

---

# Pessimistic Nonlinear Least-Squares Value Iteration for Offline Reinforcement Learning

---

Anonymous Author(s)

Affiliation

Address

email

## Abstract

1 Offline reinforcement learning, where the agent aims to learn the optimal policy  
2 based on the data collected by a behavior policy, has attracted increasing attention  
3 in recent years. While offline RL with linear function approximation has been  
4 extensively studied with optimal results achieved under certain assumptions, the the-  
5 oretical understanding of offline RL with non-linear function approximation is still  
6 limited. Specifically, most existing works on offline RL with non-linear function  
7 approximation either have a poor dependency on the function class complexity or  
8 require an inefficient planning phase. In this paper, we propose an oracle-efficient  
9 algorithm PNL-SVI for offline RL with non-linear function approximation. Our  
10 algorithmic design comprises three innovative components: (1) a variance-based  
11 weighted regression scheme that can be applied to a wide range of function classes,  
12 (2) a subroutine for variance estimation, and (3) a planning phase that utilizes a  
13 pessimistic value iteration approach. Our algorithm enjoys a regret bound that has  
14 a tight dependency on the function class complexity and achieves minimax optimal  
15 problem-dependent regret when specialized to linear function approximation. Our  
16 theoretical analysis introduces a new coverage assumption for nonlinear Q func-  
17 tion, bridging the minimum-eigenvalue assumption and the uncertainty measure  
18 widely used in online nonlinear RL. To the best of our knowledge, this is the first  
19 statistically optimal algorithm for nonlinear offline RL.

## 20 1 Introduction

21 Offline reinforcement learning (RL), also known as batch RL, is a learning paradigm where an  
22 agent learns to make decisions based on a set of pre-collected data, instead of interacting with the  
23 environment in real-time like online RL. The goal of offline RL is to learn a policy that performs well  
24 in a given task, based on historical data that was collected from an unknown environment. Recent  
25 years have witnessed significant progress in developing offline RL algorithms that can leverage large  
26 amounts of data to learn effective policies. These algorithms often incorporate powerful function  
27 approximation techniques, such as deep neural networks, to generalize across large state-action  
28 spaces. They have achieved excellent performances in a wide range of domains, including the games  
29 of Go and chess (Silver et al., 2017; Schrittwieser et al., 2020), robotics (Gu et al., 2017; Levine et al.,  
30 2018), and control systems (Degrave et al., 2022).

31 Several studies have studied the theoretical guarantees of tabular offline RL and proved near-optimal  
32 sample complexities in this setting (Xie et al., 2021b; Shi et al., 2022; Li et al., 2022). However, these  
33 algorithms cannot handle numerous real-world applications with large state spaces. Consequently,  
34 a significant body of research has shifted its focus to offline RL with function approximation. For  
35 example, several works have analyzed the sample efficiency of offline RL with linear function  
36 approximation under different MDP models, including linear MDPs and their variants (Jin et al.,  
37 2021b; Zanette et al., 2021; Min et al., 2021; Yin et al., 2022a). To handle nonlinear function class, a  
38 recent line of research considered offline RL with general function approximation (Chen and Jiang,

2019; Xie et al., 2021a; Zhan et al., 2022). While these algorithms have sample efficiency guarantees, they often require an inefficient planning phase or have a poor dependency on the function class complexity. For example, Xie et al. (2021a) proposed an information-theoretic algorithm that requires solving an optimization problem over all potential policy and corresponding version space, which includes all functions with lower Bellman error. To overcome this limitation, Xie et al. (2021a) proposed a practical implementation, as a cost, the algorithm have a poor dependency on the function class complexity. Recently, (Yin et al., 2022b) studied the general differentiable function class and propose a computation efficient algorithm (PFQL). However, their result also have an addition dependence on the dimension  $d$  of the parameter.

Therefore, a natural question arises:

*Can we design a computationally efficient algorithm that achieves the minimax optimality with respect to the complexity of nonlinear function class?*

We give an affirmative answer to the above question in this work. Our contributions are listed as follows:

- We propose a pessimism-based algorithm PNLSEVI designed for nonlinear function approximation, which strictly generalizes the existing pessimism-based algorithms for both linear and differentiable function approximation (Xiong et al., 2022; Yin et al., 2022b). Our algorithm is oracle-efficient, i.e., it is computationally efficient when there exists an efficient regression oracle and bonus oracle for the function class (e.g., generalized linear function class).
- We prove a data-dependent regret bound with the widely used  $D^2$ -divergence in online nonlinear RL regime, which is optimal with respect to the function class complexity. Our analysis closes the gap to optimality for differentiable function approximation, which was previously an open problem (Yin et al., 2022b).
- We introduce a novel uniform coverage assumption for general function approximation that is generalized over the assumption in Yin et al. (2022b). Our assumption bridges between the minimum-eigenvalue assumption used in linear models and the generalized dimension for nonlinear function class, offering new insights into the function approximation problem in RL.

**Notation:** In this work, we use lowercase letters to denote scalars and use lower and uppercase boldface letters to denote vectors and matrices respectively. For a vector  $\mathbf{x} \in \mathbb{R}^d$  and matrix  $\Sigma \in \mathbb{R}^{d \times d}$ , we denote by  $\|\mathbf{x}\|_2$  the Euclidean norm and  $\|\mathbf{x}\|_\Sigma = \sqrt{\mathbf{x}^\top \Sigma \mathbf{x}}$ . For two sequences  $\{a_n\}$  and  $\{b_n\}$ , we write  $a_n = O(b_n)$  if there exists an absolute constant  $C$  such that  $a_n \leq Cb_n$ , and we write  $a_n = \Omega(b_n)$  if there exists an absolute constant  $C$  such that  $a_n \geq Cb_n$ . We use  $\tilde{O}(\cdot)$  and  $\tilde{\Omega}(\cdot)$  to further hide the logarithmic factors. For any  $a \leq b \in \mathbb{R}$ ,  $x \in \mathbb{R}$ , let  $[x]_{[a,b]}$  denote the truncate function  $a \cdot \mathbb{1}(x \leq a) + x \cdot \mathbb{1}(a \leq x \leq b) + b \cdot \mathbb{1}(b \leq x)$ , where  $\mathbb{1}(\cdot)$  is the indicator function. For a positive integer  $n$ , we use  $[n] = \{1, 2, \dots, n\}$  to denote the set of integers from 1 to  $n$ .

## 2 Related Work

**RL with function approximation.** As one of the simplest function approximation classes, linear representation in RL has been extensively studied in recent years (Jiang et al., 2017; Dann et al., 2018; Yang and Wang, 2019; Jin et al., 2020; Wang et al., 2020c; Du et al., 2019; Sun et al., 2019; Zanette et al., 2020a,b; Weisz et al., 2021; Yang and Wang, 2020; Modi et al., 2020; Ayoub et al., 2020; Zhou et al., 2021; He et al., 2021). Several assumptions on the linear structure of the underlying MDPs have been made in these works, ranging from the *linear MDP* assumption (Yang and Wang, 2019; Jin et al., 2020; Hu et al., 2022; He et al., 2022; Agarwal et al., 2022) to the *low Bellman-rank* assumption (Jiang et al., 2017) and the *low inherent Bellman error* assumption (Zanette et al., 2020b). Extending the previous theoretical guarantees to more general problem classes, RL with nonlinear function classes has garnered increased attention in recent years (Wang et al., 2020b; Jin et al., 2021a; Foster et al., 2021; Du et al., 2021; Agarwal and Zhang, 2022; Agarwal et al., 2022). Various complexity measures of function classes have been studied including Bellman rank (Jiang et al., 2017), Bellman-Eluder dimension (Jin et al., 2021a), Decision-Estimation Coefficient (Foster et al., 2021) and generalized Eluder dimension (Agarwal et al., 2022). Among these works, the setting in our paper is most related to Agarwal et al. (2022) where  $D^2$ -divergence (Gentile et al., 2022) was introduced in RL to indicate the uncertainty of a sample with respect to a particular sample batch.

91 **Offline tabular RL.** There is a line of works integrating the principle of pessimism to develop  
 92 statistically efficient algorithms for offline tabular RL setting (Rashidinejad et al., 2021; Yin and  
 93 Wang, 2021; Xie et al., 2021b; Shi et al., 2022; Li et al., 2022). More specifically, Xie et al. (2021b)  
 94 utilized the variance of transition noise and proposed a nearly optimal algorithm based on pessimism  
 95 and Bernstein-type bonus. Subsequently, Li et al. (2022) proposed a model-based approach that  
 96 achieves minimax-optimal sample complexity without burn-in cost for tabular MDPs. Shi et al. (2022)  
 97 also contributed by proposing the first nearly minimax-optimal model-free offline RL algorithm.

98 **Offline RL with linear function approximation.** Jin et al. (2021b) presented the initial theoretical  
 99 results on offline linear MDPs. They introduced a pessimism-principled algorithmic framework for  
 100 offline RL and proposed an algorithm based on LSVI (Jin et al., 2020). Min et al. (2021) subsequently  
 101 considered offline policy evaluation (OPE) in linear MDPs, assuming independence between data  
 102 samples across time steps to obtain tighter confidence sets and proposed an algorithm with optimal  
 103  $d$  dependence. Yin et al. (2022a) took one step further and considered the policy optimization in  
 104 linear MDPs, which implicitly requires the same independence assumption. Zanette et al. (2021)  
 105 proposed an actor-critic-based algorithm that establishes pessimism principle by directly perturbing  
 106 the parameter vectors in a linear function approximation framework. Recently, Xiong et al. (2022)  
 107 proposed a novel uncertainty decomposition technique via a reference function, which leads to a  
 108 minimax-optimal sample complexity bound for offline linear MDPs without additional assumptions.

109 **Offline RL with general function approximation.** Chen and Jiang (2019) critically examined  
 110 the assumptions underlying value-function approximation methods and established an information-  
 111 theoretic lower bound. Xie et al. (2021a) introduced the concept of Bellman-consistent pessimism,  
 112 which enables sample-efficient guarantees by relying solely on the Bellman-completeness assumption.  
 113 Uehara and Sun (2021) focused on model-based offline RL with function approximation under partial  
 114 coverage, demonstrating that realizability in the function class and partial coverage are sufficient for  
 115 policy learning. Zhan et al. (2022) proposed an algorithm that achieves polynomial sample complexity  
 116 under the realizability and single-policy concentrability assumptions. Nguyen-Tang and Arora (2023)  
 117 proposed a method of random perturbations and pessimism for neural function approximation. For  
 118 differentiable function classes, Yin et al. (2022b) made advancements by improving the sample  
 119 complexity with respect to the stage  $H$ . However, their result had an additional dependence on the  
 120 dimension  $d$  of the parameter space, whereas in linear function approximation, the dependence is  
 121 typically on  $\sqrt{d}$ .

### 122 3 Preliminaries

123 In our work, we consider the inhomogeneous episodic Markov Decision Processes (MDP), which can  
 124 be denoted by a tuple of  $\mathcal{M}(\mathcal{S}, \mathcal{A}, H, \{r_h\}_{h=1}^H, \{\mathbb{P}_h\}_{h=1}^H)$ . In specific,  $\mathcal{S}$  is the state space,  $\mathcal{A}$  is the  
 125 finite action space,  $H$  is the length of each episode. For each stage  $h \in [H]$ ,  $r_h : \mathcal{S} \times \mathcal{A} \rightarrow [0, 1]$  is the  
 126 reward function<sup>1</sup> and  $\mathbb{P}_h(s'|s, a)$  is the transition probability function, which denotes the probability  
 127 for state  $s$  to transfer to next state  $s'$  with current action  $a$ . A policy  $\pi := \{\pi_h\}_{h=1}^H$  is a collection  
 128 of mappings  $\pi_h$  from a state  $s \in \mathcal{S}$  to the simplex of action space  $\mathcal{A}$ . For simplicity, we denote the  
 129 state-action pair as  $z := (s, a)$ . For any policy  $\pi$  and stage  $h \in [H]$ , we define the value function  
 130  $V_h^\pi(s)$  and the action-value function  $Q_h^\pi(s, a)$  as the expected cumulative rewards starting at stage  $h$ ,  
 131 which can be denoted as follows:

$$Q_h^\pi(s, a) = r_h(s, a) + \mathbb{E} \left[ \sum_{h'=h+1}^H r_{h'}(s_{h'}, \pi_{h'}(s_{h'})) \mid s_h = s, a_h = a \right], \quad V_h^\pi(s) = Q_h^\pi(s, \pi_h(s)),$$

132 where  $s_{h'+1} \sim \mathbb{P}_h(\cdot | s_{h'}, a_{h'})$  denotes the observed state at stage  $h' + 1$ . By this definition, the value  
 133 function  $V_h^\pi(s)$  and action-value function  $Q_h^\pi(s, a)$  are bounded in  $[0, H]$ . In addition, we define the  
 134 optimal value function  $V_h^*$  and the optimal action-value function  $Q_h^*$  as  $V_h^*(s) = \max_{\pi} V_h^\pi(s)$  and  
 135  $Q_h^*(s, a) = \max_{\pi} Q_h^\pi(s, a)$ . We denote the corresponding optimal policy by  $\pi^*$ . For any function  
 136  $V : \mathcal{S} \rightarrow \mathbb{R}$ , we denote  $[\mathbb{P}_h V](s, a) = \mathbb{E}_{s' \sim \mathbb{P}_h(\cdot | s, a)} V(s')$  and  $[\text{Var}_h V](s, a) = [\mathbb{P}_h V^2](s, a) -$   
 137  $([\mathbb{P}_h V](s, a))^2$  for simplicity. For any function  $f : \mathcal{S} \rightarrow \mathbb{R}$ , we define the Bellman operator  $\mathcal{T}_h$   
 138 as  $\mathcal{T}_h f(s_h, a_h) = \mathbb{E}_{s_{h+1} \sim \mathbb{P}_h(\cdot | s_h, a_h)} [r_h(s_h, a_h) + f(s_{h+1})]$ , where we use the shorthand  $f(s) =$   
 139  $\max_{a \in \mathcal{A}} f(s, a)$  for simplicity. Based on this definition, for every stage  $h \in [H]$  and policy  $\pi$ , we

<sup>1</sup>While we study the deterministic reward functions for simplicity, it is not difficult to generalize our results to stochastic reward functions.

140 have the following Bellman equation for value functions  $Q_h^\pi(s, a)$  and  $V_h^\pi(s)$ , as well as the Bellman  
 141 optimality equation for optimal value functions:

$$Q_h^\pi(s_h, a_h) = \mathcal{T}_h V_{h+1}^\pi(s_h, a_h), \quad Q_h^*(s_h, a_h) = \mathcal{T}_h V_{h+1}^*(s_h, a_h),$$

142 where  $V_{H+1}^\pi(s) = V_{H+1}^*(s) = 0$ . We also define the Bellman operator for second moment as  
 143  $\mathcal{T}_{2,h} f(s_h, a_h) = \mathbb{E}_{s_{h+1} \sim \mathbb{P}_h(\cdot | s_h, a_h)} \left[ (r_h(s_h, a_h) + f(s_{h+1}))^2 \right]$ . For simplicity, we omit the sub-  
 144 scripts  $h$  in the Bellman operator without causing confusion.

145 **Offline Reinforcement Learning:** In offline RL, the agent only have access to a batch-dataset  
 146  $D = \{s_h^k, a_h^k, r_h^k : h \in [H], k \in [K]\}$ , which is collected by a behavior policy  $\mu$ , and the agent  
 147 cannot interact with the environment. Given the batch dataset, the goal of offline RL is finding a  
 148 near-optimal policy  $\pi$  that minimize the sub-optimality  $V_1^*(s) - V_1^\pi(s)$ . In addition, for each stage  $h$   
 149 and behavior policy  $\mu$ , we denote the induced distribution of the state-action pair as  $d_h^\mu$ .

150 **General Function Approximation:** In this work, we focus on a special class of episodic MDPs,  
 151 where the value function satisfies the following completeness assumption.

152 **Assumption 3.1** ( $\epsilon$ -completeness under general function approximation, Agarwal et al. 2022). Given  
 153 a general function class  $\{\mathcal{F}_h\}_{h \in [H]}$ , where each function class  $\mathcal{F}_h$  is composed of functions  $f_h : \mathcal{S} \times \mathcal{A} \rightarrow [0, L]$ . We assume for each stage  $h \in [H]$ , and any function  $V : \mathcal{S} \rightarrow [0, H]$ , there exists  
 154 functions  $f_h, f_{2,h} \in \mathcal{F}_h$  such that

$$\max_{(s,a) \in \mathcal{S} \times \mathcal{A}} |f_h(s, a) - \mathcal{T}_h V(s, a)| \leq \epsilon, \quad \text{and} \quad \max_{(s,a) \in \mathcal{S} \times \mathcal{A}} |f_{2,h}(s, a) - \mathcal{T}_{2,h} V(s, a)| \leq \epsilon.$$

156 In addition, for each stage  $h \in [H]$ , we assume there exists a function  $f_h^* \in \mathcal{F}_h$  closed to the optimal  
 157 value function such that  $\|f_h^* - Q_h^*\|_\infty \leq \epsilon$ . For simplicity, we assume  $L = O(H)$  throughout the  
 158 paper and denote  $\mathcal{N} = \max_{h \in [H]} |\mathcal{F}_h|$ .

159 To deal with general function class  $\mathcal{F}$ , Agarwal et al. (2022) introduce the following measure to  
 160 capture the function class complexity for online learning.

161 **Definition 3.2** (Generalized Eluder dimension, Agarwal et al. 2022). Given  $\lambda > 0$ , a sequence of  
 162 state-action pairs  $Z = \{z_i\}_{i \in [K]}$  and a sequence of non-negative weights  $\sigma = \{\sigma_i\}_{i \in [K]}$ . Let  $\mathcal{F}$  be a  
 163 function class consisting of functions  $f : \mathcal{S} \times \mathcal{A} \rightarrow [0, L]$ . The generalized Eluder dimension of  $\mathcal{F}$  is  
 164 given by  $\dim_{\alpha, K}(\mathcal{F}) := \sup_{Z, \sigma: |Z|=K, \sigma \geq \alpha} \dim(\mathcal{F}, Z, \sigma)$ , where

$$\dim(\mathcal{F}, Z, \sigma) := \sum_{i=1}^K \min \left( 1, \frac{1}{\sigma_i^2} D_{\mathcal{F}}^2(z_i; z_{[i-1]}, \sigma_{[i-1]}) \right),$$

$$D_{\mathcal{F}}^2(z; z_{[k-1]}, \sigma_{[k-1]}) := \sup_{f_1, f_2 \in \mathcal{F}} \frac{(f_1(z) - f_2(z))^2}{\sum_{s \in [k-1]} \frac{1}{\sigma_s^2} (f_1(z_s) - f_2(z_s))^2 + \lambda}.$$

165 Here, the inequality  $\sigma \geq \alpha$  represents that  $\sigma_i \geq \alpha$  holds for all  $i \in [K]$  and we use the notation  
 166  $z_{[i-1]}, \sigma_{[i-1]}$  to represent the sequences  $\{z_s\}_{s=1}^{i-1}, \{\sigma_s\}_{s=1}^{i-1}$ .

167 However, in offline RL, the proposed Generalized Eluder dimension fails to capture the relationship  
 168 between function class  $\mathcal{F}$  and the pre-collected dataset  $\mathcal{D}$ . To generalize this definition to offline  
 169 environment, for a batch dataset  $\mathcal{D} = \{(s_h^k, a_h^k, r_h^k)\}_{h,k=1}^{H,K}$  and a function class  $\mathcal{F}_h$  consisting of  
 170 functions  $f : \mathcal{S} \times \mathcal{A} \rightarrow \mathbb{R}$ . We denote  $\mathcal{D}_h = \{(s_h^k, a_h^k, r_h^k)\}_{k \in [K]}$  as the subset of the dataset  $\mathcal{D}$  that  
 171 corresponds to the observations collected up to stage  $h$  in the MDP. Then for any weight function  
 172  $\sigma_h(\cdot, \cdot) : \mathcal{S} \times \mathcal{A} \rightarrow \mathbb{R}$ , we introduce the following  $D^2$ -divergence:

$$D_{\mathcal{F}_h}^2(z; \mathcal{D}_h; \sigma_h) = \sup_{f_1, f_2 \in \mathcal{F}_h} \frac{(f_1(z) - f_2(z))^2}{\sum_{k \in [K]} \frac{1}{(\sigma_h(z_h^k))^2} (f_1(z_h^k) - f_2(z_h^k))^2 + \lambda}.$$

173 **Data Coverage Assumption:** In offline RL, there exists a discrepancy between the state-action  
 174 distribution generated by the behavior policy and the distribution from the learned policy. Under this  
 175 situation, the distribution shift problem can cause the learned policy to perform poorly or even fail in  
 176 offline RL. Therefore, we propose the following data coverage assumption to control the distribution  
 177 shift.

---

**Algorithm 1** Pessimistic Nonlinear Least-Squares Value Iteration (PNLSVI)
 

---

**Require:** Input confidence parameters  $\beta'_{1,h}, \beta'_{2,h}, \beta_h$  and  $\epsilon > 0$ .

- 1: **Initialize:** Split the input dataset into  $\mathcal{D} = \{s_h^k, a_h^k, r_h^k\}_{k,h=1}^{K,H}$ ,  $\mathcal{D}' = \{\bar{s}_h^k, \bar{a}_h^k, \bar{r}_h^k\}_{k,h=1}^{K,H}$ ; Set the value function  $\hat{f}_{H+1}(\cdot) = \hat{f}'_{H+1}(\cdot) = 0$ .
  - 2: **for** stage  $h = H, \dots, 1$  **do**
  - 3:  $\tilde{f}'_h = \operatorname{argmin}_{f_h \in \mathcal{F}_h} \sum_{k \in [K]} \left( f_h(\bar{s}_h^k, \bar{a}_h^k) - \bar{r}_h^k - \hat{f}'_{h+1}(\bar{s}_{h+1}^k) \right)^2$ .
  - 4:  $\tilde{g}'_h = \operatorname{argmin}_{g_h \in \mathcal{F}_h} \sum_{k \in [K]} \left( g_h(\bar{s}_h^k, \bar{a}_h^k) - \left( \bar{r}_h^k + \hat{f}'_{h+1}(\bar{s}_{h+1}^k) \right)^2 \right)^2$ .
  - 5: Use the bonus oracle (Definition 4.1) to calculate the bonus function  $b'_h = \mathcal{B}(1, \mathcal{D}'_h, \mathcal{F}_h, \tilde{f}'_h, \beta'_{1,h} + \beta'_{2,h}, \lambda, \epsilon)$ ,
  - 6:  $\hat{f}'_h \leftarrow \{\tilde{f}'_h - b'_h - \epsilon\}_{[0, H-h+1]}$ ;
  - 7: **Construct** the variance estimator  $\hat{\sigma}_h^2(s, a) = \max \left\{ 1, \tilde{g}'_h(s, a) - \left( \tilde{f}'_h(s, a) \right)^2 - O \left( \frac{\sqrt{\log \mathcal{N} \mathcal{N}_b H^3}}{\sqrt{K \kappa}} \right) \right\}$ .
  - 8: **end for**
  - 9: **for** stage  $h = H, \dots, 1$  **do**
  - 10:  $\tilde{f}_h = \operatorname{argmin}_{f_h \in \mathcal{F}_h} \sum_{k \in [K]} \frac{1}{\hat{\sigma}_h^2(s_h^k, a_h^k)} \left( f_h(s_h^k, a_h^k) - r_h^k - \hat{f}_{h+1}(s_{h+1}^k) \right)^2$
  - 11: Use the bonus oracle (Definition 4.1) to calculate the bonus function  $b_h = \mathcal{B}(\hat{\sigma}_h, \mathcal{D}_h, \mathcal{F}_h, \tilde{f}_h, \beta_h, \lambda, \epsilon)$ ;
  - 12:  $\hat{f}_h \leftarrow \{\tilde{f}_h - b_h - \epsilon\}_{[0, H-h+1]}$ ;
  - 13:  $\hat{\pi}_h(\cdot | s) = \operatorname{argmax}_a \hat{f}_h(s, a)$ .
  - 14: **end for**
  - 15: **Output:**  $\hat{\pi} = \{\hat{\pi}_h\}_{h=1}^H$ .
- 

178 **Assumption 3.3** (Uniform Data Coverage). there exists a constant  $\kappa > 0$ , such that for any stage  $h$   
 179 and functions  $f_1, f_2 \in \mathcal{F}_h$ , the following inequality holds,

$$\mathbb{E}_{\mu, h} \left[ (f_1(s_h, a_h) - f_2(s_h, a_h))^2 \right] \geq \kappa \|f_1 - f_2\|_\infty^2,$$

180 where the state-action pair (at stage  $h$ )  $(s_h, a_h)$  is stochastic generated from behavior policy  $\mu$ .

181 **Remark 3.4.** Data coverage assumption is widely used in offline RL to guarantee that the collected  
 182 dataset contains enough information of the state-action space to learn an effective policy. In Yin et al.  
 183 (2022b), they studied the general differentiable function, where the function class is defined as

$$\mathcal{F} := \left\{ f(\boldsymbol{\theta}, \phi(\cdot, \cdot)) : \mathcal{S} \times \mathcal{A} \rightarrow \mathbb{R}, \boldsymbol{\theta} \in \Theta \right\}.$$

184 Under this definition, Yin et al. (2022b) introduce the following coverage assumption (Assumption  
 185 2.3) such that for all stage  $h \in [H]$ , there exists a constant  $\kappa$ ,

$$\mathbb{E}_{\mu, h} \left[ (f(\boldsymbol{\theta}_1, \phi(s, a)) - f(\boldsymbol{\theta}_2, \phi(s, a)))^2 \right] \geq \kappa \|\boldsymbol{\theta}_1 - \boldsymbol{\theta}_2\|_2^2, \forall \boldsymbol{\theta}_1, \boldsymbol{\theta}_2 \in \Theta; \quad (*)$$

$$\mathbb{E}_{\mu, h} \left[ \nabla f(\boldsymbol{\theta}, \phi(s, a)) \nabla f(\boldsymbol{\theta}, \phi(s, a))^\top \right] \succ \kappa I, \forall \boldsymbol{\theta} \in \Theta. \quad (**)$$

186 We can prove that our assumption is weaker than the first assumption (\*). For the second assumption  
 187 (\*\*), there is no direct counterpart in the general setting.

188 In addition, for the linear function class, the coverage assumption in Yin et al. (2022b) will reduce to  
 189 the following linear function coverage assumption (Wang et al., 2020a; Min et al., 2021; Yin et al.,  
 190 2022a; Xiong et al., 2022).

$$\lambda_{\min}(\mathbb{E}_{\mu, h}[\phi(s, a)\phi(s, a)^\top]) = \kappa > 0, \forall h \in [H].$$

191 Therefore, our assumption is also weaker than the linear function coverage assumption when dealing  
 192 with the linear function class. Due to space limitations, we provide the detailed proof in the appendix.

## 193 4 Algorithm

194 In this section, we provide a comprehensive and detailed description of our algorithm (PNLSVI), as  
 195 displayed in Algorithm 1. In the sequel, we introduce the key ideas of the proposed algorithm.

196 **4.1 Pessimistic Value Iteration Based Planning**

197 Our algorithm operates in two distinct phases, Variance Estimate Phase and Pessimistic Planning  
 198 Phase. At the beginning of the algorithm, the data-set is divided into two disjoint subsets  $\mathcal{D}, \mathcal{D}'$ , and  
 199 each assigned to a specific phase.

200 The basic framework of our algorithm follows the pessimistic value iteration, which was initially  
 201 introduced by Jin et al. (2021b). In details, for each stage  $h \in [H]$ , we construct the estimator value  
 202 function  $\tilde{f}_h$  by solving the following variance-weighted ridge regression (Line 11):

$$\tilde{f}_h = \operatorname{argmin}_{f_h \in \mathcal{F}_h} \sum_{k \in [K]} \frac{1}{\hat{\sigma}_h^2(s_h^k, a_h^k)} \left( f_h(s_h^k, a_h^k) - r_h^k - \hat{f}_{h+1}(s_{h+1}^k) \right)^2,$$

203 where  $\hat{\sigma}_h^2$  is the estimated variance and will be discussed in section 4.2. In Line 12, we subtract the  
 204 confidence bonus function  $b_h$  from the estimator value function  $\tilde{f}_h$  to construct the pessimistic value  
 205 function  $\hat{f}_h$ . With the help of the confidence bonus function  $b_h$ , the pessimistic value function  $\hat{f}_h$   
 206 is almost a lower bound for the optimal value function  $f_h^*$ . The details of the bonus function and bonus  
 207 oracle will be discussed in section 4.3.

208 Based on the pessimistic value function  $\hat{f}_h$  for stage  $h$ , we recursively perform the value iteration  
 209 for the stage  $h - 1$ . Finally, we use the pessimistic value function  $\hat{f}_h$  to do planning and output the  
 210 greedy policy with respect to the pessimistic value function  $\hat{f}_h$  (Line 13 - Line 15).

211 **4.2 Variance Estimate Phase**

212 In this phase, we provide a estimator for the variance  $\hat{\sigma}_h$  in the weighted ridge regression. According  
 213 to the definition of Bellman operators  $\mathcal{T}$  and  $\mathcal{T}_2$ , the variance of the function  $\hat{f}'_{h+1}$  for each state-action  
 214 pair  $(s, a)$  can be denoted by

$$[\operatorname{Var}_h \hat{f}_{h+1}](s, a) = \mathcal{T}_{2,h} \hat{f}'_{h+1}(s, a) - \left( \mathcal{T}_h \hat{f}'_{h+1}(s, a) \right)^2.$$

215 Therefore, we need the evaluate the first-order and second-order moments for  $\hat{f}'_h$ . We perform  
 216 nonlinear least-squares regression separately for each of these moments. Specifically, in Line 3, we  
 217 conduct regression to estimate the first-order moment.

$$\tilde{f}'_h = \operatorname{argmin}_{f'_h \in \mathcal{F}_h} \sum_{k \in [K]} \left( f'_h(\bar{s}_h^k, \bar{a}_h^k) - \bar{r}_h^k - \hat{f}'_{h+1}(\bar{s}_{h+1}^k) \right)^2.$$

218 In Line 4, we perform regression for the second-order moment.

$$\tilde{g}'_h = \operatorname{argmin}_{g'_h \in \mathcal{F}_h} \sum_{k \in [K]} \left( g'_h(\bar{s}_h^k, \bar{a}_h^k) - \left( \bar{r}_h^k + \hat{f}'_{h+1}(\bar{s}_{h+1}^k) \right)^2 \right)^2.$$

219 In this phase, we set the variance function to 1 for each state-action pair  $(s, a)$  and derive an estimator  
 220 with confidence radius  $\beta'_{1,h}, \beta'_{2,h}$ . Combing these two regression results and subtracting a confidence  
 221 bonus function  $b'_h$ , we create a pessimistic estimator for the variance function (Lines 6 to 7).

222 **4.3 Nonlinear Bonus Oracle**

223 As we discussed in sections 4.1 and 4.2, we introduce a uncertainty bonus function to construct a  
 224 pessimistic estimate of the value function. Unfortunately, for a general class, the uncertainty bonus  
 225 may varies greatly across different state-action pair. Under this situation, the addition uncertainty  
 226 bonus function will highly increase the complexity of the pessimistic function class, which make  
 227 it difficult to construct a accurate estimation and may significant deteriorate the final performance.  
 228 To address this issue, we assume there exists a function class  $\mathcal{W}$  with cardinality  $|\mathcal{W}| = \mathcal{N}_b$  and can  
 229 approximate the bonus function well. In addition, we assume there exists a nonlinear bonus oracle  
 230 (Agarwal and Zhang, 2022), which can output the approximate bonus function in the class  $\mathcal{W}$  for  
 231 each dataset  $\mathcal{D}_h$ .

232 **Definition 4.1** (Oracle for bonus function). For an offline dataset  $\mathcal{D} = \{s_h^k, a_h^k, r_h^k\}_{h,k=1}^{H,K}$ , given  
 233 index  $h \in [H]$ , let  $\mathcal{D}_h = \{(s_h^k, a_h^k, r_h^k)\}_{k \in [K]}$  denote the subset of the dataset  $\mathcal{D}$  that corresponds to  
 234 the observations collected up to stage  $h$  in the MDP.  $\widehat{\sigma}_h(\cdot, \cdot) : \mathcal{S} \times \mathcal{A} \rightarrow \mathbb{R}$  is a variance function.  $\mathcal{F}_h$   
 235 is a function class such that  $\widehat{f}_h \in \mathcal{F}_h$ . The parameters  $\beta_h, \lambda \geq 0$ , error parameter  $\epsilon \geq 0$ . The bonus  
 236 oracle  $\mathcal{B}(\widehat{\sigma}, \mathcal{D}_h, \mathcal{F}_h, \widehat{f}_h, \beta_h, \lambda, \epsilon)$  outputs a bonus function  $b_h(\cdot)$  such that

- 237 •  $b_h : \mathcal{S} \times \mathcal{A} \rightarrow \mathbb{R}_{\geq 0}$  belongs to function class  $\mathcal{W}$ .
- 238 •  $b_h(z_h) \geq \max \left\{ |f_h(z_h) - \widehat{f}_h(z_h)|, f_h \in \mathcal{F}_h : \sum_{k \in [K]} \frac{(f_h(z_h^k) - \widehat{f}_h(z_h^k))^2}{(\widehat{\sigma}_h(s_h^k, a_h^k))^2} \leq (\beta_h)^2 \right\}$  for any  $z_h \in \mathcal{S} \times \mathcal{A}$ .
- 239 •  $b_h(z_h) \leq C \cdot \left( D_{\mathcal{F}_h}(z_h; \mathcal{D}_h; \widehat{\sigma}_h) \cdot \sqrt{(\beta_h)^2 + \lambda} + \epsilon \beta_h \right)$  for all  $z_h \in \mathcal{S} \times \mathcal{A}$  with constant  $0 < C \leq \infty$ .

240 **Remark 4.2.** To address the concern of function class complexity, some previous studies (Xie et al.,  
 241 2021a) have approached the problem differently. Instead of introducing a pointwise bonus in the  
 242 estimated value function, they solve a complicated optimization problem to guarantee the optimism  
 243 solely in the initial state. This method can prevent the complexity from bonus function, as a cost, they  
 244 requires solving an optimization problem over all potential policy and corresponding version space,  
 245 which includes all functions with lower Bellman error.

## 246 5 Main Results

247 In this section we prove an problem-dependent regret bound of Algorithm 1.

248 **Theorem 5.1.** Under Assumption 3.3, for  $K \geq \widetilde{\Omega} \left( \frac{\log(\mathcal{N}\mathcal{N}_b)H^6}{\kappa^2} \right)$ , if we set the parameters  
 249  $\beta'_{1,h}, \beta'_{2,h} = \widetilde{O}(\sqrt{\log \mathcal{N}\mathcal{N}_b}H^2)$  and  $\beta_h = \widetilde{O}(\sqrt{\log \mathcal{N}})$  in Algorithm 1, then with probability at  
 250 least  $1 - \delta$ , for any state  $s \in \mathcal{S}$ , we have

$$V_1^*(s) - V_1^{\widehat{\pi}}(s) \leq \widetilde{O}(\sqrt{\log \mathcal{N}}) \sum_{h=1}^H \mathbb{E}_{\pi^*} [D_{\mathcal{F}_h}(z_h; \mathcal{D}_h; [\mathbb{V}_h V_{h+1}^*](\cdot, \cdot)) | s_1 = s],$$

251 where  $[\mathbb{V}_h V_{h+1}^*](s, a) = \max\{1, [\text{Var}_h V_{h+1}^*](s, a)\}$  is the truncated conditional variance.

252 **Remark 5.2.** When reduce to the linear MDP environment, the following function classes

$$\mathcal{F}_h^{\text{lin}} = \{ \langle \phi_h(\cdot, \cdot), \theta_h \rangle : \theta_h \in \mathbb{R}^d, \|\theta_h\|_2 \leq B_h \} \text{ for any } h \in [H],$$

253 satisfy the completeness assumption (Assumption 3.1) (Jin et al., 2020). Let  $\mathcal{F}_h^{\text{lin}}(\epsilon)$  be a  $\epsilon$ -net of the  
 254 linear function class  $\mathcal{F}_h^{\text{lin}}$ . In this case, the covering number satisfies  $\log |\mathcal{F}_h^{\text{lin}}(\epsilon)| = \widetilde{O}(d)$  and the  
 255 dependency of function class will reduce to  $\widetilde{O}(\sqrt{\log \mathcal{N}}) = \widetilde{O}(\sqrt{d})$ . For linear function class, Xiong  
 256 et al. (2022) proposed the following regret guarantee,

$$V_1^*(s) - V_1^{\widehat{\pi}}(s) \leq \widetilde{O}(\sqrt{d}) \cdot \sum_{h=1}^H \mathbb{E}_{\pi^*} \left[ \|\phi(s_h, a_h)\|_{\Sigma_h^*} | s_1 = s \right],$$

257 where  $\Sigma_h^* = \sum_{k \in [K]} \phi(s_h^k, a_h^k) \phi(s_h^k, a_h^k)^\top / [\mathbb{V}_h V_{h+1}^*](s_h^k, a_h^k) + \lambda \mathbf{I}$ . In comparison, we can prove  
 258 the following inequality:

$$D_{\mathcal{F}_h^{\text{lin}}(\epsilon)}(z; \mathcal{D}_h; [\mathbb{V}_h V_{h+1}^*](\cdot, \cdot)) \leq \|\phi_h(z)\|_{\Sigma_h^*}.$$

259 This shows that Theorem 5.1 matches the optimal result in Xiong et al. (2022) for linear function  
 260 class.

## 261 6 Key Techniques

262 In this section, we provide an overview of the key techniques in our algorithm design and analysis.

### 263 6.1 Variance Estimator with Nonlinear Function Class

264 The technique of variance-weighted ridge regression, first introduced in Zhou et al. (2021), has  
 265 demonstrated its effectiveness in the online RL setting with linear function approximation. For offline

266 setting, Xiong et al. (2022) modified the variance-weighted ridge regression technique, and showed  
 267 that using an accurate and independent variance estimator can improve the performance of the  
 268 pessimistic value iteration (PEVI) algorithm (Jin et al., 2021b).

269 In our work, we extend this technique to general nonlinear function class  $\mathcal{F}$ , and use the following  
 270 nonlinear least-squares regression to estimate the underlying value function:

$$\tilde{f}_h = \operatorname{argmin}_{f_h \in \mathcal{F}_h} \sum_{k \in [K]} \frac{1}{\hat{\sigma}_h^2(s_h^k, a_h^k)} \left( f_h(s_h^k, a_h^k) - r_h^k - \hat{f}_{h+1}(s_{h+1}^k) \right)^2.$$

271 For this regression, it is crucial to obtain a reliable evaluation for the variance of the estimated  
 272 cumulative reward  $r_h^k + \hat{f}_{h+1}(s_{h+1}^k)$ . According to the definition of Bellman operators  $\mathcal{T}$  and  $\mathcal{T}_2$ , the  
 273 variance of the function  $\hat{f}_{h+1}^l$  for each state-action pair  $(s, a)$  can be denoted by

$$[\operatorname{Var}_h \hat{f}_{h+1}^l](s, a) = \mathcal{T}_{2,h} \hat{f}_{h+1}^l(s, a) - \left( \mathcal{T}_h \hat{f}_{h+1}^l(s, a) \right)^2.$$

274 To evaluate the first and second moment for the Bellman operator, we perform nonlinear least-squares  
 275 regression on a separate dataset  $\mathcal{D}'$  with uniform weight ( $\hat{\sigma}_h(s, a) = 1$  for all state-action pair  $(s, a)$ ).

276 For simplicity, we denote the empirical variance as  $\mathbb{B}_h(s, a) = \tilde{g}_h'(s, a) - \left( \tilde{f}_h'(s, a) \right)^2$ , and the  
 277 difference between empirical variance  $\mathbb{B}_h(s, a)$  with actual variance  $[\operatorname{Var}_h \hat{f}_{h+1}^l](s, a)$  is upper  
 278 bound by

$$\left| \mathbb{B}_h(s, a) - [\operatorname{Var}_h \hat{f}_{h+1}^l](s, a) \right| \leq \left| \tilde{g}_h'(s, a) - \mathcal{T}_{2,h} \hat{f}_{h+1}^l(s, a) \right| + \left| \left( \tilde{f}_h'(s, a) \right)^2 - \left( \mathcal{T}_h \hat{f}_{h+1}^l(s, a) \right)^2 \right|.$$

279 For these nonlinear function estimator, the following Lemmas provide coarse concentration properties  
 280 for the first and second order Bellman operators.

281 **Lemma 6.1.** Given a stage  $h \in [H]$ , let  $\hat{f}_{h+1}^l(\cdot, \cdot) \leq H$  be the estimated value function constructed  
 282 in Algorithm 1 Line 6. By utilizing Assumption 3.1, there exists a function  $\tilde{f}_h' \in \mathcal{F}_h$ , such that  
 283  $|\tilde{f}_h'(z_h) - \mathcal{T}_h \hat{f}_{h+1}^l(z_h)| \leq \epsilon$  holds for all state-action pair  $z_h = (s_h, a_h)$ . Then with probability at least  
 284  $1 - \delta/(4H)$ , it holds that  $\sum_{k \in [K]} \left( \tilde{f}_h'(\bar{z}_h^k) - \hat{f}_{h+1}^l(\bar{z}_h^k) \right)^2 \leq (\beta'_{1,h})^2$ , where  $\beta'_{1,h} = \tilde{O}(\sqrt{\log \mathcal{N} \mathcal{N}_b H^2})$ ,  
 285 and  $\tilde{f}_h'$  is the estimated function for first-moment Bellman operator (Line 3 in Algorithm 1).

286 **Lemma 6.2.** Given a stage  $h \in [H]$ , let  $\hat{f}_{h+1}^l(\cdot, \cdot) \leq H$  be the estimated value function constructed in  
 287 Algorithm 1 Line 6. By utilizing Assumption 3.1, there exists a function  $\tilde{g}_h' \in \mathcal{F}_h$ , such that  $|\tilde{g}_h'(z_h) -$   
 288  $\mathcal{T}_{2,h} \hat{f}_{h+1}^l(z_h)| \leq \epsilon$  holds for all state-action pair  $z_h = (s_h, a_h)$ . Then with probability at least  
 289  $1 - \delta/(4H)$ , it holds that  $\sum_{k \in [K]} \left( \tilde{g}_h'(\bar{z}_h^k) - \hat{f}_{h+1}^l(\bar{z}_h^k) \right)^2 \leq (\beta'_{2,h})^2$ , where  $\beta'_{2,h} = \tilde{O}(\sqrt{\log \mathcal{N} \mathcal{N}_b H^2})$ ,  
 290 and  $\tilde{g}_h'$  is the estimated function for second-moment Bellman operator (Line 4 in Algorithm 1).

291 Notice that all of the previous analysis focuses on the estimated function  $\hat{f}_{h+1}^l$ . By leveraging  
 292 an induction procedure similar to existing works in the linear case (Jin et al., 2021b; Xiong  
 293 et al., 2022), we can control the distance between the estimated function  $\hat{f}_{h+1}^l$  and the optimal  
 294 value function  $f_h^*$ . In details, with high probability, for all stage  $h \in [H]$ , the distance is upper  
 295 bounded by  $O\left(\sqrt{\log \mathcal{N} \mathcal{N}_b H^3} / \sqrt{K \kappa}\right)$ . This result allows us to further bound  $[\operatorname{Var}_h \hat{f}_{h+1}^l](s, a)$  and  
 296  $[\operatorname{Var}_h f_{h+1}^*](s, a)$ .

297 Therefore, the concentration properties in Lemmas 6.1 and 6.2 enable us to construct the pessimistic  
 298 variance estimator, which satisfies the following property:

$$[\mathbb{V}_h V_{h+1}^*](s, a) - \tilde{O}\left(\frac{\sqrt{\log \mathcal{N} \mathcal{N}_b H^3}}{\sqrt{K \kappa}}\right) \leq \hat{\sigma}_h^2(s, a) \leq [\mathbb{V}_h V_{h+1}^*](s, a). \quad (6.1)$$

299 where  $[\mathbb{V}_h V_{h+1}^*](s, a) = \max\{1, [\operatorname{Var}_h V_{h+1}^*](s, a)\}$  is the truncated conditional variance. Compared  
 300 with the results in the linear function class, we utilize the logarithm of the covering number of the  
 301 function class as a substitute for the linear dimension  $d$ , which is a common technique in nonlinear  
 302 function approximation.



303 **6.2 Reference-Advantage Decomposition**

304 The reference-advantage decomposition is a powerful technique to tackle the challenge of additional  
 305 error from uniform concentration over whole function class  $\mathcal{F}_h$ . Such an analysis approach has been  
 306 first studied in the online RL setting Azar et al. (2017); Zhang et al. (2021); Hu et al. (2022); He et al.  
 307 (2022); Agarwal et al. (2022) and later in the offline environment by Xiong et al. (2022).

308 For offline RL, in the context of nonlinear function classes, without a explicit linear expression,  
 309 the increased complexity of the function class structure poses a significant obstacle to effectively  
 310 utilizing this technique. Previous works, such as Yin et al. (2022b), have struggled to adapt the  
 311 reference-advantage decomposition to their nonlinear function class, resulting in a parameter space  
 312 dependence that scales with  $d$ , instead of the optimal  $\sqrt{d}$ . We provide detailed insights into this  
 313 approach as follows:

$$\begin{aligned} r_h(s, a) + \widehat{f}_{h+1}(s, a) - \mathcal{T}_h \widehat{f}_{h+1}(s, a) &= \underbrace{r_h(s, a) + f_{h+1}^*(s, a) - \mathcal{T}_h f_{h+1}^*(s, a)}_{\text{Reference uncertainty}} \\ &+ \underbrace{\widehat{f}_{h+1}(s, a) - f_{h+1}^*(s, a) - ([\mathbb{P}_h \widehat{f}_{h+1}](s, a) - [\mathbb{P}_h f_{h+1}^*](s, a))}_{\text{Advantage uncertainty}}. \end{aligned}$$

314 We decompose the Bellman error into two parts: the Reference uncertainty and the Advantage  
 315 uncertainty. For the first term, the optimal value function  $f_{h+1}^*$  is fixed and not related to the pre-  
 316 collected dataset, which circumvents additional uniform concentration over the whole function class  
 317 and avoid any dependence on the function class size. For the second term, it is worth to notice that  
 318 the distance between the estimated function  $\widehat{f}_{h+1}$  and the optimal value function  $f_h^*$  is decreased as  
 319  $O(1/\sqrt{K\kappa})$ . Though, we still need to maintain the uniform convergence guarantee, the Advantage  
 320 uncertainty is dominated by the Reference uncertainty when the number of episode  $K$  is large enough.  
 321 By integrating these results, we can prove a variance-weighted concentration inequality for Bellman  
 322 operators.

323 **Lemma 6.3.** For each stage  $h \in [H]$ , assuming the variance estimator  $\widehat{\sigma}_h$  satisfies (6.1), let  
 324  $\widehat{f}_{h+1}(\cdot, \cdot) \leq H$  be the estimated value function constructed in Algorithm 1 Line 12. By utiliz-  
 325 ing Assumption 3.1, there exists a function  $\tilde{f}_h \in \mathcal{F}_h$ , such that  $|\tilde{f}_h(z_h) - \mathcal{T}_h \widehat{f}_{h+1}(z_h)| \leq \epsilon$  holds  
 326 for all state-action pair  $z_h = (s_h, a_h)$ . Then with probability at least  $1 - \delta/(4H)$ , it holds that  
 327  $\sum_{k \in [K]} \frac{1}{(\widehat{\sigma}_h(z_h^k))^2} \left( \tilde{f}_h(z_h^k) - \widehat{f}_h(z_h^k) \right)^2 \leq (\beta_h)^2$ , where  $\beta_h = \widetilde{O}(\sqrt{\log \mathcal{N}})$  and  $\tilde{f}_h$  is the estimated  
 328 function from the weighted ridge regression (Line 10 in Algorithm 1).

329 After controlling the Bellman error, with a similar argument to Jin et al. (2021b); Xiong et al. (2022),  
 330 we obtain the following lemma, which provide an upper bound for the regret.

331 **Lemma 6.4 (Regret Decomposition Property).** If  $|\mathcal{T}_h \widehat{f}_{h+1}(z) - \tilde{f}_h(z)| \leq b_h(z)$  holds for all stage  
 332  $h \in [H]$  and state-action pair  $z = (s, a) \in \mathcal{S} \times \mathcal{A}$ , then the regret of Algorithm 1 can be bounded as

$$V_1^*(s) - V_1^{\widehat{\pi}}(s) \leq 2 \sum_{h=1}^H \mathbb{E}_{\pi^*} [b_h(s_h, a_h) \mid s_1 = s].$$

333 Here, the expectation  $\mathbb{E}_{\pi^*}$  is with respect to the trajectory induced by  $\pi^*$  in the underlying MDP.

334 Combing the results in Lemmas 6.3 and 6.4, we have proved Theorem 5.1.

335 **7 Conclusion and Future Work**

336 In this paper, we present PNL-SVI, an oracle-efficient algorithm for offline RL with non-linear function  
 337 approximation. It achieves minimax optimal problem-dependent regret when specialized to linear  
 338 function approximation.

339 Regarding future work, we observe that instead of using the uniform coverage assumption, a series of  
 340 works, such as (Liu et al., 2020; Xie et al., 2021a; Uehara and Sun, 2021; Zhan et al., 2022), only  
 341 relies on partial coverage assumption. In these works, the offline data distribution only encompasses  
 342 the state-action distribution of a select high-quality comparator policy  $\pi^*$ . It would be of significant  
 343 interest to investigate whether it's possible to design practical algorithms for nonlinear function  
 344 classes under this weaker partial coverage assumption, while still preserving the inherent efficiency  
 345 found in linear function approximation.

346 **References**

- 347 AGARWAL, A., JIN, Y. and ZHANG, T. (2022). Vo  $q$  l: Towards optimal regret in model-free rl with  
348 nonlinear function approximation. *arXiv preprint arXiv:2212.06069* .
- 349 AGARWAL, A. and ZHANG, T. (2022). Model-based rl with optimistic posterior sampling: Structural  
350 conditions and sample complexity. *arXiv preprint arXiv:2206.07659* .
- 351 AYOUB, A., JIA, Z., SZEPESVARI, C., WANG, M. and YANG, L. (2020). Model-based reinforcement  
352 learning with value-targeted regression. In *International Conference on Machine Learning*. PMLR.
- 353 AZAR, M. G., OSBAND, I. and MUNOS, R. (2017). Minimax regret bounds for reinforcement  
354 learning. In *International Conference on Machine Learning*. PMLR.
- 355 CESA-BIANCHI, N. and LUGOSI, G. (2006). *Prediction, learning, and games*. Cambridge university  
356 press.
- 357 CHEN, J. and JIANG, N. (2019). Information-theoretic considerations in batch reinforcement learning.  
358 In *International Conference on Machine Learning*. PMLR.
- 359 DANN, C., JIANG, N., KRISHNAMURTHY, A., AGARWAL, A., LANGFORD, J. and SCHAPIRE, R. E. (2018). On oracle-efficient pac rl with rich observations. *Advances in neural information processing systems* **31**.
- 362 DEGRAVE, J., FELICI, F., BUCHLI, J., NEUNERT, M., TRACEY, B., CARPANESE, F., EWALDS, T., HAFNER, R., ABDOLMALEKI, A., DE LAS CASAS, D. ET AL. (2022). Magnetic control of tokamak plasmas through deep reinforcement learning. *Nature* **602** 414–419.
- 365 DU, S., KAKADE, S., LEE, J., LOVETT, S., MAHAJAN, G., SUN, W. and WANG, R. (2021). Bilinear classes: A structural framework for provable generalization in rl. In *International Conference on Machine Learning*. PMLR.
- 368 DU, S. S., KAKADE, S. M., WANG, R. and YANG, L. F. (2019). Is a good representation sufficient for sample efficient reinforcement learning? *arXiv preprint arXiv:1910.03016* .
- 370 FOSTER, D. J., KAKADE, S. M., QIAN, J. and RAKHLIN, A. (2021). The statistical complexity of interactive decision making. *arXiv preprint arXiv:2112.13487* .
- 372 GENTILE, C., WANG, Z. and ZHANG, T. (2022). Achieving minimax rates in pool-based batch active learning. In *International Conference on Machine Learning*. PMLR.
- 374 GU, S., HOLLY, E., LILICRAP, T. and LEVINE, S. (2017). Deep reinforcement learning for robotic manipulation with asynchronous off-policy updates. In *2017 IEEE international conference on robotics and automation (ICRA)*. IEEE.
- 377 HE, J., ZHAO, H., ZHOU, D. and GU, Q. (2022). Nearly minimax optimal reinforcement learning for linear markov decision processes. *arXiv preprint arXiv:2212.06132* .
- 379 HE, J., ZHOU, D. and GU, Q. (2021). Logarithmic regret for reinforcement learning with linear function approximation. In *International Conference on Machine Learning*. PMLR.
- 381 HU, P., CHEN, Y. and HUANG, L. (2022). Nearly minimax optimal reinforcement learning with linear function approximation. In *International Conference on Machine Learning*. PMLR.
- 383 JIANG, N., KRISHNAMURTHY, A., AGARWAL, A., LANGFORD, J. and SCHAPIRE, R. E. (2017). Contextual decision processes with low bellman rank are pac-learnable. In *International Conference on Machine Learning*. PMLR.
- 386 JIN, C., LIU, Q. and MIRYOOSEFI, S. (2021a). Bellman eluder dimension: New rich classes of rl problems, and sample-efficient algorithms. *Advances in neural information processing systems* **34** 13406–13418.
- 389 JIN, C., YANG, Z., WANG, Z. and JORDAN, M. I. (2020). Provably efficient reinforcement learning with linear function approximation. In *Conference on Learning Theory*. PMLR.

- 391 JIN, Y., YANG, Z. and WANG, Z. (2021b). Is pessimism provably efficient for offline rl? In  
392 *International Conference on Machine Learning*. PMLR.
- 393 LEVINE, S., PASTOR, P., KRIZHEVSKY, A., IBARZ, J. and QUILLEN, D. (2018). Learning hand-  
394 eye coordination for robotic grasping with deep learning and large-scale data collection. *The*  
395 *International journal of robotics research* **37** 421–436.
- 396 LI, G., SHI, L., CHEN, Y., CHI, Y. and WEI, Y. (2022). Settling the sample complexity of  
397 model-based offline reinforcement learning. *arXiv preprint arXiv:2204.05275* .
- 398 LIU, Y., SWAMINATHAN, A., AGARWAL, A. and BRUNSKILL, E. (2020). Provably good batch  
399 off-policy reinforcement learning without great exploration. *Advances in neural information*  
400 *processing systems* **33** 1264–1274.
- 401 MIN, Y., WANG, T., ZHOU, D. and GU, Q. (2021). Variance-aware off-policy evaluation with linear  
402 function approximation. *Advances in neural information processing systems* **34** 7598–7610.
- 403 MODI, A., JIANG, N., TEWARI, A. and SINGH, S. (2020). Sample complexity of reinforcement  
404 learning using linearly combined model ensembles. In *International Conference on Artificial*  
405 *Intelligence and Statistics*. PMLR.
- 406 NGUYEN-TANG, T. and ARORA, R. (2023). Viper: Provably efficient algorithm for offline rl  
407 with neural function approximation. In *The Eleventh International Conference on Learning*  
408 *Representations*.
- 409 RASHIDINEJAD, P., ZHU, B., MA, C., JIAO, J. and RUSSELL, S. (2021). Bridging offline rein-  
410 forcement learning and imitation learning: A tale of pessimism. *Advances in Neural Information*  
411 *Processing Systems* **34** 11702–11716.
- 412 SCHRITTWIESER, J., ANTONOGLU, I., HUBERT, T., SIMONYAN, K., SIFRE, L., SCHMITT, S.,  
413 GUEZ, A., LOCKHART, E., HASSABIS, D., GRAEPEL, T. ET AL. (2020). Mastering atari, go,  
414 chess and shogi by planning with a learned model. *Nature* **588** 604–609.
- 415 SHI, L., LI, G., WEI, Y., CHEN, Y. and CHI, Y. (2022). Pessimistic q-learning for offline  
416 reinforcement learning: Towards optimal sample complexity. In *International Conference on*  
417 *Machine Learning*. PMLR.
- 418 SILVER, D., SCHRITTWIESER, J., SIMONYAN, K., ANTONOGLU, I., HUANG, A., GUEZ, A.,  
419 HUBERT, T., BAKER, L., LAI, M., BOLTON, A. ET AL. (2017). Mastering the game of go without  
420 human knowledge. *nature* **550** 354–359.
- 421 SUN, W., JIANG, N., KRISHNAMURTHY, A., AGARWAL, A. and LANGFORD, J. (2019). Model-  
422 based rl in contextual decision processes: Pac bounds and exponential improvements over model-  
423 free approaches. In *Conference on learning theory*. PMLR.
- 424 UEHARA, M. and SUN, W. (2021). Pessimistic model-based offline reinforcement learning under  
425 partial coverage. *arXiv preprint arXiv:2107.06226* .
- 426 WANG, R., FOSTER, D. P. and KAKADE, S. M. (2020a). What are the statistical limits of offline rl  
427 with linear function approximation? *arXiv preprint arXiv:2010.11895* .
- 428 WANG, R., SALAKHUTDINOV, R. R. and YANG, L. (2020b). Reinforcement learning with general  
429 value function approximation: Provably efficient approach via bounded eluder dimension. *Advances*  
430 *in Neural Information Processing Systems* **33** 6123–6135.
- 431 WANG, Y., WANG, R., DU, S. S. and KRISHNAMURTHY, A. (2020c). Optimism in reinforcement  
432 learning with generalized linear function approximation. In *International Conference on Learning*  
433 *Representations*.
- 434 WEISZ, G., AMORTILA, P. and SZEPESVÁRI, C. (2021). Exponential lower bounds for planning  
435 in mdps with linearly-realizable optimal action-value functions. In *Algorithmic Learning Theory*.  
436 PMLR.

- 437 XIE, T., CHENG, C.-A., JIANG, N., MINEIRO, P. and AGARWAL, A. (2021a). Bellman-consistent  
438 pessimism for offline reinforcement learning. *Advances in neural information processing systems*  
439 **34** 6683–6694.
- 440 XIE, T., JIANG, N., WANG, H., XIONG, C. and BAI, Y. (2021b). Policy finetuning: Bridging sample-  
441 efficient offline and online reinforcement learning. *Advances in neural information processing*  
442 *systems* **34** 27395–27407.
- 443 XIONG, W., ZHONG, H., SHI, C., SHEN, C., WANG, L. and ZHANG, T. (2022). Nearly minimax  
444 optimal offline reinforcement learning with linear function approximation: Single-agent mdp and  
445 markov game. *arXiv preprint arXiv:2205.15512* .
- 446 YANG, L. and WANG, M. (2019). Sample-optimal parametric q-learning using linearly additive  
447 features. In *International Conference on Machine Learning*.
- 448 YANG, L. and WANG, M. (2020). Reinforcement learning in feature space: Matrix bandit, kernels,  
449 and regret bound. In *International Conference on Machine Learning*. PMLR.
- 450 YIN, M., DUAN, Y., WANG, M. and WANG, Y.-X. (2022a). Near-optimal offline reinforcement  
451 learning with linear representation: Leveraging variance information with pessimism. *arXiv*  
452 *preprint arXiv:2203.05804* .
- 453 YIN, M., WANG, M. and WANG, Y.-X. (2022b). Offline reinforcement learning with differentiable  
454 function approximation is provably efficient. *arXiv preprint arXiv:2210.00750* .
- 455 YIN, M. and WANG, Y.-X. (2021). Towards instance-optimal offline reinforcement learning with  
456 pessimism. *Advances in neural information processing systems* **34** 4065–4078.
- 457 ZANETTE, A., BRANDFONBRENER, D., BRUNSKILL, E., PIROTTA, M. and LAZARIC, A. (2020a).  
458 Frequentist regret bounds for randomized least-squares value iteration. In *International Conference*  
459 *on Artificial Intelligence and Statistics*. PMLR.
- 460 ZANETTE, A., LAZARIC, A., KOCHENDERFER, M. and BRUNSKILL, E. (2020b). Learning near  
461 optimal policies with low inherent bellman error. In *International Conference on Machine Learning*.  
462 PMLR.
- 463 ZANETTE, A., WAINWRIGHT, M. J. and BRUNSKILL, E. (2021). Provable benefits of actor-critic  
464 methods for offline reinforcement learning. *Advances in neural information processing systems* **34**  
465 13626–13640.
- 466 ZHAN, W., HUANG, B., HUANG, A., JIANG, N. and LEE, J. (2022). Offline reinforcement learning  
467 with realizability and single-policy concentrability. In *Conference on Learning Theory*. PMLR.
- 468 ZHANG, Z., JI, X. and DU, S. (2021). Is reinforcement learning more difficult than bandits? a  
469 near-optimal algorithm escaping the curse of horizon. In *Conference on Learning Theory*. PMLR.
- 470 ZHOU, D., GU, Q. and SZEPESVARI, C. (2021). Nearly minimax optimal reinforcement learning for  
471 linear mixture markov decision processes. In *Conference on Learning Theory*. PMLR.

472 **A Comparison of data coverage assumptions**

473 In Yin et al. (2022b), they studied the general differentiable function class, where the function class  
474 can be denoted by

$$\mathcal{F} := \left\{ f(\boldsymbol{\theta}, \phi(\cdot, \cdot)) : \mathcal{X} \times \mathcal{A} \rightarrow \mathbb{R}, \boldsymbol{\theta} \in \Theta \right\}.$$

475 In this definition,  $\Psi$  is a compact subset and  $\phi(\cdot, \cdot) : \mathcal{X} \times \mathcal{A} \rightarrow \Psi \subseteq \mathbb{R}^m$  is a feature map. The  
476 parameter space  $\Theta$  is a compact subset  $\Theta \subseteq \mathbb{R}^d$ . The function  $f : \mathbb{R}^d \times \mathbb{R}^m \rightarrow \mathbb{R}$  satisfies the  
477 following smoothness conditions:

- 478 • For any vector  $\phi \in \mathbb{R}^m$ ,  $f(\boldsymbol{\theta}, \phi)$  is third-time differentiable with respect to the parameter  $\boldsymbol{\theta}$ .
- 479 • Functions  $f, \partial_{\boldsymbol{\theta}} f, \partial_{\boldsymbol{\theta}}^2 f, \partial_{\boldsymbol{\theta}}^3 f$  are jointly continuous for  $(\boldsymbol{\theta}, \phi)$ .

480 Under this definition, Yin et al. (2022b) introduce the following coverage assumption (Assumption  
481 2.3) such that for all stage  $h \in [H]$ , there exists a constant  $\kappa$ ,

$$\begin{aligned} \mathbb{E}_{\mu, h} \left[ (f(\boldsymbol{\theta}_1, \phi(x, a)) - f(\boldsymbol{\theta}_2, \phi(x, a)))^2 \right] &\geq \kappa \|\boldsymbol{\theta}_1 - \boldsymbol{\theta}_2\|_2^2, \forall \boldsymbol{\theta}_1, \boldsymbol{\theta}_2 \in \Theta; (*) \\ \mathbb{E}_{\mu, h} \left[ \nabla f(\boldsymbol{\theta}, \phi(x, a)) \nabla f(\boldsymbol{\theta}, \phi(x, a))^\top \right] &\succ \kappa I, \forall \boldsymbol{\theta} \in \Theta. (**) \end{aligned}$$

482 It is worth noting that our assumption 3.3 is weaker than this assumption. For any compact sets  $\Theta, \Psi$   
483 and continuous function  $f$ , there always exist a constant  $\kappa_0 > 0$  such that  $f$  is  $\kappa_0$ -Lipschitz with  
484 respect to the parameter  $\boldsymbol{\theta}$ , i.e:

$$|f(\boldsymbol{\theta}_1, \phi) - f(\boldsymbol{\theta}_2, \phi)| \leq \kappa_0 \|\boldsymbol{\theta}_1 - \boldsymbol{\theta}_2\|_2, \forall \boldsymbol{\theta}_1, \boldsymbol{\theta}_2 \in \Theta, \phi \in \Psi.$$

485 Therefore, the coverage assumption in Yin et al. (2022b) implies that

$$\begin{aligned} \mathbb{E}_{\mu, h} \left[ (f(\boldsymbol{\theta}_1, \phi(\cdot, \cdot)) - f(\boldsymbol{\theta}_2, \phi(\cdot, \cdot)))^2 \right] &\geq \kappa \|\boldsymbol{\theta}_1 - \boldsymbol{\theta}_2\|_2^2 \\ &\geq \frac{\kappa}{\kappa_0^2} \sup_{(x, a) \in \mathcal{X} \times \mathcal{A}} (f(\boldsymbol{\theta}_1, \phi(x, a)) - f(\boldsymbol{\theta}_2, \phi(x, a)))^2. \end{aligned}$$

486 Thus, our assumption is weaker than the first assumption (\*). For the second assumption (\*\*), there  
487 is no direct counterpart in the general setting.

488 In addition, for the linear function class, the coverage assumption in Yin et al. (2022b) will reduce to  
489 the following linear function coverage assumption (Wang et al., 2020a; Min et al., 2021; Yin et al.,  
490 2022a; Xiong et al., 2022).

$$\lambda_{\min}(\mathbb{E}_{\mu, h}[\phi(x, a)\phi(x, a)^\top]) = \kappa > 0, \forall h \in [H].$$

491 Therefore, our assumption is also weaker than the linear function coverage assumption when dealing  
492 with the linear function class.

493 **B Proof of Theorem 5.1**

494 We need the following lemmas to prove Theorem 5.1. To start with, we prove the result that our data  
495 coverage assumption (Assumption 3.3) can lead to an upper bound of the  $D^2$ -divergence for large  
496 dataset.

497 **Lemma B.1.** Let  $\mathcal{D}_h$  be the dataset satisfying Assumption 3.3. When the size of data set satisfies  
498  $K \geq \tilde{\Omega} \left( \frac{\log \mathcal{N}}{\kappa^2} \right)$ , with probability at least  $1 - \delta$ , for each state-action pair  $z$ , we have

$$D_{\mathcal{F}_h}(z, \mathcal{D}_h, 1) = \tilde{O} \left( \frac{1}{\sqrt{K\kappa}} \right).$$

499 **Lemma B.2.** Let  $\mathcal{D}_h$  be a dataset satisfying Assumption 3.3. When the size of data set satisfies  
500  $K \geq \tilde{\Omega} \left( \frac{\log \mathcal{N}}{\kappa^2} \right)$ ,  $\hat{\sigma}_h \leq H$ , with probability at least  $1 - \delta$ , for each state-action pair  $z$ , we have

$$D_{\mathcal{F}_h}(z, \mathcal{D}_h, \hat{\sigma}_h) = \tilde{O} \left( \frac{H}{\sqrt{K\kappa}} \right).$$

501 The following lemmas show the confidence radius for the first and second-order Bellman error.

502 **Lemma B.3** (Restatement of Lemma 6.1). At stage  $h \in [H]$ , the estimated value function  $\widehat{f}'_{h+1}$  in  
 503 Algorithm 1 is bounded by  $H$ . According to Assumption 3.1, there exists some function  $\bar{f}'_h \in \mathcal{F}_h$ ,  
 504 such that  $|\bar{f}'_h(z_h) - \mathcal{T}_h \widehat{f}'_{h+1}(z_h)| \leq \epsilon$  for all  $z_h = (s_h, a_h)$ . Then with probability at least  $1 - \delta/(4H^2)$ ,  
 505 the following inequality holds:

$$\sum_{k \in [K]} \left( \bar{f}'_h(\bar{z}_h^k) - \widehat{f}'_h(\bar{z}_h^k) \right)^2 \leq (\beta'_{1,h})^2,$$

506 where  $\beta'_{1,h} = \widetilde{O}(\sqrt{\log \mathcal{N} \mathcal{N}_b H})$ .

507 The following lemma for second-order function approximation parallels the lemma we have proved.

508 **Lemma B.4** (Restatement of Lemma 6.2). At stage  $h \in [H]$ , the estimated value function  $\widehat{f}'_{h+1}$  in  
 509 Algorithm 1 is bounded by  $H$ . According to Assumption 3.1, there exists some functions  $\bar{g}'_h \in \mathcal{F}_h$ ,  
 510 such that  $|\bar{g}'_h(z_h) - \mathcal{T}_{2,h} \widehat{f}'_{h+1}(z_h)| \leq \epsilon$  for all  $z_h = (x_h, a_h)$ . Then with probability at least  
 511  $1 - \delta/(4H^2)$ , the following inequality holds:

$$\sum_{k \in [K]} \left( \bar{g}'_h(\bar{z}_h^k) - \widehat{g}'_h(\bar{z}_h^k) \right)^2 \leq (\beta'_{2,h})^2,$$

512 where  $\beta'_{2,h} = \widetilde{O}(\sqrt{\log \mathcal{N} \mathcal{N}_b H^2})$ .

513 Using Lemma B.3 and Lemma B.4, we can prove a high probability bound of the variance estimator.  
 514 We first recall the definition of the variance estimator.

$$\begin{aligned} \widetilde{f}'_h &= \operatorname{argmin}_{f_h \in \mathcal{F}_h} \sum_{k \in [K]} \left( f_h(\bar{s}_h^k, \bar{a}_h^k) - \bar{r}_h^k - \widehat{f}'_{h+1}(\bar{s}_{h+1}^k) \right)^2 \\ \widetilde{g}'_h &= \operatorname{argmin}_{g_h \in \mathcal{F}_h} \sum_{k \in [K]} \left( g_h(\bar{s}_h^k, \bar{a}_h^k) - \left( \bar{r}_h^k + \widehat{f}'_{h+1}(\bar{s}_{h+1}^k) \right) \right)^2. \end{aligned}$$

515 We then employ the following variance estimator:

$$\widehat{\sigma}_h^2(s, a) := \max \left\{ 1, \widetilde{g}'_h(s, a) - \left( \widetilde{f}'_h(s, a) \right)^2 - \widetilde{O} \left( \frac{\sqrt{\log \mathcal{N} \mathcal{N}_b H^3}}{\sqrt{K \kappa}} \right) \right\}.$$

516 The following lemma shows our constructed estimator is closed to the actual variance of the optimal  
 517 value function  $[\mathbb{V}_h V_{h+1}^*](s, a)$ .

518 **Lemma B.5.** with probability at least  $1 - \delta/2$ , for any  $h \in [H]$ , the variance estimator designed  
 519 above satisfies:

$$[\mathbb{V}_h V_{h+1}^*](s, a) - \widetilde{O} \left( \frac{\sqrt{\log \mathcal{N} \mathcal{N}_b H^3}}{\sqrt{K \kappa}} \right) \leq \widehat{\sigma}_h^2(s, a) \leq [\mathbb{V}_h V_{h+1}^*](s, a).$$

520 With the property of  $\widehat{\sigma}_h$  in Lemma B.5, we can prove a variance weighted version of concentration  
 521 inequality.

522 **Lemma B.6** (Restatement of Lemma 6.3). Suppose the variance function  $\widehat{\sigma}_h$  satisfies the inequality  
 523 in Lemma B.5. at stage  $h \in [H]$ , the estimated value function  $\widehat{f}'_{h+1}$  in Algorithm 1 is bounded by  $H$ .  
 524 According to Assumption 3.1, there exists some function  $\bar{f}_h \in \mathcal{F}_h$ , such that  $|\bar{f}_h(z_h) - \mathcal{T}_h \widehat{f}'_{h+1}(z)| \leq$   
 525  $\epsilon$  for all  $z_h = (s_h, a_h)$ . Then with probability at least  $1 - \delta/2$ , the following inequality holds for all  
 526 stage  $h \in [H]$  simultaneously,

$$\sum_{k \in [K]} \frac{1}{(\widehat{\sigma}_h(\bar{z}_h^k))^2} \left( \bar{f}_h(\bar{z}_h^k) - \widehat{f}_h(\bar{z}_h^k) \right)^2 \leq (\beta_h)^2.$$

527 Finally, we start the proof of Theorem 5.1.

528 *Proof of Theorem 5.1.* For any state-action pair  $z = (s, a) \in \mathcal{S} \times \mathcal{A}$ , we have

$$\begin{aligned} \left| \mathcal{T}_h \widehat{f}_{h+1}(z) - \widetilde{f}_h(z) \right| &\leq \left| \mathcal{T}_h \widehat{f}_{h+1}(z) - \widetilde{f}_h(z) \right| + \left| \widetilde{f}_h(z) - \widehat{f}_h(z) \right| \\ &\leq \epsilon + b_h(z), \end{aligned}$$

529 where we bound the first term with the Bellman completeness assumption (Assumption 3.1). For the  
530 second term, we use the bonus oracle (Definition 4.1) and Lemma B.6. Therefore, using Lemma D.2  
531 we have

$$\begin{aligned} V_1^*(s) - \widehat{V}_1(s) &\leq 2 \sum_{h=1}^H \mathbb{E}_{\pi^*} [b_h(s_h, a_h) \mid s_1 = s] + 2\epsilon H \\ &\leq \sum_{h=1}^H \mathbb{E}_{\pi^*} \left[ D_{\mathcal{F}_h}(z_h; \mathcal{D}_h; \widehat{\sigma}_h) \cdot \sqrt{(\beta_h)^2 + \lambda} \mid s_1 = s \right] + 2\epsilon H \\ &\leq \widetilde{O} \left( \sqrt{\log \mathcal{N}} \right) \sum_{h=1}^H \mathbb{E}_{\pi^*} [D_{\mathcal{F}_h}(z_h; \mathcal{D}_h; \widehat{\sigma}_h) \mid s_1 = s] \\ &\leq \widetilde{O} \left( \sqrt{\log \mathcal{N}} \right) \sum_{h=1}^H \mathbb{E}_{\pi^*} [D_{\mathcal{F}_h}(z_h; \mathcal{D}_h; [\mathbb{V}_h V_{h+1}^*](\cdot, \cdot)) \mid s_1 = s]. \end{aligned}$$

532 Here the second inequality holds because of our choice of bonus function (Definition 4.1). We use the  
533 definition of  $\beta_h = \widetilde{O}(\sqrt{\log \mathcal{N}})$  in the third inequality. Finally, due to Lemma B.5, with probability  
534 at least  $1 - \delta$ , for any  $z \in \mathcal{S} \times \mathcal{A}$ , we have  $\widehat{\sigma}_h(z) \leq [\mathbb{V}_h V_{h+1}^*](z)$ . Therefore, using the fact that  
535  $D^2$ -divergence is increasing with respect to the variance function (Definition 3.2), we have proved  
536 the last inequality.  $\square$

## 537 C Proof of the Lemmas in Section B

### 538 C.1 Proof of Lemma B.1 and Lemma B.2

539 *Proof of Lemma B.1.* From the definition of  $D^2$  divergence (Definition 3.2), we have

$$D_{\mathcal{F}_h}^2(z; \mathcal{D}_h; 1) = \sup_{f_1, f_2 \in \mathcal{F}_h} \frac{(f_1(z) - f_2(z))^2}{\sum_{k \in [K]} (f_1(z_h^k) - f_2(z_h^k))^2 + \lambda} \quad (\text{C.1})$$

540 By Hoeffding inequality (Lemma D.3), with probability at least  $1 - \delta/(\mathcal{N}^2)$ , we have

$$\sum_{k \in [K]} (f_1(z_h^k) - f_2(z_h^k))^2 - K \mathbb{E}_{\mu, h} \left[ (f_1(z_h) - f_2(z_h))^2 \right] \geq -2\sqrt{2K \log(\mathcal{N}^2/\delta)} \cdot \|f_1 - f_2\|_\infty^2.$$

541 Hence, after taking a union bound, we have with probability at least  $1 - \delta$ , for all  $f_1, f_2 \in \mathcal{F}_h$ ,

$$\begin{aligned} \sum_{k \in [K]} (f_1(z_h^k) - f_2(z_h^k))^2 &\geq K \mathbb{E}_{\mu, h} \left[ (f_1(z_h) - f_2(z_h))^2 \right] - 2\sqrt{2K \log(\mathcal{N}^2/\delta)} \cdot \|f_1 - f_2\|_\infty^2 \\ &\geq K \cdot \kappa \|f_1 - f_2\|_\infty^2 - 2\sqrt{2K \log(\mathcal{N}^2/\delta)} \cdot \|f_1 - f_2\|_\infty^2, \end{aligned} \quad (\text{C.2})$$

542 where the second inequality holds due to Assumption 3.3. Substituting (C.2) into (C.1), when the  
543 size of dataset  $K \geq \widetilde{\Omega} \left( \frac{\log \mathcal{N}}{\kappa^2} \right)$ , we have

$$D_{\mathcal{F}_h}^2(z; \mathcal{D}_h; 1) \leq \sup_{f_1, f_2 \in \mathcal{F}_h} \frac{(f_1(z) - f_2(z))^2}{\frac{1}{2}K \cdot \kappa \|f_1 - f_2\|_\infty^2 + \lambda} = \widetilde{O} \left( \frac{1}{K\kappa} \right).$$

544  $\square$

545 *Proof of Lemma B.2.* From the definition of  $D^2$  divergence, we have

$$D_{\mathcal{F}_h}^2(z; \mathcal{D}_h; \hat{\sigma}_h) = \sup_{f_1, f_2 \in \mathcal{F}_h} \frac{(f_1(z) - f_2(z))^2}{\sum_{k \in [K]} \frac{1}{(\hat{\sigma}_h(z_h^k))^2} (f_1(z_h^k) - f_2(z_h^k))^2 + \lambda} \quad (\text{C.3})$$

546 By Hoeffding inequality (Lemma D.3), with probability at least  $1 - \delta/(\mathcal{N}^2)$ ,

$$\sum_{k \in [K]} (f_1(z_h^k) - f_2(z_h^k))^2 - K \mathbb{E}_{\mu, h} [(f_1(z_h) - f_2(z_h))^2] \geq -2\sqrt{2K \log(\mathcal{N}^2/\delta)} \cdot \|f_1 - f_2\|_\infty^2.$$

547 Hence, after taking a union bound, we have with probability at least  $1 - \delta$ , for all  $f_1, f_2 \in \mathcal{F}_h$ ,

$$\begin{aligned} & \sum_{k \in [K]} \frac{1}{(\hat{\sigma}_h(z_h^k))^2} (f_1(z_h^k) - f_2(z_h^k))^2 \\ & \geq \frac{1}{H^2} \left( K \mathbb{E}_{\mu, h} [(f_1(z_h) - f_2(z_h))^2] - 2\sqrt{2K \log(\mathcal{N}^2/\delta)} \cdot \|f_1 - f_2\|_\infty^2 \right) \\ & \geq \frac{1}{H^2} \left( K \cdot \kappa \|f_1 - f_2\|_\infty^2 - 2\sqrt{2K \log(\mathcal{N}^2/\delta)} \cdot \|f_1 - f_2\|_\infty^2 \right), \end{aligned} \quad (\text{C.4})$$

548 where we use Assumption 3.3 and substituting (C.4) into (C.3), when  $K \geq \tilde{\Omega} \left( \frac{\log \mathcal{N}}{\kappa} \right)$ , we have

$$D_{\mathcal{F}_h}^2(z; \mathcal{D}_h; \hat{\sigma}_h) \leq \sup_{f_1, f_2 \in \mathcal{F}_h} \frac{H^2 (f_1(z) - f_2(z))^2}{\frac{1}{2} K \cdot \kappa \|f_1 - f_2\|_\infty^2 + \lambda} = \tilde{O} \left( \frac{H^2}{K \kappa^2} \right).$$

549

□

## 550 C.2 Proof of Lemma B.3

551 We need to prove the following concentration inequality first.

552 **Lemma C.1.** Based on the dataset  $\mathcal{D}' = \{\bar{s}_h^k, \bar{a}_h^k, \bar{r}_h^k\}_{k, h=1}^{K, H}$ , we define the filtration

$$\bar{\mathcal{H}}_h^k = \sigma(\bar{s}_1^1, \bar{a}_1^1, \bar{r}_1^1, \bar{s}_2^1, \dots, \bar{r}_H^1, \bar{s}_{H+1}^1; \bar{s}_1^2, \bar{a}_1^2, \bar{r}_1^2, \bar{s}_2^2, \dots, \bar{r}_H^2, \bar{s}_{H+1}^2; \dots, \bar{s}_1^k, \bar{a}_1^k, \bar{r}_1^k, \bar{s}_2^k, \dots, \bar{r}_h^k, \bar{s}_{h+1}^k).$$

553 For any fixed functions  $f, f' : \mathcal{S} \rightarrow [0, L]$ , we make the following definitions:

$$\begin{aligned} \bar{\eta}_h^k[f'] &:= f'(\bar{s}_{h+1}^k) - [\mathbb{P}_h f'](\bar{s}_h^k, \bar{a}_h^k) \\ \bar{D}_h^k[f, f'] &:= 2\bar{\eta}_h^k[f'] (f(\bar{z}_h^k) - \mathcal{T}_h f'(\bar{z}_h^k)). \end{aligned}$$

554 Then with probability at least  $1 - \delta/(4H^2\mathcal{N}^2\mathcal{N}_b^2)$ , the following inequality holds,

$$\sum_{k \in [K]} \bar{D}_h^k[f, f'] \leq (24L + 5)i^2(\delta) + \frac{\sum_{k \in [K]} (f(\bar{z}_h^k) - \mathcal{T}_h f'(\bar{z}_h^k))^2}{2},$$

555 where  $i(\delta) = \sqrt{2 \log \frac{\mathcal{N}\mathcal{N}_b H(2 \log(4LK) + 2)(\log(2L) + 2)}{\delta}}$ .

556 *Proof.* We use Lemma D.1, with the following conditions:

$\bar{D}_h^k[f, f']$  is adapted to the filtration  $\bar{\mathcal{H}}_h^k$  and  $\mathbb{E}[\bar{D}_h^k[f, f'] | \bar{\mathcal{H}}_h^{k-1}] = 0$ .

$$|\bar{D}_h^k[f, f']| \leq 2 |\bar{\eta}_h^k| \max_z |f(z) - \mathcal{T}_h f'(z)| \leq 4L^2 = M.$$

$$\sum_{k \in [K]} \mathbb{E} \left[ (\bar{D}_h^k[f, f'])^2 \middle| \bar{z}_h^k \right] = \sum_{k \in [K]} \mathbb{E} \left[ 4 (\bar{\eta}_h^k[f'])^2 \middle| \bar{z}_h^k \right] (f(\bar{z}_h^k) - \mathcal{T}_h f'(\bar{z}_h^k))^2 \leq (4LK)^2 = V^2.$$

557 On the other hand,

$$\begin{aligned} \sum_{k \in [K]} \mathbb{E} \left[ (\bar{D}_h^k[f, f'])^2 \middle| \bar{z}_h^k \right] &= \sum_{k \in [K]} \mathbb{E} \left[ 4 (\bar{\eta}_h^k[f'])^2 \middle| \bar{z}_h^k \right] (f(\bar{z}_h^k) - \mathcal{T}_h f'(\bar{z}_h^k))^2 \\ &\leq 8L^2 \sum_{k \in [K]} (f(\bar{z}_h^k) - \mathcal{T}_h f'(\bar{z}_h^k))^2. \end{aligned}$$



558 Then using Lemma D.1 with  $v = 1$ ,  $m = 1$ , with high probability, we have:

$$\begin{aligned} \sum_{k \in [K]} 2\bar{\eta}_h^k[f'] (f(\bar{z}_h^k) - \mathcal{T}_h f'(\bar{z}_h^k)) &\leq i(\delta) \sqrt{2(2 \cdot 8L^2) \sum_{k \in [K]} (f(\bar{z}_h^k) - \mathcal{T}_h f'(\bar{z}_h^k))^2} \\ &\quad + \frac{2}{3}i^2(\delta) + \frac{4}{3}i^2(\delta) \cdot 4L^2 \\ &\leq (24L^2 + 5)i^2(\delta) + \frac{\sum_{k \in [K]} (f(\bar{z}_h^k) - \mathcal{T}_h f'(\bar{z}_h^k))^2}{2}. \end{aligned}$$

559

□

560 *Proof of Lemma B.3.* Let  $(\beta'_{1,h})^2 = (24L^2 + 5)i^2(\delta) + 8KL\epsilon$ . We define the event  $\mathcal{E}'_{1,h} :=$   
 561  $\left\{ \sum_{k \in [K]} \left( \bar{f}'_h(\bar{z}_h^k) - \tilde{f}'_h(\bar{z}_h^k) \right)^2 > (\beta'_{1,h})^2 \right\}$ . The following inequality will be useful in our proof.

$$\begin{aligned} \sum_{k \in [K]} \left( \bar{f}'_h(\bar{z}_h^k) - \tilde{f}'_h(\bar{z}_h^k) \right)^2 &= \sum_{k \in [K]} \left[ \left( \bar{r}_h^k + \hat{f}'_{h+1}(\bar{s}_{h+1}^k) - \bar{f}'_h(\bar{z}_h^k) \right) + \left( \tilde{f}'_h(\bar{z}_h^k) - \bar{r}_h^k - \hat{f}'_{h+1}(\bar{s}_{h+1}^k) \right) \right]^2 \\ &= \sum_{k \in [K]} \left( \bar{r}_h^k + \hat{f}'_{h+1}(\bar{s}_{h+1}^k) - \bar{f}'_h(\bar{z}_h^k) \right)^2 + \sum_{k \in [K]} \left( \tilde{f}'_h(\bar{z}_h^k) - \bar{r}_h^k - \hat{f}'_{h+1}(\bar{s}_{h+1}^k) \right)^2 \\ &\quad + 2 \sum_{k \in [K]} \left( \bar{r}_h^k + \hat{f}'_{h+1}(\bar{s}_{h+1}^k) - \bar{f}'_h(\bar{z}_h^k) \right) \left( \tilde{f}'_h(\bar{z}_h^k) - \bar{r}_h^k - \hat{f}'_{h+1}(\bar{s}_{h+1}^k) \right) \\ &\leq 2 \sum_{k \in [K]} \left( \bar{r}_h^k + \hat{f}'_{h+1}(\bar{s}_{h+1}^k) - \bar{f}'_h(\bar{z}_h^k) \right)^2 \\ &\quad + 2 \sum_{k \in [K]} \left( \bar{r}_h^k + \hat{f}'_{h+1}(\bar{s}_{h+1}^k) - \bar{f}'_h(\bar{z}_h^k) \right) \left( \tilde{f}'_h(\bar{z}_h^k) - \bar{r}_h^k - \hat{f}'_{h+1}(\bar{s}_{h+1}^k) \right) \\ &\leq 2 \sum_{k \in [K]} \left( \bar{r}_h^k + \hat{f}'_{h+1}(\bar{s}_{h+1}^k) - \bar{f}'_h(\bar{z}_h^k) \right) \left( \tilde{f}'_h(\bar{z}_h^k) - \bar{f}'_h(\bar{z}_h^k) \right). \end{aligned}$$

562 Here we use our choice of  $\tilde{f}'_h$ , i.e.  $\tilde{f}'_h = \operatorname{argmin}_{f_h \in \mathcal{F}_h} \sum_{k \in [K]} \left( f_h(\bar{s}_h^k, \bar{a}_h^k) - \bar{r}_h^k - \hat{f}'_{h+1}(\bar{s}_{h+1}^k) \right)^2$ .  
 563 Next, we will use Lemma C.1. For any fixed  $h$ , let  $f = \tilde{f}'_h \in \mathcal{F}_h$ ,  $f' = \hat{f}'_{h+1} = \{f - \epsilon\}_{[0, H-h+1]}$ ,  
 564 where  $\tilde{f} = \tilde{f}'_h - b'_h \in \mathcal{F}_h - \mathcal{W}$ . Following the construction in Lemma C.1, we define

$$\begin{aligned} \bar{\eta}_h^k[f'] &= \bar{r}_h^s + f'(\bar{s}_{h+1}^k) - \mathbb{E} \left[ \bar{r}_h^k + f'(\bar{s}_{h+1}^k) | \bar{z}_h^k \right], \\ \text{and } \bar{D}_h^k[f, f'] &= 2\bar{\eta}_h^k[f'] (f(\bar{z}_h^k) - \mathcal{T}_h f'(\bar{z}_h^k)). \end{aligned}$$

565 Due to the result of Lemma C.1, taking a union bound, we have with probability at least  $1 - \delta/(4H^2)$ ,  
 566 the following inequality holds,

$$\sum_{k \in [K]} \bar{D}_h^k[f, f'] \leq (24L^2 + 5)i^2(\delta) + \frac{\sum_{k \in [K]} (f(\bar{z}_h^k) - \mathcal{T}_h f'(\bar{z}_h^k))^2}{2}. \quad (\text{C.5})$$

567 Therefore, with probability at least  $1 - \delta/(4H^2)$ , we have

$$\begin{aligned}
& 2 \sum_{k \in [K]} \left( \bar{r}_h^k + \hat{f}_{h+1}'(\bar{s}_{h+1}^k) - \bar{f}_h'(\bar{z}_h^k) \right) \left( \tilde{f}_h'(\bar{z}_h^k) - \bar{f}_h'(\bar{z}_h^k) \right) \\
&= 2 \sum_{k \in [K]} \left( \bar{r}_h^k + \hat{f}_{h+1}'(\bar{s}_{h+1}^k) - \mathcal{T}_h \hat{f}_{h+1}'(\bar{z}_h^k) \right) \left( \tilde{f}_h'(\bar{z}_h^k) - \bar{f}_h'(\bar{z}_h^k) \right) \\
&\quad + 2 \sum_{k \in [K]} \left( \mathcal{T}_h \hat{f}_{h+1}'(\bar{z}_h^k) - \bar{f}_h'(\bar{z}_h^k) \right) \left( \tilde{f}_h'(\bar{z}_h^k) - \bar{f}_h'(\bar{z}_h^k) \right) \\
&\leq 2 \sum_{k \in [K]} \left( \bar{r}_h^k + \hat{f}_{h+1}'(\bar{s}_{h+1}^k) - \mathcal{T}_h \hat{f}_{h+1}'(\bar{z}_h^k) \right) \left( \tilde{f}_h'(\bar{z}_h^k) - \bar{f}_h'(\bar{z}_h^k) \right) + 4KL\epsilon \\
&\leq (24L^2 + 5)i^2(\delta) + 4KL\epsilon + \frac{\sum_{k \in [K]} \left( \tilde{f}_h'(\bar{z}_h^k) - \mathcal{T}_h \hat{f}_{h+1}'(\bar{z}_h^k) \right)^2}{2} \\
&\leq (24L^2 + 5)i^2(\delta) + 8KL\epsilon + \frac{\sum_{k \in [K]} \left( \bar{f}_h'(\bar{z}_h^k) - \tilde{f}_h'(\bar{z}_h^k) \right)^2}{2} \\
&\leq \frac{(\beta'_{1,h})^2}{2} + \frac{\sum_{k \in [K]} \left( \bar{f}_h'(\bar{z}_h^k) - \tilde{f}_h'(\bar{z}_h^k) \right)^2}{2}.
\end{aligned}$$

568 Here the second inequality holds because of the Bellman completeness assumption (Assumption 3.1).  
569 The third inequality arises from (C.5). The last inequality holds due to the choice of

$$\beta'_{1,h} = \sqrt{2(24L^2 + 5)i^2(\delta) + 16KL\epsilon} = \tilde{O}\left(\sqrt{\log \mathcal{N} \mathcal{N}_b H}\right).$$

570 But conditioned on the event  $\mathcal{E}'_{1,h}$ , we have

$$\begin{aligned}
& \sum_{k \in [K]} \left( \bar{r}_h^k + \hat{f}_{h+1}'(\bar{s}_{h+1}^k) - \bar{f}_h'(\bar{z}_h^k) \right) \left( \tilde{f}_h'(\bar{z}_h^k) - \bar{f}_h'(\bar{z}_h^k) \right) \\
&\geq \sum_{k \in [K]} \left( \bar{f}_h'(\bar{z}_h^k) - \tilde{f}_h'(\bar{z}_h^k) \right)^2 \\
&> \frac{(\beta'_{1,h})^2}{2} + \frac{\sum_{k \in [K]} \left( \bar{f}_h'(\bar{z}_h^k) - \tilde{f}_h'(\bar{z}_h^k) \right)^2}{2}.
\end{aligned}$$

571 Thus, we have  $\mathbb{P}[\mathcal{E}'_{1,h}] \leq \delta/(4H^2)$ . □

### 572 C.3 Proof of Lemma B.4

573 To prove this lemma, we need a lemma similar to Lemma C.1

574 **Lemma C.2.** On dataset  $\mathcal{D}' = \{\bar{s}_h^k, \bar{a}_h^k, \bar{r}_h^k\}_{k,h=1}^{K,H}$ , we define the filtration

$$\bar{\mathcal{H}}_h^k = \sigma(\bar{s}_1^1, \bar{a}_1^1, \bar{r}_1^1, \bar{s}_2^1, \dots, \bar{r}_H^1, \bar{s}_{H+1}^1; \bar{s}_1^2, \bar{a}_1^2, \bar{r}_1^2, \bar{s}_2^2, \dots, \bar{r}_H^2, \bar{s}_{H+1}^2; \dots, \bar{s}_1^k, \bar{a}_1^k, \bar{r}_1^k, \bar{s}_2^k, \dots, \bar{r}_h^k, \bar{s}_{h+1}^k).$$

575 For any fixed function  $f, f' : \mathcal{S} \rightarrow [0, L]$ , we make the following definitions:

$$\begin{aligned}
\bar{\eta}_h^k[f'] &:= \left( \bar{r}_h^k + f'(\bar{s}_{h+1}^k) \right)^2 - \left[ \mathbb{P}_h(\bar{r}_h + f')^2 \right] (\bar{s}_h^k, \bar{a}_h^k) \\
\bar{D}_h^k[f, f'] &:= 2\bar{\eta}_h^k[f'] \left( f(\bar{z}_h^k) - \mathcal{T}_{2,h} f'(\bar{z}_h^k) \right).
\end{aligned}$$

576 Then with probability at least  $1 - \delta/(4H^2 \mathcal{N}^2 \mathcal{N}_b^2)$ , the following inequality holds,

$$\sum_{k \in [K]} \bar{D}_h^k[f, f'] \leq (24L + 5)i^2(\delta) + \frac{\sum_{k \in [K]} \left( f(\bar{z}_h^k) - \mathcal{T}_{2,h} f'(\bar{z}_h^k) \right)^2}{2},$$

577 where  $i^2(\delta) = \sqrt{4 \log \frac{\mathcal{N} \mathcal{N}_b H (2 \log(4LK) + 2) (\log(4L) + 2)}{\delta}}$ .

578 *Proof.* We use Lemma D.1, with the following conditions:

$\bar{D}_h^k[f, f']$  is adapted to the filtration  $\bar{\mathcal{H}}_h^k$  and  $\mathbb{E}[\bar{D}_h^k[f, f'] \mid \bar{\mathcal{H}}_h^{k-1}] = 0$ .

$|\bar{D}_h^k[f, f']| \leq 2|\bar{\eta}_h^k| \max_z |f(z) - \mathcal{T}_{2,h}f'(z)| \leq 4L^2 = M$ .

$$\sum_{k \in [K]} \mathbb{E} \left[ (\bar{D}_h^k[f, f'])^2 \mid \bar{\mathcal{H}}_h^k \right] = \sum_{k \in [K]} \mathbb{E} [4(\bar{\eta}_h^k[f'])^2 \mid \bar{\mathcal{H}}_h^k] (f(\bar{z}_h^k) - \mathcal{T}_{2,h}f'(\bar{z}_h^k))^2 \leq (4L^2K)^2 = V^2.$$

579 On the other hand,

$$\begin{aligned} \sum_{k \in [K]} \mathbb{E} \left[ (\bar{D}_h^k[f, f'])^2 \mid \bar{\mathcal{H}}_h^k \right] &= \sum_{k \in [K]} \mathbb{E} \left[ 4(\bar{\eta}_h^k[f'])^2 \mid \bar{\mathcal{H}}_h^k \right] (f(\bar{z}_h^k) - \mathcal{T}_h f'(\bar{z}_h^k))^2 \\ &\leq 8L^4 \sum_{k \in [K]} (f(\bar{z}_h^k) - \mathcal{T}_{2,h}f'(\bar{z}_h^k))^2. \end{aligned}$$

580 Then using Lemma D.1 with  $v = 1, m = 1$ , we have:

$$\begin{aligned} \sum_{k \in [K]} 2\bar{\eta}_h^k[f'] (f(\bar{z}_h^k) - \mathcal{T}_{2,h}f'(\bar{z}_h^k)) &\leq i'(\delta) \sqrt{2(2 \cdot 8L^4) \sum_{k \in [K]} (f(\bar{z}_h^k) - \mathcal{T}_{2,h}f'(\bar{z}_h^k))^2} \\ &\quad + \frac{2}{3}i'^2(\delta) + \frac{4}{3}i'^2(\delta) \cdot 4L^2 \\ &\leq (20L^4 + 5)i'^2(\delta) + \frac{\sum_{k \in [K]} (f(\bar{z}_h^k) - \mathcal{T}_h f'(\bar{z}_h^k))^2}{2} \end{aligned}$$

581

□

582 *Proof of Lemma B.4.* Let  $(\beta'_{2,h})^2 = 2(20L^4 + 5)i'^2(\delta) + 16KL\epsilon$ . We define the event  $\mathcal{E}'_{2,h} :=$

583  $\left\{ \sum_{k \in [K]} (\bar{g}'_h(\bar{z}_h^k) - \tilde{g}'_h(\bar{z}_h^k))^2 > (\beta'_{2,h})^2 \right\}$ . The following inequality will be useful in our proof.

$$\begin{aligned} \sum_{k \in [K]} (\bar{g}'_h(\bar{z}_h^k) - \tilde{g}'_h(\bar{z}_h^k))^2 &= \sum_{k \in [K]} \left[ \left( (\bar{r}_h^k + \hat{f}'_{h+1}(\bar{s}_{h+1}^k))^2 - \bar{g}'_h(\bar{z}_h^k) \right) + \left( \tilde{g}'_h(\bar{z}_h^k) - (\bar{r}_h^k + \hat{f}'_{h+1}(\bar{s}_{h+1}^k))^2 \right) \right]^2 \\ &= \sum_{k \in [K]} \left( (\bar{r}_h^k + \hat{f}'_{h+1}(\bar{s}_{h+1}^k))^2 - \bar{g}'_h(\bar{z}_h^k) \right)^2 + \sum_{k \in [K]} \left( \tilde{g}'_h(\bar{z}_h^k) - (\bar{r}_h^k + \hat{f}'_{h+1}(\bar{s}_{h+1}^k))^2 \right)^2 \\ &\quad + 2 \sum_{k \in [K]} \left( (\bar{r}_h^k + \hat{f}'_{h+1}(\bar{s}_{h+1}^k))^2 - \bar{g}'_h(\bar{z}_h^k) \right) \left( \tilde{g}'_h(\bar{z}_h^k) - (\bar{r}_h^k + \hat{f}'_{h+1}(\bar{s}_{h+1}^k))^2 \right) \\ &\leq 2 \sum_{k \in [K]} \left( (\bar{r}_h^k + \hat{f}'_{h+1}(\bar{s}_{h+1}^k))^2 - \bar{g}'_h(\bar{z}_h^k) \right)^2 \\ &\quad + 2 \sum_{k \in [K]} \left( (\bar{r}_h^k + \hat{f}'_{h+1}(\bar{s}_{h+1}^k))^2 - \bar{g}'_h(\bar{z}_h^k) \right) \left( \tilde{g}'_h(\bar{z}_h^k) - (\bar{r}_h^k + \hat{f}'_{h+1}(\bar{s}_{h+1}^k))^2 \right) \\ &\leq 2 \sum_{k \in [K]} \left( (\bar{r}_h^k + \hat{f}'_{h+1}(\bar{s}_{h+1}^k))^2 - \bar{g}'_h(\bar{z}_h^k) \right) \left( \tilde{g}'_h(\bar{z}_h^k) - \bar{g}'_h(\bar{z}_h^k) \right). \quad (\text{C.6}) \end{aligned}$$

584 Here we use our choice of  $\tilde{g}'_h$ , i.e.  $\tilde{g}'_h = \operatorname{argmin}_{g_h \in \mathcal{F}_h} \sum_{k \in [K]} \left( g_h(\bar{s}_h^k, \bar{a}_h^k) - (\bar{r}_h^k + \hat{f}'_{h+1}(\bar{s}_{h+1}^k))^2 \right)^2$ .

585 Next, we will use Lemma C.2. For any fixed  $h$ , let  $f = \tilde{g}'_h \in \mathcal{F}_h$ ,  $f' = \hat{f}'_{h+1} = \{\tilde{f} - \epsilon\}_{[0, H-h+1]}$ ,

586 where  $\tilde{f} = \hat{f}'_h - b'_h \in \mathcal{F}_h - \mathcal{W}$ . Following the construction in Lemma C.1, we define

$$\begin{aligned} \bar{\eta}_h^k[f'] &:= (\bar{r}_h^k + f'(\bar{s}_{h+1}^k))^2 - [\mathbb{P}_h(\bar{r}_h + f')]^2(\bar{s}_h^k, \bar{a}_h^k) \\ \text{and } \bar{D}_h^k[f, f'] &:= 2\bar{\eta}_h^k[f'] (f(\bar{z}_h^k) - \mathcal{T}_{2,h}f'(\bar{z}_h^k)). \end{aligned}$$

587 Due to the result of Lemma C.2, taking a union bound, we have with probability at least  $1 - \delta/(4H^2)$ ,  
588 the following inequality holds,

$$\sum_{k \in [K]} \bar{D}_h^k[f, f'] \leq (20L^4 + 5)i'^2(\delta) + \frac{\sum_{k \in [K]} (f(\bar{z}_h^k) - \mathcal{T}_{2,h}f'(\bar{z}_h^k))^2}{2}. \quad (\text{C.7})$$

589 Therefore, with probability at least  $1 - \delta/(4H^2)$ , we have

$$\begin{aligned}
& 2 \sum_{k \in [K]} \left( (\bar{r}_h^k + \hat{f}_{h+1}^k(s_{h+1}^k))^2 - \bar{g}_h'(z_h^k) \right) (\tilde{g}_h'(z_h^k) - \bar{g}_h'(z_h^k)) \\
&= 2 \sum_{k \in [K]} \left( (\bar{r}_h^k + \hat{f}_{h+1}^k(s_{h+1}^k))^2 - \mathcal{T}_{2,h} \hat{f}_{h+1}^k(z_h^k) \right) (\tilde{g}_h'(z_h^k) - \bar{g}_h'(z_h^k)) \\
&\quad + 2 \sum_{k \in [K]} \left( \mathcal{T}_{2,h} \hat{f}_{h+1}^k(z_h^k) - \bar{g}_h'(z_h^k) \right) (\tilde{g}_h'(z_h^k) - \bar{g}_h'(z_h^k)) \\
&\leq 2 \sum_{k \in [K]} \left( (\bar{r}_h^k + \hat{f}_{h+1}^k(s_{h+1}^k))^2 - \mathcal{T}_{2,h} \hat{f}_{h+1}^k(z_h^k) \right) (\tilde{g}_h'(z_h^k) - \bar{g}_h'(z_h^k)) + 4KL\epsilon \\
&\leq (20L^4 + 5)i'^2(\delta) + 4KL\epsilon + \frac{\sum_{k \in [K]} \left( \tilde{g}_h'(z_h^k) - \mathcal{T}_{2,h} \hat{f}_{h+1}^k(z_h^k) \right)^2}{2} \\
&\leq (20L^4 + 5)i'^2(\delta) + 8KL\epsilon + \frac{\sum_{k \in [K]} \left( \bar{g}_h'(z_h^k) - \tilde{g}_h'(z_h^k) \right)^2}{2} \\
&\leq \frac{(\beta'_{2,h})^2}{2} + \frac{\sum_{k \in [K]} \left( \bar{g}_h'(z_h^k) - \tilde{g}_h'(z_h^k) \right)^2}{2}.
\end{aligned}$$

590 Here the second inequality holds because of the Bellman completeness assumption (Assumption 3.1).

591 The third inequality arises from (C.7). The last inequality holds due to the choice of

$$\beta'_{2,h} = \sqrt{2(20L^4 + 5)i'^2(\delta) + 16KL\epsilon} = \tilde{O}(\sqrt{\log \mathcal{N} \mathcal{N}_b H^2}).$$

592 But conditioned on the event  $\mathcal{E}'_{2,h}$ , we have

$$\begin{aligned}
& \sum_{k \in [K]} \left( (\bar{r}_h^k + \hat{f}_{h+1}^k(s_{h+1}^k))^2 - \bar{g}_h'(z_h^k) \right) (\tilde{g}_h'(z_h^k) - \bar{g}_h'(z_h^k)) \\
&\geq \sum_{k \in [K]} \left( \bar{g}_h'(z_h^k) - \tilde{g}_h'(z_h^k) \right)^2 \\
&> \frac{(\beta'_{2,h})^2}{2} + \frac{\sum_{k \in [K]} \left( \bar{g}_h'(z_h^k) - \tilde{g}_h'(z_h^k) \right)^2}{2}.
\end{aligned}$$

593 Here we use (C.6). Thus, we have  $\mathbb{P}[\mathcal{E}'_{2,h}] \leq \delta/(4H^2)$ . □

#### 594 C.4 Proof of Lemma B.5

595 *Proof of Lemma B.5.* We write  $\mathbb{B}_h(s, a) = \tilde{g}_h'(s, a) - \left( \tilde{f}_h(s, a) \right)^2$ . We first bound the difference

596 between  $\mathbb{B}_h(s, a)$  and  $[\text{Var}_h \hat{f}_{h+1}^k](s, a)$ . By the definition of conditional variance, we have

$$\left| \mathbb{B}_h(s, a) - [\text{Var}_h \hat{f}_{h+1}^k](s, a) \right| \leq \left| \tilde{g}_h(s, a) - \mathcal{T}_{2,h} \hat{f}_{h+1}^k(s, a) \right| + \left| \left( \tilde{f}_h(s, a) \right)^2 - \left( \mathcal{T}_h \hat{f}_{h+1}^k(s, a) \right)^2 \right|,$$

597 where we use our definition of Bellman operators. By the Bellman completeness assumption, there

598 exists  $\bar{f}'_h \in \mathcal{F}_h$ ,  $\bar{g}'_h \in \mathcal{F}_h$ , such that  $\left| \bar{f}'_h(s, a) - \mathcal{T}_h \hat{f}_{h+1}^k(s, a) \right| \leq \epsilon$ ,  $\left| \bar{g}'_h(s, a) - \mathcal{T}_{2,h} \hat{f}_{h+1}^k(s, a) \right| \leq \epsilon$

599 for all  $(s, a)$ . Then by Lemma B.3 we can see that with probability at least  $1 - \delta/(4H^2)$ , the following inequality holds

$$\sum_{k \in [K]} \left( \bar{f}'_h(z_h^k) - \tilde{f}_h(z_h^k) \right)^2 \leq (\beta'_{1,h})^2. \quad (\text{C.8})$$

601 Similarly, for the second order term, using Lemma B.4, we can see that with probability at least  
602  $1 - \delta/(4H^2)$ , the following inequality holds

$$\sum_{k \in [K]} \left( \bar{g}'_h(z_h^k) - \tilde{g}_h(z_h^k) \right)^2 \leq (\beta'_{2,h})^2. \quad (\text{C.9})$$

603 After taking a union bound, we have that with probability at least  $1 - \delta/(2H)$ , (C.8) and (C.9) hold  
 604 for all  $h \in [H]$  simultaneously. Under this high-probability event, we have

$$\begin{aligned}
& \left| \tilde{g}'_h(s, a) - \mathcal{T}_{2,h} \hat{f}'_{h+1}(s, a) \right| + \left| \left( \tilde{f}_h(s, a) \right)^2 - \left( \mathcal{T}_h \hat{f}'_{h+1}(s, a) \right)^2 \right| \\
& \leq \epsilon + |\tilde{g}'_h(s, a) - \bar{g}'_h(s, a)| + O(H) \cdot \left| \tilde{f}'_h(s, a) - \bar{f}'_h(s, a) \right| + \epsilon \\
& \leq O(H) \cdot \epsilon + \frac{|\tilde{g}'_h(s, a) - \bar{g}'_h(s, a)|}{\sqrt{\sum_{k \in [K]} (\bar{g}'_h(z_h^k) - \tilde{g}'_h(z_h^k))^2 + \lambda}} \cdot \sqrt{\sum_{k \in [K]} (\bar{g}'_h(z_h^k) - \tilde{g}'_h(z_h^k))^2 + \lambda} \\
& \quad + O(H) \cdot \frac{|\tilde{f}'_h(s, a) - \bar{f}'_h(s, a)|}{\sqrt{\sum_{k \in [K]} (\bar{f}'_h(z_h^k) - \tilde{f}'_h(z_h^k))^2 + \lambda}} \cdot \sqrt{\sum_{k \in [K]} (\bar{f}'_h(z_h^k) - \tilde{f}'_h(z_h^k))^2 + \lambda} \\
& \leq O(H) \cdot \epsilon + \frac{|\tilde{g}'_h(s, a) - \bar{g}'_h(s, a)|}{\sqrt{\sum_{k \in [K]} (\bar{g}'_h(z_h^k) - \tilde{g}'_h(z_h^k))^2 + \lambda}} \cdot \sqrt{(\beta'_{2,h})^2 + \lambda} \\
& \quad + O(H) \cdot \frac{|\tilde{f}'_h(s, a) - \bar{f}'_h(s, a)|}{\sqrt{\sum_{k \in [K]} (\bar{f}'_h(z_h^k) - \tilde{f}'_h(z_h^k))^2 + \lambda}} \cdot \sqrt{(\beta'_{1,h})^2 + \lambda} \\
& \leq \tilde{O}(\sqrt{\log \mathcal{N} \mathcal{N}_b H^2}) \cdot D_{\mathcal{F}_h}(z, \mathcal{D}'_h, 1) \\
& \leq \tilde{O}\left(\frac{\sqrt{\log \mathcal{N} \mathcal{N}_b H^2}}{\sqrt{K \kappa}}\right),
\end{aligned}$$

605 where the first inequality holds due to the completeness assumption. The third inequality holds  
 606 because of (C.8) and (C.9). The fourth inequality holds due to the definition of  $D^2$ -divergence.  
 607 Finally we use Lemma B.1.

608 To further bound the difference between  $[\text{Var}_h \hat{f}'_{h+1}](s, a)$  and  $[\text{Var}_h V_{h+1}^*](s, a)$  under the event  
 609 when (C.8) and (C.9) hold for all  $h \in [H]$  simultaneously, we first prove  $\|\hat{f}'_{h+1} - V_{h+1}^*\|_\infty \leq$   
 610  $\tilde{O}\left(\frac{\sqrt{\log \mathcal{N} \mathcal{N}_b H^3}}{\sqrt{K \kappa}}\right)$  by induction.

611 At stage  $H + 1$ ,  $\hat{f}'_{H+1} = V_{H+1}^* = 0$ , the inequality holds naturally. At stage  $H$ , we have

$$\begin{aligned}
Q_H^*(s, a) &= \mathcal{T}_H V_{H+1}^*(s, a) \\
&= \mathcal{T}_H \hat{f}'_{H+1}(s, a) \\
&\geq \tilde{f}'_H(s, a) - |\mathcal{T}_H \hat{f}'_{H+1}(s, a) - \tilde{f}'_H(s, a)| \\
&\geq \tilde{f}'_H(s, a) - (\epsilon + |\tilde{f}'_H(s, a) - \bar{f}'_H(s, a)|) \\
&\geq \tilde{f}'_H(s, a) - b'_H(s, a) - \epsilon \\
&= \hat{f}'_H(s, a).
\end{aligned}$$

612 Here we use the definition of  $\hat{f}'_H$  in Algorithm 1 Line 6. Lemma B.3 shows

$$\sum_{k \in [K]} \left( \bar{f}'_h(z_h^k) - \tilde{f}'_h(z_h^k) \right)^2 \leq (\beta'_{1,h})^2.$$

613 Then the fifth inequality follows the bonus oracle assumption (Definition 4.1). Therefore,  $V_H^*(s) \geq$   
 614  $\hat{f}'_H(s)$  for all  $s \in \mathcal{S}$ .

615 We also have

$$\begin{aligned}
V_H^*(s) - \widehat{f}_H(s) &= \langle Q_H^*(s, \cdot) - \widehat{f}_H(s, \cdot), \pi^*(\cdot|s) \rangle_{\mathcal{A}} + \langle \widehat{f}_H(s, \cdot), \pi_H^*(\cdot|s) - \widehat{\pi}_H(\cdot|s) \rangle_{\mathcal{A}} \\
&\leq \langle Q_H^*(s, \cdot) - \widehat{f}_H(s, \cdot), \pi^*(\cdot|s) \rangle_{\mathcal{A}} \\
&= \langle \mathcal{T}_H V_H^*(s, \cdot) - \widehat{f}_H(s, \cdot) + b'_H(s, \cdot), \pi^*(\cdot|s) \rangle_{\mathcal{A}} \\
&= \langle \mathcal{T}_H \widehat{f}_{H+1}'(s, \cdot) - \widehat{f}_H(s, \cdot) + b'_H(s, \cdot), \pi^*(\cdot|s) \rangle_{\mathcal{A}} \\
&\quad + \langle \mathcal{T}_H V_{H+1}^*(s, \cdot) - \mathcal{T}_H \widehat{f}_{H+1}'(s, \cdot), \pi_H^*(\cdot|s) \rangle_{\mathcal{A}} \\
&\leq 2 \langle b'_H(s, \cdot), \pi_H^*(\cdot, s) \rangle_{\mathcal{A}} + \epsilon \\
&\leq \widetilde{O} \left( \frac{\sqrt{\log \mathcal{N} \mathcal{N}_b H}}{\sqrt{K \kappa}} \right),
\end{aligned}$$

616 where the second inequality holds due to the selection of policy  $\widehat{\pi}_H$ . In the fifth inequality, we use  
617 the Bellman completeness assumption:

$$\left| \widehat{f}_H(z) - \mathcal{T}_H \widehat{f}_{H+1}'(z) \right| \leq \epsilon, \forall z \in \mathcal{S} \times \mathcal{A}.$$

618 and Lemma B.3. The last inequality holds because of Definition 4.1 and Lemma B.1.

619 We define  $R_h = \widetilde{O} \left( \frac{\sqrt{\log \mathcal{N} \mathcal{N}_b H}}{\sqrt{K \kappa}} \right) \cdot (H - h + 1)$ . To use the method of induction, we define the  
620 induction assumption as follows: Suppose with the probability of  $1 - \delta_{h+1}$ , the event  $\mathcal{E}_{h+1} = \{0 \leq$   
621  $V_{h+1}^*(s) - \widehat{V}_{h+1}'(s) \leq R_{h+1}\}$  holds. Then we want to prove that with the probability of  $1 - \delta_h$ , the  
622 event  $\mathcal{E}_h = \{0 \leq V_h^*(s) - \widehat{V}_h'(s) \leq R_h\}$  holds.

623 Conditioned on the event  $\mathcal{E}_{h+1}$ , using similar argument to stage  $H$ , we have

$$\begin{aligned}
Q_h^*(s, a) &= \mathcal{T}_h V_{h+1}^*(s, a) \\
&\geq \mathcal{T}_h \widehat{f}_{h+1}'(s, a) \\
&\geq \widehat{f}_h'(s, a) - |\mathcal{T}_h \widehat{f}_{h+1}'(s, a) - \widehat{f}_h'(s, a)| \\
&\geq \widehat{f}_h'(s, a) - \left( \epsilon + |\widehat{f}_h'(s, a) - \widetilde{f}_h'(s, a)| \right) \\
&\geq \widetilde{f}_h'(s, a) - b'_h(s, a) \\
&= \widehat{f}_h'(s, a).
\end{aligned}$$

624 Therefore,  $V_h^*(\cdot) \geq \widehat{f}_h'(\cdot)$ .

625 On the other hand, similar to the case at stage  $H$ , we have with probability at least  $1 - \delta_h - \delta/(2H^2)$ ,

$$\begin{aligned}
V_h^*(s) - \widehat{f}_h(s) &= \langle Q_h^*(s, \cdot) - \widehat{f}_h(s, \cdot), \pi_h^*(\cdot|s) \rangle_{\mathcal{A}} + \langle \widehat{f}_h(s, \cdot), \pi_h^*(\cdot|s) - \widehat{\pi}_h(\cdot|s) \rangle_{\mathcal{A}} \\
&\leq \langle Q_h^*(s, \cdot) - \widehat{f}_h(s, \cdot), \pi_h^*(\cdot|s) \rangle_{\mathcal{A}} \\
&= \langle \mathcal{T}_h V_{h+1}^*(s, \cdot) - \widehat{f}_h(s, \cdot) + b'_h(s, a), \pi_h^*(\cdot|s) \rangle_{\mathcal{A}} \\
&= \langle \mathcal{T}_h \widehat{f}_{h+1}'(s, \cdot) - \widehat{f}_h(s, \cdot) + b'_h(s, a), \pi_h^*(\cdot|s) \rangle_{\mathcal{A}} \\
&\quad + \langle \mathcal{T}_h V_{h+1}^*(s, \cdot) - \mathcal{T}_h \widehat{f}_{h+1}'(s, \cdot), \pi_h^*(\cdot|s) \rangle_{\mathcal{A}} \\
&\leq 2 \langle b'_h(s, \cdot), \pi_h^*(\cdot, s) \rangle_{\mathcal{A}} + \epsilon + R_{h+1} \\
&\leq R_{h+1} + \widetilde{O} \left( \frac{\sqrt{\log \mathcal{N} \mathcal{N}_b H}}{\sqrt{K \kappa}} \right) \\
&\leq \widetilde{O} \left( \frac{\sqrt{\log \mathcal{N} \mathcal{N}_b H}}{\sqrt{K \kappa}} \right) \cdot (H - h + 1) = R_h.
\end{aligned}$$

626 The induction shows we can choose  $\delta_h = h\delta/(2H^2)$ . Thus, taking a union bound over all  $h \in [H]$ ,  
627 we prove that with probability at least  $1 - \delta/2$ , the following inequality

$$0 \leq V_{h+1}^*(\cdot) - \widehat{f}_{h+1}'(\cdot) \leq \widetilde{O} \left( \frac{\sqrt{\log \mathcal{N} \mathcal{N}_b H^2}}{\sqrt{K \kappa}} \right) \quad (\text{C.10})$$

628 holds for all  $h \in [H]$  simultaneously.

629 Conditioned on this event, we can further bound the difference between  $[\text{Var}_h \hat{f}'_{h+1}](s, a)$  and  
 630  $[\text{Var}_h V_{h+1}^*](s, a)$ .

$$\begin{aligned} \left| [\text{Var}_h \hat{f}'_{h+1}](s, a) - [\text{Var}_h V_{h+1}^*](s, a) \right| &\leq \left| [\mathbb{P}_h \hat{f}'_{h+1}{}^2](s, a) - [\mathbb{P}_h V_{h+1}^{*2}](s, a) \right| \\ &\quad + \left| \left( [\mathbb{P}_h \hat{f}'_{h+1}](s, a) \right)^2 - \left( [\mathbb{P}_h V_{h+1}^*](s, a) \right)^2 \right| \\ &\leq O(H) \cdot \left\| V_{h+1}^* - \hat{f}'_{h+1} \right\|_\infty \\ &\leq \tilde{O} \left( \frac{\sqrt{\log \mathcal{N} \mathcal{N}_b H^3}}{\sqrt{K \kappa}} \right). \end{aligned}$$

631 The last inequality arises from (C.10). Therefore, for any  $(s, a) \in \mathcal{S} \times \mathcal{A}$ , we have

$$\begin{aligned} \left| \mathbb{B}_h(s, a) - [\text{Var}_h V_{h+1}^*](s, a) \right| &\leq \left| \mathbb{B}_h(s, a) - [\text{Var}_h \hat{f}'_{h+1}](s, a) \right| \\ &\quad + \left| [\text{Var}_h \hat{f}'_{h+1}](s, a) - [\text{Var}_h V_{h+1}^*](s, a) \right| \\ &\leq \tilde{O} \left( \frac{\sqrt{\log \mathcal{N} \mathcal{N}_b H^3}}{\sqrt{K \kappa}} \right). \end{aligned}$$

632 Thus, for any  $(s, a) \in \mathcal{S} \times \mathcal{A}$ , we have

$$\mathbb{B}_h(s, a) - \tilde{O} \left( \frac{\sqrt{\log \mathcal{N} \mathcal{N}_b H^3}}{\sqrt{K \kappa}} \right) \leq [\text{Var}_h V_{h+1}^*](s, a).$$

633 Finally, using the fact that the function  $\max\{1, \cdot\}$  is increasing and nonexpansive, we finish the proof  
 634 of Lemma B.5, which is

$$[\mathbb{V}_h V_{h+1}^*](s, a) - \tilde{O} \left( \frac{\sqrt{\log \mathcal{N} \mathcal{N}_b H^3}}{\sqrt{K \kappa}} \right) \leq \hat{\sigma}_h^2(s, a) \leq [\mathbb{V}_h V_{h+1}^*](s, a).$$

635

□

### 636 C.5 Proof of Lemma B.6

637 To prove this result, we need the following lemmas.

638 **Lemma C.3.** Based on the dataset  $\mathcal{D} = \{s_h^k, a_h^k, r_h^k\}_{k,h=1}^{K,H}$ , we define the filtration  $\mathcal{H}_h^k =$   
 639  $\sigma(s_1^1, a_1^1, r_1^1, s_2^1, \dots, r_H^1, s_{H+1}^1; x_1^2, a_1^2, r_1^2, s_2^2, \dots, r_H^2, s_{H+1}^2; \dots, s_1^k, a_1^k, r_1^k, s_2^k, \dots, r_h^k, s_{h+1}^k)$ . For  
 640 any fixed function  $f, f' : \mathcal{S} \rightarrow \mathbb{R}$ , we define the following random variables:

$$\begin{aligned} \eta_h^k &:= V_{h+1}^*(s_{h+1}^k) - [\mathbb{P}_h V_{h+1}^*](s_h^k, a_h^k) \\ D_h^s[f, f'] &:= 2 \frac{\eta_h^k}{(\hat{\sigma}_h(z_h^k))^2} (f(z_h^k) - f'(z_h^k)), \end{aligned}$$

641 Suppose the variance function  $\hat{\sigma}_h$  satisfies the inequality in Lemma B.5, where

$$[\mathbb{V}_h V_{h+1}^*](s, a) - \tilde{O} \left( \frac{\sqrt{\log \mathcal{N} \mathcal{N}_b H^3}}{\sqrt{K \kappa}} \right) \leq \hat{\sigma}_h^2(s, a) \leq [\mathbb{V}_h V_{h+1}^*](s, a).$$

642 Then, with probability at least  $1 - \delta/(4H^2 \mathcal{N}^2)$ , the following inequality holds,

$$\sum_{k \in [K]} D_h^k[f, f'] \leq \frac{4}{3} v(\delta) \sqrt{\lambda} + \sqrt{2} v(\delta) + 30 v^2(\delta) + \frac{1}{v(\delta)} \sqrt{\sum_{k \in [K]} \frac{1}{(\hat{\sigma}_h(z_h^k))^2} (f(z_h^k) - f'(z_h^k))^2} + \lambda,$$

643 where  $v(\delta) = \sqrt{2 \log \frac{HN(2 \log(18LT)+2)(\log(18L)+2)}{\delta_h}}$ .

644 *Proof.* We use Lemma D.1, with the following conditions:

$$D_h^k[f, f'] \text{ is adapted to the filtration } \mathcal{H}_h^k \text{ and } \mathbb{E}[D_h^k[f, f'] \mid \mathcal{H}_h^{k-1}] = 0.$$

$$|D_h^k[f, f']| \leq 2|\eta_h^k| \max_z |f(z) - f'(z)| \leq 8LH = M.$$

$$\sum_{k \in [K]} \mathbb{E} \left[ (D_h^k[f, f'])^2 \mid z_h^k \right] = 4 \sum_{k \in [K]} \frac{\mathbb{E}[(\eta_h^k)^2 \mid z_h^k]}{(\hat{\sigma}_h(z_h^k))^4} (f(z_h^k) - f'(z_h^k)).$$

645 On the other hand,

$$\begin{aligned} \sum_{k \in [K]} \mathbb{E} \left[ (D_h^k[f, f'])^2 \mid z_h^k \right] &= 4 \sum_{k \in [K]} \frac{\mathbb{E}[(\eta_h^k)^2 \mid z_h^k]}{(\hat{\sigma}_h(z_h^k))^4} (f(z_h^k) - f'(z_h^k))^2 \\ &\leq 8 \sum_{k \in [K]} \frac{1}{(\hat{\sigma}_h(z_h^k))^2} (f(z_h^k) - f'(z_h^k))^2, \end{aligned}$$

646 where the last inequality holds because of the inequality in Lemma B.5:

$$\begin{aligned} \mathbb{E}[(\eta_h^k)^2 \mid z_h^k] &= [\text{Var}_h V_{h+1}^*](s_h^k, a_h^k) \\ &\leq [\mathbb{V}_h V_{h+1}^*](s_h^k, a_h^k) \\ &\leq (\hat{\sigma}_h(z_h^k))^2 + \tilde{O}\left(\frac{\sqrt{\log \mathcal{N} \mathcal{N}_b H^3}}{\sqrt{K \kappa}}\right) \\ &\leq 2(\hat{\sigma}_h(z_h^k))^2, \end{aligned}$$

647 where we use the requirement that  $K \geq \tilde{\Omega}\left(\frac{\log \mathcal{N} \mathcal{N}_b H^6}{\kappa}\right)$ .

648 Moreover, for any  $k \in [K]$ ,

$$\begin{aligned} |D_h^k[f, f']| &\leq 2 \left| \frac{\eta_h^k}{(\hat{\sigma}_h(z_h^k))^2} \right| |f(z_h^k) - f'(z_h^k)| \\ &\leq 4H \sqrt{D_{\mathcal{F}_h}^2(z_h^k, \mathcal{D}_h, \hat{\sigma}_h) \left( \sum_{k \in [K]} \frac{1}{(\hat{\sigma}_h(z_h^k))^2} (f(z_h^k) - f'(z_h^k))^2 + \lambda \right)} \\ &\leq \tilde{O}\left(\frac{4H^2}{\sqrt{K \kappa}}\right) \sqrt{\sum_{k \in [K]} \frac{1}{(\hat{\sigma}_h(z_h^k))^2} (f(z_h^k) - f'(z_h^k))^2 + \lambda} \\ &\leq \frac{1}{v(\delta)} \sqrt{\sum_{k \in [K]} \frac{1}{(\hat{\sigma}_h(z_h^k))^2} (f(z_h^k) - f'(z_h^k))^2 + \lambda}. \end{aligned}$$

649 The second inequality holds because of the definition of  $D^2$  divergence (Definition 3.2). The  
650 third inequality holds due to Lemma B.2. The last inequality holds because of the choice of  
651  $K \geq \tilde{\Omega}\left(\frac{v^2(\delta)H^4}{\kappa}\right)$ .

652 Then using Lemma D.1 with  $v = 1, m = 1$ , we have

$$\begin{aligned} \sum_{k \in [K]} 2 \frac{\eta_h^k}{(\hat{\sigma}_h(z_h^k))^2} (f(z_h^k) - f'(z_h^k)) &\leq v(\delta) \sqrt{16 \sum_{k \in [K]} \frac{1}{(\hat{\sigma}_h(z_h^k))^2} (f(z_h^k) - f'(z_h^k))^2 + 2 + \frac{2}{3}v^2(\delta)} \\ &\quad + \frac{4}{3}v(\delta) \sqrt{\sum_{k \in [K]} \frac{1}{(\hat{\sigma}_h(z_h^k))^2} (f(z_h^k) - f'(z_h^k))^2 + \lambda} \\ &\leq \frac{4}{3}v(\delta)\sqrt{\lambda} + \sqrt{2}v(\delta) + 30v^2(\delta) \\ &\quad + \frac{\sum_{k \in [K]} \frac{1}{(\hat{\sigma}_h(z_h^k))^2} (f(z_h^k) - f'(z_h^k))^2}{4}. \end{aligned}$$



654 **Lemma C.4.** Based on the dataset  $\mathcal{D} = \{s_h^k, a_h^k, r_h^k\}_{k,h=1}^{K,H}$ , we define the following filtration  $\mathcal{H}_h^k =$   
 655  $\sigma(s_1^1, a_1^1, r_1^1, s_2^1, \dots, r_H^1, s_{H+1}^1; x_1^2, a_1^2, r_1^2, s_2^2, \dots, r_H^2, s_{H+1}^2; \dots, s_1^k, a_1^k, r_1^k, s_2^k, \dots, r_h^k, s_{h+1}^k)$ . For  
 656 any fixed functions  $f, \tilde{f} : \mathcal{S} \rightarrow [0, L]$  and  $f' : \mathcal{S} \rightarrow [0, H]$ , we define the following random  
 657 variables

$$\begin{aligned} \xi_h^k[f'] &:= f'(s_{h+1}^k) - V_{h+1}^*(s_{h+1}^k) - [\mathbb{P}_h(f' - V_{h+1}^*)](s_h^k, a_h^k), \\ \Delta_h^k[f, \tilde{f}, f'] &:= 2 \frac{\xi_h^k[f']}{(\hat{\sigma}_h(z_h^k))^2} (f(z_h^k) - \tilde{f}(z_h^k)), \end{aligned}$$

658 Suppose the variance function  $\hat{\sigma}_h$  satisfies the inequality in Lemma B.5, where

$$[\mathbb{V}_h V_{h+1}^*](s, a) - \tilde{O} \left( \frac{\sqrt{\log \mathcal{N} \mathcal{N}_b H^3}}{\sqrt{K \kappa}} \right) \leq \hat{\sigma}_h^2(s, a) \leq [\mathbb{V}_h V_{h+1}^*](s, a).$$

659 Then, with probability at least  $1 - \delta/(4H^2 \mathcal{N}^3 \mathcal{N}_b)$ , the following inequality holds,

$$\begin{aligned} \sum_{k \in [K]} \Delta_h^k[f, \tilde{f}, f'] &\leq \left( \frac{4}{3} \iota(\delta) \sqrt{\lambda} + \sqrt{2} \iota(\delta) \right) \|f' - V_{h+1}^*\|_\infty^2 + \frac{2}{3} \iota^2(\delta) / \log \mathcal{N}_b \\ &\quad + 30 \iota^2(\delta) \|f' - V_{h+1}^*\|_\infty^2 + \frac{\sum_{k \in [K]} \frac{1}{(\hat{\sigma}_h(z_h^k))^2} (f(z_h^k) - f'(z_h^k))^2}{4}. \end{aligned}$$

660 where  $\iota(\delta) = \sqrt{3 \log \frac{H \mathcal{N} \mathcal{N}_b (2 \log(18LT) + 2) (\log(18L) + 2)}{\delta}}$ .

661 *Proof.*  $\Delta_h^k[f, \tilde{f}, f']$  is adapted to the filtration  $\mathcal{H}_h^k$  and  $\mathbb{E}[\Delta_h^k[f, \tilde{f}, f'] | \mathcal{H}_h^{k-1}] = 0$ . We also have

$$\begin{aligned} \sum_{k \in [K]} \mathbb{E}[(\Delta_h^k[f, \tilde{f}, f'])^2 | z_h^k] &= 4 \sum_{k \in [K]} \frac{\mathbb{E}[(\xi_h^k[f'])^2 | z_h^k]}{(\hat{\sigma}_h(z_h^k))^4} (f(z_h^k) - f'(z_h^k))^2 \\ &\leq 8 \sum_{k \in [K]} \frac{\|f' - V_{h+1}^*\|_\infty^2}{(\hat{\sigma}_h(z_h^k))^2} (f(z_h^k) - f'(z_h^k))^2. \end{aligned}$$

662 Moreover, for any  $k \in [K]$ ,

$$\begin{aligned} |\Delta_h^k[f, \tilde{f}, f']| &\leq 2 \left| \frac{\xi_h^k[f']}{(\hat{\sigma}_h(z_h^k))^2} \right| |f(z_h^k) - f'(z_h^k)| \\ &\leq 4 \|f' - V_{h+1}^*\|_\infty \sqrt{D_{\mathcal{F}_h}^2(z_h^k, \mathcal{D}_h, \hat{\sigma}_h) \left( \sum_{k \in [K]} \frac{1}{(\hat{\sigma}_h(z_h^k))^2} (f(z_h^k) - f'(z_h^k))^2 + \lambda \right)} \\ &\leq \tilde{O} \left( \frac{H}{\sqrt{K \kappa}} \right) \cdot \|f' - V_{h+1}^*\|_\infty \sqrt{\sum_{k \in [K]} \frac{1}{(\hat{\sigma}_h(z_h^k))^2} (f(z_h^k) - f'(z_h^k))^2 + \lambda} \\ &\leq \frac{\|f' - V_{h+1}^*\|_\infty}{\iota(\delta)} \sqrt{\sum_{k \in [K]} \frac{1}{(\hat{\sigma}_h(z_h^k))^2} (f(z_h^k) - f'(z_h^k))^2 + \lambda} \end{aligned}$$

663 The second inequality holds because of the definition of  $D^2$  divergence (Definition 3.2). The  
 664 third inequality holds due to Lemma B.2. The last inequality holds because of the choice of  
 665  $K \geq \tilde{\Omega} \left( \frac{\iota^2(\delta) H^4}{\kappa} \right)$ .

666 Then using Lemma D.1 with  $v = 1$ ,  $m = 1/\log \mathcal{N}_b$ , we have

$$\begin{aligned}
& \sum_{k \in [K]} 2 \frac{\xi_h^k[f']}{(\hat{\sigma}_h(z_h^k))^2} \left( f(z_h^k) - \tilde{f}(z_h^k) \right) \leq \iota(\delta) \sqrt{8 \sum_{k \in [K]} \frac{\|f' - V_{h+1}^*\|_\infty^2}{(\hat{\sigma}_h(z_h^k))^2} (f(z_h^k) - f'(z_h^k))^2} + 2 \\
& \quad + \frac{2}{3} \iota^2(\delta) / \log \mathcal{N}_b + \frac{4}{3} \iota(\delta) \|f' - V_{h+1}^*\|_\infty \sqrt{\sum_{k \in [K]} \frac{1}{(\hat{\sigma}_h(z_h^k))^2} (f(z_h^k) - f'(z_h^k))^2} + \lambda \\
& \leq \left( \frac{4}{3} \iota(\delta) \sqrt{\lambda} + \sqrt{2} \iota(\delta) \right) \|f' - V_{h+1}^*\|_\infty + \frac{2}{3} \iota^2(\delta) / \log \mathcal{N}_b + 30 \iota^2(\delta) \|f' - V_{h+1}^*\|_\infty^2 \\
& \quad + \frac{\sum_{k \in [K]} \frac{1}{(\hat{\sigma}_h(z_h^k))^2} (f(z_h^k) - f'(z_h^k))^2}{4}.
\end{aligned}$$

667

□

668 *Proof of Lemma B.6.* We define the event  $\mathcal{E}_h := \left\{ \sum_{k \in [K]} \frac{1}{(\hat{\sigma}(z_h^k))^2} \left( \bar{f}_h(z_h^k) - \tilde{f}_h(z_h^k) \right)^2 > (\beta_h)^2 \right\}$ .

669 The following inequality will be useful in our proof.

$$\begin{aligned}
& \sum_{k \in [K]} \frac{1}{(\hat{\sigma}(z_h^k))^2} \left( \bar{f}_h(z_h^k) - \tilde{f}_h(z_h^k) \right)^2 \\
& = \sum_{k \in [K]} \frac{1}{(\hat{\sigma}(z_h^k))^2} \left[ \left( r_h^k + \hat{f}_{h+1}(s_{h+1}^k) - \bar{f}_h(z_h^k) \right) + \left( \tilde{f}_h(z_h^k) - r_h^k - \hat{f}_{h+1}(s_{h+1}^k) \right) \right]^2 \\
& = \sum_{k \in [K]} \frac{1}{(\hat{\sigma}(z_h^k))^2} \left( r_h^k + \hat{f}_{h+1}(s_{h+1}^k) - \bar{f}_h(z_h^k) \right)^2 + \sum_{k \in [K]} \frac{1}{(\hat{\sigma}(z_h^k))^2} \left( \tilde{f}_h(z_h^k) - r_h^k - \hat{f}_{h+1}(s_{h+1}^k) \right)^2 \\
& \quad + 2 \sum_{k \in [K]} \frac{1}{(\hat{\sigma}(z_h^k))^2} \left( r_h^k + \hat{f}_{h+1}(s_{h+1}^k) - \bar{f}_h(z_h^k) \right) \left( \tilde{f}_h(z_h^k) - r_h^k - \hat{f}_{h+1}(s_{h+1}^k) \right) \\
& \leq 2 \sum_{k \in [K]} \frac{1}{(\hat{\sigma}(z_h^k))^2} \left( r_h^k + \hat{f}_{h+1}(s_{h+1}^k) - \bar{f}_h(z_h^k) \right)^2 \\
& \quad + 2 \sum_{k \in [K]} \frac{1}{(\hat{\sigma}(z_h^k))^2} \left( r_h^k + \hat{f}_{h+1}(s_{h+1}^k) - \bar{f}_h(z_h^k) \right) \left( \tilde{f}_h(z_h^k) - r_h^k - \hat{f}_{h+1}(s_{h+1}^k) \right) \\
& \leq 2 \sum_{k \in [K]} \frac{1}{(\hat{\sigma}(z_h^k))^2} \left( r_h^k + \hat{f}_{h+1}(s_{h+1}^k) - \bar{f}_h(z_h^k) \right) \left( \tilde{f}_h(z_h^k) - \bar{f}_h(z_h^k) \right). \tag{C.11}
\end{aligned}$$

670 In the third inequality, we use our choice of  $\tilde{f}_h$  in Algorithm 1 Line 10,

$$\tilde{f}_h = \operatorname{argmin}_{f_h \in \mathcal{F}_h} \sum_{k \in [K]} \frac{1}{(\hat{\sigma}(z_h^k))^2} \left( f_h(s_h^k, a_h^k) - r_h^k - \hat{f}_{h+1}(s_{h+1}^k) \right)^2.$$

671 We first use Lemma C.3 at stage  $H$ . Let  $f = \tilde{f}_H \in \mathcal{F}_H$ ,  $f' = \bar{f}_H \in \mathcal{F}_H$ . We define

$$\begin{aligned}
\eta_H^k & := V_{H+1}^*(s_{H+1}^k) - [\mathbb{P}_H V_{H+1}^*](z_H^k) \\
D_H^k[f, f'] & := 2 \frac{\eta_H^k}{(\hat{\sigma}_H(z_H^k))^2} (f(z_H^k) - f'(z_H^k)).
\end{aligned}$$

672 Taking a union bound, we have with probability at least  $1 - \delta/(4H^2)$ , the following inequality holds,

$$\begin{aligned}
\sum_{k \in [K]} 2 \frac{\eta_H^k}{(\hat{\sigma}_H(z_H^k))^2} \left( \tilde{f}(z_H^k) - \bar{f}(z_H^k) \right) & \leq \frac{4}{3} v(\delta) \sqrt{\lambda} + \sqrt{2} v(\delta) + 30 v^2(\delta) \\
& \quad + \frac{\sum_{k \in [K]} \frac{1}{(\hat{\sigma}_H(z_H^k))^2} (\tilde{f}(z_H^k) - \bar{f}(z_H^k))^2}{4}. \tag{C.12}
\end{aligned}$$

673 Then we use Lemma C.4 at stage  $H$ . Let  $f = \tilde{f}_H \in \mathcal{F}_H$ ,  $\tilde{f} = \bar{f}_H \in \mathcal{F}_H$ ,  $f' = \hat{f}_{H+1} = 0$ . We  
674 define:

$$\begin{aligned}\xi_H^k[f'] &:= f'(s_{H+1}^k) - V_{H+1}^*(s_{H+1}^k) - [\mathbb{P}_H(f' - V_{H+1}^*)](z_H^k) \\ \Delta_H^k[f, \tilde{f}, f'] &:= 2 \frac{\xi_H^k[f']}{(\hat{\sigma}_H(z_H^k))^2} \left( f(z_H^k) - \tilde{f}(z_H^k) \right).\end{aligned}$$

675 Therefore, taking a union bound, we have with probability at least  $1 - \delta/(4H^2)$ , we have

$$\begin{aligned}\sum_{k \in [K]} 2 \frac{\xi_H^k[\hat{f}_{H+1}]}{(\hat{\sigma}_H(z_H^k))^2} \left( \tilde{f}_H(z_H^k) - \bar{f}_H(z_H^k) \right) &\leq \left( \frac{4}{3} \iota(\delta) \sqrt{\lambda} + \sqrt{2} \iota(\delta) \right) \|f' - V_{H+1}^*\|_\infty^2 \\ &+ \frac{2}{3} \iota^2(\delta) / \sqrt{\log \mathcal{N}_b} + 30 \iota^2(\delta) \|\hat{f}_{H+1} - V_{H+1}^*\|_\infty^2 + \frac{\sum_{k \in [K]} \frac{1}{(\hat{\sigma}_H(z_H^k))^2} \left( \tilde{f}_H(z_H^k) - \bar{f}_H(z_H^k) \right)^2}{4}.\end{aligned}\tag{C.13}$$

676 Combining (C.12) and (C.13), with probability at least  $1 - \delta/(2H^2)$ , we have

$$\begin{aligned}2 \sum_{k \in [K]} \frac{1}{(\hat{\sigma}_H(z_H^k))^2} \left( r_H^k + \hat{f}_{H+1}(s_{H+1}^k) - \bar{f}_H(z_H^k) \right) \left( \tilde{f}_H(z_H^k) - \bar{f}_H(z_H^k) \right) \\ = 2 \sum_{k \in [K]} \frac{1}{(\hat{\sigma}_H(z_H^k))^2} \left( r_H^k + \hat{f}_{H+1}(s_{H+1}^k) - \mathcal{T}_H \hat{f}_{H+1}(z_H^k) \right) \left( \tilde{f}_H(z_H^k) - \bar{f}_H(z_H^k) \right) \\ + 2 \sum_{k \in [K]} \frac{1}{(\hat{\sigma}_H(z_H^k))^2} \left( \mathcal{T}_H \hat{f}_{H+1}(z_H^k) - \bar{f}_H(z_H^k) \right) \left( \tilde{f}_H(z_H^k) - \bar{f}_H(z_H^k) \right) \\ \leq 2 \sum_{k \in [K]} \frac{1}{(\hat{\sigma}_H(z_H^k))^2} \left( r_H^k + \hat{f}_{H+1}(s_{H+1}^k) - \mathcal{T}_H \hat{f}_{H+1}(z_H^k) \right) \left( \tilde{f}_H(z_H^k) - \bar{f}_H(z_H^k) \right) + 4KL\epsilon \\ \leq \frac{4}{3} v(\delta) \sqrt{\lambda} + \sqrt{2} v(\delta) + 30 v^2(\delta) + \left( \frac{4}{3} \iota(\delta) \sqrt{\lambda} + \sqrt{2} \iota(\delta) \right) \|f' - V_{H+1}^*\|_\infty^2 + \frac{2}{3} \iota^2(\delta) / \log \mathcal{N}_b \\ + 30 \iota^2(\delta) \|\hat{f}_{H+1} - V_{H+1}^*\|_\infty^2 + 8KL\epsilon + \frac{\sum_{k \in [K]} \frac{1}{(\hat{\sigma}_H(z_H^k))^2} \left( \bar{f}_H(z_H^k) - \tilde{f}_H(z_H^k) \right)^2}{2} \\ \leq \frac{(\beta_H)^2}{2} + \frac{\sum_{k \in [K]} \frac{1}{(\hat{\sigma}_H(z_H^k))^2} \left( \bar{f}_H(z_H^k) - \tilde{f}_H(z_H^k) \right)^2}{2}.\end{aligned}$$

677 In the last inequality, we use that fact  $\hat{f}_{H+1} = V_{H+1}^* = 0$  and our choice of  $\beta_H$ .

$$\begin{aligned}\beta_H &= \sqrt{2 \left( \frac{4}{3} v(\delta) \sqrt{\lambda} + \sqrt{2} v(\delta) + 30 v^2(\delta) + \frac{2}{3} \iota^2(\delta) / \log \mathcal{N}_b + 8KL\epsilon \right)} \\ &= \tilde{O}(\sqrt{\log \mathcal{N}}).\end{aligned}$$

678 But conditioned on the event  $\mathcal{E}_H$ , we have

$$\begin{aligned}\sum_{k \in [K]} \frac{1}{(\hat{\sigma}_H(z_H^k))^2} \left( r_H^k + \hat{f}_{H+1}(s_{H+1}^k) - \bar{f}_H(z_H^k) \right) \left( \tilde{f}_H(z_H^k) - \bar{f}_H(z_H^k) \right) \\ \geq \sum_{k \in [K]} \frac{1}{(\hat{\sigma}_H(z_H^k))^2} \left( \bar{f}_H(z_H^k) - \tilde{f}_H(z_H^k) \right)^2 \\ > \frac{(\beta_H)^2}{2} + \frac{\sum_{k \in [K]} \frac{1}{(\hat{\sigma}_H(z_H^k))^2} \left( \bar{f}_H(z_H^k) - \tilde{f}_H(z_H^k) \right)^2}{2}.\end{aligned}$$

679 Here we use (C.11). We finally prove that  $\mathbb{P}[\mathcal{E}_H] \geq 1 - \delta/2H^2$ .

680 Suppose the event  $\mathcal{E}_H$  holds, we can prove the following result.

$$\begin{aligned}
Q_H^*(s, a) &= \mathcal{T}_H V_{H+1}^*(s, a) \\
&= \mathcal{T}_H \widehat{f}_{H+1}(s, a) \\
&\geq \widetilde{f}_H(s, a) - \left| \mathcal{T}_H \widehat{f}_{H+1}(s, a) - \widetilde{f}_H(s, a) \right| \\
&\geq \widetilde{f}_H(s, a) - \left( \epsilon + |\bar{f}_H(s, a) - \widetilde{f}_H(s, a)| \right) \\
&\geq \widetilde{f}_H(s, a) - b_H(s, a) - \epsilon \\
&= \widehat{f}_H(s, a).
\end{aligned}$$

681 Here we use the definition of  $\widehat{f}_H$  in Algorithm 1 Line 12. Lemma B.6 shows

$$\sum_{k \in [K]} \frac{1}{(\widehat{\sigma}_h(z_h^k))^2} \left( \bar{f}_h(z_h^k) - \widetilde{f}_h(z_h^k) \right)^2 \leq (\beta_h)^2.$$

682 Then the fifth inequality follows the bonus oracle assumption (Definition 4.1). Therefore,  $V_H^*(s) \geq$   
683  $\widehat{f}_H(s)$  for all  $s \in \mathcal{S}$ .

684 We also have

$$\begin{aligned}
V_H^*(s) - \widehat{f}_H(s) &= \langle Q_H^*(s, \cdot) - \widehat{f}_H(s, \cdot), \pi^*(\cdot|s) \rangle_{\mathcal{A}} + \langle \widehat{f}_H(s, \cdot), \pi_H^*(\cdot|s) - \widehat{\pi}_H(\cdot|s) \rangle_{\mathcal{A}} \\
&\leq \langle Q_H^*(s, \cdot) - \widehat{f}_H(s, \cdot), \pi^*(\cdot|s) \rangle_{\mathcal{A}} \\
&= \langle \mathcal{T}_H V_H^*(s, \cdot) - \widehat{f}_H(s, \cdot) + b_H(s, a), \pi^*(\cdot|s) \rangle_{\mathcal{A}} \\
&= \langle \mathcal{T}_H \widehat{f}_{H+1}(s, \cdot) - \widetilde{f}_H(s, \cdot) + b_H(s, a), \pi^*(\cdot|s) \rangle_{\mathcal{A}} \\
&\quad + \langle \mathcal{T}_H V_{H+1}^*(s, \cdot) - \mathcal{T}_H \widehat{f}_{H+1}(s, \cdot), \pi_H^*(\cdot|s) \rangle_{\mathcal{A}} \\
&\leq 2 \langle b_H(s, \cdot), \pi_H^*(\cdot|s) \rangle_{\mathcal{A}} + \epsilon \\
&\leq \widetilde{O} \left( \frac{\sqrt{\log \mathcal{N} H^2}}{\sqrt{K \kappa}} \right).
\end{aligned}$$

685 Here the second inequality holds because of the definition of  $\widehat{\pi}$ . The fifth inequality holds due to we  
686 the Bellman completeness assumption (Assumption 3.1):

$$\left| \bar{f}_H(z) - \mathcal{T}_H \widehat{f}_{H+1}(z) \right| \leq \epsilon, \forall z \in \mathcal{S} \times \mathcal{A}.$$

687 We also use Definition 4.1 and Lemma B.2.

688 Then we do the induction step. Let  $R_h = \widetilde{O} \left( \frac{\sqrt{\log \mathcal{N} H^2}}{\sqrt{K \kappa}} \right) \cdot (H - h + 1)$ ,  $\delta_h = h\delta/(4H^2)$ . We define  
689 another event  $\mathcal{E}_h^{\text{ind}}$  for induction.

$$\mathcal{E}_h^{\text{ind}} = \{0 \leq V_h^*(s) - \widehat{f}_h(s) \leq R_h, \forall s \in \mathcal{S}\}.$$

690 The above analysis shows that  $\mathcal{E}_H \subseteq \mathcal{E}_H^{\text{ind}}$  and  $\mathbb{P}[\mathcal{E}_H] \geq 1 - 2\delta_H$ . Moreover,  $\mathbb{P}[\mathcal{E}_H^{\text{ind}}] \geq 1 - 2\delta_H$

691 We conduct the induction in the following way. At stage  $h$ , if  $\mathbb{P}[\mathcal{E}_{h+1}] \geq 1 - 2\delta_{h+1}$  and  $\mathbb{P}[\mathcal{E}_{h+1}^{\text{ind}}] \geq$   
692  $1 - 2\delta_{h+1}$ , we prove that  $\mathbb{P}[\mathcal{E}_h] \geq 1 - 2\delta_h$  and  $\mathbb{P}[\mathcal{E}_h^{\text{ind}}] \geq 1 - 2\delta_h$ .

693 Suppose at stage  $h$ ,  $\mathbb{P}[\mathcal{E}_{h+1}] \geq 1 - 2\delta_{h+1}$  and  $\mathbb{P}[\mathcal{E}_{h+1}^{\text{ind}}] \geq 1 - 2\delta_{h+1}$ . We first use Lemma C.3. Let  
694  $f = \widetilde{f}_h \in \mathcal{F}_h$ ,  $f' = \bar{f}_h \in \mathcal{F}_h$ . We define

$$\begin{aligned}
\eta_h^k &:= V_{h+1}^*(s_{h+1}^k) - [\mathbb{P}_h V_{h+1}^*](z_h^k) \\
D_h^k[f, f'] &:= 2 \frac{\eta_h^k}{(\widehat{\sigma}_h(z_h^k))^2} (f(z_h^k) - f'(z_h^k)).
\end{aligned}$$

695 After taking a union bound, we have with probability at least  $1 - \delta/(4H^2)$ , the following inequality  
696 holds,

$$\begin{aligned} \sum_{k \in [K]} 2 \frac{\eta_h^k}{(\widehat{\sigma}_h(z_h^k))^2} \left( \widetilde{f}(z_h^k) - \bar{f}(z_h^k) \right) &\leq \frac{4}{3} v(\delta) \sqrt{\lambda} + \sqrt{2} v(\delta) + 30v^2(\delta) \\ &+ \frac{\sum_{k \in [K]} \frac{1}{(\widehat{\sigma}_h(z_h^k))^2} \left( \widetilde{f}(z_h^k) - \bar{f}(z_h^k) \right)^2}{4}. \end{aligned} \quad (\text{C.14})$$

697 Next, we use Lemma C.4 at stage  $h$ . Let  $f = \widetilde{f}_h \in \mathcal{F}_h$ ,  $\widetilde{f} = \bar{f}_h \in \mathcal{F}_h$ ,  $f' = \widehat{f}_{h+1} = \{\widetilde{b}\}_{[0, H-h+1]}$ ,  
698 where  $\widetilde{b} = \widetilde{f}_h - b_h \in \mathcal{F}_h - \mathcal{W}$ . We define:

$$\begin{aligned} \xi_h^k[f'] &:= f'(s_{h+1}^k) - V_{h+1}^*(s_{h+1}^k) - [\mathbb{P}_h(f' - V_{h+1}^*)](z_h^k) \\ \Delta_h^k[f, \widetilde{f}, f'] &:= 2 \frac{\xi_h^k[f']}{(\widehat{\sigma}_h(z_h^k))^2} \left( f(z_h^k) - \widetilde{f}(z_h^k) \right), \end{aligned}$$

699 After taking a union bound, we have with probability at least  $1 - \delta/(4H^2)$ , we have

$$\begin{aligned} \sum_{k \in [K]} 2 \frac{\xi_h^k[\widehat{f}_{h+1}]}{(\widehat{\sigma}_h(z_h^k))^2} \left( \widetilde{f}_h(z_h^k) - \bar{f}_h(z_h^k) \right) &\leq \left( \frac{4}{3} \iota(\delta) \sqrt{\lambda} + \sqrt{2} \iota(\delta) \right) \|f' - V_{h+1}^*\|_\infty^2 \\ &+ \frac{2}{3} \iota^2(\delta) / \sqrt{\log \mathcal{N}_b} + 30\iota^2(\delta) \|\widehat{f}_{h+1} - V_{h+1}^*\|_\infty^2 + \frac{\sum_{k \in [K]} \frac{1}{(\widehat{\sigma}_h(z_h^k))^2} (\widetilde{f}_h(z_h^k) - \bar{f}_h(z_h^k))^2}{4}. \end{aligned} \quad (\text{C.15})$$

700 Let  $U_h$  be the event that (C.14) and (C.15) holds simultaneously. On the event  $U_h \cap \mathcal{E}_{h+1}^{\text{ind}}$ , which  
701 satisfies  $\mathbb{P}[U_h \cap \mathcal{E}_{h+1}^{\text{ind}}] \geq 1 - 2\delta_{h+1} - 2\delta/H^2 = 1 - 2\delta_h$ , we have

$$\begin{aligned} &2 \sum_{k \in [K]} \frac{1}{(\widehat{\sigma}_h(z_h^k))^2} \left( r_h^k + \widehat{f}_{h+1}(s_{h+1}^k) - \bar{f}_h(z_h^k) \right) \left( \widetilde{f}_h(z_h^k) - \bar{f}_h(z_h^k) \right) \\ &= 2 \sum_{k \in [K]} \frac{1}{(\widehat{\sigma}_h(z_h^k))^2} \left( r_h^k + \widehat{f}_{h+1}(s_{h+1}^k) - \mathcal{T}_h \widehat{f}_{h+1}(z_h^k) \right) \left( \widetilde{f}_h(z_h^k) - \bar{f}_h(z_h^k) \right) \\ &\quad + 2 \sum_{k \in [K]} \frac{1}{(\widehat{\sigma}_h(z_h^k))^2} \left( \mathcal{T}_h \widehat{f}_{h+1}(z_h^k) - \bar{f}_h(z_h^k) \right) \left( \widetilde{f}_h(z_h^k) - \bar{f}_h(z_h^k) \right) \\ &\leq 2 \sum_{k \in [K]} \frac{1}{(\widehat{\sigma}_h(z_h^k))^2} \left( r_h^k + \widehat{f}_{h+1}(s_{h+1}^k) - \mathcal{T}_h \widehat{f}_{h+1}(z_h^k) \right) \left( \widetilde{f}_h(z_h^k) - \bar{f}_h(z_h^k) \right) + 4KL\epsilon \\ &\leq \frac{4}{3} v(\delta) \sqrt{\lambda} + \sqrt{2} v(\delta) + 30v^2(\delta) + \left( \frac{4}{3} \iota(\delta) \sqrt{\lambda} + \sqrt{2} \iota(\delta) \right) \|\widehat{f}_{h+1} - V_{h+1}^*\|_\infty^2 \\ &\quad + \frac{2}{3} \iota^2(\delta) / \log \mathcal{N}_b + 30\iota^2(\delta) \|\widehat{f}_{h+1} - V_{h+1}^*\|_\infty^2 + 8KL\epsilon + \frac{\sum_{k \in [K]} \frac{1}{(\widehat{\sigma}_h(z_h^k))^2} \left( \bar{f}_h(z_h^k) - \widetilde{f}_h(z_h^k) \right)^2}{2} \\ &\leq \frac{(\beta_h)^2}{2} + \frac{\sum_{k \in [K]} \frac{1}{(\widehat{\sigma}_h(z_h^k))^2} \left( \bar{f}_h(z_h^k) - \widetilde{f}_h(z_h^k) \right)^2}{2}, \end{aligned}$$

702 where the third inequality holds because of (C.14) and (C.15). The last inequality holds because  
703 on the event of  $\mathcal{E}_{h+1}^{\text{ind}}$ ,  $0 \leq V_{h+1}^* - \widehat{f}_{h+1} \leq R_{h+1} = \widetilde{O}\left(\frac{H^2}{\sqrt{K\kappa}}\right) \cdot (H - h)$  and the choice of  
704  $K \geq \widetilde{\Omega}\left(\frac{\iota(\delta)^2 H^6}{\kappa}\right)$ . We also use our choice of  $\beta_h = \widetilde{O}(\sqrt{\log \mathcal{N}})$ .

705 However, on the event of  $\mathcal{E}_h^c$ , we have

$$\begin{aligned} & 2 \sum_{k \in [K]} \frac{1}{(\widehat{\sigma}(z_h^k))^2} \left( r_h^k + \widehat{f}_{h+1}(s_{h+1}^k) - \bar{f}_h(z_h^k) \right) \left( \widetilde{f}_h(z_h^k) - \bar{f}_h(z_h^k) \right) \\ & \geq \sum_{k \in [K]} \frac{1}{(\widehat{\sigma}(z_h^k))^2} \left( \bar{f}_h(z_h^k) - \widetilde{f}_h(z_h^k) \right)^2 \\ & > \frac{(\beta_h)^2}{2} + \frac{\sum_{k \in [K]} \frac{1}{(\widehat{\sigma}(z_h^k))^2} \left( \bar{f}_h(z_h^k) - \widetilde{f}_h(z_h^k) \right)^2}{2}. \end{aligned}$$

706 We conclude that  $U_h \cap \mathcal{E}_{h+1}^{\text{ind}} \subseteq \mathcal{E}_h$ , thus  $\mathbb{P}[\mathcal{E}_h] \geq 1 - 2\delta_h$ .

707 Next we prove  $\mathbb{P}[\mathcal{E}_h^{\text{ind}}] \geq 1 - 2\delta_h$ . Suppose the event  $U_h \cap \mathcal{E}_{h+1}^{\text{ind}}$  holds, the above conclusion shows  
708 that

$$\sum_{k \in [K]} \frac{1}{(\widehat{\sigma}_h(z_h^k))^2} \left( \bar{f}_h(z_h^k) - \widetilde{f}_h(z_h^k) \right)^2 > (\beta_h)^2.$$

709 We can prove the following result.

$$\begin{aligned} Q_h^*(s, a) &= \mathcal{T}_h V_{h+1}^*(s, a) \\ &\geq \mathcal{T}_h \widehat{f}_{h+1}(s, a) \\ &\geq \widetilde{f}_h(s, a) - |\mathcal{T}_h \widehat{f}_{h+1}(s, a) - \widetilde{f}_h(s, a)| \\ &\geq \widetilde{f}_h(s, a) - (\epsilon + |\bar{f}_h(s, a) - \widetilde{f}_h(s, a)|) \\ &\geq \widetilde{f}_h(s, a) - b_h(s, a) \\ &= \widehat{f}_h(s, a), \end{aligned}$$

710 where the second inequality holds because the event  $\mathcal{E}_h^{\text{ind}}$  holds. The fourth inequality holds because  
711 of the Bellman completeness assumption (Assumption 3.1). From Lemma B.6, we have

$$\sum_{k \in [K]} \frac{1}{(\widehat{\sigma}_h(z_h^k))^2} \left( \bar{f}_h(z_h^k) - \widetilde{f}_h(z_h^k) \right)^2 \leq (\beta_h)^2.$$

712 Then the fifth inequality holds due to the bonus oracle (Definition 4.1). Therefore,  $V_h^*(s) \geq \widehat{f}_h(s)$   
713 for all  $s \in \mathcal{S}$ .

714 We also have

$$\begin{aligned} V_h^*(s) - \widehat{f}_h(s) &= \langle Q_h^*(s, \cdot) - \widehat{f}_h(s, \cdot), \pi^*(\cdot|s) \rangle_{\mathcal{A}} + \langle \widehat{f}_h(s, \cdot), \pi_h^*(\cdot|s) - \widehat{\pi}_h(\cdot|s) \rangle_{\mathcal{A}} \\ &\leq \langle Q_h^*(s, \cdot) - \widehat{f}_h(s, \cdot), \pi^*(\cdot|s) \rangle_{\mathcal{A}} \\ &= \langle \mathcal{T}_h V_{h+1}^*(s, \cdot) - \widetilde{f}_h(s, \cdot) + b_h(s, a), \pi^*(\cdot|s) \rangle_{\mathcal{A}} \\ &= \langle \mathcal{T}_h \widehat{f}_{h+1}(s, \cdot) - \widetilde{f}_h(s, \cdot) + b_h(s, a), \pi^*(\cdot|s) \rangle_{\mathcal{A}} \\ &\quad + \langle \mathcal{T}_h V_{h+1}^*(s, \cdot) - \mathcal{T}_h \widehat{f}_{h+1}(s, \cdot), \pi_h^*(\cdot|s) \rangle_{\mathcal{A}} \\ &\leq 2 \langle b_h(s, \cdot), \pi_h^*(\cdot, s) \rangle_{\mathcal{A}} + \epsilon + R_{h+1} \\ &\leq \widetilde{O} \left( \frac{\sqrt{\log \mathcal{N} H^2}}{\sqrt{K \kappa}} \right) \cdot (H - h + 1) = R_h. \end{aligned}$$

715 The first equality holds because of our choice of the policy  $\widehat{\pi}_h$ . In the fifth inequality, we use  
716 Assumption 3.1

$$\left\| \bar{f}_h(\cdot, \cdot) - \mathcal{T}_h \widehat{f}_{h+1}(\cdot, \cdot) \right\|_{\infty} \leq \epsilon,$$

717 and the oracle of bonus function (Definition 4.1) with

$$\sum_{k \in [K]} \frac{1}{(\widehat{\sigma}_h(z_h^k))^2} \left( \bar{f}_h(z_h^k) - \widetilde{f}_H(z_h^k) \right)^2 \leq (\beta_h)^2,$$

718 which holds by Lemma B.6. Therefore, we have  $U_h \cap \mathcal{E}_{h+1}^{\text{ind}} \subseteq \mathcal{E}_h^{\text{ind}}$  and  $\mathbb{P}[\mathcal{E}_h^{\text{ind}}] \geq 1 - 2\delta_h$ . We also  
 719 use the induction assumption. Thus we complete the proof of induction.

720 Finally, taking the union bound of all the  $\mathcal{E}_h$ , we get the result that with probability at least  $1 - \delta/2$ ,  
 721 the event  $\cup_{h=1}^H \mathcal{E}_h$  holds, i.e for any  $h \in [H]$  simultaneously, we have

$$\sum_{k \in [K]} \frac{1}{(\hat{\sigma}_h(z_h^k))^2} \left( \bar{f}_h(z_h^k) - \tilde{f}_h(z_h^k) \right)^2 \leq (\beta_h)^2.$$

722 Therefore, we complete the proof of Lemma B.6. □

## 723 D Auxiliary lemmas

724 **Lemma D.1** (Agarwal et al. 2022). Let  $M > 0$ ,  $V > v > 0$  be constants, and  
 725  $\{x_i\}_{i \in [t]}$  be a stochastic process adapted to a filtration  $\{\mathcal{H}_i\}_{i \in [t]}$ . Suppose  $\mathbb{E}[x_i | \mathcal{H}_{i-1}] = 0$ ,  
 726  $|x_i| \leq M$  and  $\sum_{i \in [t]} \mathbb{E}[x_i^2 | \mathcal{H}_{i-1}] \leq V^2$  almost surely. Then for any  $\delta, \epsilon > 0$ , let  $\iota =$   
 727  $\sqrt{\log \frac{(2 \log(V/v)+2) \cdot (\log(M/m)+2)}{\delta}}$ , we have

$$\mathbb{P} \left( \sum_{i \in [t]} x_i > \iota \sqrt{2 \left( 2 \sum_{i \in [t]} \mathbb{E}[x_i^2 | \mathcal{H}_{i-1}] + v^2 \right)} + \frac{2}{3} \iota^2 \left( 2 \max_{i \in [t]} |x_i| + m \right) \right) \leq \delta.$$

728 **Lemma D.2** (Regret Decomposition Property, Jin et al. 2021b). Suppose the following inequality  
 729 holds,

$$|\mathcal{T}_h \hat{f}_{h+1}(z) - \tilde{f}_h(z)| \leq b_h(z), \forall z = (s, a) \in \mathcal{S} \times \mathcal{A}, \forall h \in [H],$$

730 the regret of Algorithm 1 can be bounded as

$$V_1^*(s) - V_1^{\hat{\pi}}(s) \leq 2 \sum_{h=1}^H \mathbb{E}_{\pi^*} [b_h(s_h, a_h) | s_1 = s].$$

731 Here  $\mathbb{E}_{\pi^*}$  is with respect to the trajectory induced by  $\pi^*$  in the underlying MDP.

732 **Lemma D.3** (Azuma-Hoeffding inequality, Cesa-Bianchi and Lugosi 2006). Let  $\{x_i\}_{i=1}^n$  be a  
 733 martingale difference sequence with respect to a filtration  $\{\mathcal{G}_i\}$  satisfying  $|x_i| \leq M$  for some  
 734 constant  $M$ ,  $x_i$  is  $\mathcal{G}_{i+1}$ -measurable,  $\mathbb{E}[x_i | \mathcal{G}_i] = 0$ . Then for any  $0 < \delta < 1$ , with probability at least  
 735  $1 - \delta$ , we have

$$\sum_{i=1}^n x_i \leq M \sqrt{2n \log(1/\delta)}.$$