paper, all sets are multisets, i.e., a single element can appear multiple times.

Markov Decision Processes (MDPs) Let $\mathcal{M} = (\mathcal{S}, \mathcal{A}, H, P, R)$ be an MDP, where \mathcal{S} is the (possibly uncountable) state space, \mathcal{A} is the finite action space with $|\mathcal{A}| = K$, $H \in \mathbb{Z}_+$ is the planning horizon, $P : \mathcal{S} \times \mathcal{A} \rightarrow \triangle(\mathcal{S})$ is the transition function and $R : \mathcal{S} \times \mathcal{A} \rightarrow \triangle(\mathbb{R})$ is the reward distribution.

A (stochastic) policy $\pi : \mathcal{S} \rightarrow \Delta(\mathcal{A})$ prescribes a distribution over actions for each state. Without loss of generality, we assume a fixed start state s_1 .¹ The policy π induces a random trajectory $s_1, a_1, r_1, s_2, a_2, r_2, \dots, s_H, a_H, r_H$ where $r_1 \sim R(s_1, a_1)$, $s_2 \sim P(s_1, a_1)$, $a_2 \sim \pi(s_2)$, etc. For a given policy π , we use \mathcal{D}_h^π to denote the distribution over \mathcal{S}_h induced by executing policy π .

To streamline our analysis, we denote $\mathcal{S}_h \subseteq \mathcal{S}$ to be the set of states at level h . Similar to previous theoretical reinforcement learning results, we also assume $r_h \geq 0$ for all $h \in [H]$ and $\sum_{h=1}^H r_h \leq 1$ [17]. Our goal is to find a policy π that maximizes the expected reward $\mathbb{E} \left[\sum_{h=1}^H r_h \mid \pi \right]$. We use π^* to denote the optimal policy.

Given a policy π , a level $h \in [H]$ and a state-action pair $(s, a) \in \mathcal{S}_h \times \mathcal{A}$, the Q -function is defined as $Q^\pi(s, a) = \mathbb{E} \left[\sum_{h'=h}^H r_{h'} \mid s_h = s, a_h = a, \pi \right]$. It will also be useful to define the value function of a given state $s \in \mathcal{S}_h$ as $V^\pi(s) = \mathbb{E} \left[\sum_{h'=h}^H r_{h'} \mid s_h = s, \pi \right]$. For simplicity, we denote $Q^*(s, a) = Q^{\pi^*}(s, a)$ and $V^* = V^{\pi^*}(s)$. Recall that if we know Q^* , we can just choose the action greedily: $\pi^*(s) = \operatorname{argmax}_{a \in \mathcal{A}} Q^*(s, a)$. In this paper, we make the following assumption about the variation of the suboptimality of policies [12].

Assumption 3.1 (Bounded Coefficient of Variation of Policy Sub-optimality). *There exists a constant $1 \leq C < \infty$, such that for any fixed level $h \in [H]$ and deterministic policy π ,*

$$\mathbb{E}_{s \sim \mathcal{D}_h^\pi} \left[|V^\pi(s) - V^*(s)|^2 \right] \leq C \left(\mathbb{E}_{s \sim \mathcal{D}_h^\pi} [|V^\pi(s) - V^*(s)|] \right)^2.$$

Intuitively, this assumption says the variation due to the randomness over states is not too large comparing to the mean. For example, if the transition is deterministic, then this assumption holds with $C = 1$.

Our paper also relies on the following fine-grained characterization of the MDP.

Definition 3.1 (Suboptimality Gaps). *Given $s \in \mathcal{S}$ and $a \in \mathcal{A}$, the gap is defined as $\operatorname{gap}(s, a) = V^*(s) - Q^*(s, a)$. The minimum gap is defined as $\gamma \triangleq \min_{s \in \mathcal{S}, a \in \mathcal{A}} \{\operatorname{gap}(s, a) : \operatorname{gap}(s, a) > 0\}$.*

This notion has been extensively studied in the bandit literature to obtain fine-grained bounds [4]. Recently, Simchowitz et al. [28] derived regret bounds in tabular MDPs based on this notion. In this paper we assume $\gamma > 0$, and the sample complexity of our algorithm depends polynomially on $1/\gamma$. Notice that assuming γ is strictly positive is not a restrictive assumption for the *finite action setting* considered in this paper. First, in the contextual linear bandit literature, this assumption is widely discussed. See, e.g., [1, 8]. The notion, context, in the bandit literature is essentially $\phi(s)$ in our paper and the number of contexts can also be infinite. Second, there are many natural environments in RL which satisfy this assumption. For example, in many environments, states can be classified as good states and bad states. In these environments, an agent can obtain a reward only if it is in a good state. There are also two kinds of actions: good actions and bad actions. If the agent is in a good state and chooses a good action, the agent will transit to a good state. If the agent chooses a bad action, the agent will transit to a bad state. If the agent is in a bad state, whatever action the agent chooses, the agent will transit to a bad state. Note that for this kind of environments, there is a strictly positive gap between good actions and bad actions when the agent is in good states and there is no difference between good actions and bad actions when the agent is in bad states. In this case, γ is strictly positive, since by Definition 3.1, we take the minimum over all state-action pairs with *strictly* positive gap. These environments are natural generalizations of the combination lock environment [20]. Some Atari games, e.g. Freeway, have a similar flavor as these environments.

Function Approximation When the state space is large, we need structures on the state space so that reinforcement learning methods can generalize. We constrain the optimal Q -function to a pre-specified function class \mathcal{Q} [7], e.g., the class of linear functions. In this paper we associate each $h \in [H]$ and $a \in \mathcal{A}$ with a Q -function $f_h^a \in \mathcal{Q}$. We make the following assumption.

Assumption 3.2. *For every $(h, a) \in [H] \times \mathcal{A}$, its associated optimal Q -function is in \mathcal{Q} .*

¹Some papers assume the starting state is sampled from a distribution P_1 . Note this is equivalent to assuming a fixed state s_1 , by setting $P(s_1, a) = P_1$ for all $a \in \mathcal{A}$ and now our s_2 is equivalent to the starting state in their assumption.

This is a widely used assumption in the theoretical reinforcement learning literature [17]. Note that without this assumption, we cannot hope to obtain optimal policy using functions in \mathcal{Q} as the Q -function.

The focus of this paper is about linear function class which is one of the most popular function classes used in practice. This function class depends on a feature extractor $\phi : \mathcal{S} \rightarrow \mathbb{R}^d$ which can be a hand-crafted feature extractor or a pre-trained neural network that transforms a state to a d -dimension embedding. For $s_h \in \mathcal{S}_h$ and $a \in \mathcal{A}$, our estimated optimal Q -function admits the form $f_h^a(s) = \phi(s)^\top \hat{\theta}_h^a$ where $\hat{\theta}_h^a \in \mathbb{R}^d$ only depends on the level $h \in [H]$ and $a \in \mathcal{A}$. Therefore, we only need to learn $K \cdot H$ d -dimension vectors (linear coefficients), since by Assumption 3.2, for each $h \in [H]$ and $a \in \mathcal{A}$, there exists $\theta_h^a \in \mathbb{R}^d$ such that for all $s_h \in \mathcal{S}_h$, $Q^*(s_h, a) = \phi(s_h)^\top \theta_h^a$.

The aim of this paper is to obtain polynomial sample complexity bounds. To this end, we also need some regularity conditions.

Assumption 3.3. For all $s \in \mathcal{S}$, its feature is bounded $\|\phi(s)\|_2 \leq 1$. For all $h \in [H]$, $a \in \mathcal{A}$, the true linear predictor is bounded $\|\theta_h^a\|_2 \leq 1$.

4 Distribution Shift Error Checking Oracle

As we have discussed in Section 1, in reinforcement learning, we often need to know whether a predictor learned from samples generated from one distribution \mathcal{D}_1 can predict well on another distribution \mathcal{D}_2 . This is related to off-policy learning for which one often needs to bound the probability density ratio between \mathcal{D}_1 and \mathcal{D}_2 on all state-action pair. When function approximation scheme is used, we naturally arrive at the following oracle.

Oracle 4.1 (Distribution Shift Error Checking Oracle $(\mathcal{D}_1, \mathcal{D}_2, \epsilon_1, \epsilon_2, \Lambda)$). For two given distributions $\mathcal{D}_1, \mathcal{D}_2$ over \mathcal{S} , two real numbers ϵ_1 and ϵ_2 , and a regularizer $\Lambda : \mathcal{Q} \times \mathcal{Q} \rightarrow \mathbb{R}$, define

$$v = \max_{f_1, f_2 \in \mathcal{Q}} \mathbb{E}_{s \sim \mathcal{D}_2} \left[(f_1(s) - f_2(s))^2 \right]$$

$$\text{s.t. } \mathbb{E}_{s \sim \mathcal{D}_1} \left[(f_1(s) - f_2(s))^2 \right] + \Lambda(f_1, f_2) \leq \epsilon_1.$$

The oracle returns True if $v \geq \epsilon_2$, and False otherwise.

To motivate this oracle, let f_2 be the optimal Q -function and f_1 is a predictor we learned using samples generated from distribution \mathcal{D}_1 . In this scenario, we know f_1 has a small expected error ϵ_1 on distribution \mathcal{D}_1 . Note since we maximize over the entire function class \mathcal{Q} , v is an upper bound on the expected error of f_1 on distribution \mathcal{D}_2 . If v is large enough, say larger than ϵ_2 , then it could be the case that we cannot predict well on distribution \mathcal{D}_2 . On the other hand, if v is small, we are certain that f_1 has small error on \mathcal{D}_2 . Here we add a regularization term $\Lambda(f_1, f_2)$ to prevent pathological cases. The concrete choice of Λ will be given later.

In practice, it is impossible to get access to the underlying distributions \mathcal{D}_1 and \mathcal{D}_2 . Thus, we use samples generated from these two distributions instead.

Oracle 4.2 (Sample-based Distribution Shift Error Checking Oracle $(\mathcal{D}_1, \mathcal{D}_2, \epsilon_1, \epsilon_2, \Lambda)$). For two set of states $\mathcal{D}_1, \mathcal{D}_2 \subseteq \mathcal{S}$, two real numbers ϵ_1 and ϵ_2 , and a regularizer $\Lambda : \mathcal{Q} \times \mathcal{Q} \rightarrow \mathbb{R}$, define

$$v = \max_{f_1, f_2 \in \mathcal{Q}} \frac{1}{|\mathcal{D}_2|} \sum_{t_i \in \mathcal{D}_2} \left[(f_1(t_i) - f_2(t_i))^2 \right]$$

$$\text{s.t. } \frac{1}{|\mathcal{D}_1|} \sum_{s_i \in \mathcal{D}_1} \left[(f_1(s_i) - f_2(s_i))^2 \right] + \Lambda(f_1, f_2) \leq \epsilon_1.$$

The oracle returns True if $v \geq \epsilon_2$ and False otherwise. If $\mathcal{D}_1 = \emptyset$, the oracle simply returns True.

An interesting property of Oracle 4.2 is that it only depends on the states and does not rely on the reward values.

5 Difference Maximization Q -learning

Now we describe our algorithm. We maintain three sets of global variables.

Algorithm 1 Difference Maximization Q -learning (DMQ)

Output: A near-optimal policy π .

- 1: **for** $h = H, H - 1, \dots, 1$ **do**
 - 2: Run Algorithm 2 on input h .
 - 3: Return $\hat{\pi}$, the greedy policy with respect to $\{f_h^a\}_{a \in \mathcal{A}, h \in [H]}$.
-

1. $\{f_h^a\}_{a \in \mathcal{A}, h \in [H]}$. These are our estimated Q -functions for all actions $a \in \mathcal{A}$ and all levels $h \in [H]$.
2. $\{\Pi_h\}_{h \in [H]}$. For each level $h \in [H]$, Π_h is a set of exploration policies for level h , which we use to collect data.
3. $\{D_h\}_{h \in [H]}$. For each $h \in [H]$, $D_h = \{s_{h,i}\}_{i=1}^N$ is a set of states in \mathcal{S}_h .

We initialize these global variables in the following manner. For $\{f_h^a\}_{a \in \mathcal{A}, h \in [H]}$, we initialize them arbitrarily. For each $h \in [H]$, we initialize Π_h to be a single purely random exploration policy, i.e., $\Pi_h = \{\pi\}$, where $\pi(s) = \text{unif}(\mathcal{A})$ for all $s \in \mathcal{S}$. We initialize $\{D_h\}_{h \in [H]}$ to be empty sets.

Algorithm 1 uses Algorithm 2 to learn predictors for each level $h \in [H]$. Algorithm 2 takes $h \in [H]$ as input, tries to learn predictors $\{f_h^a\}_{a \in \mathcal{A}}$ at level h . Algorithm 3 takes $h \in [H]$ and $a \in \mathcal{A}$ as inputs, and checks whether the predictors learned for later levels $h' > h$ are accurate enough under the current policy.

Now we explain Algorithm 2 and Algorithm 3 in more detail. Algorithm 2 iterates all actions, and for each action $a \in \mathcal{A}$, it uses Algorithm 3 to check whether we can learn the Q -function that corresponds to a well. After executing Algorithm 3, we are certain that we can learn f_h^a well (we will explain this in the next paragraph), and thus construct a set of new policies $\Pi_h^a = \{\pi_h^a\}_{\pi_h \in \Pi_h}$, in the following way. For each policy $\pi_h \in \Pi_h$, we define π_h^a as

$$\pi_h^a(s_{h'}) = \begin{cases} \pi_h(s_{h'}) & \text{if } h' < h \\ a & \text{if } h' = h \\ \arg\max_{a' \in \mathcal{A}} f_{h'}^{a'}(s_{h'}) & \text{if } h' > h \end{cases} \quad (1)$$

This policy uses π_h as the roll-in policy till level h , chooses action a at level h and uses greedy policy with respect to $\{f_{h'}^a\}_{h' > h, a \in \mathcal{A}}$, the current estimates of Q -functions at level $h + 1, \dots, H$ as the roll-out policy. In each iteration, we sample one policy π uniformly at random from Π_h^a , and use it to collect (s, y) , where $s \in \mathcal{S}_h$ and $y \in \mathbb{R}$ is the on-the-go reward. In total we collect a dataset D_h^a with size $N \cdot |\Pi_h^a|$, and we use regression to learn a predictor on these data. Formally, we calculate

$$f_h^a = \arg\min_{f \in \mathcal{Q}} \left[\frac{1}{N \cdot |\Pi_h^a|} \sum_{(s,y) \in D_h^a} (f(s) - y)^2 + \Gamma(f) \right]. \quad (2)$$

Here, $\Gamma(f)$ represents a regularization term on f . Finally, we update D_h by using each $\pi_h \in \Pi_h$ to collect N states in \mathcal{S}_h .

Now we explain Algorithm 3. For each $\pi_h \in \Pi_h$, we use π_h^a defined in (1) to collect N trajectories. For each $h' = h + 1, \dots, H$, we set $\tilde{D}_{\pi_h^a, h'} = \{s_{h',i}\}_{i=1}^N$, where $s_{h',i}$ is the state at level h' in the i -th trajectory. Next, for each $h' = H, \dots, h + 1$, we invoke Oracle 4.2 on input $D_{h'}$ and $\tilde{D}_{\pi_h^a, h'}$. Note that $D_{h'}$ was collected when we execute Algorithm 2 to learn the predictors at level h' . The oracle will return whether our current predictors at level h' can still predict well on the distribution that generates $\tilde{D}_{\pi_h^a, h'}$. If not, then we add π_h^a to our policy set $\Pi_{h'}$, and we execute Algorithm 2 to learn the predictors at level h' once again. Note it is crucial to iterate h' from H to $h + 1$, so that we will always make sure the predictors at later levels are correct.

6 Provably Efficient Q -learning with Linear Function Approximation

Now we instantiate our algorithm to the linear function class. For the regression problem in (2), we set $\Gamma(\theta) = \lambda_{\text{ridge}} \|\theta\|_2^2$. The concrete choice of the parameter λ_{ridge} will be given later. In this case,

Algorithm 2

Input: $h \in [H]$, a target level.

- 1: **for** $a \in \mathcal{A}$ **do**
- 2: Execute Algorithm 3 on input (h, a) .
- 3: Initialize $D_h^a = \emptyset$.
- 4: Construct a policy set Π_h^a according to (1).
- 5: **for** $i = 1, \dots, N \cdot |\Pi_h^a|$ **do**
- 6: Sample $\pi \sim \text{unif}(\Pi_h^a)$.
- 7: Use π to collect (s_i, y_i) , where $s_i \in \mathcal{S}_h$ and y_i is the on-the-go reward.
- 8: Add (s_i, y_i) into D_h^a .
- 9: Learn a predictor $f_h^a = \text{argmin}_{f \in \mathcal{Q}} \left[\frac{1}{N \cdot |\Pi_h^a|} \sum_{(s,y) \in D_h^a} (f(s) - y)^2 + \Gamma(f) \right]$.
- 10: Set $D_h = \emptyset$.
- 11: **for** $\pi_h \in \Pi_h$ **do**
- 12: Use π_h to collect a set of states $\{s_{\pi_h, i}\}_{i=1}^N$, where $s_{\pi_h, i} \in \mathcal{S}_h$.
- 13: Add all states $\{s_{\pi_h, i}\}_{i=1}^N$ into D_h .

Algorithm 3

Input: target level $h \in [H]$ and an action $a \in \mathcal{A}$.

- 1: **for** $\pi_h \in \Pi_h$ **do**
- 2: Collect N trajectories using policy π_h^a defined in (1).
- 3: **for** $h' = H, H-1, \dots, h+1$ **do**
- 4: Let $\tilde{D}_{\pi_h^a, h'} = \{s_{h', i}\}_{i=1}^N$ be the states at level h' on the N trajectories collected using π_h^a .
- 5: Invoke Oracle 4.2 on input $(D_{h'}, \tilde{D}_{\pi_h^a, h'}, \frac{\epsilon_s}{|\Pi_{h'}|}, \epsilon_t, \Lambda_{\Pi_{h'}})$.
- 6: **if** Oracle 4.2 returns True **then**
- 7: $\Pi_{h'} = \Pi_{h'} \cup \{\pi_h^a\}$.
- 8: Execute Algorithm 2 on input h' .

the regression program represents the ridge regression estimator

$$\hat{\theta}_h^a = \left(\frac{1}{|D_h^a|} \sum_{(s,y) \in D_h^a} \phi(s)\phi(s)^\top + \lambda_{\text{ridge}} \cdot I \right)^{-1} \left(\frac{1}{|D_h^a|} \sum_{(s,y) \in D_h^a} y \cdot \phi(s) \right),$$

and $f_h^a(s_h) = \phi(s_h)^\top \hat{\theta}_h^a$ for $s_h \in \mathcal{S}_h$.

For Oracle 4.2, we choose $\Lambda_{\Pi_{h'}}(\theta_1, \theta_2) = \lambda_r / |\Pi_{h'}| \cdot \|\theta_1 - \theta_2\|_2^2$. The concrete choice of the parameter λ_r will be given later. Since \mathcal{Q} is the linear function class, the optimization problem is equivalent to the following program

$$\begin{aligned} & \max_{\theta_1, \theta_2} \frac{1}{|D_2|} \sum_{t_i \in D_2} ((\theta_1 - \theta_2)^\top \phi(t_i))^2 \\ & \text{s.t. } \frac{1}{|D_1|} \sum_{s_i \in D_1} ((\theta_1 - \theta_2)^\top \phi(s_i))^2 + \lambda_r / |\Pi_{h'}| \cdot \|\theta_1 - \theta_2\|_2^2 \leq \epsilon_1. \end{aligned}$$

We let $M_1 = \frac{1}{|D_1|} \sum_{s_i \in D_1} \phi(s_i)\phi(s_i)^\top + \lambda_r / |\Pi_{h'}| \cdot I$, $M_2 = \frac{1}{|D_2|} \sum_{t_i \in D_2} \phi(t_i)\phi(t_i)^\top$, and let $\tilde{\theta} \triangleq \frac{1}{\sqrt{\epsilon_1}} M_1^{1/2} (\theta_1 - \theta_2)$, then the optimization problem can be further reduced to

$$\max_{\tilde{\theta}} \tilde{\theta}^\top \left(\epsilon_1 M_1^{-\frac{1}{2}} M_2 M_1^{-\frac{1}{2}} \right) \tilde{\theta} \quad \text{s.t. } \|\tilde{\theta}\|_2 \leq 1,$$

which is equivalent to compute the top eigenvalue of $\epsilon_1 M_1^{-\frac{1}{2}} M_2 M_1^{-\frac{1}{2}}$. Therefore, the regression problem in (2) and Oracle 4.2 can be efficiently implemented. Our main result is the following theorem.

Theorem 6.1 (Provably Efficient Q -Learning with Linear Function Approximation). *Let $\epsilon \leq \text{poly}(\gamma, 1/C, 1/d, 1/H, 1/K)$ be the target accuracy parameter. Under Assumption 3.1, 3.2 and 3.3, then using at most $\text{poly}(1/\epsilon)$ trajectories, with high probability, Algorithm 1 returns a policy $\hat{\pi}$ that satisfies $V^{\hat{\pi}}(s_1) \geq V^*(s_1) - \epsilon$.*

This theorem demonstrates that if the true Q -function is linear, then it is actually possible to learn a near-optimal policy with polynomial number of samples. We refer readers to the Proof of Theorem 6.1 for the specific values of $\epsilon_t, \epsilon_s, \epsilon_N, \lambda_{\text{ridge}}, \lambda_r, N$. Furthermore, our algorithm also runs in polynomial time. Therefore, this is the first provably efficient algorithm for Q -learning with function approximation in the stochastic setting.

Now we briefly sketch the proof of Theorem 6.1. The full proof is deferred to Section A. Our proof follows directly from the design of our algorithm. First, through classical analysis of linear regression, we know the learned predictor $\hat{\theta}_h^a$ can predict well on the distribution induced by π_h^a . Second, Oracle 4.2 guarantees that if it returns False, then the learned predictors at level h' can predict well on the distribution over \mathcal{S}_h induced by the policy π_h^a . Therefore, the labels we used to learn θ_a^h have only small bias, and thus, we can learn θ_a^h well. Now the trickiest part of the proof is to show Oracle 4.2 returns True at most polynomial number of times. To establish this, for each $h \in [H]$, we construct a potential function in terms of covariance matrices induced by the policies in Π_h . We show whenever a new policy is added to Π_h , this potential function must be increased by a multiplicative factor. We further show this potential function is at always polynomially upper bounded by the size of the policy set. Therefore, we can conclude the size of Π_h is polynomially upper bounded. See Lemma A.5 for details.

7 Discussion

By giving a provably efficient algorithm for Q -learning with function approximation, this paper paves the way for rigorous studies of modern model-free reinforcement learning methods with function approximation. Now we list some future directions.

Regret Bound This paper presents a PAC bound but no regret bound. Note that we assume the gap between the on-the-go reward of the best action and the rest is strictly positive. In the tabular setting, previous work showed that under this assumption, one can obtain $\log T$ regret bound [28, 38]. We believe it would be a very strong result to prove (or disprove) $\log T$ regret bound in the setting considered in this paper.

Q -learning with General Function Class While the main theorem in this paper is about the linear function class, the DSEC oracle and the general algorithmic framework applies to any function classes. From an information-theoretic point of view, given Oracle 4.2, can we use it to design algorithms for general function class with polynomial sample complexity guarantees? For example, if the Q -function class has a bounded VC-dimension, can Algorithm 1 give a polynomial sample complexity guarantee? We believe a generalization of Lemma A.5 is required to resolve this question. Another interesting problem is to generalize our algorithm to the case that the Q -function is not exactly linear but can only be approximated by a linear function.

From the computational point of view, can we characterize the function classes for which we have an efficient solver for Oracle 4.2? For those we do not have such exact solvers, can we develop a relaxed version of Oracle 4.2 which, possibly sacrificing the sample efficiency, makes the optimization problem tractable. This idea was used in the sparse learning literature [34]. Another interesting problem is to improve the computational efficiency of our algorithm to make it fast enough to be used in practice.

Toward a Rigorous Theory for DQN Deep Q -learning (DQN) is one of the most popular model-free methods in modern reinforcement learning. Recent studies established that over-parameterized neural networks are equivalent to kernel predictors [15, 3] with multi-layer kernel functions. Since kernel predictors can be viewed as linear predictors in infinite dimensional feature spaces, can we adapt our algorithm to over-parameterized neural networks and multi-layer kernels, and prove polynomial sample complexity guarantees when, e.g., the true Q -function has a small reproducing Hilbert space norm?

Acknowledgements

The authors would like to thank Nan Jiang, Akshay Krishnamurthy, Wen Sun, Yining Wang and Lin F. Yang for useful discussions. The paper was initiated while S. S. Du was an intern at MSR NYC and a Ph.D. student at Carnegie Mellon University. Part of this work was done while S. S. Du and R. Wang were visiting Simons Institute.

References

- [1] Yasin Abbasi-Yadkori, Dávid Pál, and Csaba Szepesvári. Improved algorithms for linear stochastic bandits. In *Advances in Neural Information Processing Systems*, pages 2312–2320, 2011.
- [2] Shipra Agrawal and Randy Jia. Posterior sampling for reinforcement learning: worst-case regret bounds. In *NIPS*, 2017.
- [3] Sanjeev Arora, Simon S Du, Wei Hu, Zhiyuan Li, Ruslan Salakhutdinov, and Ruosong Wang. On exact computation with an infinitely wide neural net. *arXiv preprint arXiv:1904.11955*, 2019.
- [4] Jean-Yves Audibert and Sébastien Bubeck. Best arm identification in multi-armed bandits. In *COLT-23th Conference on learning theory-2010*, pages 13–p, 2010.
- [5] Mohammad Gheshlaghi Azar, Ian Osband, and Rémi Munos. Minimax regret bounds for reinforcement learning. *arXiv preprint arXiv:1703.05449*, 2017.
- [6] K. Azizzadenesheli, E. Brunskill, and A. Anandkumar. Efficient exploration through bayesian deep Q-networks. In *2018 Information Theory and Applications Workshop (ITA)*, pages 1–9, Feb 2018.
- [7] Dimitri P Bertsekas and John N Tsitsiklis. *Neuro-dynamic programming*, volume 5. Athena Scientific Belmont, MA, 1996.
- [8] Varsha Dani, Thomas P Hayes, and Sham M Kakade. Stochastic linear optimization under bandit feedback. In *Conference on Learning Theory*, 2008.
- [9] Christoph Dann, Nan Jiang, Akshay Krishnamurthy, Alekh Agarwal, John Langford, and Robert E Schapire. On polynomial time PAC reinforcement learning with rich observations. *arXiv preprint arXiv:1803.00606*, 2018.
- [10] Christoph Dann, Tor Lattimore, and Emma Brunskill. Unifying PAC and regret: Uniform PAC bounds for episodic reinforcement learning. In *Proceedings of the 31st International Conference on Neural Information Processing Systems, NIPS’17*, pages 5717–5727, USA, 2017. Curran Associates Inc.
- [11] Simon S Du, Akshay Krishnamurthy, Nan Jiang, Alekh Agarwal, Miroslav Dudík, and John Langford. Provably efficient RL with rich observations via latent state decoding. *arXiv preprint arXiv:1901.09018*, 2019.
- [12] Brian Everitt. *The Cambridge dictionary of statistics*. Cambridge University Press, Cambridge, UK; New York, 2002.
- [13] Meire Fortunato, Mohammad Gheshlaghi Azar, Bilal Piot, Jacob Menick, Matteo Hessel, Ian Osband, Alex Graves, Volodymyr Mnih, Remi Munos, Demis Hassabis, Olivier Pietquin, Charles Blundell, and Shane Legg. Noisy networks for exploration. In *International Conference on Learning Representations*, 2018.
- [14] Daniel Hsu, Sham M Kakade, and Tong Zhang. Random design analysis of ridge regression. In *Conference on learning theory*, pages 9–1, 2012.
- [15] Arthur Jacot, Franck Gabriel, and Clément Hongler. Neural tangent kernel: Convergence and generalization in neural networks. In *Advances in neural information processing systems*, pages 8571–8580, 2018.

- [16] Thomas Jaksch, Ronald Ortner, and Peter Auer. Near-optimal regret bounds for reinforcement learning. *Journal of Machine Learning Research*, 11(Apr):1563–1600, 2010.
- [17] Nan Jiang, Akshay Krishnamurthy, Alekh Agarwal, John Langford, and Robert E Schapire. Contextual decision processes with low bellman rank are PAC-learnable. In *Proceedings of the 34th International Conference on Machine Learning-Volume 70*, pages 1704–1713. JMLR. org, 2017.
- [18] Chi Jin, Zeyuan Allen-Zhu, Sebastien Bubeck, and Michael I Jordan. Is Q-learning provably efficient? In *Advances in Neural Information Processing Systems*, pages 4863–4873, 2018.
- [19] Sham Kakade, Mengdi Wang, and Lin Yang. Variance reduction methods for sublinear reinforcement learning. 02 2018.
- [20] Sham Machandranath Kakade et al. *On the sample complexity of reinforcement learning*. PhD thesis, University of London London, England, 2003.
- [21] Michael Kearns and Satinder Singh. Near-optimal reinforcement learning in polynomial time. *Mach. Learn.*, 49(2-3):209–232, November 2002.
- [22] Akshay Krishnamurthy, Alekh Agarwal, and John Langford. PAC reinforcement learning with rich observations. In *Advances in Neural Information Processing Systems*, pages 1840–1848, 2016.
- [23] Zachary Chase Lipton, Xiujun Li, Jianfeng Gao, Lihong Li, Faisal Ahmed, and Li Deng. BBQ-networks: Efficient exploration in deep reinforcement learning for task-oriented dialogue systems. In *AAAI*, 2018.
- [24] Francisco S Melo and M Isabel Ribeiro. Q-learning with linear function approximation. In *International Conference on Computational Learning Theory*, pages 308–322. Springer, 2007.
- [25] Ian Osband, Benjamin Van Roy, and Zheng Wen. Generalization and exploration via randomized value functions. In *Proceedings of the 33rd International Conference on International Conference on Machine Learning - Volume 48, ICML’16*, pages 2377–2386. JMLR.org, 2016.
- [26] Jason Pavis and Ronald Parr. PAC optimal exploration in continuous space markov decision processes. In *Proceedings of the Twenty-Seventh AAAI Conference on Artificial Intelligence, AAAI’13*, pages 774–781. AAAI Press, 2013.
- [27] A. L. Samuel. Some studies in machine learning using the game of checkers. *IBM Journal of Research and Development*, 3(3):210–229, July 1959.
- [28] Max Simchowitz and Kevin Jamieson. Non-asymptotic gap-dependent regret bounds for tabular MDPs. 05 2019.
- [29] Zhao Song and Wen Sun. Efficient model-free reinforcement learning in metric spaces. *arXiv preprint arXiv:1905.00475*, 2019.
- [30] Alexander L Strehl, Lihong Li, Eric Wiewiora, John Langford, and Michael L Littman. PAC model-free reinforcement learning. In *Proceedings of the 23rd international conference on Machine learning*, pages 881–888. ACM, 2006.
- [31] Wen Sun, Nan Jiang, Akshay Krishnamurthy, Alekh Agarwal, and John Langford. Model-based reinforcement learning in contextual decision processes. *arXiv preprint arXiv:1811.08540*, 2018.
- [32] Richard S. Sutton. Open theoretical questions in reinforcement learning. In *EuroCOLT*, 1999.
- [33] Joel A Tropp et al. An introduction to matrix concentration inequalities. *Foundations and Trends® in Machine Learning*, 8(1-2):1–230, 2015.
- [34] Vincent Q Vu, Juhee Cho, Jing Lei, and Karl Rohe. Fantope projection and selection: A near-optimal convex relaxation of sparse PCA. In *Advances in neural information processing systems*, pages 2670–2678, 2013.

- [35] Christopher JCH Watkins and Peter Dayan. Q-learning. *Machine learning*, 8(3-4):279–292, 1992.
- [36] Zheng Wen and Benjamin Van Roy. Efficient exploration and value function generalization in deterministic systems. In *Advances in Neural Information Processing Systems*, pages 3021–3029, 2013.
- [37] Lin F Yang, Chengzhuo Ni, and Mengdi Wang. Learning to control in metric space with optimal regret. *arXiv preprint arXiv:1905.01576*, 2019.
- [38] Andrea Zanette and Emma Brunskill. Tighter problem-dependent regret bounds in reinforcement learning without domain knowledge using value function bounds. *arXiv preprint arXiv:1901.00210*, 2019.
- [39] Shaofeng Zou, Tengyu Xu, and Yingbin Liang. Finite-sample analysis for SARSA and Q-learning with linear function approximation. *arXiv preprint arXiv:1902.02234*, 2019.

Supplementary Material for “Provably Efficient Q -learning with Function Approximation via Distribution Shift Error Checking Oracle”

A Proof of Theorem 6.1

In this section we give the proof of Theorem 6.1.

Proof of Theorem 6.1. In the proof we set $\epsilon_t = \frac{\gamma^2 \epsilon}{5H}$, $\epsilon_s = 96C \cdot \epsilon^2 d \log(d/\epsilon)$, $\epsilon_N = \epsilon^2$, $\lambda_{\text{ridge}} = \epsilon^2$, $\lambda_r = \epsilon^6$, $B = 12d \log(d/\epsilon)$ and $N = \frac{d}{\lambda_r^2} \text{polylog}(\frac{1}{\epsilon})$. First, by Lemma A.6, we know with high probability over the generating process of $\{D_h\}_{h \in [H]}$, we have $|\Pi_h| \leq B$ for all $h \in [H]$. Note this also shows our algorithm ends in polynomial time. In the following we condition on this event.

We will prove $\hat{\pi}$ satisfies

$$\mathbb{P}_{s_h \sim \mathcal{D}_h^{\hat{\pi}}} [\hat{\pi}(s_h) \neq \pi^*(s_h)] \leq \frac{\epsilon}{H}$$

for all $h \in [H]$. By Lemma A.1, we know this implies the main conclusion.

To prove this property, it suffices to show our estimated predictors satisfy

$$\mathbb{P}_{s_h \sim \mathcal{D}_h^{\hat{\pi}}} \left[|f_h^a(s_h) - Q^*(s_h, a)| \leq \frac{\gamma}{2} \right] \leq \frac{\epsilon}{H}$$

for all $h \in [H]$ and $a \in \mathcal{A}$. Since $f_h^a(s_h) = \phi(s_h)^\top \hat{\theta}_h^a$, by Markov's inequality, we only need to show

$$\mathbb{E}_{s_h \sim \mathcal{D}_h^{\hat{\pi}}} \left[\left(\left(\hat{\theta}_h^a \right)^\top \phi(s_h) - Q^*(s_h, a) \right)^2 \right] \leq \frac{\gamma^2 \epsilon}{4H}. \quad (3)$$

We prove the following two invariants regarding the algorithm.

1. Each time we update f_h^a (and thus $\hat{\theta}_h^a$) in Line 9 of Algorithm 2, for all $\pi \in \Pi_h$, it holds that

$$\mathbb{E}_{s_h \sim \mathcal{D}_h^\pi} \left[\left(\left(\hat{\theta}_h^a \right)^\top \phi(s_h) - Q^*(s_h, a) \right)^2 \right] \leq \frac{\gamma^2 \epsilon}{4H}$$

$$\text{and } \left\| \hat{\theta}_h^a \right\|_2 \leq 1/\lambda_{\text{ridge}}.$$

2. Each time Oracle 4.2 returns False in Line 5 of Algorithm 3, it holds that for all actions $a' \in \mathcal{A}$,

$$\mathbb{E}_{s_{h'} \sim \mathcal{D}_{h'}^{\pi_h^a}} \left[\left(\left(\hat{\theta}_{h'}^{a'} \right)^\top \phi(s_{h'}) - Q^*(s_{h'}, a') \right)^2 \right] \leq \frac{\gamma^2 \epsilon}{4H}.$$

These two invariants imply that for the policy $\hat{\pi}$ returned by Algorithm 1, (3) holds for all $h \in [H]$ and $a \in \mathcal{A}$, which also implies the correctness of our algorithm. It remains to prove these two invariants.

We first prove the first invariant. We fix a level $h \in [H]$ and an action $a \in \mathcal{A}$. Let $f_h^a \in \mathcal{Q}$ be the predictor calculated in Line 9 of Algorithm 2, and $\hat{\theta}_h^a \in \mathbb{R}^d$ be the corresponding linear coefficients. Since D_h^a is collected after executing Line 2 of Algorithm 2, by induction, for all policies $\pi_h^a \in \Pi_h^a$ defined in (1), $h' > h$ and $a' \in \mathcal{A}$, we have

$$\mathbb{E}_{s_{h'} \sim \mathcal{D}_{h'}^{\pi_h^a}} \left[\left(\left(\hat{\theta}_{h'}^{a'} \right)^\top \phi(s_{h'}) - Q^*(s_{h'}, a') \right)^2 \right] \leq \frac{\gamma^2 \epsilon}{4H}.$$

It follows that for all policies $\pi_h^a \in \Pi_h^a$, $h' > h$ and $a' \in \mathcal{A}$, we have

$$\mathbb{P}_{s_{h'} \sim \mathcal{D}_{h'}^{\pi_h^a}} \left[\left| \left(\hat{\theta}_{h'}^{a'} \right)^\top \phi(s_{h'}) - Q^*(s_{h'}, a') \right| \geq \gamma/2 \right] \leq \epsilon/H.$$

Thus, by Lemma A.1

$$\mathbb{E}_{s_{h+1} \sim \mathcal{D}_{h+1}^{\pi_h^a}} [V^{\pi_h^a}(s_{h+1})] \geq \mathbb{E}_{s_{h+1} \sim \mathcal{D}_{h+1}^{\pi_h^a}} [V^*(s_{h+1})] - \epsilon.$$

By Assumption 3.1, for all $\pi_h^a \in \Pi_h^a$, we have

$$\mathbb{E}_{s_{h+1} \sim \mathcal{D}_{h+1}^{\pi_h^a}} \left[\left(V^{\pi_h^a}(s_{h+1}) - V^*(s_{h+1}) \right)^2 \right] \leq C\epsilon^2,$$

which implies

$$\mathbb{E}_{\pi_h^a \sim \text{unif}(\Pi_h^a), s_{h+1} \sim \mathcal{D}_{h+1}^{\pi_h^a}} \left[\left(V^{\pi_h^a}(s_{h+1}) - V^*(s_{h+1}) \right)^2 \right] \leq C\epsilon^2,$$

For each $(s_i, y_i) \in D_h^a$, we have

$$y_i = \phi(s_i)^\top \theta_h^a + b_i + \xi_i,$$

where $\mathbb{E}[b_i^2] \leq C\epsilon^2$, $|\xi_i| \leq 1$ almost surely and $\mathbb{E}[\xi_i] = 0$.

By Lemma A.3,

$$\left(\hat{\theta}_h^a - \theta_h^a \right)^\top \mathbb{E}_{\pi_h \sim \text{unif}(\Pi_h), s_h \sim \mathcal{D}_h^{\pi_h}} [\phi(s_h) \phi(s_h)^\top] \left(\hat{\theta}_h^a - \theta_h^a \right) \leq 4(C\epsilon^2 + \epsilon_N + \lambda_{\text{ridge}}),$$

which implies for all $\pi_h \in \Pi_h$,

$$\left(\hat{\theta}_h^a - \theta_h^a \right)^\top \mathbb{E}_{s_h \sim \mathcal{D}_h^{\pi_h}} [\phi(s_h) \phi(s_h)^\top] \left(\hat{\theta}_h^a - \theta_h^a \right) \leq 4(C\epsilon^2 + \epsilon_N + \lambda_{\text{ridge}}) \cdot B \leq \frac{\gamma^2 \epsilon}{4H}.$$

By Lemma A.4, we have $\|\hat{\theta}_h^a\|_2 \leq 1/\lambda_{\text{ridge}}$. Thus, the first invariant holds.

Now we can prove the second invariant. By the first invariant, using Lemma A.2 and Lemma A.4, with high probability, we have

$$\begin{aligned} & \left(\hat{\theta}_{h'}^a - \theta_{h'}^a \right)^\top \left(\lambda_r I + \sum_{\pi_{h'} \in \Pi_{h'}} \sum_{i=1}^N \frac{1}{N} [\phi(s_{i,\pi_{h'}}) \phi(s_{i,\pi_{h'}})^\top] \right) \left(\hat{\theta}_{h'}^a - \theta_{h'}^a \right) \\ & \leq 5(C\epsilon^2 + \epsilon_N + \lambda_{\text{ridge}} + \lambda_r/\lambda_{\text{ridge}}^2) |\Pi_{h'}| \leq \epsilon_s. \end{aligned}$$

Since Oracle 4.2 returns False, we know

$$\left(\hat{\theta}_{h'}^a - \theta_{h'}^a \right)^\top \left(\sum_{i=1}^N \frac{1}{N} [\phi(s_{h',i}) \phi(s_{h',i})^\top] \right) \left(\hat{\theta}_{h'}^a - \theta_{h'}^a \right) \leq \epsilon_t.$$

By Lemma A.2,

$$\left(\hat{\theta}_h^a - \theta_h^a \right)^\top \left(\mathbb{E}_{s_{h'} \sim \mathcal{D}_{h'}^{\pi_h^a}} [\phi(s_{h'}) \phi(s_{h'})^\top] \right) \left(\hat{\theta}_h^a - \theta_h^a \right) \leq \epsilon_t + \lambda_r(1 + 1/\lambda_{\text{ridge}}^2) \leq \frac{\gamma^2 \epsilon}{4H}.$$

This finishes the proof. \square

Lemma A.1 (Policy Correctness). *Given fixed level $h \in [H]$ and a policy π , suppose for all $h' = h, \dots, H$,*

$$\mathbb{P}_{s_{h'} \sim \mathcal{D}_{h'}^\pi} [\pi(s_{h'}) \neq \pi^*(s_{h'})] \leq \epsilon/H.$$

Then for all $h' = h, \dots, H$,

$$\mathbb{E}_{s_{h'} \sim \mathcal{D}_{h'}^\pi} [V^\pi(s_{h'})] \geq \mathbb{E}_{s_{h'} \sim \mathcal{D}_{h'}^\pi} [V^*(s_{h'})] - \epsilon.$$

Proof of Lemma A.1. Consider the random trajectory $s_1, a_1, r_1, s_2, a_2, r_2, \dots, s_H, a_H, r_H$ induced by policy π . With probability at least $1 - \epsilon$, we have $\pi(s_{h'}) = \pi^*(s_{h'})$ for all $h' = h, \dots, H$. We prove the claim by using $\sum_{h=1}^H r_h \leq 1$. \square

Lemma A.2 (Covariance Concentration Bound [33]). *Suppose $M_1, \dots, M_N \in \mathbb{R}^{d \times d}$ are i.i.d. drawn from a distribution \mathcal{D} over positive semi-definite matrices. If $\|M_t\|_F \leq 1$ almost surely and $N = \Omega\left(\frac{d \log(d/\delta)}{\epsilon^2}\right)$, then with probability at least $1 - \delta$,*

$$\left\| \frac{1}{N} \sum_{t=1}^N M_t - \mathbb{E}_{M \sim \mathcal{D}}[M] \right\|_{\text{op}} \leq \epsilon.$$

Lemma A.3 (Ridge Regression with Bias). *Suppose*

$$(s_1, y_1), (s_2, y_2), \dots, (s_N, y_N)$$

are i.i.d. drawn from a distribution \mathcal{D} and satisfy

$$y_i = \theta^\top \phi(s_i) + b_i + \xi_i,$$

where $\mathbb{E}_{(s_i, y_i) \sim \mathcal{D}}[b_i^2] \leq \bar{b}^2$ for some $0 \leq \bar{b} \leq 1$, $|\xi_i| \leq 1$ almost surely and $\mathbb{E}[\xi_i] = 0$. Let

$$S = [\phi(s_1)^\top; \dots; \phi(s_N)^\top] \in \mathbb{R}^{N \times d},$$

$$y = [y_1; \dots; y_N] \in \mathbb{R}^N,$$

and

$$\hat{\theta} = \left(\frac{S^\top S}{N} + \lambda_{\text{ridge}} \cdot I \right)^{-1} \frac{S^\top y}{N}$$

be the ridge regression estimator. If $N = \Omega\left(\frac{d}{\epsilon_N^2} \log\left(\frac{d}{\delta}\right)\right)$, then with probability at least $1 - \delta$,

$$\mathbb{E}_{s \sim \mathcal{D}} \left[\left((\theta - \hat{\theta})^\top \phi(s) \right)^2 \right] \leq 4 \left(\bar{b}^2 + \epsilon_N + \lambda_{\text{ridge}} \right).$$

Proof of Lemma A.3. Let

$$b = [b_1; \dots; b_N] \in \mathbb{R}^N.$$

By Chernoff bound, with probability at least $1 - \delta/3$, $\|b\|_2^2/N \leq \bar{b}^2 + \epsilon_N/2$.

$$\begin{aligned} & \hat{\theta} - \theta \\ &= \left(\frac{S^\top S}{N} + \lambda_{\text{ridge}} \cdot I \right)^{-1} \frac{S^\top y}{N} - \theta \\ &= \left(\frac{S^\top S}{N} + \lambda_{\text{ridge}} \cdot I \right)^{-1} \frac{S^\top (S\theta + b + \xi)}{N} - \theta \\ &= \left(\left(\frac{S^\top S}{N} + \lambda_{\text{ridge}} \cdot I \right)^{-1} \frac{S^\top S}{N} - I \right) \theta + \left(\frac{S^\top S}{N} + \lambda_{\text{ridge}} \cdot I \right)^{-1} \frac{S^\top b}{N} + \left(\frac{S^\top S}{N} + \lambda_{\text{ridge}} \cdot I \right)^{-1} \frac{S^\top \xi}{N} \\ &\triangleq I_1 + I_2 + I_3. \end{aligned}$$

Thus,

$$\begin{aligned} & \frac{1}{N} \left\| S (\hat{\theta} - \theta) \right\|_2^2 \\ &= (\hat{\theta} - \theta)^\top \frac{S^\top S}{N} (\hat{\theta} - \theta) \\ &= (I_1 + I_2 + I_3)^\top \frac{S^\top S}{N} (I_1 + I_2 + I_3) \\ &\leq 3 \left(I_1^\top \frac{S^\top S}{N} I_1 + I_2^\top \frac{S^\top S}{N} I_2 + I_3^\top \frac{S^\top S}{N} I_3 \right). \end{aligned}$$

For the first term, we have

$$\begin{aligned} I_1^\top \frac{S^\top S}{N} I_1 &\leq \|\theta\|_2^2 \cdot \left\| \left(\left(\frac{S^\top S}{N} + \lambda_{\text{ridge}} \cdot I \right)^{-1} \frac{S^\top S}{N} - I \right)^\top \frac{S^\top S}{N} \left(\left(\frac{S^\top S}{N} + \lambda_{\text{ridge}} \cdot I \right)^{-1} \frac{S^\top S}{N} - I \right) \right\|_{\text{op}} \\ &\leq \lambda_{\text{ridge}} \|\theta\|_2^2 \leq \lambda_{\text{ridge}}. \end{aligned}$$

For the second term, we have

$$I_2^\top \frac{S^\top S}{N} I_2 \leq \frac{\|b\|_2^2}{N} \left\| \frac{1}{N} \left(\left(\frac{S^\top S}{N} + \lambda_{\text{ridge}} \cdot I \right)^{-1} S^\top \right)^\top \frac{S^\top S}{N} \left(\left(\frac{S^\top S}{N} + \lambda_{\text{ridge}} \cdot I \right)^{-1} S^\top \right) \right\|_{\text{op}} \leq \frac{\|b\|_2^2}{N}.$$

Using Lemma 29 of [14], we know $I_3^\top \frac{S^\top S}{N} I_3 \leq \frac{\epsilon_N}{2}$ with probability at least $1 - \delta/3$. Finally, applying the standard empirical process method, we can bound the generalization error and thus finish the proof. \square

Lemma A.4 (Ridge Regression Gives Upper Bound on the Norm). *Suppose*

$$(\phi(s_1), y_1), (\phi(s_2), y_2), \dots, (\phi(s_N), y_N) \in \mathbb{R}^d \times \mathbb{R}$$

satisfy $|y_i| \leq 1$ and $\|\phi(s_i)\|_2 \leq 1$ for all $i \in [N]$. Let $S = [\phi(s_1)^\top; \dots; \phi(s_N)^\top] \in \mathbb{R}^{N \times d}$, $y = [y_1; \dots; y_N] \in \mathbb{R}^N$ and $\hat{\theta} = \left(\frac{S^\top S}{N} + \lambda_{\text{ridge}} \cdot I \right)^{-1} \frac{S^\top y}{N}$ be the ridge regression estimator. Then we have

$$\|\hat{\theta}\|_2 \leq \frac{1}{\lambda_{\text{ridge}}}.$$

Proof of Lemma A.4. By triangle inequality, $\left\| \frac{S^\top y}{N} \right\|_2 \leq 1$. Furthermore,

$$\left\| \left(\frac{S^\top S}{N} + \lambda_{\text{ridge}} \cdot I \right)^{-1} \right\|_{\text{op}} \leq 1/\lambda_{\text{ridge}}.$$

Thus,

$$\|\hat{\theta}\|_2 \leq \frac{1}{\lambda_{\text{ridge}}}.$$

\square

Lemma A.5. *Consider the following process. Initially $\mathcal{M} = \emptyset$. Let ϵ_s and ϵ_t be two real numbers such that $0 < \epsilon_s \leq \frac{\epsilon_t}{d}$. For $t = 1, 2, \dots$, we receive a positive semi-definite matrix $M_t \in \mathbb{R}^{d \times d}$ with $\|M_t\|_F \leq 1$. If there exists $x \in \mathbb{R}^d$ such that $x^\top M_t x \geq \epsilon_t$ and $x^\top (\lambda_r I + \sum_{M \in \mathcal{M}} M) x \leq \epsilon_s$, then we add M_t into \mathcal{M} . It holds that $|\mathcal{M}| \leq 2d \log \left(\frac{d}{\lambda_r} \right)$ throughout the process.*

Proof of Lemma A.5. We first show that if $\mathcal{M} \neq \emptyset$, then after adding M_t into \mathcal{M} , we must have

$$\det \left(\lambda_r I + \sum_{M \in \mathcal{M}} M \right) \geq \left(1 + \frac{\epsilon_t}{d\epsilon_s} \right) \det \left(\lambda_r I + \sum_{M \in \mathcal{M} \setminus \{M_t\}} M \right) \geq 2 \det \left(\lambda_r I + \sum_{M \in \mathcal{M} \setminus \{M_t\}} M \right).$$

Let

$$A = \lambda_r I + \sum_{M \in \mathcal{M} \setminus \{M_t\}} M,$$

and

$$A = \sum_{j=1}^d \lambda_j v_j v_j^\top$$

be its spectral decomposition. For the positive semi-definite matrix M_t , we write $M_t = UU^\top$. By matrix determinant lemma, we have

$$\det(A + M_t) = \det(I + U^\top A^{-1}U) \det(A).$$

Therefore, it suffices to prove the largest eigenvalue of $U^\top A_i^{-1}U$ is larger than $\frac{\epsilon_t}{d\epsilon_t} \geq 1$.

Since we add M_t into \mathcal{M} , there exists x such that

$$\|Ux\|_2^2 \geq \epsilon_t$$

and

$$\sum_{j=1}^d \lambda_j (v_j^\top x)^2 \leq \epsilon_s.$$

Let $z = Ux / \|Ux\|$ be a unit vector such that $z^\top Ux = \|Ux\|_2$. Let $u = Uz$. We have

$$\begin{aligned} z^\top U^\top A_i^{-1}Uz &= u^\top \left(\sum_{j=1}^d \frac{1}{\lambda_j} v_j v_j^\top \right) u \\ &= \sum_{j=1}^d \frac{1}{\lambda_j} (v_j^\top u)^2 \\ &= \sum_{j=1}^d (v_j^\top u)^2 (v_j^\top x)^2 \frac{1}{\lambda_j \cdot (v_j^\top x)^2} \\ &\geq \frac{1}{\epsilon_s} \sum_{j=1}^d (v_j^\top u)^2 (v_j^\top x)^2 \\ &\geq \frac{1}{\epsilon_s d} \left(\sum_{j=1}^d u^\top v_j v_j^\top x \right)^2 \\ &= \frac{1}{\epsilon_s d} (z^\top Ux)^2 \\ &= \frac{1}{\epsilon_s d} \|Ux\|_2^2 \\ &\geq \frac{\epsilon_t}{d\epsilon_s}, \end{aligned}$$

which implies

$$\det \left(\lambda_r I + \sum_{M \in \mathcal{M}} M \right) \geq 2 \det \left(\lambda_r I + \sum_{M \in \mathcal{M} \setminus \{M_t\}} M \right).$$

It follows that

$$\det \left(\lambda_r I + \sum_{M \in \mathcal{M}} M \right) \geq 2^{|\mathcal{M}|-1} \lambda_r^d.$$

On the other hand, we have

$$\det \left(\lambda_r I + \sum_{M \in \mathcal{M}} M \right) \leq (|\mathcal{M}| + 1)^d,$$

since $\|M\|_F \leq 1$ for all $M \in \mathcal{M}$.

Thus,

$$2^{|\mathcal{M}|-1} \lambda_r^d \leq (|\mathcal{M}| + 1)^d,$$

which implies $|\mathcal{M}| \leq 2d \log \left(\frac{d}{\lambda_r} \right)$. □

Lemma A.6 (Polynomially Bounded Policy Set). *If $N \geq \frac{d}{\lambda_r^2} \cdot B^2 \cdot \text{polylog}(1/\epsilon)$, then with high probability we have $|\Pi_h| \leq B$ for all $h \in [H]$.*

Proof of Lemma A.6. Consider a fixed $h' \in [H]$. We will add a new policy π_h^a into $\Pi_{h'}$ only when Oracle 4.2 returns True in Line 6 of Algorithm 3. Since Oracle 4.2 returns True in Line 6 of Algorithm 3, there must exist $x = \theta_1 - \theta_2$ such that

$$x^\top \left(\lambda_r / |\Pi_{h'}| \cdot I + \frac{1}{N |\Pi_{h'}|} \sum_{\pi_{h'} \in \Pi_{h'}} \sum_{i=1}^N \phi(s_{\pi_{h'}, i}) \phi(s_{\pi_{h'}, i})^\top \right) x \leq \epsilon_s / |\Pi_{h'}|.$$

Recall that $D_{h'} = \{s_{\pi_{h'}, i}\}_{\pi_{h'} \in \Pi_{h'}, i \in [N]}$ is a set of states generated using policies in $\Pi_{h'}$ (cf. Line 13 of Algorithm 2). It follows that

$$x^\top \left(\lambda_r \cdot I + \sum_{\pi_{h'} \in \Pi_{h'}} \frac{1}{N} \sum_{i=1}^N \phi(s_{\pi_{h'}, i}) \phi(s_{\pi_{h'}, i})^\top \right) x \leq \epsilon_s.$$

Thus, we have

$$\|x\|_2^2 \leq \epsilon_s / \lambda_r.$$

By Lemma A.2, for each $\pi_{h'} \in \Pi_{h'}$, with high probability,

$$\left| x^\top \left(\frac{1}{N} \sum_{i=1}^N \phi(s_{\pi_{h'}, i}) \phi(s_{\pi_{h'}, i})^\top - \mathbb{E}_{s_{\pi_{h'}} \sim \mathcal{D}_{h'}^{\pi_{h'}}} [\phi(s_{\pi_{h'}}) \phi(s_{\pi_{h'}})^\top] \right) x \right| \leq \epsilon_s / B.$$

Therefore, with high probability, it is satisfied that

$$x^\top \left(\lambda_r I + \sum_{\pi_{h'} \in \Pi_{h'}} \mathbb{E}_{s_{\pi_{h'}} \sim \mathcal{D}_{h'}^{\pi_{h'}}} [\phi(s_{\pi_{h'}}) \phi(s_{\pi_{h'}})^\top] \right) x \leq 2\epsilon_s.$$

Moreover, since Oracle 4.2 returns True in Line 6 of Algorithm 3, we must have

$$x^\top \left(\frac{1}{N} \sum_{i=1}^N [\phi(s_{h', i}) \phi(s_{h', i})^\top] \right) x \geq \epsilon_t.$$

Recall that $\tilde{D}_{\pi_h^a, h'} = \{s_{h', i}\}_{i=1}^N$ are the states at level h' on the N trajectories collected using π_h^a (cf. Line 4 of Algorithm 3). Again by Lemma A.2, with high probability we have

$$x^\top \left(\mathbb{E}_{s_{\pi_{h'}} \sim \mathcal{D}_{h'}^{\pi_h^a}} [\phi(s_{\pi_{h'}}) \phi(s_{\pi_{h'}})^\top] \right) x \geq \frac{\epsilon_t}{2}.$$

Thus, if we use \mathcal{M} to denote

$$\left\{ \mathbb{E}_{s_{\pi_{h'}} \sim \mathcal{D}_{h'}^{\pi_{h'}}} [\phi(s_{\pi_{h'}}) \phi(s_{\pi_{h'}})^\top] \right\}_{\pi_{h'} \in \Pi_{h'}},$$

and M_t to denote

$$\mathbb{E}_{s_{\pi_{h'}} \sim \mathcal{D}_{h'}^{\pi_h^a}} [\phi(s_{\pi_{h'}}) \phi(s_{\pi_{h'}})^\top],$$

then this is exactly the process described in Lemma A.5, and thus the upper bound on $|\Pi_{h'}|$ follows. \square