Agnostic *Q*-learning with Function Approximation in Deterministic Systems: Near-Optimal Bounds on Approximation Error and Sample Complexity

Anonymous Author(s) Affiliation Address email

Abstract

| 1 | The current paper studies the problem of agnostic Q -learning with function approx- |
|----|-------------------------------------------------------------------------------------------------------------------|
| 2 | imation in deterministic systems where the optimal Q-function is approximable |
| 3 | by a function in the class \mathcal{F} with approximation error $\delta \geq 0$. We propose a novel |
| 4 | recursion-based algorithm and show that if $\delta = O(\rho/\sqrt{\dim E})$, then one can find |
| 5 | the optimal policy using $O(\dim_E)$ trajectories, where ρ is the gap between the |
| 6 | optimal Q -value of the best actions and that of the second-best actions and \dim_E |
| 7 | is the Eluder dimension of \mathcal{F} . Our result has two implications: |
| 8 | 1. In conjunction with the lower bound in [Du et al., 2020], our upper bound |
| 9 | suggests that the condition $\delta = \Theta \left(\rho / \sqrt{\dim_E} \right)$ is necessary and sufficient for |
| 10 | algorithms with polynomial sample complexity. |
| 11 | 2. In conjunction with the obvious lower bound in the tabular case, our upper |
| 12 | bound suggests that the sample complexity $\Theta(\dim_E)$ is tight in the agnostic |
| 13 | setting. |
| 14 | Therefore, we help address the open problem on agnostic Q-learning proposed |
| 15 | in [Wen and Van Roy, 2013]. We further extend our algorithm to the stochastic |
| 16 | reward setting and obtain similar results. |
| | |

17 **1 Introduction**

Q-learning is a fundamental approach in reinforcement learning [Watkins and Dayan, 1992]. Empiri-18 cally, combining Q-learning with function approximation schemes has lead to tremendous success 19 on various sequential decision-making problems. However, theoretically, we only have a good 20 understanding of Q-learning in the tabular setting. Strehl et al. [2006], Jin et al. [2018] show that 21 with certain exploration techniques, Q-learning provably finds a near-optimal policy with sample 22 complexity polynomial in the number of states, number of actions and the planning horizon. However, 23 modern reinforcement learning applications often require dealing with large state space where the 24 polynomial dependency on the number of states is not acceptable. 25

Recently, there has been great interest in designing and analyzing *Q*-learning algorithms with linear function approximation [Wen and Van Roy, 2013, Du et al., 2019]. Under various additional assumptions, these works show that one can obtain a near-optimal policy using *Q*-learning with sample complexity polynomial in the feature dimension *d* and the planning horizon, if the optimal

Q-function is an exact linear function of the d-dimensional features of the state-action pairs.

A major drawback of these works is that the algorithms can only be applied in the well-specified case,

i.e., the optimal Q-function is an exact linear function. In practice, the optimal Q-function is usually

³³ linear up to small approximation errors instead of being exactly linear. In this paper, we focus on

Submitted to 34th Conference on Neural Information Processing Systems (NeurIPS 2020). Do not distribute.

the agnostic setting, i.e., the optimal Q-function can only be approximated by a function class with

approximation error δ , which is closer to practical scenarios. Indeed, designing a provably efficient

 $_{36}$ Q-learning algorithm in the agnostic setting is an open problem posed by Wen and Van Roy [2013].

Technically, the agnostic setting is arguably more challenging than the exact setting. As recently 37 shown by Du et al. [2020], for the class of linear functions, when the approximation error $\delta =$ 38 $\Omega(\sqrt{\operatorname{poly}(H)/d})$ where H is the planning horizon, any algorithm needs to sample exponential 39 number of trajectories to find a near-optimal policy even in deterministic systems. Therefore, for 40 algorithms with polynomial sample complexity, additional assumptions are needed to bypass the 41 hardness result. For the exact setting $\delta = 0$, Wen and Van Roy [2013] show that one can find an 42 optimal policy using polynomial number of trajectories for linear functions in deterministic systems, 43 which implies that the agnostic setting could be exponentially harder than the exact setting. 44

⁴⁵ Due to the technical challenges, for the agnostic setting, previous papers mostly focus on the bandit ⁴⁶ setting or reinforcement learning with a generative model [Lattimore and Szepesvari, 2019, Van Roy ⁴⁷ and Dong, 2019, Neu and Olkhovskaya, 2020], and much less is known for the standard reinforcement ⁴⁸ learning setting. In this paper, we design *Q*-learning algorithms with provable guarantees in the ⁴⁹ agnostic case for the standard reinforcement learning setting.

50 1.1 Our Contributions

⁵¹ Our main contribution is a provably efficient *Q*-learning algorithm for the agnostic setting with ⁵² general function approximation in deterministic systems. Our results help address the open problem ⁵³ posed by Wen and Van Roy [2013].

Theorem 1.1 (Informal). For a given episodic deterministic system and a function class \mathcal{F} , suppose there exists $f \in \mathcal{F}$ such that the optimal Q-function Q^* satisfies $|f(s, a) - Q^*(s, a)| \leq \delta$ for any state-action pair (s, a). Suppose $\rho = \Omega(\sqrt{\dim_E}\delta)$, where the optimality gap ρ is the gap between the optimal Q-value of the best action and that of the second-best action (formally defined in Definition 3.1) and \dim_E is the Eluder dimension of \mathcal{F} (see Definition 3.5), our algorithm finds the optimal policy using $O(\dim_E)$ trajectories.

⁶⁰ Our main assumption is that the optimality gap ρ satisfies $\rho = \Omega(\sqrt{\dim_E}\delta)$. Below we discuss the ⁶¹ necessity of this assumption and its connection with the recent hardness result in Du et al. [2020].

In Du et al. [2020], it has been proved that in deterministic systems, if the optimality gap $\rho = 1$ and the optimal *Q*-function can be approximated by linear functions with approximation error $\delta = \Omega(\sqrt{\text{poly}(H)/d})$, any algorithm needs to sample exponential number of trajectories to find a near-optimal policy even in deterministic systems. Here *d* is the input dimension of the linear functions. Using the same technique as in [Du et al., 2020], we show the following hardness result for *Q*-learning with linear function approximation in the agnostic setting.

Proposition 1.2 (Generalization of Theorem 4.1 in [Du et al., 2020]). For any $\rho \leq 1$, there exists a family of deterministic systems where the optimality gap is ρ and the optimal Q-function can be approximated by linear functions with approximation error $\delta = O(C/\sqrt{d} \cdot \rho)$, such that any

algorithm that returns a $\rho/2$ -optimal policy needs to sample $\Omega(2^C)$ trajectories.

By setting $C = O(\log(Hd))$ such that $2^C = \operatorname{poly}(Hd)$, Proposition 1.2 implies that for any 72 algorithm with polynomial sample complexity, the approximation error δ that can be handled is at 73 most $O(\rho/\sqrt{d})$. Recall that the Eluder dimension of linear functions is O(d). Theorem 1.1 suggests 74 that as long as $\rho = \tilde{\Omega}(\sqrt{d\delta})$, our algorithm finds the optimal policy using polynomial number of 75 samples. Note that this applies to every pair of (ρ, δ) that satisfies the condition. Proposition 1.2 76 suggests that there exist environments with $\rho = \Omega(\sqrt{d\delta})$ which require exponential number of 77 samples to find a near-optimal policy. Therefore, combining Theorem 1.1 and Proposition 1.2, we 78 give a tight characterization (up to logarithmic factors) on the quantitative relation between ρ and δ 79 under which one can use polynomial number of samples to find the optimal policy. 80 Our result is in the same spirit as the results in [Lattimore and Szepesvari, 2019, Van Roy and 81

⁸¹ Our result is in the same spirit as the results in [Lattinore and Szepesvari, 2019, van Roy and
⁸² Dong, 2019], which also demonstrate the tightness of the hardness result in [Du et al., 2020].
⁸³ However, as will be made clear, technically our result significantly deviates from those in [Lattimore
⁸⁴ and Szepesvari, 2019, Van Roy and Dong, 2019]. See Section 2 for more detailed comparison
⁸⁵ with [Lattimore and Szepesvari, 2019, Van Roy and Dong, 2019].

Note that the sample complexity of our algorithm is linear in the Eluder dimension of the function 86 class. For the tabular setting, the Eluder dimension is as large as the cardinality of the state-action 87 space [Russo and Van Roy, 2013]. This cardinality is also a sample complexity lower bound, i.e., 88 for the tabular setting, the sample complexity lower bound is $\Omega(\dim_E)$. Therefore, our sample 89 complexity is also tight. 90 Finally, we show how to generalize our results to handle stochastic rewards. Under the same 91 assumption that $\rho = \Omega(\sqrt{\dim_E}\delta)$, our algorithm finds an optimal policy using $\frac{\text{poly}(\dim_E, H)}{\rho^2} \log(1/p)$ trajectories with failure probability p. We would like to remark that the $\log(1/p)/\rho^2$ dependency is 92

93

necessary for finding optimal policies even in the bandit setting [Mannor and Tsitsiklis, 2004]. 94

Organization In Section 2, we review related work. In Section 3, we introduce necessary notations, 95 definitions and assumptions. In Section 4, we discuss the special case where \mathcal{F} is the class of 96 linear functions to demonstrate the high-level approach of our algorithm and the intuition behind the 97 analysis. We then present the result for general function classes in Section 5. We conclude in Section 98 6 and defer proofs to the supplementary material. 99

Related Work 2 100

Classical theoretical reinforcement learning literature studies asymptotic behavior of concrete algo-101 rithms or finite sample complexity bounds for Q-learning algorithms under various assumptions [Melo 102 and Ribeiro, 2007, Zou et al., 2019]. These works usually assume the initial policy has certain benign 103 properties, which may not hold in practical applications. Another line of work focuses on sample 104 complexity and regret bound in the tabular setting [Lattimore and Hutter, 2012, Azar et al., 2013, 105 Sidford et al., 2018a,b, Agarwal et al., 2019, Jaksch et al., 2010, Agrawal and Jia, 2017, Azar et al., 106 2017, Kakade et al., 2018]. Strehl et al. [2006], Jin et al. [2018] show that with certain exploration 107 techniques, Q-learning provably finds a near-optimal with polynomial sample complexity. However, 108 these works have sample complexity at least linearly depends on the number of states, which is 109 necessary without additional assumptions [Jaksch et al., 2010]. 110

Various exploration algorithms are proposed for Q-learning with function approximation [Azizzade-111 nesheli et al., 2018, Fortunato et al., 2018, Lipton et al., 2018, Osband et al., 2016, Pazis and Parr, 112 2013]. However, none of these algorithms have polynomial sample complexity guarantees. Li et al. 113 [2011] propose a Q-learning algorithm which requires the Know-What-It-Knows oracle. However, it 114 is unknown how to implement such oracle in general. Wen and Van Roy [2013] propose an algorithm 115 for Q-learning with function approximation in deterministic systems which works for a family of 116 function classes in the exact setting. For the agnostic setting, the algorithm in [Wen and Van Roy, 117 2013] can only be applied to a special case called "state aggregation case". See Section 4.3 in [Wen 118 and Van Roy, 2013] for more details. Indeed, as stated in the conclusion of [Wen and Van Roy, 2013], 119 designing provably efficient algorithm for agnostic Q-learning with general function approximation 120 is a challenging open problem. 121

Du et al. [2019] propose an algorithm for Q-learning with linear function approximation in the exact 122 setting. The algorithm in [Du et al., 2019] further requires conditions on the optimality gap ρ and a 123 low-variance condition on the transition. Our algorithms also requires conditions on the optimality 124 125 gap ρ and shares similar recursion-based structures as the algorithm in [Du et al., 2019]. However, our algorithm handles general function classes with bounded Eluder dimension and with approximation 126 error, neither of which can be handled by the algorithm in [Du et al., 2019]. 127

Recently, Du et al. [2020] proved lower bounds for Q-learning algorithm in the agnostic setting. As 128 mentioned in the introduction, our algorithm complements the lower bounds in [Du et al., 2020] 129 and demonstrates the tightness of their lower bound. Lattimore and Szepesvari [2019], Van Roy and 130 Dong [2019] also give algorithms in the agnostic setting to demonstrate the tightness of the lower 131 bound in [Du et al., 2020] from other perspectives. Technically, our results are different from those 132 in [Lattimore and Szepesvari, 2019, Van Roy and Dong, 2019] in the following ways. First, we 133 study the standard reinforcement learning setting, where Van Roy and Dong [2019] focus on the 134 bandit setting and Lattimore and Szepesvari [2019] study both the bandit setting and reinforcement 135 learning with a generative model. Second, for the reinforcement learning result in [Lattimore and 136 Szepesvari, 2019], it is further assumed that Q-functions induced by all polices can be approximated 137 by linear functions, while in this paper we only assume the optimal Q-function can be approximated 138

by a function class with bounded Eluder dimension, which is much weaker than the assumption in [Lattimore and Szepesvari, 2019]. In conjunction with the lower bound in [Du et al., 2020], we give a tight condition $\delta = \widetilde{\Theta} \left(\rho / \sqrt{\dim_E} \right)$ under which there is an algorithm with polynomial sample complexity to find the optimal policy.

Recently, a line of work study *Q*-learning in the linear MDP setting [Yang and Wang, 2019b,a, Jin et al., 2019, Wang et al., 2019]. In the linear MDP setting, it is assumed that both the reward function and the transition operator is linear, which is stronger than the assumption that the optimal *Q*-function is linear studied in this paper. For the linear MDP setting, algorithms with polynomial sample complexity are known, and these algorithms can usually handle approximation errors on the reward function and the transition operator.

149 **3** Preliminaries

Notations We write [n] to denote the set $\{1, 2, ..., n\}$. We use $\|\cdot\|_p$ to denote the ℓ_p norm of a vector. For any finite set S, we write $\triangle(S)$ to denote the probability simplex.

152 3.1 Episodic Reinforcement Learning

In this paper, we consider Markov Decision Processes with deterministic transition and stochastic reward. Formally, let $\mathcal{M} = (S, \mathcal{A}, H, P, R)$ be a Markov Decision Process (MDP) where S is the state space, \mathcal{A} is the action space, $H \in \mathbb{Z}_+$ is the planning horizon, $P : S \times \mathcal{A} \to S$ is the deterministic transition function which takes a state-action pair and returns a state, and $R : S \times \mathcal{A} \to \Delta(\mathbb{R})$ is the reward distribution. When the reward is deterministic, we may regard $R : S \times \mathcal{A} \to \mathbb{R}$ as a function instead of a distribution. We assume there is a fixed initial state s_1 .

A policy $\pi : S \to \triangle(A)$ prescribes a distribution over actions for each state. The policy π induces a (random) trajectory $s_1, a_1, r_1, s_2, a_2, r_2, \ldots, s_H, a_H, r_H$ where $a_1 \sim \pi(s_1), r_1 \sim R(s_1, a_1), s_2 = P(s_1, a_1), a_2 \sim \pi(s_2)$, etc. To streamline our analysis, for each $h \in [H]$, we use $S_h \subseteq S$ to denote the set of states at level h, and we assume S_h do not intersect with each other.¹ We also assume $\sum_{h=1}^{H} r_h \in [0, 1]$. Our goal is to find a policy π that maximizes the expected total reward $\mathbb{E}\left[\sum_{h=1}^{H} r_h \mid \pi\right]$. We use π^* to denote the optimal policy.

165 **3.2** *Q*-function, *V*-function and the Optimality Gap

An important concept in RL is the Q-function. Given a policy π , a level $h \in [H]$ and a state-action 166 pair $(s, a) \in S_h \times A$, the Q-function is defined as $Q_h^{\pi}(s, a) = \mathbb{E}\left[\sum_{h'=h}^{H} r_{h'} \mid s_h = s, a_h = a, \pi\right]$. For simplicity, we denote $Q_h^*(s, a) = Q_h^{\pi^*}(s, a)$. It will also be useful to define the value function 167 168 of a given state $s \in S_h$ as $V_h^{\pi}(s) = \mathbb{E}\left[\sum_{h'=h}^{H} r_{h'} \mid s_h = s, \pi\right]$. For simplicity, we denote $V_h^*(s) = V_h^*(s)$ 169 $V_h^{\pi^*}(s)$. Throughout the paper, for the Q-function Q_h^{π} and Q_h^* and the value function V_h^{π} and V_h^* , 170 we may omit h from the subscript when it is clear from the context. 171 In addition to these definitions, we list below an important concept, the optimality gap, which is 172 widely used in reinforcement learning and bandit literature. 173 **Definition 3.1** (Optimality Gap). The optimality gap ρ is defined as $\rho = \inf_{Q^*(s,a) \neq V^*(s)} V^*(s) - Q^*(s) = 0$ 174 $Q^*(s,a).$ 175

In words, ρ is the smallest reward-to-go difference between the best set of actions and the rest. In this paper we need ρ to be strictly positive. We remark that this is not a restrictive assumption. This assumption is widely used in bandit problems Abbasi-Yadkori et al. [2011], Dani et al. [2008], Lattimore and Szepesvári [2018]. Recently, Du et al. [2019] gave a provably efficient *Q*-learning algorithm based on this assumption, Simchowitz and Jamieson [2019] showed that with this condition, the agent only incurs logarithmic regret in the tabular setting and Zanette et al. [2019] showed that under this condition, one can remove all horizon dependencies in the sample complexity. Empirically,

¹This assumption is only for the sake of presentation. Our result can be easily generalized to the case when this assumption does not hold.

arguably all environments with a finite action set satisfy the optimality gap conditions. In Atari-games, e.g., Freeway, the optimal Q value is often distinctive from the rest of actions. For board games, e.g. tic-tac-toe, Chess, etc, most states have zero rewards except for the winning states. Hence, every optimal action has a Q-value of 1 and the rest actions have a Q-value of 0, in which case $\rho = 1$ by Definition 3.1.

188 3.3 Function Approximation and Eluder Dimension

When the state space is large, we need structures on the state space so that reinforcement learning methods can generalize. For a given function class \mathcal{F} , each $f \in \mathcal{F}$ is a function that maps a stateaction pair to a real number. For a given MDP and a function class \mathcal{F} , we define the approximation error to the optimal Q-function as follow.

Definition 3.2 (Approximation Error). For a given MDP and a function class \mathcal{F} , the approximation error δ is defined to be $\delta = \inf_{f \in \mathcal{F}} \sup_{(s,a) \in \mathcal{S} \times \mathcal{A}} |f(s,a) - Q^*(s,a)|.$

Here, the approximation error δ characterizes how well the given function class \mathcal{F} approximates the optimal Q-function. When $\delta = 0$, then optimal Q-function can be perfectly predicted by the function class, which has been studied in previous papers [Wen and Van Roy, 2013, Du et al., 2019]. In this paper, we focus the case $\delta > 0$.

An important function class is the class of linear functions. We assume the agent is given a feature extractor $\phi : S \times A \to \mathbb{R}^d$ where $\|\phi(s, a)\|_2 \leq 1$ for all state-action pairs. The feature extractor can be hand-crafted or a pre-trained neural network that transforms a state-action pair to a *d*-dimensional embedding. Given the feature extractor ϕ , we define the class of linear functions as follow.

Definition 3.3. For a vector $\theta \in \mathbb{R}^d$, we define $f_{\theta}(s, a) = \theta^{\top} \phi(s, a)$. The class of linear functions is defined as $\mathcal{F} = \{f_{\theta} \mid ||\theta||_2 \leq 1\}$.

Here we assume $\|\theta\|_2 \leq 1$ only for normalization purposes.

For general function classes, an important concept is the *Eluder dimension*, for which we first need to introduce the concept of ϵ -dependence.

Definition 3.4 (ϵ -dependence [Russo and Van Roy, 2013]). For a function class \mathcal{F} , we say a stateaction pair (s, a) is ϵ -dependent on state-action pairs $\{(s_1, a_1), \ldots, (s_n, a_n)\} \subset \mathcal{S} \times \mathcal{A}$ with respect to \mathcal{F} if for all $f_1, f_2 \in \mathcal{F}$,

$$\sum_{i=1}^{n} |f_1(s_i, a_i) - f_2(s_i, a_i)|^2 \le \epsilon^2 \implies |f_1(s, a) - f_2(s, a)|^2 \le \epsilon^2.$$

Further, (s, a) is ϵ -independent of state-action pairs $\{(s_1, a_1), \dots, (s_n, a_n)\}$ if (s, a) is not ϵ dependent on state-action pairs $\{(s_1, a_1), \dots, (s_n, a_n)\}$.

Now, we recall the definition of ϵ -Eluder dimension as introduced in Russo and Van Roy [2013].

Definition 3.5 (ε -Eluder Dimension). For a function class \mathcal{F} , the ϵ -Eluder dimension dim_E(\mathcal{F}, ϵ) is the length of the longest sequence of elements in $\mathcal{S} \times \mathcal{A}$ such that every element is ϵ' -independent of its predecessors for some $\epsilon' \geq \epsilon$.

As an example, when \mathcal{F} is the class of linear functions with norm $\|\theta\|_2 \leq 1$ and $\|\phi(s, a)\|_2 \leq 1$, the ε -Eluder dimension $\dim_E(\mathcal{F}, \epsilon)$ is $O(d \log(1/\epsilon))$ as noted in Example 4 in Russo and Van Roy [2013]. We refer interested readers to Russo and Van Roy [2013] for more examples.

We remark that in this paper, the sample complexity of our algorithm depends on the ε -Eluder dimension introduced in Russo and Van Roy [2013] instead of the the Eluder dimension introduced in Wen and Van Roy [2013], since the Eluder dimension introduced in Wen and Van Roy [2013] is defined for the exact case and therefore cannot handle approximation errors.

224 4 Algorithm for Linear Functions

In this section, we consider the special case where \mathcal{F} is the class of linear functions to demonstrate the high-level approach of our algorithm and the intuition behind the analysis. For simplicity, we also

Algorithm 1 Main Algorithm

Initialize the current policy π arbitrarily
 set C = ρ²/16 · I ∈ ℝ^{d×d}
 set Y = 0 ∈ ℝ^d
 invoke Explore(s₁)
 return π

Algorithm 2 Explore(s)

1: for $a \in \mathcal{A}$ do if $\phi(s,a)^{\top}C^{-1}\phi(s,a) \leq 1$ then 2: set $\hat{Q}(s,a) = \phi(s,a)^{\top} C^{-1} Y$ 3: 4: else let s' = P(s, a)5: set 6: $\hat{Q}(s,a) = \begin{cases} r(s,a) & \text{if } s \in \mathcal{S}_H \\ \mathsf{Explore}(s') + r(s,a) & \text{otherwise} \end{cases}$ set $C = C + \phi(s, a)\phi(s, a)^{\top}$, $Y = Y + \phi(s, a)\hat{Q}(s, a)$ 7: end if 8: 9: end for 10: set $\pi(s) = \operatorname{argmax}_{a \in \mathcal{A}} \hat{Q}(s, a)$. 11: return $r(s, \pi(s)) + \operatorname{Explore}(P(s, \pi(s)))$

assume that the size of action space A is bounded by a constant and the reward is deterministic. We show how to remove these assumptions in the following sections.

Our goal is to show when $\rho = \Omega(\delta \sqrt{d \log(1/\rho)})$, Algorithm 1 learns the optimal policy π^* using nearly linear number of trajectories.

Theorem 4.1. Suppose $\rho \ge 4\delta(\sqrt{2d\log(16/\rho^2)} + 1)$. Algorithm 1 returns the optimal policy π^* using at most $O(d\log(1/\rho))$ trajectories.

The complete proof is provided in the supplementary material. On a high level, our algorithm is divided into two parts: Algorithm 1 in which we define the main loop and Algorithm 2 in which we define a recursion-based subroutine Explore(s) to calculate the optimal values. Intuitively, the subroutine Explore(s) should return $V^*(s)$, and upon the termination of Explore(s) we should have $\pi(s) = \pi^*(s)$.

In our algorithm, we maintain a dataset to store the features of a subset of the state-action pairs $\phi(s, a)$ and their optimal Q-values $Q^*(s, a)$. Here, the matrix $C \in \mathbb{R}^d$ is the covariance of the dataset, i.e., $C = \sum \phi(s, a)\phi(s, a)^{\top}$ and $Y = \sum \phi(s, a)Q^*(s, a)$. In order to predict the optimal Q-value of an unseen state-action pair (s, a) using least squares, we may directly calculate $\phi(s, a)^{\top}C^{-1}Y$ if C is invertible. We use a ridge term of $\rho^2/16$ to make sure C is always invertible.

The high-level idea behind our algorithm is simple: we use least squares to predict the optimal Q-value whenever possible, and use recursions to figure out the optimal Q-value otherwise. One technical subtlety here is: What condition should we check to decide whether we can calculate the optimal Q-value directly by least squares or we need to make recursive calls? This condition needs to be chosen carefully, since if we make too many recursive calls, the overall sample complexity will be unbounded, and if we make too few recursive calls, the optimal Q-values estimated by linear squares will be inaccurate which affects the correctness of the algorithm.

In Line 2 of Explore(s), we check whether $\phi(s, a)^{\top} C^{-1} \phi(s, a) \leq 1$, which is the condition we use 250 to decide whether we should make recursive calls or calculate the optimal Q-value directly by least 251 squares. Here $\phi(s, a)^{\top} C^{-1} \phi(s, a)$ is the variance of the prediction, which is common in UCB-type 252 algorithm for linear contextual bandit (see e.g. Li et al. [2010]). In our algorithm, instead of using 253 $\phi(s,a)^{\top}C^{-1}\phi(s,a)$ as an uncertainty bonus, we directly check its magnitude to decide whether 254 the linear predictor learned on the collected dataset generalizes well on the new data $\phi(s, a)$ or not. 255 The effectiveness of such a choice follows from the following lemma which bounds the number of 256 recursive calls made by our algorithm. 257

Lemma 4.2. Line 7 is executed for at most $2d \log(16/\rho^2)$ times.

A proof is provided in the supplementary material. Moreover, in order to make sure that the value

returned by Explore(s) is accurate, in Line 11 of Explore(s), we make recursive calls instead of using the estimated Q-values \hat{Q} . As will be shown in the supplementary material, such a choice guarantees

that the value returned by Explore(s) always equals $V^*(s)$.

Lastly, we want to remark that if we use a $\rho' < \rho$ in the algorithm, the algorithm is still correct and the sample complexity will be $O(d \log(1/\rho'))$. For unknown ρ , one can use an exponential search in a suitable range which will only increase the sample complexity by a logarithmic factor.

266 5 General Result

In this section, we consider the general case where \mathcal{F} is an arbitrary function class and provide a provably efficient algorithm which is a generalization of the algorithm in Section 4. Note that we make no assumptions on the action space \mathcal{A} . For simplicity, we assume that the reward is deterministic. We show how to remove this assumption in the supplementary material. We first define the Maximum Uncertainty Oracle which allows us to work with arbitrary action space.

272 5.1 Maximum Uncertainty Oracle

As discussed the previous section, it is useful to identify actions for which we can not accurately compute the optimal Q-value using the least-squares predictor. We formalize this intuition to arrive at the following oracle which finds the action with largest "uncertainty" for a given state s. We note that similar oracles were also used in [Du et al., 2019].

Definition 5.1 (Oracle (s, δ, Y)). *Given a state* $s \in S$, $\delta \ge 0$ and a set of state-action pairs $Y \subseteq S \times A$, define

$$(\hat{a}, \hat{f}_1, \hat{f}_2) = \operatorname*{argmax}_{a \in A, f_1, f_2 \in \mathcal{F}} |f_1(s, a) - f_2(s, a)|^2$$
(1)

s.t.
$$\frac{1}{|Y|} \sum_{(s',a') \in Y} |f_1(s',a') - f_2(s',a')|^2 \le \delta^2.$$
 (2)

279 The oracle returns $(\hat{a}, |\hat{f}_1(s, \hat{a}) - \hat{f}_2(s, \hat{a})|^2)$.

To motivate this oracle, suppose f_2 is the function that gives the best approximation of the optimal Q-function, i.e., the optimizer f in Definition 3.2. In this scenario, we know f_1 predicts well on state-action pairs $(s', a') \in Y$ which is implied by the constraint. Note that since we maximize over the entire function class \mathcal{F} , \hat{a} is the action with largest uncertainty. If $|\hat{f}_1(s, \hat{a}) - \hat{f}_2(s, \hat{a})|^2$ is small, then we can predict well on state s for all actions. Otherwise, if we cannot predict well on state s for some action, so we need to explore and return the action with largest uncertainty.

Remark 1. When \mathcal{F} is the class of linear functions, evaluating the oracle's response amounts to solving:

$$(\hat{a}, \hat{\theta}_1, \hat{\theta}_2) = \underset{a \in A, \theta_1, \theta_2 \in \mathcal{F}}{\operatorname{argmax}} |(\theta_1 - \theta_2)^\top \phi(s, a)|^2$$
s.t.
$$(\theta_1 - \theta_2)^\top \left(\frac{1}{|Y|} \sum_{(s', a') \in Y} \phi(s', a') \phi(s', a')^\top \right) (\theta_1 - \theta_2) \le \delta^2.$$

In this case, using the notation in the algorithm in Section 4, it can be seen that the oracle returns the action $a \in A$ which maximizes $\phi(s, a)^\top C^{-1} \phi(s, a)$.

290 5.2 Algorithm

In this section, we present the high level intuition for the Algorithm 3. Our goal is to show that when $\rho = \Omega(\delta \sqrt{\dim_E(\mathcal{F}, \rho)})$, our algorithm learns the optimal policy π^* using linear number of trajectories (in terms of Eluder dimension).

Algorithm 3 Main Algorithm

1: Initialize the current policy π and f arbitrarily.

2: set $Y = \{\}$

- 3: **invoke** $Explore(s_1)$
- 4: return π

Algorithm 4 Explore(*s*)

1: set $(a, r) = \text{Oracle}(s, 2\delta, Y)$ 2: while $r > |\frac{\rho}{2} - \delta|$ do 3: set $Y = Y \cup \{(s, a, \text{Explore}(P(s, a)) + r(s, a))\}$ 4: set $(a, r) = \text{Oracle}(s, 2\delta, Y)$ 5: end while 6: set $f = \operatorname{argmin}_{f \in \mathcal{F}} \sum_{(s_i, a_i, y_i) \in Y} |f(s_i, a_i) - y_i|^2$ 7: set $\pi(s) = \operatorname{argmax}_{a \in \mathcal{A}} f(s, a)$ 8: return $r(s, \pi(s)) + \text{Explore}(P(s, \pi(s)))$

294 Theorem 5.1. Suppose

$$\rho \ge 6\sqrt{2}\delta\sqrt{\dim_E(\mathcal{F},\frac{\rho}{4})}.$$
(3)

Then Algorithm 3 returns the optimal policy π^* using at most $O(\dim_E(\mathcal{F}, \rho/4))$ trajectories.

The complete proof is provided in the supplementary material. Similar to the algorithm for linear functions given in Section 4, the algorithm for general function class is divided into two parts: Algorithm 3 and a subroutine Explore(s). Intuitively, the subroutine Explore(s) should return $V^*(s)$, and upon the termination of Explore(s), we should have $\pi(s) = \pi^*(s)$.

In our algorithm, we maintain a dataset to store the state-action pairs (s, a) and their optimal Q-values $Q^*(s, a)$. In order to predict the optimal Q-value of an unseen state-action pair (s, a), we find the best predictor on the dataset using least squares, and use it to predict on (s, a).

Similar to the algorithm in Section 4, the high level idea is that we use least squares to predict the optimal Q-value whenever possible, and otherwise we explore the environment. In Line 2, we check for a state s, whether the Maximum Uncertainty Oracle reports an uncertainty $r > |\rho/2 - \delta|$. Such a choice guarantees that the value returned by Explore(s) always equals $V^*(s)$ and also, as we prove, upper bounds the number of times we explore, i.e., execute Line 3, by the Eluder dimension of function class \mathcal{F} .

Lemma 5.2. For any constant c > 1, suppose $\rho \ge 4\delta \sqrt{\frac{c \dim_E(F, \frac{\rho}{4}) - 1}{c-1}} + 2\delta$. Then we have $|Y| \le c \dim_E(F, \frac{\rho}{4})$.

A proof is provided in the supplementary material. The proof relies on definition of the Eluder dimension and the Maximum Uncertainty Oracle. We remark that when applied to linear functions, using the notation in the algorithm in Section 4, the subroutine Explore(s) keeps finding an action $a \in \mathcal{A}$ which maximizes $\phi(s, a)^{\top} C^{-1} \phi(s, a)$ (see Remark 1) until $\phi(s, a)^{\top} C^{-1} \phi(s, a)$ is below a threshold for all actions $a \in \mathcal{A}$. Therefore, our algorithm is a generalization of the algorithm in Section 4.

Again, we remark that while Algorithm 3 depends on both ρ and δ , one can use an exponential search for ρ and δ , and the sample complexity will increase mildly.

319 6 Conclusion

In this paper, we propose a novel provably efficient recursion-based algorithm for agnostic *Q*-learning with general function approximation in deterministic systems. We obtain a sharp characterization on the relation between the approximation error and the optimality gap, and also a tight sample complexity. We help address the open problem raised by Wen and Van Roy [2013].

324 Broader Impact

The focus of this paper is purely theoretical, and thus a broader impact discussion is not applicable.

326 **References**

- 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.
- Alekh Agarwal, Sham Kakade, and Lin F Yang. On the optimality of sparse model-based planning for markov decision processes. *arXiv preprint arXiv:1906.03804*, 2019.
- Shipra Agrawal and Randy Jia. Optimistic posterior sampling for reinforcement learning: worst-case regret bounds. In *Advances in Neural Information Processing Systems*, pages 1184–1194, 2017.
- Mohammad Gheshlaghi Azar, Rémi Munos, and Hilbert J Kappen. Minimax PAC bounds on the
 sample complexity of reinforcement learning with a generative model. *Machine learning*, 91(3):
 325–349, 2013.
- Mohammad Gheshlaghi Azar, Ian Osband, and Rémi Munos. Minimax regret bounds for reinforce ment learning. In *Proceedings of the 34th International Conference on Machine Learning*, pages
 263–272, 2017.
- 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, 2018.
- Varsha Dani, Thomas P Hayes, and Sham M Kakade. Stochastic linear optimization under bandit
 feedback. 2008.
- Simon S Du, Yuping Luo, Ruosong Wang, and Hanrui Zhang. Provably efficient *Q*-learning
 with function approximation via distribution shift error checking oracle. In *Advances in Neural Information Processing Systems*, pages 8058–8068, 2019.
- Simon S Du, Sham M Kakade, Ruosong Wang, and Lin F Yang. Is a good representation sufficient for
 sample efficient reinforcement learning? In *International Conference on Learning Representations*,
 2020.
- 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*
- 352 *Representations*, 2018.
- Thomas Jaksch, Ronald Ortner, and Peter Auer. Near-optimal regret bounds for reinforcement learning. *Journal of Machine Learning Research*, 11(Apr):1563–1600, 2010.
- 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.
- Chi Jin, Zhuoran Yang, Zhaoran Wang, and Michael I Jordan. Provably efficient reinforcement
 learning with linear function approximation. *arXiv preprint arXiv:1907.05388*, 2019.
- Sham Kakade, Mengdi Wang, and Lin F Yang. Variance reduction methods for sublinear reinforcement learning. *arXiv preprint arXiv:1802.09184*, 2018.
- Tor Lattimore and Marcus Hutter. PAC bounds for discounted mdps. In *International Conference on Algorithmic Learning Theory*, pages 320–334. Springer, 2012.
- ³⁶³ Tor Lattimore and Csaba Szepesvári. Bandit algorithms. *preprint*, page 28, 2018.
- Tor Lattimore and Csaba Szepesvari. Learning with good feature representations in bandits and in RL with a generative model. *arXiv preprint arXiv:1911.07676*, 2019.
- Lihong Li, Wei Chu, John Langford, and Robert E Schapire. A contextual-bandit approach to personalized news article recommendation. In *Proceedings of the 19th international conference on World wide web*, pages 661–670, 2010.

- Lihong Li, Michael L Littman, Thomas J Walsh, and Alexander L Strehl. Knows what it knows: a framework for self-aware learning. *Machine learning*, 82(3):399–443, 2011.
- ³⁷¹ 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.
- Shie Mannor and John N Tsitsiklis. The sample complexity of exploration in the multi-armed bandit problem. *Journal of Machine Learning Research*, 5(Jun):623–648, 2004.
- Francisco S Melo and M Isabel Ribeiro. Q-learning with linear function approximation. In *Interna- tional Conference on Computational Learning Theory*, pages 308–322, 2007.
- Gergely Neu and Julia Olkhovskaya. Efficient and robust algorithms for adversarial linear contextual
 bandits. *arXiv preprint arXiv:2002.00287*, 2020.
- 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*, pages 2377–2386, 2016.
- Jason Pazis and Ronald Parr. PAC optimal exploration in continuous space markov decision processes.
 In *Proceedings of the Twenty-Seventh AAAI Conference on Artificial Intelligence*, pages 774–781, 2013.
- Daniel Russo and Benjamin Van Roy. Eluder dimension and the sample complexity of optimistic
 exploration. In *Advances in Neural Information Processing Systems*, pages 2256–2264, 2013.
- Aaron Sidford, Mengdi Wang, Xian Wu, Lin Yang, and Yinyu Ye. Near-optimal time and sample
 complexities for solving markov decision processes with a generative model. In *Advances in Neural Information Processing Systems*, pages 5186–5196, 2018a.
- Aaron Sidford, Mengdi Wang, Xian Wu, and Yinyu Ye. Variance reduced value iteration and faster
 algorithms for solving markov decision processes. In *Proceedings of the Twenty-Ninth Annual ACM-SIAM Symposium on Discrete Algorithms*, pages 770–787. SIAM, 2018b.
- Max Simchowitz and Kevin G Jamieson. Non-asymptotic gap-dependent regret bounds for tabular mdps. In *Advances in Neural Information Processing Systems*, pages 1151–1160, 2019.
- 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.
- Benjamin Van Roy and Shi Dong. Comments on the Du-Kakade-Wang-Yang lower bounds. *arXiv preprint arXiv:1911.07910*, 2019.
- Yining Wang, Ruosong Wang, Simon S Du, and Akshay Krishnamurthy. Optimism in reinforcement
 learning with generalized linear function approximation. *arXiv preprint arXiv:1912.04136*, 2019.
- 403 Christopher JCH Watkins and Peter Dayan. Q-learning. *Machine learning*, 8(3-4):279–292, 1992.
- 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.
- Lin F. Yang and Mengdi Wang. Reinforcement leaning in feature space: Matrix bandit, kernels, and regret bound. *arXiv preprint arXiv:1905.10389*, 2019a.
- Lin F. Yang and Mengdi Wang. Sample-optimal parametric q-learning using linearly additive features.
 In *International Conference on Machine Learning*, pages 6995–7004, 2019b.
- Andrea Zanette, Mykel J Kochenderfer, and Emma Brunskill. Almost horizon-free structure-aware
 best policy identification with a generative model. In *Advances in Neural Information Processing Systems*, pages 5626–5635, 2019.
- Shaofeng Zou, Tengyu Xu, and Yingbin Liang. Finite-sample analysis for SARSA with linear
 function approximation. In *Advances in Neural Information Processing Systems*, pages 8665–8675,
 2019.

417 A Proof of Proposition 1.2

In this section, we briefly discuss how to generalize the results in [Du et al., 2020] to prove Proposition 1.2. We first recall Theorem 4.1 in [Du et al., 2020].

Proposition A.1 (Theorem 4.1 in [Du et al., 2020]). There exists a family of deterministic systems \mathcal{M} such that for any $M \in \mathcal{M}$, the following conditions hold. There exists a feature extractor $\phi: S \times \mathcal{A} \to \mathbb{R}^d$ and $\theta_1, \theta_2, \ldots, \theta_H \in \mathbb{R}^d$ such that $d = O(H/\delta^2)$, and for any $h \in [H]$ and any $(s, a) \in S_h \times \mathcal{A}$,

$$|Q^*(s,a) - \theta_h^\top \phi(s,a)| \le \delta.$$

⁴²⁴*Moreover, for the deterministic systems in* \mathcal{M} *, any algorithm that returns a* 1/2*-optimal policy with* ⁴²⁵*probability* 0.9 *needs to sample* $\Omega(2^H)$ *trajectories.*

We first note that the assumption in Proposition A.1 is slightly different from ours. In this paper, we assume there exists a single vector $\theta \in \mathbb{R}^d$ such that for any $(s, a) \in S \times A$,

$$|Q^*(s,a) - \theta^\top \phi(s,a)| \le \delta.$$

However, the lower bound in [Du et al., 2020] can still be generalized to hold under our assumption, if one breaks the feature space into H blocks so that each block contains d/H coordinates, and for any state $s_1 \in S_1$ and $a \in A$, $\phi(s_1, a)$ contains non-zero entries only in the first block, and for any state $s_2 \in S_2$ and $a \in A$, $\phi(s_2, a)$ contains non-zero entries only in the second block, etc. By doing so, we need to change the condition $d = O(H/\delta^2)$ to $d = O(H^2/\delta^2)$.

Moreover, in order to prove an $\Omega(2^C)$ sample complexity lower bound, one only needs to use the first *C* levels in the family of deterministic systems in Proposition A.1, and add H - C dummy levels so that there are *H* levels in total. In this case, Proposition A.1 requires $d = O(C^2/\delta^2)$, or equivalently, $\delta = \Omega(C/\sqrt{d})$.

Finally, by scrutinizing the construction in [Du et al., 2020], it can be seen that the optimality gap $\rho = 1$. In general, for a given value $\rho \leq 1$, we can scale all reward values and the vector θ in the original construction by ρ . By doing so, the approximation error $\delta = \Omega(C/\sqrt{d} \cdot \rho)$.

440 **B** Missing Proofs in Section 4

441 Proof of Theorem 4.1. Recall that by Definition 3.2 and Definition 3.3, there exists $\theta \in \mathbb{R}^d$ with 442 $\|\theta\|_2 \leq 1$ such that $|Q^*(s, a) - \theta^\top \phi(s, a)| \leq \delta$ for all state-action pairs (s, a).

Since the sample complexity of our algorithm equals the number of times we execute Line 5 in Explore(s), following Lemma 4.2, the sample complexity of our algorithm is $O(d \log(1/\rho))$.

To complete the proof, it is sufficient to prove the following induction hypothesis for all levels $h \in [H]$.

447 Induction Hypothesis.

- I When Line 6 is executed for any state $s \in S_h$, $\hat{Q}(s, a) = Q^*(s, a)$.
- II Each time Line 10 in Explore(s) is executed for any state $s \in S_h$, we have $\pi(s) = \pi^*(s)$, and the value returned by Explore(s) equals $V^*(s)$.

For the above induction hypothesis, the base case h = H is clearly true. Now we assume the induction hypothesis holds for all levels $H, \ldots, h + 1$ and prove it holds for all levels $h \in [H]$.

Induction Hypothesis I. This follows from Induction Hypothesis II for level h+1 and the Bellman equations.

Induction Hypothesis II. By Induction Hypothesis I and Definition 3.1, we only need to show when Line 3 is executed, we have $|\hat{Q}(s,a) - Q^*(s,a)| \le \rho/2$, in which case we have $\pi(s) = \pi^*(s)$. To verify this, note that

$$|\phi(s,a)^{\top}C^{-1}Y - Q^{*}(s,a)| \le |\phi(s,a)^{\top}C^{-1}Y - \theta^{\top}\phi(s,a)| + |Q^{*}(s,a) - \theta^{\top}\phi(s,a)|.$$

The second term is bounded by δ . For the first term, we write Φ to be a matrix whose *i*-th column is the *i*-th $\phi(s, a)$ vector in the summation. Recall that

$$C = \left(\sum \phi(s, a)\phi(s, a)^{\top}\right) + \rho^2/16 \cdot I = \Phi \Phi^{\top} + \rho^2/16 \cdot I$$

460 and

$$Y = \sum \phi(s, a) Q^*(s, a)$$

461 by Induction Hypothesis I. Moreover,

$$Y = \sum \phi(s, a)(\phi(s, a)^{\top}\theta + b(s, a))$$

where $|b(\cdot, \cdot)| \leq \delta$. Thus, the first term can be upper bounded by

$$\left\|\phi(s,a)^{\top}C^{-1}\Phi\right\|_{1}\cdot\delta+\left|\phi(s,a)^{\top}(C^{-1}\Phi\Phi^{\top}-I)\theta\right|.$$

For the first term, by Lemma 4.2 there are at most $2d \log(16/\rho^2)$ columns in Φ . When Line 3 is executed, we must have $\phi(s, a)^{\top} C^{-1} \phi(s, a) \leq 1$. Using Lemma B.1 we have

$$\begin{split} &\|\phi(s,a)^{\top}C^{-1}\Phi\|_{1} \\ \leq &\sqrt{2d\log(16/\rho^{2})} \cdot \|\phi(s,a)^{\top}C^{-1}\Phi\|_{2} \\ &= &\sqrt{2d\log(16/\rho^{2})} \cdot \sqrt{\phi(s,a)^{\top}C^{-1}\Phi\Phi^{\top}C^{-1}\phi(s,a)} \\ \leq &\sqrt{2d\log(16/\rho^{2})}. \end{split}$$

For the second term, since $\|\theta\|_2 \leq 1$ and $\phi(s,a)^\top C^{-1}\phi(s,a) \leq 1$, by Cauchy-Schwarz and Lemma B.1, we have

$$|\phi(s,a)^{\top} (C^{-1} \Phi^{\top} \Phi - I)\theta| \le \|\phi(s,a)^{\top} (C^{-1} \Phi^{\top} \Phi - I)\|_{2} \le \rho/4.$$

467 All together we get

$$|\phi(s,a)^{\top}C^{-1}Y - Q^*(s,a)| \le \rho/2$$

468 which completes the proof.

Proof of Lemma 4.2. Suppose Line 7 has been executed for T times, since $\|\phi(s,a)\|_2 \leq 1$, the trace of $\phi(s,a)\phi(s,a)^{\top}$ is upper bounded by $\|\phi(s,a)\|_2^2 \leq 1$. By additivity of trace, the trace of C is upper bounded by

$$T + d \cdot \rho^2 / 16$$

since initially the trace of C is $d \cdot \rho^2 / 16$. By AM-GM,

$$\det(C) \le (T/d + \rho^2/16)^d.$$

However, each time Line 7 is executed, by matrix determinant lemma, det(C) will be increased by a factor of

$$1 + \phi(s_h, a) \cdot C^{-1} \phi(s_h, a) \ge 2$$

475 Moreover, initially $\det(C) = (\rho^2/16)^d$. Thus,

$$2^T (\rho^2/16)^d \le (T/d + \rho^2/16)^d,$$

476 which proves the lemma.

Lemma B.1. For any positive semi-definite $M \in \mathbb{R}^{d \times d}$, $\alpha > 0$ and $x \in \mathbb{R}^d$ such that $x^{\top}(M + \alpha \cdot I)^{-1}x \leq 1$, we have

- 479 $||(M(M + \alpha \cdot I)^{-1} I)x||_2 \le \alpha;$
- $\bullet \ x^\top (M+\alpha\cdot I)^{-1}M(M+\alpha\cdot I)^{-1}x\leq 1.$

Proof. We use $M = U^T \Lambda U$ to denote the spectral decomposition of M, where Λ is a diagonal matrix with non-negative entries. We use Λ_i to denote the *i*-th diagonal entry of Λ and let y = Ux.

483 By the assumption, it holds that

$$\sum_{i=1}^{d} \frac{y_i^2}{\Lambda_i + \alpha} \le 1.$$

484 Clearly,

$$\|(M(M+\alpha \cdot I)^{-1} - I)x\|_2^2$$

= $\sum_{i=1}^d y_i^2 \cdot \left(\frac{\Lambda_i}{\Lambda_i + \alpha} - 1\right)^2 = \sum_{i=1}^d y_i^2 \cdot \left(\frac{\alpha}{\Lambda_i + \alpha}\right)^2 \le \alpha$

485 and

486

$$x^{\top} (M + \alpha \cdot I)^{-1} M (M + \alpha \cdot I)^{-1} x$$
$$= \sum_{i=1}^{d} y_i^2 \cdot \frac{\Lambda_i}{(\Lambda_i + \alpha \cdot I)^2} \le 1.$$

487 C Missing Proofs in Section 5

488 Proof of Theorem 5.1. Firstly, using Lemma 5.2 with c = 18 we have

$$|Y| \le 18 \dim_E(\mathcal{F}, \frac{\rho}{4}),\tag{4}$$

i.e. Line 3 is executed for at most $18 \dim_E(F, \rho/4)$ times and therefore the sample complexity of our algorithm is $O(\dim_E(\mathcal{F}, \rho/4))$.

To complete the proof, it is sufficient to prove the following induction hypothesis for all levels $h \in [H]$.

493 Induction Hypothesis.

- I For any state $s \in S_h$, when Line 6 in Explore(s) is executed, we have $y_i = Q^*(s_i, a_i)$ for all $(s_i, a_i, y_i) \in Y$.
- II For any state $s \in S_h$, when Line 7 in Explore(s) is executed, we have $\pi(s) = \pi^*(s)$, and the value returned by Explore(s) is $V^*(s)$.

For the above induction hypothesis, the base case h = H is clearly true. Now we assume the induction hypothesis holds for all levels $H, \ldots, h + 1$ and prove it holds for all levels $h \in [H]$.

Induction Hypothesis I. From Induction Hypothesis II for level h+1, it follows that value returned by Explore(P(s, a)) is $V^*(P(s, a))$ for all $a \in A$. Then, Induction Hypothesis I follows from the Bellman equations.

Induction Hypothesis II. It suffices to show that for any state $s \in S_h$, when Line 7 in Explore(s) is executed, for all actions $a \in A$

$$|f(s,a) - Q^*(s,a)| \le \frac{\rho}{2}.$$
 (5)

First, there exists $f^* \in \mathcal{F}$ such that for all $(s_i, a_i, y_i) \in Y$,

$$|f^*(s_i, a_i) - Q^*(s_i, a_i)| \le \delta.$$
(6)

From Induction Hypothesis I, for all $(s_i, a_i, y_i) \in Y$

$$y_i = Q^*(s_i, a_i). \tag{7}$$

507 From Equation (6) and (7), it follows that

$$\sum_{(s_i, a_i, y_i) \in Y} |f^*(s_i, a_i) - y_i|^2 \le |Y|\delta^2.$$
(8)

Since, we execute Line 6 and $f^* \in \mathcal{F}$, from Equation (8), it follows that

$$\sum_{(s_i, a_i, y_i) \in Y} |f(s_i, a_i) - y_i|^2 \le |Y|\delta^2.$$
(9)

- 509 We split the analysis into two cases:
- 510 (1) we consider actions for which we execute Line 3 and
- 511 (2) we consider rest of the actions.
- **Case 1:** We now prove Equation (5) for all actions a for which we execute Line 3. Using Equation (4), (7) and (9), we get that for actions a for which we executed Line 3 (since then we added it to Y)

$$|f(s,a) - Q^*(s,a)| \le \sqrt{18 \dim_E(F,\frac{\rho}{4})} \delta \le \frac{\rho}{2}$$
 (10)

- where the last step follows from our assumption on ρ (Equation (3)).
- **Case 2:** We now prove this for rest of the actions *a*. From Equation (6), (7), (9) and triangle inequality for the ℓ_2 norm, we get

$$\sum_{(s_i, a_i, y_i) \in Y} |f^*(s_i, a_i) - f(s_i, a_i)|^2 \le 4|Y|\delta^2.$$
(11)

Also, since we did not add this action to Y, by the definition of the oracle (Definition 5.1), we get

$$|f^*(s,a) - f(s,a)| \le \frac{\rho}{2} - \delta.$$
 (12)

518 Therefore,

$$|Q^*(s,a) - f(s,a)| \le \frac{\rho}{2}$$
(13)

- 519 which completes the proof.
- 520 Proof of Lemma 5.2. For some n > 0, assume

$$Y = \{(s_1, a_1, y_1), \dots, (s_n, a_n, y_n)\}\$$

We will show that n is upper bounded by Eluder dimension. When we add (s_j, a_j, y_j) to Y at Line 3,

- 1. The condition at Line 2 must be True i.e. from Equation (1), there exists $f_1, f_2 \in F$ such that $|f_1(s_j, a_j) - f_2(s_j, a_j)| > \frac{\rho}{2} - \delta$.
- 2. Observe that for any subsequence $B \subset \{(s_1, a_1), \dots, (s_{j-1}, a_{j-1})\}$ where (s_j, a_j) is $(\frac{\rho}{2} - \delta)$ -dependent on B (Definition 3.4),

$$\sum_{(s,a)\in B} |f_1(s,a) - f_2(s,a)|^2 \ge (\frac{\rho}{2} - \delta)^2.$$
(14)

3. Therefore, if there are K disjoint subsequences in $\{(s_1, a_1), \dots, (s_{j-1}, a_{j-1})\}$ such that (s_j, a_j) is $(\frac{\rho}{2} - \delta)$ -dependent on all of them, then

$$\sum_{i=1}^{j-1} |f_1(s_i, a_i) - f_2(s_i, a_i)|^2 \ge K(\frac{\rho}{2} - \delta)^2.$$
(15)

4. However, using Equation 2, we have that

$$\sum_{i=1}^{j-1} |f_1(s_i, a_i) - f_2(s_i, a_i)|^2 \le (j-1)(2\delta)^2.$$
(16)

Therefore, we can upper bound for any state-action pair $(s_j, a_j) \in \{(s_1, a_1), \dots, (s_n, a_n)\}$, the number of disjoint subsequences K in $\{(s_1, a_1), \dots, (s_{j-1}, a_{j-1})\}$ that (s_j, a_j) is $(\frac{\rho}{2} - \delta)$ -dependent on, i.e.

$$K \le \frac{(j-1)(2\delta)^2}{(\frac{\rho}{2}-\delta)^2}.$$

Moreover, it follows from the proof of Proposition 3 in [Russo and Van Roy, 2013] that for any sequence of state-action pairs say $\{(s_1, a_1), \dots, (s_n, a_n)\}$, there exists a (s_j, a_j) which is $(\frac{\rho}{2} - \delta)$ -dependent on at least $\frac{n}{\dim_E(F, \frac{\rho}{2} - \delta)} - 1$ disjoint subsequences in $\{(s_1, a_1), \dots, (s_{j-1}, a_{j-1})\}$. Therefore,

$$\frac{n}{\dim_E(F,\frac{\rho}{2}-\delta)} - 1 \le K \le \frac{(j-1)(2\delta)^2}{(\frac{\rho}{2}-\delta)^2}$$
(17)

536 and thus

528

$$n \le \dim_E(F, \frac{\rho}{2} - \delta) \left(\frac{(n-1)(2\delta)^2}{(\frac{\rho}{2} - \delta)^2} + 1 \right).$$
 (18)

537 As $\rho > 4\delta$, we get

$$n \le \dim_E(F, \frac{\rho}{4}) \left(\frac{(n-1)(2\delta)^2}{(\frac{\rho}{2} - \delta)^2} + 1 \right)$$
 (19)

- which follows from definition of Eluder dimension since a < b implies $\dim_E(F, a) \ge \dim_E(F, b)$.
- 539 For any ρ and c > 1 such that

$$\rho \ge 2\left(2\sqrt{\frac{c\dim_E(F,\frac{\rho}{4})-1}{c-1}}+1\right)\delta\tag{20}$$

540 we get from Equation (19) that

$$n \le c \dim_E(F, \frac{\rho}{4}). \tag{21}$$

541

542 **D** Extension to Stochastic Rewards

Algorithm 5 Main Algorithm

| 1: Initialize the current policy π and f arbitrarily | |
|----------------------------------------------------------|--|
| 2: set $Y = \{\}$ | |
| 3: invoke $Explore(s_1)$ | |
| | |

In this section, we extend our algorithm and analysis to stochastic rewards, i.e., reward $r(s, a) \sim R(s, a)$ is a random variable with expectation $\bar{r}(s, a)$ and $r(s, a) \in [0, 1]$.

545 D.1 Algorithm

We modify Explore(s) such that whenever previously we used r(s, a), we use the empirical mean $\hat{r}(s, a)$ of n samples from R(s, a) to get a good estimate of the expected reward $\bar{r}(s, a)$. For our algorithm, we set

$$n = \frac{H^2}{2\delta_r^2} \log \frac{18 \dim_E(\mathcal{F}, \rho/4)H}{p},$$
(22)

where δ_r is a parameter to be chosen and p is the failure probability of the algorithm.

Algorithm 6 Explore(*s*)

1: set $(a, r) = \text{Oracle}(s, 2(\delta + \delta_r), Y)$ 2: while $r > |\frac{\rho}{2} - \delta|$ do 3: set $\hat{r}(s, a)$ to be the empirical mean of $n = \frac{H^2}{2\delta_r^2} \log \frac{18 \dim_E(\mathcal{F}, \rho/4)H}{p}$ samples from R(s, a)4: set $Y = \begin{cases} Y \cup \{(s, a, \hat{r}(s, a))\} & s \in S_H \\ Y \cup \{(s, a, \text{Explore}(P(s, a)) + \hat{r}(s, a))\} & \text{otherwise} \end{cases}$ 5: set $(a, r) = \text{Oracle}(s, 2(\delta + \delta_r), Y)$ 6: end while 7: set $f = \operatorname{argmin}_{f \in \mathcal{F}} \sum_{(s_i, a_i, y_i) \in Y} |f(s_i, a_i) - y_i|^2$ 8: set $\pi(s) = \operatorname{argmax}_{a \in \mathcal{A}} f(s, a)$ 9: return $\begin{cases} \hat{r}(s, \pi(s)) & s \in S_H \\ \hat{r}(s, \pi(s)) + \text{Explore}(P(s, \pi(s))) & \text{otherwise} \end{cases}$

550 D.2 Analysis

551 Theorem D.1. Suppose

$$\rho \ge 6\sqrt{2}(\delta + \delta_r)\sqrt{\dim_E(\mathcal{F}, \rho/4)} + 2\delta_r.$$
(23)

- 552 Algorithm 5 returns the optimal policy π^* with probability 1 p.
- 553 **Remark 2.** Note that by setting

$$\delta_r = \frac{\rho}{24\sqrt{2\dim_E(\mathcal{F},\rho/4)}} \quad and \quad \rho \ge 12\sqrt{2}\delta\sqrt{\dim_E(\mathcal{F},\rho/4)}, \tag{24}$$

Theorem D.1 implies that Algorithm 5 returns the optimal policy π^* with probability 1 - p using at most most

$$\frac{\operatorname{poly}(\dim_E(\mathcal{F},\rho/4),H)}{\rho^2}\log(1/p)$$

556 trajectories.

- 557 Now we formally prove Theorem D.1.
- *Proof of Theorem D.1.* Firstly, for c = 18, following Lemma D.2, we have

$$|Y| \le 18 \dim_E(\mathcal{F}, \rho/4), \tag{25}$$

- i.e. Line 4 is executed for at most $18 \dim_E(F, \rho/4)$ times.
- To complete the proof, it is sufficient to prove the following induction hypothesis for all levels $h \in [H]$.

563 Induction Hypothesis.

1. For any state
$$s \in S_h$$
, when Line 7 in Explore(s) is executed, we have

$$y_i \in \left[Q^*(s_i, a_i) - \frac{H - h + 1}{H}\delta_r, Q^*(s_i, a_i) + \frac{H - h + 1}{H}\delta_r\right]$$

for all $(s_i, a_i, y_i) \in Y$.

2. For any state $s \in S_h$, when Line 8 in Explore(s) is executed, we have $\pi(s) = \pi^*(s)$, and the value returned by Explore(s) is in

$$\left[V^*(s) - \frac{H-h+1}{H}\delta_r, V^*(s) + \frac{H-h+1}{H}\delta_r\right]$$

568

566

567

560

Note that the base case h = H is true by Lemma D.3 and union bound. Now we assume the induction hypothesis holds for all levels $H, \ldots, h + 1$ and prove it holds for level h. Induction Hypothesis 1. From Induction Hypothesis 2 for level h+1, it follows that value returned by Explore(P(s, a)) is in

$$\left[V^*(P(s,a)) - \frac{H-h}{H}\delta_r, V^*(P(s,a)) + \frac{H-h}{H}\delta_r\right]$$

for all $a \in A$. Then, Induction Hypothesis 1 follows from Lemma D.3 and union bound.

Induction Hypothesis 2. It suffices to show that for any state $s \in S_h$, when Line 8 in Explore(s) is executed, then for all actions $a \in A$

$$|f(s,a) - Q^*(s,a)| \le \frac{\rho}{2}.$$
 (26)

576 Similar to proof of Theorem 5.1, we get

$$\sum_{s_i, a_i, y_i) \in Y} |f(s_i, a_i) - y_i|^2 \le |Y| (\delta + \delta_r)^2.$$
(27)

577 We split the analysis in two cases:

1. we consider actions for which we execute Line 4 and

(

579 2. we consider rest of the actions.

Case 1: We now prove Equation (26) for all actions *a* for which we execute Line 4. Similar to proof of Theorem 5.1, we get

$$|f(s,a) - Q^*(s,a)| \le \sqrt{18 \dim_E(\mathcal{F}, \rho/4)} (\delta + \delta_r) + \delta_r \le \frac{\rho}{2}.$$
(28)

Case 2: We now prove this for rest of the actions *a*. Similar to proof of Theorem 5.1, we get

$$\sum_{(s_i, a_i, y_i) \in Y} |f^*(s_i, a_i) - f(s_i, a_i)|^2 \le 4|Y|(\delta + \delta_r)^2.$$
(29)

Also, since we did not add this action to Y, by the definition of the oracle (Definition 5.1), we get

$$|Q^*(s,a) - f(s,a)| \le \frac{\rho}{2},$$
(30)

⁵⁸⁴ which completes the proof.

585 **Lemma D.2.** For any constant c > 1, if

$$\rho \ge 4(\delta + \delta_r) \sqrt{\frac{c \dim_E(\mathcal{F}, \rho/4) - 1}{c - 1}} + 2\delta,\tag{31}$$

586 then

$$|Y| \le c \dim_E(\mathcal{F}, \rho/4). \tag{32}$$

Proof. Let $Y = \{(s_1, a_1, y_1), \dots, (s_n, a_n, y_n)\}$. Similar to proof of Lemma 5.2, we can upper bound for any state-action pair $(s_j, a_j) \in \{(s_1, a_1), \dots, (s_n, a_n)\}$, the number of disjoint subsequences Kin $\{(s_1, a_1), \dots, (s_{j-1}, a_{j-1})\}$ that (s_j, a_j) is $(\frac{\rho}{2} - \delta)$ -dependent on, i.e.

$$K \leq \frac{(j-1)(2(\delta+\delta_r))^2}{(\frac{\rho}{2}-\delta)^2}$$

Also, for any sequence of state-action pairs say $\{(s_1, a_1), \ldots, (s_n, a_n)\}$, there exists a (s_j, a_j) which is $(\frac{\rho}{2} - \delta)$ -dependent on at least $\frac{n}{\dim_E(F, \frac{\rho}{2} - \delta)} - 1$ disjoint subsequences in $\{(s_1, a_1), \ldots, (s_{j-1}, a_{j-1})\}$. Therefore,

$$\frac{n}{\dim_E(F,\frac{\rho}{2}-\delta)} - 1 \le K \le \frac{(j-1)(2(\delta+\delta_r))^2}{(\frac{\rho}{2}-\delta)^2}.$$
(33)

593 That is, for any ρ and c > 1 such that

$$\rho \ge 2\left(2(\delta + \delta_r)\sqrt{\frac{c\dim_E(\mathcal{F}, \rho/4) - 1}{c - 1}} + \delta\right),\tag{34}$$

594 we get

$$n \le c \dim_E(\mathcal{F}, \rho/4). \tag{35}$$

595

⁵⁹⁶ A simple concentration bound gives the following lemma:

Lemma D.3. For any fixed state s and action a, consider $n \ge \frac{H^2}{2\delta_r^2} \log \frac{1}{p}$ random independent samples $\{r_i(s,a)\}_{i=1}^n$ of random variable R(s,a) with expectation $\bar{r}(s,a)$ and $r_i(s,a) \in [0,1]$. Then,

$$\left|\frac{1}{n}\sum_{i=1}^{n}r_{i}(s,a)-\bar{r}(s,a)\right| \leq \frac{\delta_{r}}{H}$$

599 with probability at least 1 - p.