Strategic Decision-Making in the Presence of Information Asymmetry: Provably Efficient RL with Algorithmic Instruments

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Abstract

We study offline reinforcement learning under a novel model called strategic MDP, which characterizes the strategic interactions between a principal and a sequence of myopic agents with private types. Due to the bilevel structure and private types, strategic MDP involves information asymmetry between the principal and the agents. We focus on the offline RL problem where the goal is to learn the optimal policy of the principal concerning a target population of agents, based on a pre-collected dataset that consists of historical interactions. The unobserved private types confound such a dataset as they affect both the rewards and observations received by the principal. We propose a novel algorithm, *pessimistic policy learning with algorithmic instruments (PLAN)*, which leverages the ideas of instrumental variable regression and the pessimism principle to learn a near-optimal principal’s policy in the context of general function approximation. Our algorithm is based on the critical observation that the principal’s actions serve as valid instrumental variables. In particular, under a partial coverage assumption on the offline dataset, we prove that PLAN outputs a $1/\sqrt{K}$-optimal policy with $K$ being the number of collected trajectories. We further apply our framework to some special cases of strategic MDP, including strategic regression (Harris et al., 2021b), strategic bandit, and noncompliance in recommendation systems (Robins, 1998).

1 Introduction

In multi-agent decision-making systems (Ferber and Weiss, 1999), at each step, each agent chooses an action based on its local information gathered so far, where the local information contains both the public information that is shared by every agent, and the private information that is only known to itself. The actions taken by all the agents then determine the state of the underlying environment and the observations received by each agent at the next step. The goal of each agent is to maximize its own expected cumulative rewards via taking a sequence of actions that leverage her private information, in the presence of other agents.

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Multi-agent systems with private information find wide applications in economics (Laffont and Martimort, 2009), social science (Sabater and Sierra, 2005), robotics (Farinelli et al., 2004; Yan et al., 2013), and cognitive science (Sun et al., 2006). The private information of the agent often include hidden states that represent the agent’s own type information or part of information about the environment that other agents are ignorant of, and hidden actions taken or local observation received by the agent that are not observed by others.

In this work, we aim to study reinforcement learning in the presence of private information. Motivated by the principal-agent framework in contract theory (Bolton and Dewatripont, 2004; Laffont and Martimort, 2009), we propose a stylized bilevel multi-agent decision-making model where a principal interacts with a sequence of myopic agents with private information. Such a model specifies an information asymmetry — the agents have private information unknown to the principal, while the principal’s policy is known to the agents. In specific, such a model can be viewed as a bilevel Stackelberg game (Ba¸sar and Olsder, 1998) where the principal first announces her policy, and the agents then choose their best-response actions — actions that maximize their immediate rewards — based on their private information. Here the private information includes both the private types and actions of the agent, which are unknown to the principal. The type of agent reflects its personal preference and is part of the agent’s reward function. In contrast, the principal aims to maximize its expected cumulative rewards, assuming the agents always adopt the best response policies. Such a model is called the strategic Markov decision process (MDP), as it models the interaction between the principal and a sequence of agents that strategically respond to the principal.

In strategic MDP, the private types of agents influence the game structure in two ways. First, the actions taken by the agents implicitly depend on the private types. While the principal does not observe these actions, the agents generate available observations which affect the principal’s immediate rewards. Second, the state transitions depend on both the actions of the principal and the private types of agents. As a result, the optimal policy of the principal also implicitly depends on the private types of the agents. In other words, the principal should adopt different policies targeting at different types of agents.

Strategic MDP is motivated by the notion of performative prediction (Perdomo et al., 2020), which refers to the setting where the prediction given by the classifier causes a distributional change in the targeted variables. Such a performative distributional shift is ubiquitous in strategic machine learning problems where the agents strategically modify the data distribution in response to the announced machine learning model, in order to improve their outcomes. As a concrete example, consider the scenario of the college application, the requirements on the scores of the standardized tests (e.g., SAT) incentivize the applicants to make additional efforts (e.g., taking multiple tests) to improve their scores (Goodman et al., 2020). Strategic MDP captures such a strategic/performative setting by assuming the agents strategically choose best-response actions to maximize their rewards, while these actions, in turn, change the distribution of the observations. More importantly, strategic MDP brings strategic interactions into the context of sequential decision-making by introducing Markovian state transitions, which helps model more complex strategic behaviors involving dynamic structures.
In this paper, we study the offline RL problem (Levine et al., 2020) in strategic MDP, where the goal is to learn the optimal policy of the principal based on an offline dataset collected a priori. Specifically, since the principal’s optimal policy depends on the agents’ private types, we consider learning the optimal policy for a targeted population of agents, where a population refers to a distribution over the private type. Moreover, the offline dataset is generated by interacting with an arbitrary population of agents with a possibly suboptimal behavior policy and only consists of the variables available to the principal. In other words, the agents’ private types and actions are not recorded in the offline dataset.

Compared with the standard MDP model, offline RL in strategic MDP involves the confounding issue brought by the private types, which is absent in MDP, and a more involved challenge of distributional shift. Specifically, the private actions taken by the agents affect the state transitions and the principal’s observations and rewards stored in the dataset. Moreover, these private actions are determined implicitly by the private types of the agents from the best-response policies. As a result, the private types are unobserved confounders and thus directly applying standard offline RL methods to learn the transition model and reward functions would incur a considerable bias. Furthermore, the offline dataset involves two kinds of distributional shifts. First, the dataset is collected by interacting with some population of agents while we are interested in the optimal policy concerning the target population. Second, in data generation, the principal’s policy is fixed to some behavior policy which can be very different from our desired optimal policy. As a result, any successful learning algorithm needs to handle the challenges due to the offline dataset’s unobserved confounder and distributional shift.

To this end, we propose a novel algorithm, pessimistic policy learning with algorithmic instruments (PLAN), which resolves the above two challenges by leveraging the ideas of instrumental variable regression and the pessimism principle (Buckman et al., 2020; Jin et al., 2021b). Specifically, although the private types are absent in the offline dataset, we prove that the actions taken by the principal serve as instrumental variables that help identify their causal effect. That is, both the reward function and transition kernel can be written as the solutions to some conditional moment equations given the states and actions of the principal. Intuitively, the principal’s actions directly affect how the agents take the best-response actions in each step. Moreover, they indirectly affect the observations presented to the principals via the agents’ actions. Thus, the principal’s actions serve as instrumental variables. Such a fundamental property enables us to construct a loss function based on the offline data via minimax estimation, where the global minimizer of the population loss corresponds to the true model. Meanwhile, the construction of the minimax loss function can readily incorporate general function approximators. Furthermore, to handle the distributional shift, we follow the pessimism principle by (i) constructing a high-confidence region containing the true model based on the level sets of loss functions and (ii) returning the optimal policy of the most pessimistic candidate model in the confidence region. Under proper assumptions, we prove that PLAN outputs a $1/\sqrt{K}$-optimal policy when the offline dataset satisfies a mild partial coverage assumption, where $K$ is the number of trajectories in the offline dataset. We also instantiate our results to specific function classes, including kernel and neural network functions. Besides, as concrete examples, we apply the results for strategic MDP to particular cases, including strategic
regression (Harris et al., 2021b), strategic bandit, and noncompliance in recommendation systems (Robins, 1998).

**Main Contributions**

Our contribution is several-fold. First, we propose a general framework named strategic MDP for modeling the interaction between a principal and a sequence of myopic agents with private information. Such a model captures many strategic decision-making problems as special cases, such as strategic regression, strategic bandit, Stackelberg game, and etc. Second, for offline RL in strategic MDP, we propose a novel algorithm, PLAN, which leverages instrumental variable regression to handle the confounding issue caused by the agents’ private information and adopts the idea of pessimism to handle the distributional shift of the offline data. Specifically, the instruments are the state variables and the actions of the principal sampled from the behavior policy during data collection. Third, under mild assumptions on the offline dataset and the function classes employed in statistical estimation, we prove that PLAN outputs a near optimal policy with statistical accuracy. Meanwhile, we also apply the theoretical results to special cases of strategic MDP, including strategic regression and strategic bandits, to showcase the efficacy of PLAN.

**1.1 Related Work**

**Pessimism in offline RL.** There exists a large body of literature on offline RL. Assuming the offline dataset has sufficient coverage over all target policies, many existing works establish the statistical rates of convergence for various offline RL methods with function approximation. See, e.g., (Antos et al., 2007; Munos and Szepesvári, 2008; Antos et al., 2008; Farahmand et al., 2010, 2016; Busoniu et al., 2017; Fan et al., 2019; Chen and Jiang, 2019; Duan et al., 2021) and the references therein. Our work mainly builds upon the recent line of works that develop offline RL algorithms based on the pessimism principle. Leveraging pessimism, these works prove that various RL algorithms are provably efficient when the offline datasets merely satisfy a partial coverage condition (Liu et al., 2020; Kidambi et al., 2020; Yu et al., 2020; Buckman et al., 2020; Xie et al., 2021; Jin et al., 2021b; Uehara and Sun, 2021; Shi et al., 2022; Rashidinejad et al., 2021; Zanette et al., 2021; Li et al., 2022; Yan et al., 2022a; Lu et al., 2022). Among these contributions, our work is particularly related to Lu et al. (2022), which studies offline RL in partially observable MDPs, where the offline dataset is collected by a behavior policy that has access to the latent states. In Lu et al. (2022), the observations and actions in the dataset are confounded by the latent states. To handle the confounding issue, Lu et al. (2022) assume the existence of confounding bridge functions and leverage proximal causal inference (Lipsitch et al., 2010; Tchetgen et al., 2020) to construct pessimistic estimates of the bridge functions. In contrast, strategic MDP is a different problem, and our PLAN algorithm is based on instrumental variable estimation. Besides, we consider general function approximators with kernel and neural networks as special cases. Whereas Lu et al. (2022) only focuses on the linear setting.

**RL with confounders.** Our work is also related to the works that propose RL methods in the presence of confounded data. In particular, a line of research studies RL methods for dynamic treat-
ment regimes (DTR) (Chakraborty and Murphy, 2014) under the sequential ignorability condition (Murphy et al., 2001; Robins, 2004; Schulte et al., 2014) ensures that all confounders are measured. When there exist unmeasured confounders, Chen and Zhang (2021) utilize a time-varying instrumental variable to establish a novel estimation framework for DTR. Compared with Chen and Zhang (2021), although our work also uses instrumental variables to address the confounding issue, they study a different model and thus are not directly comparable. In addition, there is also a line of research on learning the optimal policies of various confounded MDP models (Zhang and Bareinboim, 2016; Liao et al., 2021; Lu et al., 2021; Wang et al., 2021). Among these works, our work is most relevant to the work of Liao et al. (2021), which proposes a value iteration algorithm that leverages instrumental variable regression to learn the value functions. In particular, in terms of value function estimation, the work of Liao et al. (2021) focuses on the setting of linear function approximation and assumes the dataset has uniform coverage. In contrast, our work considers general function classes and only assumes a partial coverage of the offline dataset. Furthermore, a growing body of literature leverages causal inference tools for the off-policy evaluation (OPE) problem in partially observable MDPs. See, e.g., Tennenholtz et al. (2020); Kallus and Zhou (2020); Namkoong et al. (2020); Shi et al. (2021); Chen et al. (2021); Bennett et al. (2021); Bennett and Kallus (2021); Hu and Wager (2021); Chen and Qi (2022) and the references therein. These works aim to evaluate a history-dependent policy where the offline dataset is collected by a behavior policy that has access to the latent states. Thus the observations and actions in the dataset are confounded. In comparison, we focus on learning the optimal policy, which involves evaluating each policy within the policy class as a special case. The fact that the offline dataset has merely partial coverage motivates our pessimism approach, whereas pessimism seems unnecessary in these works on OPE.

1.2 Notation

We introduce some useful notation before proceeding. We let \([N]\) denote \(\{1, 2, \ldots, N\}\) for any positive integer \(N\). For any random variable \(X \sim P\) and \(q \geq 0\), we use \(\|X\|_q\) to represent the \(\ell_q\)-norm of \(X\) under a probability measure \(P\), i.e., \(\|X\|_q = (E_P[X^q])^{1/q}\). In addition, we let \(\|X\|_{q,K}\) be the sample version of \(\|X\|_q\), namely, \(\|X\|_{q,K} = (1/K \sum_{i=1}^K X_i^q)^{1/q}\). For two positive sequences \(\{a_n\}_{n \geq 1}, \{b_n\}_{n \geq 1}\), we write \(a_n = O(b_n)\) or \(a_n \lesssim b_n\) if there exists a positive constant \(C\) such that \(a_n \leq C \cdot b_n\) and we write \(a_n = o(b_n)\) if \(a_n/b_n \to 0\). In addition, we write \(a_n = \Omega(b_n)\) or \(a_n \gtrsim b_n\) if \(a_n/b_n \geq c\) with some constant \(c > 0\). We use \(a_n = \Theta(b_n)\) if \(a_n = O(b_n)\) and \(a_n = \Omega(b_n)\). If a function class \(\mathcal{F}\) is star-shaped, it holds that \(\forall f \in \mathcal{F}, \alpha f \in \mathcal{F}, \forall \alpha \in [0, 1]\). Moreover, a function class \(\mathcal{F}\) is assumed to be symmetric when \(\forall f \in \mathcal{F},\ we \ have -f \in \mathcal{F}\). The star hull of a function class \(\mathcal{X}\) is defined as the minimal star-shaped function class that contains \(\mathcal{X}\).

1.3 Roadmap

The rest of this paper is organized as follows. We provide some preliminary knowledge in §2. We then describe the problem setting in §3 and introduce the PLAN algorithm in §4. In addition, in §5, we establish the theoretical guarantees of PLAN and prove that PLAN is provably efficient. Finally,
we discuss related applications of the strategic MDP model in §6.

2 Preliminaries

In this section, we present some preliminary background to set up a theme and to introduce some notation. Specifically, we introduce the episodic Markov decision process and some basic concepts on empirical process in §2.1 and §2.2, respectively.

2.1 Episodic Markov Decision Process (MDP)

An episodic MDP \((S, A, H, P, r)\) consists of a state space \(S\), an action space \(A\), a time horizon \(H\), a transition kernel \(P = \{P^*_h\}_{h=1}^H\) and a reward function \(r = \{R^*_h\}_{h=1}^H\).

Without loss of generality, we consider bounded reward function with \(R^*_h \in [0, 1]\) for all \(h \in [H]\). For any policy \(\pi = \{\pi_h : S \rightarrow \Delta(A)\}_{h=1}^H\), we define the Q-function (action-value function) \(Q^\pi_h(s, a)\) and (state-)value function \(V^\pi_h(s)\) at each step as follows:

\[
Q^\pi_h(s, a) = E_\pi \left[ \sum_{i=h}^{H} R^*_i(s_i, a_i) \big| s_i = s, a_i = a \right],
\]
\[
V^\pi_h(s) = E_\pi \left[ \sum_{i=h}^{H} R^*_i(s_i, a_i) \big| s_h = s \right].
\]

Here the expectation is taken with respect to the randomness induced by \(\pi\) and the transition kernel \(P^*_h\), which is obtained by taking \(a_h \sim \pi_h(\cdot|s_h)\) at state \(s_h\) and obtaining the next state \(s_{h+1} \sim P^*_h(\cdot|s_h, a_h), \forall h \in [H]\). Suppose the initial state \(s_1\) is sampled from a distribution \(\rho_0\), the optimal policy for our cumulative reward is defined as

\[
\pi^* := \arg\max_{\pi \in \Pi} E_{s \sim \rho_0}[V^\pi_1(s)],
\]

where \(\Pi\) is a class of policies such that \(\Pi := \{\pi = (\pi_1, \cdots, \pi_H), \pi_h : S \rightarrow \Delta(A), \forall h \in [H]\}\).

2.2 Local Rademacher Complexity and Critical Radius

The (empirical) local Rademacher complexity quantifies the complexity of a bounded function class locally around the ground truth with a given radius (Bartlett et al., 2005; Wainwright, 2019).

**Definition 2.1** (Empirical Local Rademacher Complexity). The local Rademacher complexity of a function class \(\mathcal{F} : V \rightarrow [-L, L]\) and its empirical counterpart are defined respectively as follows:

\[
\mathcal{R}_K(\delta, \mathcal{F}) = E_{\epsilon, V} \left[ \sup_{f \in \mathcal{F}, \|f\|_2 \leq \delta} \left| \frac{1}{K} \sum_{i=1}^{K} \epsilon_i f(v_i) \right| \right],
\]
\[
\mathcal{R}_{K, s}(\delta, \mathcal{F}) = E_{\epsilon} \left[ \sup_{f \in \mathcal{F}, \|f\|_{2,K} \leq \delta} \left| \frac{1}{K} \sum_{i=1}^{K} \epsilon_i f(v_i) \right| \right],
\]

where \(\mathcal{F}\) is a class of functions. The empirical counter part is defined similarly by replacing \(\epsilon\) with \(\epsilon_s\).
where \( \{v_i\}_{i=1}^K \) are i.i.d. observations sampled from some distribution \( V \), and \( \{\epsilon_i\}_{i=1}^K \) are i.i.d. Rademacher random variables taking values in \( \{-1, 1\} \) with equal probability. Here \( \mathbb{E}_{\epsilon,V} \) means the expectation is taken with respect to both random variables \( \{\epsilon_i\}_{i=1}^K \) and \( \{v_i\}_{i=1}^K \), whereas \( \mathbb{E}_\epsilon \) means the expectation is only taken with respect to \( \{\epsilon_i\}_{i=1}^K \).

Based on the definition of local Rademacher complexity, we introduce the critical radius of a function class as follows.

**Definition 2.2** (Critical Radius). The critical radius \( \delta_K \) of a function class \( F : V \rightarrow [-L, L] \) is defined as the minimal \( \delta \) that satisfies

\[
\mathcal{R}_K(\delta, F) \leq \frac{\delta^2}{L}.
\]  

(2.1)

If the function class \( F \) is star-shaped, then \( \mathcal{R}_K(\delta, F)/\delta \) is a decreasing function over \( \delta \). Thus, the solution to \( \mathcal{R}_K(\delta, F) \leq \frac{\delta^2}{L} \) always exists (Bartlett et al., 2005; Wainwright, 2019).

### 3 Problem Setting

In this section, we introduce the model formulation, data collection process and the learning objectives in our problem setting.

#### 3.1 Model Formulation

We consider a framework that models the interaction between a principal and a sequence of agents. Given the principal’s action, the agents are myopically rational and strategic. Specifically, they always maximize their immediate rewards based on their private types and generate observations for the principal. The principal then collects an immediate reward and future state through the interaction with these agents. This results in a strategic MDP as follows.

**Definition 3.1** (Strategic MDP). The strategic MDP model is formulated as follows.

- **Principal’s action:** Given the environmental state \( s_h \), the principal takes an action \( a_h \) which may depend on the whole history instead of only \( s_h \). Without loss of generality, we assume the initial state is generated from a fixed distribution \( \rho_0 \).

- **Agent’s action:** For any stage \( h \), an agent comes to system whose private type \( i_h \sim \mathbb{P}_h(\cdot) \) is sampled independently from an unknown distribution \( \mathbb{P}_h(\cdot) \). The agent then takes the action

\[
b_h := \arg\max_b R^*_a(s_h, a_h, i_h, b)
\]

to maximize its immediate private reward \( R^*_a(\cdot) \) that depends on the current state \( s_h \), principal’s action \( a_h \), its private type \( i_h \) and available actions. The principal can not observe the private type \( i_h \) and action \( b_h \).
• Observation (manipulated feature): The principal receives an observation $o_h$ sampled from an observation channel $F_h$, namely,

$$o_h \sim F_h(\cdot \mid s_h, a_h, i_h) := F_{ah}(\cdot \mid s_h, i_h, b_h).$$

Intuitively, here $o_h$ is regarded as part of the feature manipulated by the strategic agent based on the current state $s_h$, its own private type $i_h$, and principal’s action $a_h$ (through $b_h$).

• Reward: Principal receives an immediate reward $r_h = R_h^*(s_h, a_h, o_h) + g_h$, where $g_h$ is an unobserved noise correlated with the agent’s private type $i_h$. For simplicity, we assume $g_h = f_{1h}(i_h) + \epsilon_h$ is a zero mean, subgaussian random variable. Here $\epsilon_h$ is assumed to be a random variable independent of all other variables.

• Transition: The environment then transits to the next state, $s_{h+1} \sim G_h^*(s_h, a_h, o_h) + \xi_h$. Here $\xi_h$ is also assumed to be correlated with $i_h$. Without loss of generality, we let $\xi_h = f_{2h}(i_h) + \eta_h$. Here $\eta_h$ is a Gaussian random variable $N(0, \sigma^2 I)$ with an known covariance $\sigma^2 I$ and is independent of all other random variables. In short, we have

$$s_{h+1} \sim \mathbb{P}_h^*(\cdot \mid s_h, a_h, o_h, i_h) \sim N(G_h^*(s_h, a_h, o_h) + f_{2h}(i_h), \sigma^2 I). \quad (3.1)$$

For the simplicity of our notation, we use $\mathbb{P}_h^*(\cdot \mid s_h, a_h, o_h, i_h)$ to represent this transition kernel.

To summarize, strategic MDP models the interactions between a principal and a sequence of strategic agents with private information. Given the principal’s action $a_h$ and current state variable $s_h$, the agent then strategically manipulates principal’s observation $o_h$ through its action $b_h$ and private type $i_h$. These factors then affect the reward received by the principal and also lead to the next state of the system. It is worth noting that this framework can be viewed as a version of the bilevel Stackelberg game ( Başar and Olsder, 1998), where the principal first takes an action and the agent then chooses its action that maximizes its reward based on the principal’s policy and its private type. Especially, when there does not exist strategic agents (i.e., the agents report their actions $a_h = b_h$ that is independent with their private type), this formulation reduces to standard Stackelberg stochastic game ( Başar and Olsder, 1998). Moreover, our model also generalizes recently studies on strategic classification and regression ( Miller et al., 2020; Harris et al., 2021b; Shavit et al., 2020), where the principal only interacts with the strategic agents in one round with no state transition.

**Remark 3.1.** Here we consider the most general case where the reward and transition functions depend on all variables $(s_h, a_h, o_h)$. Generally speaking, throughout this paper, for all $h \in [H]$, these functions $R_h^*(\cdot), G_h^*(\cdot), \forall j \in [d_1]$ map an embedding of the space of $(s_h, a_h, o_h)$ to the Euclidean space, in the sense that $R_h^*(\cdot), G_h^*(\cdot) : \phi_x(s_h, a_h, o_h) \in \mathbb{R}^d \rightarrow \mathbb{Y} \subset \mathbb{R}$ with some known $\phi_x(\cdot)$. In the following, for simplicity of our notation, we omit the embedding function $\phi_x(\cdot)$ and use $(s_h, a_h, o_h)$ to represent $\phi_x(s_h, a_h, o_h)$ without specification.

Next, we use a real-world example of the existence of noncompliant agents in recommendation systems ( Robins, 1998; Ngo et al., 2021) to digest this setting.
**Example 3.1** (Noncompliant Agents in Recommendation Systems). For every stage $h$, the principal obtains the state variable $s_h$, which represents the current environment condition (e.g., inventory level, the operation condition of the company). A new agent comes to the system, and the principal recommends $a_h$ (recommends some new products) based on the current state variable. However, the agent is noncompliant and may choose another action $b_h$ (such as buying some other products) instead of only relying on the recommended action. The principal then observes the true action $o_h = b_h$ and receives the revenue $r_h = R^*_h(s_h, b_h) + g_h$ from this purchase. The system finally transits to the next state $s_{h+1} = G^*_h(s_h, b_h) + \xi_h$.

This example serves as a particular case of our strategic MDP, namely, the principal observes the actual action $o_h = b_h$ the strategic agent chooses. However, in some situations, such as a clinical trial, the noncompliant agent may not report the real action $b_h$ but the manipulated observation $o_h$ instead (Pearl, 2009). This is also captured by our model.

In the offline RL problem in strategic MDP, the goal is to learn the optimal policy of the principal through some historical (offline) data in the face of a sequence of strategic agents from a certain population who always take their best responses. Thus, in the following subsections, we describe the data generation process and introduce the learning objectives, respectively.

### 3.2 Offline Data Collection

In this subsection, we describe the offline setting for the data collection process. We sample $K$ trajectories $\{(s_h^{(k)}, a_h^{(k)}, o_h^{(k)}, r_h^{(k)})\}_{k=1}^{K,H}$ independently, in which every trajectory $\{(a_h, s_h, o_h)\}_{h=1}^H$ is sampled from a joint distribution $\rho : \{(S_h \times A_h \times O_h)\}_{h=1}^H \rightarrow \mathbb{R}$. The dynamics are the same with those in Definition 3.1 and we summarize it as follows:

$$a_h \sim \pi_h, \text{ a behavior policy that may depend on past information } \{s_i, a_i, o_i\}_{i=1}^{h-1} \cup \{s_h\},$$

$$i_h \sim P_h(\cdot), \text{ an agent with private type } i_h \text{ comes into the system},$$

$$o_h \sim F_h(\cdot \mid s_h, a_h, i_h), \text{ with } b_h = \arg\max_b R^*_ah(s_h, a_h, i_h, b),$$

$$r_h \sim R^*_h(s_h, a_h, o_h) + g_h, \text{ with } g_h = f_1h(i_h) + \epsilon_h,$$

$$s_{h+1} \sim G^*_h(s_h, a_h, o_h) + \xi_h, \text{ with } \xi_h = f_2h(i_h) + \eta_h, \forall h \in [H].$$

Here, we assume that distributions $F_h(\cdot \mid s_h, a_h, i_h)$, $R^*_ah(\cdot)$, $P_h(\cdot)$ and functions $f_{1h}(\cdot), f_{2h}(\cdot)$ in Definition 3.1 are unknown in the data collection process. Moreover, these functions are not necessarily the same as those in our planning stage discussed in §3.3 below. Furthermore, we highlight that during the data collection process, the action $a_h$ may depend on all past information (i.e., following some non-Markovian policies) instead of only relying on $s_h$ for all $h \in [H]$.

### 3.3 Evaluation (Planning): Personalized Policy Optimization

In this subsection, we discuss the planning process for our strategic MDP, where we learn the optimal policy of the principal, targeting at a specific population of agents.

More specifically, in the planning stage, we assume the distribution of private type $i_h \sim P_h(\cdot)$, private reward functions $R^*_ah(\cdot)$ and $f_{1h}(\cdot), f_{2h}(\cdot), o_h \sim F_h(\cdot \mid s_h, a_h, i_h), \forall h \in [H]$ are known to the
principal. The motivation behind this is that the aforementioned quantities affect the optimal policy but are never observed through the data. Therefore, one only hopes to return policy for a target population and take these terms related to agents’ private types as input. Quantitatively, this is equivalent to learning the optimal policy for the aggregated MDP, which marginalizes the effect of agents. To be clear, we next define a new MDP \((S, A, H, \{\bar{P}^*_h\}_{h=1}^H, \{\bar{R}^*_h\}_{h=1}^H)\) which takes the distribution of a specific population of agents into account in the planning stage.

We define a new (marginalized) true reward function \(\bar{R}^*_h: S \times A \to \mathbb{R}, h \in [H]\) and transition kernel \(\bar{P}^*_h: S \to \mathbb{R}, h \in [H]\) in the \(h\)-th step as follows:

\[
\bar{R}^*_h(s_h, a_h) = \int_{o_h, i_h} \left[ R^*_h(s_h, a_h, o_h) + f_{1h}(i_h) \right] dF_h(o_h \mid s_h, a_h, i_h) dP_h(i_h), \tag{3.5}
\]

\[
\bar{P}^*_h(\cdot \mid s_h, a_h) = \int_{o_h, i_h} \bar{P}^*_h(\cdot \mid s_h, a_h, o_h, i_h) dF_h(o_h \mid s_h, a_h, i_h) dP_h(i_h), \tag{3.6}
\]

where \(\bar{P}^*_h(\cdot \mid s_h, a_h, o_h, i_h)\) is given in (3.1). Finally, we have the actual underlying model of our aggregated MDP as \(\{\bar{R}^*_h(s_h, a_h), \bar{P}^*_h(\cdot \mid s_h, a_h)\}_{h=1}^H\) in the planning stage.

For any given \(h \in [H]\), we next define its associated \(Q\)-function \(\bar{Q}^*_h: S \times A \to \mathbb{R}\) and value function \(\bar{V}^*_h: S \to \mathbb{R}\) under any given policy \(\pi\) as follows:

\[
\bar{Q}^*_h(s, a) = \mathbb{E}_\pi \left[ \sum_{j=h}^H \bar{R}^*_j(s_j, a_j) \mid s_h = s, a_h = a \right],
\]

\[
\bar{V}^*_h(s) = \mathbb{E}_\pi \left[ \sum_{j=h}^H \bar{R}^*_j(s_j, a_j) \mid s_h = s \right].
\]

Here the expectation is taken with respect to the randomness of the state-action sequence \(\{s_i, a_i\}_{i=h}^H\) with \(\{s_i, a_i\}_{i=h}^H\) following the dynamics induced by \(\pi\) and transition kernel \(\bar{P}^*_h(\cdot \mid s_h, a_h)\). The associated Bellman equation is

\[
\bar{Q}^*_h(s, a) = \bar{R}^*_h(s_h, a_h) + \mathbb{E}_{s_{h+1} \sim \bar{P}^*_h(\cdot \mid s_h, a_h)} \bar{V}^*_h(s_{h+1}), \\
\bar{V}^*_h(s) = \langle \bar{Q}^*_h(s, \cdot), \pi_h(\cdot \mid s) \rangle, \bar{V}^*_\pi H+1(\cdot) = 0. \tag{3.7}
\]

It is worth noting that we only need to study the Markovian policy class \(\Pi := \{\pi = (\pi_1, \cdots, \pi_H), \pi_h : S \to \Delta(A), \forall h \in [H]\}\) in the planning stage thanks to the Markov property.

Recall that we assume the initial state is generated from a fixed distribution \(\rho_0\) in Definition 3.1. Then, for any given policy \(\pi \in \Pi\), the expected total rewards of the principal under the true model \(M^* := \{(\bar{R}^*_h, \bar{P}^*_h)\}_{h=1}^H\) is denoted by \(J(M^*, \pi)\), with \(J(M^*, \pi) := \mathbb{E}_{s_0 \sim \rho_0} [\bar{V}^*_\pi(s)]\). The optimal policy is given by \(\pi^* = \arg\max_{\pi \in \Pi} J(M^*, \pi)\). Recall that when the agents come from a specific population, learning the optimal policy of the aforementioned aggregated MDP is equivalent to studying the principal’s planning problem with \(J(M^*, \pi)\) being the principal’s total rewards. This is also equivalent to minimizing the suboptimality, which quantifies the loss we get by implementing our policy \(\pi\) versus implementing the optimal policy \(\pi^*\), namely,

\[
\text{SubOpt}(\pi) = J(M^*, \pi^*) - J(M^*, \pi). \tag{3.8}
\]
In the next section, we provide a detailed algorithm for constructing a policy $\pi$ that optimizes the suboptimality based on the collected offline data.

4 The PLAN Algorithm

This section introduces the algorithm to optimize the policy for our strategic MDP using pre-collected datasets and a model-based algorithm. We first provide a detailed explanation of the challenges of our model in §4.1. We then design our algorithm that tackles these challenges for strategic MDP §4.2 and §4.3.

4.1 A Peek into Strategic MDP: Why Challenging?

Before proceeding to analyze the challenges in learning the strategic MDP, we first rigorously define the notion of confounders.

**Definition 4.1 (Confounders).** A random variable $u$ is a confounder with respect to $(X, Y)$ if both of $(X, Y)$ are caused by $u$.

The first challenge in studying strategic MDP is the existence of unobserved confounders. We observe that $i_h$ affects both principal’s observed feature $o_h$, immediate reward $r_h$ and future state $s_{h+1}$ for all $h \in [H]$ according to Definition 3.1. Therefore, for any $h \in [H]$, we see that the private information $i_h$ serves as an unobserved confounding variable to $(r_h, o_h)$ and $(s_{h+1}, o_h)$ by Definition 4.1. In the scenario, we have $E[g_h | s_h, a_h, o_h]$ and $E[\xi_h | s_h, a_h, o_h] \neq 0$, and we fail to identify the true reward function $R^*_h(\cdot)$ or transition function $G^*_h(\cdot)$ via well-used square loss.

There exist a series of works which study offline RL using the model-based method. They first learn the model (reward functions and transition kernels) and then optimize their policy (Azar et al., 2017; Agarwal et al., 2020; Uehara and Sun, 2021; Zanette et al., 2021; Li et al., 2022). Thus, a tempting way to solving our strategic MDP is to apply standard model-based RL techniques by treating $(o_h, s_h)$ as the observed state variable, such as using MLE to estimate the model and then plan using the estimated model. However, as we mentioned above, due to the unobserved confounders $i_h, h \in [H]$, these standard techniques will result in biased estimators for rewards and transition kernels (Pearl, 2009; Hernández and Robins, 2010). In the worst scenario, the error caused by the bias is lower bounded by a constant level, leading to a considerable loss in optimality.

There are two additional challenges, namely, distribution shift (insufficient data coverage) and the existence of an enormous number of states and actions, in studying our strategic MDP.

In terms of the distribution shift, there are two implications. First, the distribution of state-action pairs induced by the behavior policy may not cover the distribution induced by some other policies in the planning stage. Second, we are interested in learning the policy for a target population of agents, whose distribution is also not necessarily the same as that in the data generation process. These result in the existence of distribution shift between our collected data and the target population.

The third challenge arises due to an enormous number of states and actions in reinforcement learning (RL) applications. In this case, traditional tabular RL is inefficient in modeling, and spe-
cific function approximation is necessary to approximate the value function or the policy. Unlike most existing works studying offline RL in finite actions and states (tabular MDP) or assuming particular constraints on the models (linear MDP), we consider using general function approximation, especially under the existence of latent confounders in the paper.

To tackle these challenges, in the following subsection, we introduce the ideas of instrumental variable regression and the pessimism principle.

4.2 Ideas for Addressing These Challenges

In this subsection, we address the aforementioned challenges on latent confounder, insufficient data coverage and function approximation in §4.2.1 and §4.2.2, respectively.

4.2.1 Dealing with the Latent Confounder: Instrumental Variables (IV)

We first tackle the challenge due to latent confounders by leveraging instrumental variables (IV). We define instrumental variables and illustrate why IV remedies the curse of latent confounder in strategic MDP.

**Definition 4.2 (Instrumental Variables).** A random variable $Z$ is an instrumental variable with respective to $(X,Y)$, if it is satisfies the following two conditions:

- $Z$ is not independent with $X$.
- $Z$ only affects $Y$ through $X$, and is independent with all other variables that has influence on $Y$ but are not mediated by $X$.

To utilize the instrumental variables, we present an assumption on the latent variables $i_h$. Recall that $i_h$ represents the private type of the agent at step $h$.

**Assumption 4.1.** We assume $\{i_h\}_{h=1}^H$ are independent random variables. Moreover, for any given $h \in [H]$, $i_h$ is also assumed to be independent of $\{(s_t, a_t)\}_{t=1}^h$.

This assumption requires the private type $i_h$ involved in every stage does not share confounding variables across different stages $h \in [H]$ and is independent of past states and actions $\{(s_t, a_t)\}_{t=1}^h$. This is satisfied by the example discussed in §3.1, where we have a sequence of agents whose private types are drawn independently from some distribution and are independent of past states and actions. This assumption can also be satisfied when the principal is only interacting with a single agent until stage $H$, where for different $h \in [H]$, $i_h$ is independent with each other by representing the private type of that agent from various aspects. For example, in a job interview with multiple stages, the hiring manager would like to test the agent’s ability from different aspects (such as leadership and technical capabilities) in these stages. Thus, the underlying skills $\{i_h\}_{h=1}^H$ of the agent satisfy Assumption 4.1.

According to Definition 4.2, we observe that $(s_h, a_h)$ serves as an instrumental variable for $(x_h, r_h)$ and $(x_h, s_{h+1})$. Here $x_h = \phi_x(s_h, a_h, o_h)$ with $\phi_x$ being a fixed and known embedding function. We next summarize this property in Lemma 4.1.
Lemma 4.1. Under our model settings given in §3.1 and Assumption 4.1, \( z_h := (s_h, a_h) \) is an instrumental variable for \((x_h, r_h)\) and \((x_h, s_{h+1})\) where \( x_h = \phi_x(s_h, a_h, o_h) \) with \( \phi_x \) being a fixed and known embedding function.

Figure 1: Causal graph of the \( h \)-stage of strategic MDP. Here \( z_h = (s_h, a_h) \) denotes the instrumental variable and \( x_h = \phi_x(s_h, a_h, o_h) \) is our covariate. Moreover, \( y_h \) represents the response variable (reward \( r_h \) or next state \( s_{h+1} \)) and \( i_h \) is the hidden confounder variable.

Next, we utilize the IV \((s_h, a_h)\) to identify the strategic MDP model from the confounded offline data. Therefore, \( R_h^*(\cdot), G_h^*(\cdot) \) satisfy the following moment equations (4.1) and (4.2):

\[
\mathbb{E}_\rho[R_h^*(s_h, a_h, o_h) - r_h | s_h, a_h] = 0, \tag{4.1}
\]

\[
\mathbb{E}_\rho[G_h^*(s_h, a_h, o_h) - s_{h+1} | s_h, a_h] = 0, \tag{4.2}
\]

as \( \mathbb{E}_\rho[\xi_h | s_h, a_h] = 0 \) and \( \mathbb{E}_\rho[g_h | s_h, a_h] = 0 \) by our model formulation and Assumption 4.1.

Thus, in order to identify \( R_h^*(\cdot) \), one then minimizes the following loss function

\[
\min_{R_h \in L^2(\mathcal{X})} L(R_h) = \min_{R_h \in L^2(\mathcal{X})} \mathbb{E}_\rho \left[ \mathbb{E}_\rho[R_h(s_h, a_h, o_h) - r_h | s_h, a_h] \right]^2, \tag{4.3}
\]

which is a projected least squares loss function. By (4.1), we see \( R_h^*(\cdot) \) is a minimizer of this loss. It is worth noting that we are also able to use \( \psi_z(s_h, a_h) \) with some known embedding function \( \psi_z(\cdot) \) as the instrumental variable. Similar to Remark 3.1, for the simplicity of our notation, we also omit \( \psi_z(\cdot) \) without specification.

In this subsection, we utilize algorithmic instrumental variables to identify our model and thus tackle the first challenge on latent confounding variables. In the following subsection, we introduce the idea of pessimism for handling the distribution shift.

4.2.2 Handling Distribution Shift: Pessimism Principle

In this subsection, we will provide some intuition of using pessimism to handle distribution shift. At a high level, for all \( \pi \in \Pi \), we want to construct a data-driven \( \hat{J}(\pi) \) which serves as a pessimistic
estimate of \( J(M^*, \pi) \), in the sense that
\[
\hat{J}(\pi) \leq J(M^*, \pi), \text{ for all } \pi \in \Pi. \tag{4.4}
\]
Here \( M^* \) denotes the true model defined in §3.3. We then choose the optimal policy with respect to such a pessimistic estimate, namely,
\[
\hat{\pi} := \arg\max_{\pi \in \Pi} \hat{J}(\pi). \tag{4.5}
\]
In this scenario, the suboptimality of \( \hat{\pi} \) is bounded by
\[
\text{SubOpt}(\hat{\pi}) = J(M^*, \pi^*) - J(M^*, \hat{\pi}) = J(M^*, \pi^*) - \hat{J}(\pi^*) + \hat{J}(\hat{\pi}) - J(M^*, \pi^*) \leq J(M^*, \pi^*) - \hat{J}(\pi^*) \leq J(M^*, \pi^*) - \hat{J}(\pi^*). \tag{4.6}
\]
The first inequality follows from our construction of \( \hat{\pi} \) given in (4.5) and the second inequality follows from (4.4). One observes that (4.6) reflects the bias due to pessimism. As it only depends on the trajectory induced by \( \pi^* \), it is small as long as the dataset has good coverage over \( \pi^* \).

To solve the third challenge, we leverage general function approximation to accommodate this issue. Using general function approximation admits many merits. It allows more flexible function classes than tabular and linear cases, see §4.3 for more details. Moreover, we are also able to handle the function class misspecification which will be discussed in §5.2.

Next, we combine all pieces and provide our algorithm for solving strategic MDP. In specific, we construct such pessimistic value functions using lower level sets of the IV-assisted loss functions with general function approximation.

### 4.3 Putting All Pieces Together: Pessimistic Strategic MDP with General Function Approximation

In this subsection, we propose a novel algorithm, namely, pessimistic policy learning with algorithmic instruments (PLAN), which resolves the aforementioned challenges by leveraging the ideas of pessimism principle and instrumental variable regression with general function approximation.

#### 4.3.1 A Glimpse of the PLAN Algorithm

As we mentioned in §4.2.2, to leverage pessimism, we need to construct a data-driven pessimistic function \( \hat{J}(\pi) \) such that \( \hat{J}(\pi) \leq J(M^*, \pi) \), for all \( \pi \in \Pi \). For any confidence region \( \mathcal{M} \) of \( M^* = \{(\bar{R}_h^*, \bar{P}_h^*)\}_{h=1}^H \), which is constructed based on data, and any given policy \( \pi \), we let \( \hat{J}(\pi) := \min_{M \in \mathcal{M}} J(M, \pi) \). Here \( J(M, \pi) \) represents the total value function evaluated by policy \( \pi \) under model \( M = \{(\bar{R}_h, \bar{P}_h)\}_{h=1}^H \). Then it can be shown that \( \hat{J}(\pi) = \min_{M \in \mathcal{M}} J(M, \pi) \leq J(M^*, \pi) \) as long as \( \mathcal{M} \) contains \( M^* \). In this scenario, we then construct the estimated policy \( \hat{\pi} \) as we discussed in §4.2.2, namely,
\[
\hat{\pi} = \arg\max_{\pi \in \Pi} \min_{M \in \mathcal{M}} J(M, \pi). \tag{4.7}
\]
As a consequence, by (4.6), we have

\[ \text{SubOpt}(\hat{\pi}) \leq J(M^*, \pi^*) - \tilde{J}(\pi^*) = J(M^*, \pi^*) - \min_{M \in \mathcal{M}} J(M, \pi^*). \]

Next, we construct the confidence region \( \mathcal{M} \) of \( M^* = \{(\hat{R}^*_h, \hat{\pi}^*_h)\}_{h=1}^H \).

### 4.3.2 Construction of Confidence Sets

In this subsection, we construct the confidence sets \( \mathcal{M} := \{\hat{\mathcal{R}}_h, \hat{G}_h\}_{h=1}^H \) for \( \{\hat{R}^*_h, \hat{\pi}^*_h\}_{h=1}^H \) via lower level sets of the sample loss functions, where the loss functions are derived from minimax estimation.

First, we introduce the sample version of the loss functions. Recall that the model identification is derived in §4.2.1 via the loss function in (4.3) which admits \( R^*_h \) as a minimizer. Note that (4.3) can not be directly estimated from the data due to the conditional expectation inside the square function. By Fenchel duality (Rockafellar and Wets, 2009; Shapiro et al., 2021), the loss in (4.3) is equivalent to the following minimax loss function that can be estimated via data:

\[
\min_{R_h \in L^2(\mathcal{X})} L(R_h) = 2 \min_{R_h \in L^2(\mathcal{X})} \max_{f \in L^2(S \times A)} \mathbb{E}_{\rho} [(r_h - R_h(s_h, a_h, o_h))f(s_h, a_h)] - \mathbb{E}_{\rho} [f^2(s_h, a_h)].
\]

Here \( L^2(\mathcal{X}) \) denotes the \( \ell_2 \)-integrable functions on domain \( \mathcal{X} \) under probability measure \( \rho \).

Next, we derive confidence sets \( \hat{\mathcal{R}}_h \) and \( \hat{G}_h \) for \( \hat{R}^*_h \) and \( \hat{\pi}^*_h \), respectively, by leveraging the sample version of the loss function and the offline dataset in §3.2. First, we construct a Wilk’s type confidence set (Wilks, 1938) for \( \hat{R}^*_h \) by letting

\[
\mathcal{R}_h = \left\{ R_h \in \mathbb{R}_h : \mathcal{L}_K(\hat{R}_h) - \mathcal{L}_K(\hat{R}_h) \lesssim c^2_{r,h,K} \right\},
\]

(4.8)

where we define \( \mathcal{L}_K \) and \( \hat{R}_h \) respectively as

\[
\mathcal{L}_K(R_h) = \sup_{f \in \mathcal{F}} \left\{ \frac{1}{K} \sum_{k=1}^{K} \left( r_h - R_h(s_h^{(k)}, a_h^{(k)}, o_h^{(k)}) \right) f(s_h^{(k)}, a_h^{(k)}) - \frac{1}{2K} \sum_{k=1}^{K} f^2(s_h^{(k)}, a_h^{(k)}) \right\}, \quad \text{and}
\hat{R}_h = \text{argmin}_{R_h \in \mathbb{R}_h} \mathcal{L}_K(R_h).
\]

Here \( \mathbb{R}_h := \{R_h : \mathcal{X} \rightarrow [-L, L]\} \) with \( R^*_h \in \mathbb{R}_h \) and \( \mathcal{F} := \{f : S \times A \rightarrow [-L, L]\} \). Moreover, \( c_{r,h,K} \in \mathbb{R} \) is a threshold that will be specified later. By properly choosing this threshold, we can prove that \( \mathcal{R}_h \) contains \( R^*_h \) with high probability. In other words, the confidence set \( \mathcal{R}_h \) is valid.

For our aggregated MDP discussed in §3.3, we define the high-confidence set for \( \mathcal{R}_h \) in (3.5) as a transformation of \( \mathcal{R}_h \) according to the target population of agents:

\[
\bar{\mathcal{R}}_h = \left\{ \bar{R}_h : \bar{R}_h = \int_{o_h, i_h} [R_h(s_h, a_h, o_h) + f_{1h}(i_h)] dF_h(o_h | s_h, a_h, i_h) dP_h(i_h), R_h \in \mathcal{R}_h \right\}.
\]

Here we recall that \( F_h(\cdot | s_h, a_h, i_h) \) is the known conditional distribution of \( o_h \) given \( (s_h, a_h, i_h) \) in the planning stage. Observe that when \( R^*_h \in \mathcal{R}_h \), we have \( \bar{R}^*_h \in \bar{\mathcal{R}}_h \).
Similarly, the confidence set for the $j$-th coordinate of function $G^*_h : \mathcal{X} \to \mathbb{R}^{d_1}$ is defined as

$$\mathcal{G}_{h,j} = \left\{ G_{h,j} \in \mathcal{G}_{h,j} : \mathcal{L}_K(G_{h,j}) - \mathcal{L}_K(\hat{G}_{h,j}) \lesssim c_{h,g,K}^2 \right\}. \quad (4.9)$$

Here $\mathcal{G}_{h,j} := \{G_{h,j} : \mathcal{X} \to [-L, L]\}$, with $G^*_{h,j} \in \mathcal{G}_{h,j} \forall j \in [d_1]$. In addition, with slight abuse of notation, we define $\mathcal{L}_K$ and $\hat{G}_{h,j}$ as

$$\mathcal{L}_K(G_{h,j}) = \sup_{f \in \mathcal{F}} \left\{ \frac{1}{K} \sum_{k=1}^K (s_{h+1,j}^{(k)} - G_{h,j}(s_{h}^{(k)}, a_{h}^{(k)}, o_{h}^{(k)})) f(s_{h}^{(k)}, a_{h}^{(k)}) - \frac{1}{2K} \sum_{k=1}^K f(s_{h}^{(k)}, a_{h}^{(k)})^2 \right\},$$

$$\hat{G}_{h,j} = \arg\min_{G_{h,j} \in \mathcal{G}_{h,j}} \mathcal{L}_K(G_{h,j}).$$

Similarly, we define $\bar{G}_{h,j}$ as the confidence set for $\bar{G}^*_h$:

$$\bar{\mathcal{G}}_{h,j} = \left\{ \mathbb{P}_{h,j}(\cdot | s_{h}, a_{h}) : \mathbb{P}_{h,j}(\cdot | s_{h}, a_{h}) = \int_{o_{h}, i_{h}} \mathbb{P}_{h,j}(\cdot | s_{h}, a_{h}, o_{h}, i_{h}) dF_{h}(o_{h} | s_{h}, a_{h}, i_{h}) dP_{i}(i_{h}), \right\},$$

$$\mathbb{P}_{h,j}(\cdot | s_{h}, a_{h}, o_{h}, i_{h}) \sim N(G_{h,j}(s_{h}, a_{h}, o_{h}) + f_{2h,j}(i_{h}), \sigma^2), \text{ with } G_{h,j}(\cdot) \in \mathcal{G}_{h,j}. \right\}.$$

Combining these confidence sets together, we achieve that $\mathcal{M} = \{(\bar{R}_h, \bar{G}_h)\}_{h=1}^H$ contains the true model $M^*$ with high probability.

It is worth noting that most existing literature only studies tabular or linear MDP using pessimism-based ideas with no hidden confounders (Jin et al., 2021b; Rashidinejad et al., 2021; Shi et al., 2022; Yan et al., 2022a). However, our algorithm PLAN works for a general class of non-parametric reward and transition kernels and even permits the existence of hidden confounding variables. In the next section, we provide more details on the theoretical guarantees of PLAN.

## 5 Theoretical Results

In this section, we present theoretical guarantees for PLAN in §4. We next analyze our policy optimization results with well-specified function classes in §5.1 and misspecified ones in §5.2, respectively.

### 5.1 Theoretical Results for Suboptimality under Well-Specified Function Class.

In this subsection, we provide theoretical guarantees for the suboptimality of our estimated policy (4.7). Here $\bar{R}_h, \bar{G}_{h,j}$ are correctly specified, containing $R^*_h$ and $G^*_{h,j}$.

Before proceeding to the theoretical analysis, we first present several assumptions. The first assumption ensures that the sampling distribution $\rho$ satisfies a partial coverage condition.
Assumption 5.1 (Concentrability Coefficients of Partial Coverage). There exists a constant $C_{\pi^*} > 0$ such that
\[
\sup_{R_h \in \{R_h \rightarrow R_h^*\}} \frac{\mathbb{E}_{\rho} [R_h^2(s_h, a_h, o_h)]}{\mathbb{E}_{\rho(s_h, a_h, o_h)}[R_h^2(s_h, a_h, o_h)]} \leq C_{\pi^*}^2, \forall h \in [H],
\]
\[
\sup_{G_{h,j} \in \{G_{h,j} \rightarrow G_{h,j}^*\}} \frac{\mathbb{E}_{\rho} [G_{h,j}^2(s_h, a_h, o_h)]}{\mathbb{E}_{\rho(s_h, a_h, o_h)}[G_{h,j}^2(s_h, a_h, o_h)]} \leq C_{\pi^*}^2, \forall j \in [d_1], \forall h \in [H],
\]
where we define $R_h - R_h^* = \{ (R_h - R_h^*)(\cdot), R_h(\cdot) \in R_h \}, G_{h,j} - G_{h,j}^* = \{ (G_{h,j} - G_{h,j}^*)(\cdot), G_{h,j}(\cdot) \in G_{h,j} \}. In addition, we define $d(\pi^*, \theta^*)(s_h, a_h, o_h)$ as the joint distribution of $(s_h, a_h, o_h)$ at stage $h$ induced by $\pi^* = \{ \pi^*_j(a_j | s_j) \}_{j=1}^h$ and $\mathbb{P} = \{ \mathbb{P}_j(o_j | s_j, a_j) \}_{j=1}^h$, where $\mathbb{P}_j(\cdot | s_j, a_j) := \int_{i_j} F_j(\cdot | i_j, a_j, s_j) dP_2(i_j)$ is the known marginal distribution of $o_j$ given $(s_j, a_j)$ in the $j$-th planning stage.

In this assumption, we let the ratio of the square loss under two distributions, namely, the distribution $d(\pi^*, \theta^*)(\cdot)$ induced by the optimal policy with “population-specific” agents and the sample distribution $\rho$, be bounded by a concentrability coefficients $C_{\pi^*}$. This notion is adapted from Uehara and Sun (2021). A sufficient condition for this assumption is when the ratio of these two densities $\sup_{(s_h, a_h, o_h)} f(\pi^*, \theta^*)(s_h, a_h, o_h)/f_\rho(s_h, a_h, o_h)$ is upper bounded by $C_{\pi^*}^2$. Therefore, Assumption 5.1 is mild in a sense that it only requires partial coverage of the sample distribution $\rho(\cdot)$ (i.e., covering $d(\pi^*, \theta^*)(\cdot)$ induced by the optimal policy $\pi^*$ instead of all $\pi$).

Furthermore, as we utilize IV regression in PLAN, analysis of IV regression enables us to bounded projected MSE (PMSE) $\mathbb{E}_\rho[\mathbb{E}_\rho[(R_h - R_h^*)(s_h, a_h, o_h) | s_h, a_h]^2], which is measured in the space of instrumental variable, as opposed to the more desired MSE $\mathbb{E}_\rho[R_h - R_h^*]^2(s_h, a_h, o_h)].$ Transforming the PMSE to MSE, acting as a discontinuous mapping, results in an ill-posed inverse problem (Horowitz, 2013). Thus, we next present an ill-posed condition, which measures the difficulty of such an inverse problem.

Assumption 5.2 (Ill-posed Condition). We assume there exist coefficients $\tau_{r,h,K}$ and $\tau_{G,h,K}$ depending on $K, h, and function classes $\mathcal{R}_h, \mathcal{G}_h$ such that the following conditions hold:
\[
\sup_{R_h \in \{R_h \rightarrow R_h^*\}} \frac{\mathbb{E}_{\rho(s_h, a_h, o_h)}[R_h^2(s_h, a_h, o_h)]}{\mathbb{E}_{\rho(s_h, a_h, o_h)}[R_h(s_h, a_h, o_h) | s_h, a_h]^2]} \leq \tau_{r,h,K}^2, \forall h \in [H],
\]
\[
\sup_{G_{h,j} \in \{G_{h,j} \rightarrow G_{h,j}^*\}} \frac{\mathbb{E}_{\rho(s_h, a_h, o_h)}[G_{h,j}^2(s_h, a_h, o_h)]}{\mathbb{E}_{\rho(s_h, a_h, o_h)}[G_{h,j}(s_h, a_h, o_h) | s_h, a_h]^2]} \leq \tau_{G,h,K}^2, \forall j \in [d_1], \forall h \in [H].
\]

It is worth noting that the ill-posed condition is a standard assumption in the literature of (nonparametric) instrumental regression. See, e.g., Chen and Reiss (2011); Darolles et al. (2011); Horowitz (2013); Dikkala et al. (2020) for more details.

Next, to ensure that the minimax estimation procedure given in §4.3.2 is valid, we impose an assumption on the employed function classes.

Assumption 5.3. Let $\mathcal{F} := \{ f : Z \rightarrow [-L, L] \}, \mathcal{R}_h = \{ R_h : \mathcal{X} \rightarrow [-L, L] \}, \mathcal{G}_{h,j} = \{ G_{h,j} : \mathcal{X} \rightarrow [-L, L] \}, \forall j \in [d_1], \forall h \in [H]$ be function classes given in (4.8) and (4.9) with $R_h^* \in \mathcal{R}_h, G_{h,j}^* \in \mathcal{G}_{h,j}$
\( \mathbb{G}_{h,j} \forall j \in [d_1] \). Moreover, we assume that for all \( R_h \in \mathbb{R}_h \) and \( \mathbb{G}_{h,j} \in \mathbb{G}_{h,j} \), it holds that
\[
\mathbb{T}(R_h - R_h^*) (z) := \mathbb{E}_p[R_h(o_h, a_h, s_h) - R_h^*(o_h, a_h, s_h) \mid (a_h, s_h) = z] \in \mathcal{F},
\]
\[
\mathbb{T}(G_{h,j} - G_{h,j}^*) (z) := \mathbb{E}_p[G_{h,j}(o_h, a_h, s_h) - G_{h,j}^*(o_h, a_h, s_h) \mid (a_h, s_h) = z] \in \mathcal{F}, \forall h \in [H], \forall j \in [d_1].
\]
Furthermore, \( \mathcal{F} \) is assumed to be a symmetric and star-shaped function class.

In this assumption, we assume function classes \( \mathcal{F}, \mathbb{R}_h, \mathbb{G}_{h,j}, \forall j \in [d_1], \forall h \in [H] \) given in (4.8) and (4.9) are well-specified in the sense that \( R_h^* \in \mathbb{R}_h, G_{h,j}^* \in \mathbb{G}_{h,j} \) and \( \mathcal{F} \) contains the projected function classes
\[
\mathcal{P}(R, h) := \{ \mathbb{T}(R_h - R_h^*) (z), R_h \in \mathbb{R}_h \}
\]
and
\[
\mathcal{P}(G, h, j) := \{ \mathbb{T}(G_{h,j} - G_{h,j}^*) (z), G_{h,j} \in \mathbb{G}_{h,j} \}, \forall j \in [d_1], h \in [H].
\]
Recall that the confidence sets for \( R_h^* \) and \( G_{h,j}^* \) are constructed in (4.8) and (4.9). We now specify the corresponding thresholding parameters \( c_{h,r,K} \) and \( c_{h,G,K} \). We set \( c_{h,r,K} = \mathcal{O}(\delta_{R,h,\delta}) \) with \( \delta_{R,h,\delta} = \mathcal{O}(\mathcal{O}(\delta_{R,h,\delta}) + \sqrt{\log(H/\delta)/K}) \). Here \( \delta_{R,h} \) is the maximum critical radii of \( \mathcal{F} \) and the following function class
\[
\mathcal{R}_h^* := \{ c(R_h - R_h^*) (x) \cdot \mathbb{T}(R_h - R_h^*) (z) : \mathcal{X} \times \mathcal{Z} \rightarrow \mathbb{R}; \forall c \in [0, 1], h \in [H] \}. \quad (5.1)
\]
Here \( \mathcal{R}_h^* \) is the star hull of the function class which is the product of \( (\mathbb{R}_h^* - R_h^*) \) and its projections in \( \mathcal{P}(R, h) \). The upper bound of the critical radii of \( \mathcal{R}_h^* \) and \( \mathcal{F} \) measures the maximal complexity of function classes \( \mathcal{R}_h^* \) and \( \mathcal{F} \), respectively.

Similarly, we define \( c_{h,G,K} := \mathcal{O}(\delta_{G,h,\delta}) \) with \( \delta_{G,h,\delta} = \mathcal{O}(\mathcal{O}(\delta_{G,h,\delta} + \sqrt{\log(Hd_1/\delta)/K}) \) and \( \delta_{G,h} \) being the maximum critical radii of \( \mathcal{F} \) and the following function class
\[
\mathcal{G}_{h,j}^* := \{ c(G_{h,j} - G_{h,j}^*) (x) \cdot \mathbb{T}(G_{h,j} - G_{h,j}^*) (z) : \mathcal{X} \times \mathcal{Z} \rightarrow \mathbb{R}; G_{h,j} \in \mathbb{G}_{h,j}, \forall c \in [0, 1] \}, \quad (5.2)
\]
\( \forall j \in [d_1] \). Here we recall that \( d_1 \) is the dimension of the state variable. With these necessary assumptions at hand, we bound the suboptimality in the following theorem.

**Theorem 5.1.** Under Assumptions 5.1, 5.2, and 5.3, with probability \( 1 - \delta - 1/K \), the suboptimality of \( \hat{\pi} \) returned by \( \text{PLAN} \) is upper bounded by
\[
\text{SubOpt}(\hat{\pi}) \lesssim C_\pi \left[ H \sum_{h=1}^{H} \tau_{G,h,K} \sqrt{d_1} L_{K,d_1} \delta_{G,h,\delta} + \sum_{h=1}^{H} \tau_{R,h,K} L_{K,1} \delta_{R,h,\delta} \right],
\]
where \( L_{K,x} = L + \sigma \sqrt{\log(H + 1) \log(Kx)} \), with \( x \in \{1, d_1\} \), \( \delta_{R,h,\delta} = \delta_{R,h} + \sqrt{\log(H/\delta)/K} \), and \( \delta_{G,h,\delta} = \delta_{G,h} + \sqrt{\log(d_1 H/\delta)/K} \). Here \( L \) is the upper bound of bounded functions in \( \mathcal{F}, \mathbb{R}_h, \mathbb{G}_{h,j}, \forall h \in [H], \forall j \in [d_1] \) mentioned in Assumption 5.3 in \( \ell_\infty \)-norm. Besides, \( \delta_{G,h} \) is the maximum critical radii of \( \mathcal{F}, \mathcal{G}_{h,j}^*, \forall j \in [d_1] \), and \( \delta_{R,h} \) is an upper bound of the critical radii of \( \mathcal{F}, \mathcal{R}_h^* \).
Theorem 5.1 provides an upper bound for the suboptimality of $\hat{\pi}$ under mild conditions. This upper bound involves critical radii, measuring the complexity of function classes $\mathcal{F}$ and $\mathbb{R}_h, h \in [H]$, time horizon $H$, and concentrability and ill-posed coefficients. For every single stage, we achieve a fast statistical rate with order $O(\sqrt{1/K})$ under many function classes; see §5.1.1 and §5.1.2 for more details. This matches the well-known regression rate and thus is minimax optimal up to ill-posed coefficients for general instrumental regression problems.

Compared with existing literature that studies strategic regression (Harris et al., 2021b), our contribution is two-fold. First, we extend the strategic regression to the decision-making problem where the principal interacts with strategic agents in multiple stages. In contrast, strategic regression only involves single-stage decision making. Moreover, we consider general function classes and utilize the method of moments and pessimism to tackle the technique difficulty, whereas Harris et al. (2021b) only consider the linear function class and use point estimators.

Compared with existing works studying offline MDP, we propose a new framework, namely, strategic MDP, that captures strategic interactions between a sequence of agents and a principal. In specific, the agents have private types, acting as latent confounders, affect both principal’s observation, immediate reward and future state. We propose a model-based algorithm and develop novel proof frameworks by leveraging IV regression, pessimism via lower level sets, and general function approximation to eliminate the technical challenges. We achieve similar statistical rates of suboptimality with standard model-based RL (without latent confounders) with function approximation to eliminate the technical challenges. We achieve similar statistical rates of suboptimality with standard model-based RL (without latent confounders) with function approximation (Duan et al., 2020; Uehara and Sun, 2021), which is minimax optimal up to $H$ factors.

We next provide two instantiations of Theorem 5.1 with linear and kernel functions, respectively.

### 5.1.1 Example: Linear Function Class

In this subsection, we provide an instantiation of Theorem 5.1 when $R^*_h, G^*_h, j \in [d_1]$ lie in linear spaces with finite dimensions. Throughout this subsection, we let $x_h := \phi(x_h, a_h, o_h) \in \mathcal{X}$ and $z_h := \psi(s_h, a_h) \in \mathcal{Z}$ with $\phi(x)$ and $\psi(z)$ being some embedding mappings. For all $h \in [H]$, we define proper linear function classes $\mathcal{F}, \mathbb{R}_h$, and $\mathcal{G}_{h,j}$ as

$$\mathcal{F} = \{ \langle \beta, z \rangle : \mathcal{Z} \to \mathbb{R} ; \beta \in \mathbb{R}^{m}, \| \beta \|_2 \leq U \},$$

$$\mathbb{R}_h = \mathcal{G}_{h,j} = \{ \langle \theta, x \rangle : \mathcal{X} \to \mathbb{R} ; \theta \in \mathbb{R}^{n_h}, \| \theta \|_2 \leq B \}. \quad (5.4)$$

Here we assume the covariate $x_h$ has dimension $n_h, h \in [H]$ and instrumental variable has dimension $m$. We next summarize necessary assumptions on our true models in the following Assumption 5.4.

**Assumption 5.4.** Suppose $R^*_h(x_h) = \langle x_h, \theta^* \rangle, G^*_{h,j}(x_h) = \langle x_h, \theta^*_j \rangle, j \in [d_1]$ with $\| \theta^* \|_2 \leq B, \| \theta^*_j \|_2 \leq B$. We assume $\mathbb{E}[x_h | z_h] = W_h z_h$ with $W_h \in \mathbb{R}^{n_h \times m}$ and $\| W_h \|_F \leq B_F, \forall h \in [H]$.

In Assumption 5.4, we assume every dimension of $x_h$ conditional on $z_h$ is a linear function of $z_h$. Under this assumption, we have $\mathbb{E}[R_h(x_h) - R^*_h(x_h) | z_h = z] = \langle \theta - \theta^*, W_h z \rangle = \langle \beta_h, z \rangle \in \mathcal{F}$, for any $R_h \in \mathbb{R}_h$ with $\beta_h = W_h^T(\theta - \theta^*)$, if the constant $U$ given in (5.3) is large enough. Similar situation also works for every coordinate of $G_h$. Thus, Assumption 5.3 given in §5.1 holds in this
case. Following (5.1) and (5.2), we have
\[ R^*_h = \left\{ \langle \theta - \theta^*, x \rangle \langle \beta, z \rangle : \mathcal{X} \times \mathcal{Z} \rightarrow \mathbb{R}; ||\theta - \theta^*||_2 \leq B, ||\beta||_2 \leq U \right\}, \]
(5.5)
\[ G^*_{h,j} = \left\{ \langle \theta - \theta_j, x \rangle \langle \beta, z \rangle : \mathcal{X} \times \mathcal{Z} \rightarrow \mathbb{R}; ||\theta - \theta_j^*||_2 \leq B, ||\beta||_2 \leq U \right\}. \]
(5.6)

Next, we discuss the corresponding ill-posed condition defined in Assumption 5.2 when both \( R^*_h(\cdot) \) and \( G^*_h(\cdot) \) fall in linear function classes.

**Assumption 5.5** (Ill-posed condition). We assume \( 0/0 = 0 \) and
\[
\sup_{x \in \mathbb{R}^d} x^\top \mathbb{E}_{x \sim \rho(x)} x_h x_h^\top \mathbb{E}_{z \sim \rho(z)} W_h z_h z_h^\top W_h^\top \leq \tau_h^2, \]
(5.7)

It is worth noting that Assumption 5.5 does not imply that the matrix \( \mathbb{E}_{x \sim \rho(x)} W_h z_h z_h^\top W_h^\top \) is invertible. With the convention \( 0/0 = 0 \), this assumption holds when the eigenspace of \( Z := \mathbb{E}_{z \sim \rho(z)} W_h z_h z_h^\top W_h^\top \) with respect to nonzero eigenvalues contains that of \( X := \mathbb{E}_{x \sim \rho(x)} x_h x_h^\top \).

Imagine an extreme case, where \( x_h = z_h \), we have the ill-posed coefficient is equal to 1 and this does not imply the invertibility of \( Z = E[x_h x_h^\top] \).

We observe from Theorem 5.1 that the suboptimality upper bound only involves the critical radius of \( F, R^*_h \) and \( G^*_h \), \( \forall j \in [d_1] \). As \( F \) is a linear space with finite dimension, its critical radius is of the order \( O(\sqrt{m/K}) \) (Wainwright, 2019). Meanwhile, as \( R^*_h \) can be viewed as the product of two linear spaces, each with finite dimensions, its critical radius is of order \( \delta_{R,h} = O(\sqrt{\max\{m,n_h\} \log K/K}) \) (Wainwright, 2019). Similar results also holds for \( G^*_h \forall j \in [d_1] \).

Plugging these results into the upper bound of Theorem 5.1, we obtain the following Corollary 5.1.

**Corollary 5.1.** Let \( F, R_h, G_h, R^*_h, G^*_h \) be defined as in (5.3),(5.4), (5.5) and (5.6), respectively. Assume that we construct confidence sets \( R_h, G_h \) and policy \( \hat{\pi} \) according to PLAN. Under Assumption 5.5, with probability \( 1 - \delta - 1/K \), we obtain
\[
\text{SubOpt}(\hat{\pi}) \leq \sum_{h=1}^{H} \tau_h C_{\pi^*}(H \cdot \sqrt{d_1 L_{K,d_1} + L_{K,1}}) \left( \sqrt{\max\{m,n_h\} \log K} + \sqrt{\frac{\log(Hd_1/\delta)}{K}} \right).
\]
Here \( L_{K,x} = L + \sigma \sqrt{\log(1 + \log K x)} \) with \( x \in \{1, d_1\} \) and \( L \) is the upper bound of all functions in \( R_h, G_{h,j}, \forall h \in [H], j \in [d_1] \) in \( \ell_\infty \)-norm.

**5.1.2 Example: Kernel Function Class**

In this subsection, we study an instantiation of Theorem 5.1 when \( R^*_h, G^*_h \forall j \in [d_1] \) lie in a RKHS. Before continuing, we first give a brief introduction to RKHS.

An RKHS is associated with a positive semidefinite kernel \( K : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R} \). Under mild regularity conditions, Mercer’s theorem guarantees that \( K \) admits an eigenexpansion of the form
\[
K(x, x') = \sum_{i=1}^{\infty} \mu_i \phi_i(x) \phi_i(x'),
\]
for a sequence of nonnegative eigenvalues \( \{\mu_i\}_{i \geq 1} \) and eigenfunctions \( \{\phi_i\}_{i \geq 1} \) which are orthogonal in \( L^2(\mathbb{P}) \). Here \( \mathbb{P}(\cdot) \) is some probability measure. Given such an expansion, the RKHS norm can be written as

\[
\|f\|_{\mathcal{H}}^2 = \sum_{i=1}^{\infty} \frac{\theta_i^2}{\mu_i} \quad \text{with} \quad \theta_i = \int_{\mathcal{X}} f(x)\phi_i(x) d\mathbb{P}(x).
\]

Thus, the induced RKHS by kernel \( K \) is written as

\[
\mathcal{H} := \left\{ f = \sum_{i=1}^{\infty} \theta_i \phi_i \mid \sum_{i=1}^{\infty} \frac{\theta_i^2}{\mu_i} < \infty \right\}.
\]

with the inner product

\[
\langle f, g \rangle_{\mathcal{H}} = \sum_{i=1}^{\infty} \frac{\langle f, \phi_i \rangle \langle g, \phi_i \rangle}{\mu_i}.
\]

Here \( \langle \cdot, \cdot \rangle \) denotes the inner product in \( L^2(\mathcal{X}, \mathbb{P}) \).

We assume \( R^*_h, G^*_h, j \in [d_1], \forall h \in [H] \) lie in the Reproducing Kernel Hilbert spaces (RKHS) \( \mathcal{H}_\mathcal{R}, \mathcal{H}_G \) with kernels \( K_\mathcal{R}(\cdot, \cdot) \) and \( K_\mathcal{G}(\cdot, \cdot) \) that are bounded in \( \ell_\infty \)-norm, respectively. The associated probability measure is the sampling probability measure \( \rho \). Moreover, in this subsection, we define covariate \( x_h := \phi_x(s_h, a_h, \omega_h) \in \mathcal{X} \) and instrumental variable \( z_h := \psi(s_h, a_h) \in \mathcal{Z} \) with some known embedding functions \( \phi_x(\cdot), \psi_z(\cdot) \).

To begin with, we define the function classes that contains \( r^*_h, G^*_h, j \in [d_1] \) as:

\[
\mathbb{R}_h = \left\{ R_h \in \mathcal{H}_\mathcal{R} : \mathcal{X} \rightarrow \mathbb{R}; \|R_h\|_{\mathcal{H}_\mathcal{R}}^2 \leq C_h^2 \right\},
\]

\[
\mathbb{G}_{h,j} = \left\{ G_{h,j} \in \mathcal{H}_G : \mathcal{X} \rightarrow \mathbb{R}; \|G_{h,j}\|_{\mathcal{H}_G}^2 \leq C_h^2 \right\}, \forall j \in [d_1],
\]

where \( C_h^2 \) is a constant only depending on \( h \). In addition, the test function class \( \mathcal{F} \) in RKHS \( \mathcal{H}_\mathcal{F} \) with \( \ell_\infty \)-bounded kernel \( K_\mathcal{F} \) is given as follows:

\[
\mathcal{F} = \left\{ f \in \mathcal{H}_\mathcal{F} : \mathcal{Z} \rightarrow \mathbb{R}; \|f\|_{\mathcal{H}_\mathcal{F}}^2 \leq C_1^2 \right\},
\]

in which \( C_1 \) is an absolute constant.

Similar to Assumption 5.3, in the example with RKHS, the test function class \( \mathcal{F} \) with kernel \( K_\mathcal{F} \) is also assumed to contain the projected functions from \( \mathbb{R}_h, \mathbb{G}_{h,j}, \forall h \in [H], j \in [d_1] \). In addition, we deduce

\[
\mathcal{R}^*_h = \{(R_h - R^*_h)(x)\mathbb{T}(R_h - R^*_h)(z) : R_h \in \mathcal{H}_\mathcal{R}, \|R_h - R^*_h\|_{\mathcal{H}_\mathcal{R}}^2 \leq C_3^2 \},
\]

and

\[
\mathcal{G}^*_{h,j} = \{(G_{h,j} - G^*_{h,j})(x)\mathbb{T}(G_{h,j} - G^*_{h,j})(z) : G_{h,j} \in \mathcal{H}_\mathcal{G}, \|G_{h,j} - G^*_{h,j}\|_{\mathcal{H}_\mathcal{G}}^2 \leq C_3^2 \},
\]

\( \forall h \in [H], \forall j \in [d_1] \), from (5.1), (5.2), respectively.
According to the Proposition 12.31 of Wainwright (2019), the space $\mathcal{R}_h^*, \forall h \in [H]$ also admits a reproducing kernel, defined as

$$K_{\mathcal{R}_h^*}((x, z), (x^*, z^*)) = K(x, x^*)K(z, z^*),$$

if the inner product of $\mathcal{R}_h^*$ is defined as $\langle R_h f_h, \tilde{R}_h f_h \rangle_{\mathcal{R}_h^*} = \langle R_h, \tilde{R}_h \rangle_{\mathcal{H}_K} (f_h, \tilde{f}_h)_{\mathcal{H}_F}$. Similar situation also holds for $G_{h,j}^*, \forall j \in [d_1], h \in [H]$.

Finally, we discuss the ill-posed condition in RKHS as follows.

**Assumption 5.6.** We assume

$$\max_{R_h \in \mathbb{R} : \mathbb{E}_p[\mathbb{T}(R_h-R_h^*)^2(z_h)] \leq x^2} \mathbb{E}_p\left[\left(R_h - R_h^*\right)^2(x_h)\right] \leq \tau_r^2(x), \forall h \in [H],$$

$$\max_{G_{h,j} \in \mathbb{R} : \mathbb{E}_p[\mathbb{T}(G_{h,j}-G_{h,j}^*)^2(z_h)] \leq x^2} \mathbb{E}_p\left[\left(G_{h,j} - G_{h,j}^*\right)^2(x_h)\right] \leq \tau_G^2(x), \forall h \in [H], j \in [d_1],$$

where $\tau_r(x), \tau_G(x)$ are fixed functions that only depends on $x$ and the associated probability measure is the sample distribution $\rho$.

**Remark 5.1.** In this remark, we provide more details on functions $\tau_r(\cdot)$, as $\tau_G(\cdot)$ can be analyzed in the same way. Let $I = \{1, \ldots, m\}$, $Z_{m,h} = \mathbb{E}[\mathbb{E}[e_I(x_h) | z_h] \mathbb{E}[e_I(x_h) | z_h]^T]$, where $e_I(x_h)$ is the first $m$ eigenfunctions of RKHS with kernel $K_{\mathcal{R}}$. If

- $\lambda_{\min}(Z_{m,h}) \geq \tau_m$,
- $\forall i \leq m < j$, $|\mathbb{E}[\mathbb{E}[e_i(x_h) | z_h] \mathbb{E}[e_j(x_h) | z_h]^T]| \lesssim \tau_m$,

then it holds that $\tau_r^2(\delta) \lesssim \min_m \left( \frac{4m^2}{\tau_m^2} + C\lambda_{m+1} \right)$, where $\lambda_{m+1}$ is the $(m+1)$-th eigenvalue of $K_{\mathcal{R}}$, by Lemma 11 in Dikkala et al. (2020). Specifically, we have the following explicit results on $\tau_r^2(\delta)$.

- If $\lambda_m \sim m^{-b}, \tau_m \geq m^{-a}, a, b > 0$, we have $\tau_r^2(\delta) \sim \delta^{\frac{2a}{a+b}}$.
- If $\lambda_m \sim e^{-m}, \tau_m \geq m^{-a}, a > 0$, we have $\tau_r^2(\delta) \sim \delta^2 \log(1/\delta)^{a}$.
- If $\lambda_m \sim e^{-bm}, \tau_m \geq e^{-am}, a > 0$, we have $\tau_r^2(\delta) \sim \delta^{\frac{2b}{a+b}}$.
- If $\lambda_m \sim m^{-b}, \tau_m \geq e^{-m}$, we have $\tau_r^2(\delta) \sim 1/\log(1/\delta)^{2b}$.

The aforementioned remark illustrates that the ill-conditioned coefficient in every stage $h$ is determined by the relative decaying speed of eigenvalues of $K_{\mathcal{R}}$ and $Z_m,h$. With these necessary components at hand, we present the corollary of Theorem 5.1 for the kernel setting as follows.

**Corollary 5.2.** Suppose $R_h^*$ and $G_{h,j}^*, \forall j \in [d_1]$ lie in the function classes (5.8) and (5.9). Under Assumptions 5.1 and 5.3, by constructing our policy $\hat{\pi}$ using the same way with (4.7), with function classes defined above, we obtain
If the eigenvalues of all kernels $K_{R^*_h}, K_{G^*_h}, K_{\mathcal{F}}$ defined in this section decay exponentially, with rate $\exp(-i)$, with probability $1 - \delta - 1/K$, we obtain

$$
\text{SubOpt}(\tilde{\pi}) \lesssim \sum_{h=1}^{H} C_{\pi^*} \left[ H \sqrt{d_1} \tau_G \left( L_{K,d_1} \left( \sqrt{\log \frac{K}{K}} + \sqrt{\frac{\log(d_1/\delta)}{K}} \right) \right) 
\right.
\left. + \tau_r \left( L_{K,1} \left( \sqrt{\log \frac{K}{K}} + \sqrt{\frac{\log(d_1/\delta)}{K}} \right) \right) \right].
$$

If the eigenvalues of all kernels decay polynomially, with rate $i^{-\alpha}, \alpha > 1$, with probability $1 - \delta - 1/K$, we have

$$
\text{SubOpt}(\tilde{\pi}) \lesssim \sum_{h=1}^{H} C_{\pi^*} \left[ H \sqrt{d_1} \tau_G \left( L_{K,d_1} \left( \sqrt{\log \frac{K}{K^{\alpha/(\alpha+1)}}} + \sqrt{\frac{\log(d_1/\delta)}{K}} \right) \right) 
\right.
\left. + \tau_r \left( L_{K,1} \left( \sqrt{\log \frac{K}{K^{\alpha/(\alpha+1)}}} + \sqrt{\frac{\log(d_1/\delta)}{K}} \right) \right) \right].
$$

Here $L_{K,x} = L + \sigma \sqrt{(\log H + 1) \log(Kx)}$ with $x \in \{1, d_1\}$ and $L$ being the upper bound of all functions in $\mathbb{R}_h, \mathcal{G}_{h,j}, \forall h \in [H], \forall j \in [d_1]$ in $\ell_\infty$-norm.

In aforementioned examples, results are established based on the realizability of function classes, which could be restrictive. In the following, we relax such case by allowing function class misspecification.

### 5.2 Suboptimality under Misspecified Functional Classes

In this subsection, we establish theoretical guarantees for PLAN under function class misspecification. We utilize function classes $\tilde{R}_h, \tilde{G}_{h,j}$, which may not contain the true reward and transition functions, to estimate the model and solve the planning problem.

In specific, we let

$$
\tilde{\pi}^M = \argmax_{\pi \in \Pi} \min_{M \in \mathcal{M}^M} J(M, \pi)
$$

where $\mathcal{M}^M := \{ (\tilde{\mathcal{G}}_h^M, \tilde{R}_h^M) \}_{h=1}^{H}$ are confidence sets constructed in the same way as §4.3.2 via function classes $\tilde{\mathcal{R}}_h, \tilde{\mathcal{G}}_{h,j}, j \in [d_1], h \in [H]$.

In terms of theoretical analysis, we characterize two kinds of the misspecification errors in the following assumption.

**Assumption 5.7.** We present two approximation errors on both primal and dual function classes:

- (Primal Function Class) For all $h \in [H], j \in [d_1]$, we have

$$
\min_{R_h \in \tilde{R}_h} \| R_h(\cdot) - R^*_h(\cdot) \|_\infty \leq \eta_{r,h,K},
$$

$$
\min_{G_{h,j} \in \tilde{G}_{h,j}} \| G_{h,j}(\cdot) - G^*_h(\cdot) \|_\infty \leq \eta_{G,h,K}.
$$

Moreover, we assume the corresponding elements that achieve the minimum approximation error to $R^*_h(\cdot), G^*_h(\cdot)$ in $\ell_\infty$-norm exist and are denoted by $R^0_h(\cdot), G^0_{h,j}(\cdot), \forall h \in [H], j \in [d_1]$, respectively.
• (Dual Function Class) We assume $\mathcal{F} := \{ f : \mathcal{Z} \to [-L, L]\}$ is a symmetric and star-shaped function class and

$$
\forall R_h \in \tilde{R}_h, \min_{f \in \mathcal{F}} \| f(s_h, a_h) - \mathbb{T}(R_h - R_h^0)(s_h, a_h) \|_2 \leq \xi_{r, h, K},
$$

$$
\forall j \in [d_1], \forall G_{h,j} \in \tilde{G}_{h,j}, \min_{f \in \mathcal{F}} \| f(s_h, a_h) - \mathbb{T}(G_{h,j} - G_{h,j}^0)(s_h, a_h) \|_2 \leq \xi_{G_{h,j}, h},
$$

in which the probability measure is $\rho$.

For all $R_h \in \mathbb{R}_h, G_{h,j} \in \mathbb{G}_{h,j}$, we let $f_{R_h} = \arg\min_{f \in \mathcal{F}} \| f - \mathbb{T}(R_h - R_h^0) \|_2, f_{G_{h,j}} = \arg\min_{f \in \mathcal{F}} \| f - \mathbb{T}(G_{h,j} - G_{h,j}^0) \|_2$. Meanwhile, for all $h \in [H]$, we denote

$$
\tilde{R}^*_h := \left\{ c(R_h - R_h^0)(x) \cdot f_{R_h}(z) : \mathcal{X} \times \mathcal{Z} \to \mathbb{R}; R_h \in \tilde{R}_h, \forall c \in [0, 1] \right\},
$$

(5.12)

$$
\tilde{G}^*_{h,j} := \left\{ c(G_{h,j} - G_{h,j}^0)(x) \cdot f_{G_{h,j}}(z) : \mathcal{X} \times \mathcal{Z} \to \mathbb{R}; G_{h,j} \in \tilde{G}_{h,j}, \forall c \in [0, 1] \right\}, \forall j \in [d_1].
$$

(5.13)

The corresponding thresholding parameters $c_{r,h,K}$ and $c_{G,h,K}$ involved in the high-confidence sets given in §4.3.2 are specified as $c_{r,h,K} = O(\delta_{R,h,\delta} + \eta_{r,h,K}) = O(\delta_{R,h} + \sqrt{\log(H/\delta)/K} + \eta_{r,h,K})$ and $c_{G,h,K} := O(\delta_{G,h,\delta} + \eta_{G,h,K}) = O(\delta_{G,h} + \sqrt{\log(Hd_1/\delta)/K} + \eta_{G,h,K})$, respectively. Here $\delta_{R,h}$ is maximum the critical radii of $\mathcal{F}$, $\tilde{R}^*_h$, and $\delta_{G,h}$ is the maximum critical radii of $\mathcal{F}$ and $\tilde{G}^*_{h,j}$, $\forall j \in [d_1]$.

Combining all assumptions mentioned above, we present the following theorem on the suboptimality of $\tilde{\pi}^*$.

**Theorem 5.2.** Under Assumptions 5.1, 5.2 (with replacing $R^*_h, G^*_{h,j}$ by $R^0_h$ and $G^0_{h,j}$, $\forall h \in [H], j \in [d_1]$), and Assumption 5.7, with probability $1 - \delta - 1/K$, the suboptimality is upper bounded by

$$
\text{SubOpt}(\tilde{\pi}^*) \lesssim C_{\pi^*} \left[ \sum_{h=1}^{H} \tau_{K,h} \sqrt{d_1} L_{K,d_1} \left( \delta_{G,h,\delta} + \xi_{G,h,K} + \frac{\eta_{G,h,K}^2}{\delta_{R,h,\delta}} + \eta_{G,h,K} \right) 
\right]^2,
$$

$$
+ \sum_{h=1}^{H} \tau_{K,h} L_{K,1} \left( \delta_{r,h,\delta} + \xi_{r,h,K} + \frac{\eta_{r,h,K}^2}{\delta_{G,h,\delta}} + \eta_{r,h,K} \right)
$$

where $L_{K,x} = L + \sigma \sqrt{\log(H + 1) \log(Kx)}$, with $x \in \{1, d_1\}$, $\delta_{R,h,\delta} = \delta_{R,h} + \sqrt{\log(H/\delta)/K}$, and $\delta_{G,h,\delta} = \delta_{G,h} + \sqrt{\log(Hd_1/\delta)/K}$. Moreover, if we choose proper function classes such that $\delta_{G,h,\delta} = \Theta(\eta_{G,h,K})$ and $\delta_{R,h,\delta} = \Theta(\eta_{r,h,K})$, the aforementioned upper bound reduces to

$$
\text{SubOpt}(\tilde{\pi}^*) \lesssim C_{\pi^*} \left[ \sum_{h=1}^{H} \tau_{K,h} \sqrt{d_1} L_{K,d_1} \left( \delta_{G,h,\delta} + \xi_{G,h,K} \right) \sum_{h=1}^{H} \tau_{K,h} L_{K,1} \left( \delta_{R,h,\delta} + \xi_{r,h,K} \right) \right].
$$

Theorem 5.2 presents an upper bound for the suboptimality under misspecified function classes. Besides the critical radii of involved function classes, the upper bound also involves the approximation errors induced by misspecification. If one chooses approximation function classes properly, one is able to balance the bias and variance and achieve minimax optimal statistical rates of estimating functions in the true function class. To illustrate this idea, we provide a concrete example using the class of neural networks to approximate the Sobolev ball in Appendix §E.2.1.
6 Applications

This section discusses two applications of strategic MDP, including strategic regression, strategic bandits.

6.1 Strategic Regression

In this subsection, we show that the strategic regression proposed by Harris et al. (2021b), where the principal interacts with an agent in one round with no state transition, is a special case of the strategic MDP. Their setting admits a specific example on college exams:

- The principal (school) announces some information on evaluation criterion $a$ before the final exam, such as “At least 50% of problems in the final exam are about math”.

- The agent (student) maximizes its reward by taking some action $b \in \mathbb{R}^d$, such as reviewing math knowledge given the information $a \in \mathbb{R}^d$ and its private information $i := (z, W)$. Here $z \in \mathbb{R}^d$ denotes the baseline ability of that student, and $W \in \mathbb{R}^{d \times d}$ represents the effort transition matrix. In specific, the agent takes

$$b = \arg\max_b R_a(b, a, i),$$

where $R_a(b, a, i) = (z + Wb)^\top a - \frac{1}{2} \|b\|_2^2$. In simple terms, we have $b = W^\top a$.

- Principal observes the feature manipulated by the student $o = (z + Wb) = (z + WW^\top a)$.

- Principal obtains reward $r = o^\top \theta^* + g$ which represents the overall score the student obtain (including math). Here $g$ is a mean zero random variable that is correlated with the baseline ability $z$ of that student but is independent with $a$.

We next design a policy of the principal to maximize overall score $\mathbb{E}[r]$ for a specific population of agents (e.g., overall score of students who major in literature). In this scenario, the distribution $P(\cdot)$ of private information $i$ of this population is assumed to be known in the planning stage. When faced with such a population, the marginalized reward function of the principal is given by:

$$\bar{R}(a) = \mathbb{E}_{o \sim P(\cdot | a)}[o^\top \theta | a] = \mathbb{E}_{(z, W) \sim P(\cdot)}[(z + W W^\top a)^\top \theta | a],$$

where $P(o | a)$ is the conditional distribution of $o$ given $a$ when $i \sim P(\cdot)$. Moreover, the function class that contains the true reward function $R^*(\cdot) = \langle \cdot, \theta^* \rangle$ is defined as:

$$\mathbb{R}_1 = \left\{ \langle \theta, o \rangle : o \to \mathbb{R}; \|\theta\|_2 \leq B, \theta \in \mathbb{R}^d \right\},$$

which is a special case of our example in §5.1.1. In this scenario, the value function evaluated by policy $\pi$ under the true model $\bar{R}^*(a) = \mathbb{E}_{o \sim P(\cdot | a)}[o^\top \theta^* | a]$ reduces to

$$J(\bar{R}^*, \pi) := \mathbb{E}_{a \sim \pi}[\bar{R}^*(a)].$$
Let $\pi^*$ be the optimal policy that maximizes $J(\bar{R}^*, \pi)$. Therefore, for any given policy $\pi \in \Delta(\mathcal{A})$, the suboptimality of $\pi$ is given by

$$\text{SubOpt}(\pi) = J(\bar{R}^*, \pi^*) - J(\bar{R}^*, \pi).$$

(6.1)

Our goal is to design a certain policy that minimizes this suboptimality.

In this application, we assume the offline data $\{a_t, o_t, r_t\}_{t=1}^K$ are collected i.i.d. with $(a_t, o_t) \sim \rho(a, o)$. By our model formulation and Definition 4.2, we see that $a$ serves as the instrumental variable for $(o, r)$ (Harris et al., 2021b).

Next, we apply $\text{PLAN}$ with $H = 1$ and linear functions (introduced in §5.1.1), covariate $x = a$, and instrumental variable $z = a$ to derive a policy $\hat{\pi}$. It is worth noting that the ill-posed coefficient under the setting reduces to

$$\sup_{x \in \mathbb{R}^d} x^T \mathbb{E}_{o \sim \rho(o)} [oo^T] x \leq \tau_1^2.$$

With these necessary tools at hand, we summarize our conclusion in the following Proposition 6.1.

**Proposition 6.1.** Given the settings in §6.1 and Assumptions 5.1 and 5.5, with probability $1 - \delta - 1/K$, we have

$$\text{SubOpt}(\hat{\pi}) \lesssim \tau_1 C_{\pi^*} L_K \left( \sqrt{\frac{d \log K}{K}} + \sqrt{\frac{\log(c_0/\delta)}{K}} \right).$$

Here $L_K = L + \sigma \sqrt{\log(K)}$ with $L$ being the upper bound of all functions in $\mathbb{R}_1$ in $\ell_\infty$-norm.

We deduce from Proposition 6.1 that the suboptimality is proportional to $O(\sqrt{d/K})$, which is minimax optimal in the linear class.

### 6.2 Strategic Bandit

In this section, we apply $\text{PLAN}$ to strategic bandit problem where the principal interacts with the agents by taking actions in two rounds. One possible real-world application is the interaction between some information providers (stock information provider, medical treatment specialist, insurance company, and etc) and strategic agents (Sayin and Ba¸sar, 2018). For example, in the stock market, if some information provider distributes some information about the future stock market, the strategic agents will manipulate their features by selling or buying more stocks given such information. In this scenario, the information provider will profit by taking a second action based on the agents’ manipulated features. Besides, other real-world examples such as the interaction between a medical treatment provider or an insurance company and strategic agents also fit in this setting.

We call this framework as strategic bandit mathematically and formulate it as follows.

**Definition 6.1** (Strategic Bandit). The interaction protocol is specified as follows:

- The principal first announces an action $a_1$. 


• Given the principal’s first action $a_1$, a myopic agent with private type $i \sim P(\cdot)$ takes an action to maximize its immediate reward: $b = \arg\max_b R^\pi_1(a_1, i, b)$.

• The principal receives an observation $o \sim F(\cdot | a_1, i) := F(a_\cdot | b, i)$ that is the feature generated by the agent based on its private type $i$ and the principal’s action $a_1$ (through $b$).

• The principal takes the second action $a_2$ based on observation $o$ and receives a reward $r = R^*(o, a_2) + g$, where $g$ is a mean zero random variable but is affected by the private information $i$ of the agent.

Our goal is learning the optimal policy of the principal i.e., maximizing the principal’s expected reward $E[r]$ for a specific population of agents, whose distribution of private type $P(\cdot)$, private reward function $R^*(\cdot)$ and $F(\cdot | a_1, i)$ are known to the principal in the planning stage.

We consider the function class $R, \pi \in \mathbb{R}_1$. For any given reward model $R(\cdot) \in \mathbb{R}_1$ and policy $\pi \in \Pi = \{\pi_1 \times \pi_2 : \pi_1 \in \Delta(A_1), \pi_2 : O \rightarrow \Delta(A_2)\}$, under a specific population of agents, the value function is defined as follows:

$$J(R, \pi) = \int [R(o, a_2) | o] d\pi(a_2 | o)dF(o | a_1, i)dP(i)d\pi(a_1).$$

Let $\pi^*$ be the optimal policy that maximizes $J(R^*, \pi)$. For any given policy $\pi$, we define the suboptimality as

$$\text{SubOpt}(\pi) = J(\tilde{R}^*, \pi^*) - J(R^*, \pi). \quad (6.2)$$

In this application, we assume our offline data $\{a_{t1}, a_{t2}, r_t\}_{t=1}^K$ is collected i.i.d. with $(a_{t1}, a_{t2}) \sim \rho(a_1, o, a_2)$. From the statement of model formulation given above, one observes that $a_1$ serves as an instrumental variable for $(o_t, a_1, r)$ by Lemma 4.1 based on Definition 4.2.

The way of constructing confidence sets and policy $\hat{\pi}$ are almost the same with that in §4.3.2, by treating $(o, a_2)$ as the covariate and $a_1$ as the instrumental variable. Therefore, we omit the relevant details. We next state the assumptions on concentrability coefficient in order to establish theoretical guarantees for $\hat{\pi}$.

**Assumption 6.1 (Concentrability Coefficients).** We assume

$$\sup_{a_1, a_2, o} \frac{f_{\pi^*}(a_2 | o)f_p(o | a_1)f_{\pi^*}(a_1)}{f_{\rho}(o, a_1, a_2)} \leq C_{\pi^*}^2.$$

In this assumption, we let the ratio of two densities, namely, the joint density of $(a_1, o, a_2)$ induced by the optimal policy for a specific population of agents and the sampling density $f_{\rho}$, be bounded by a concentrability coefficients $C_{\pi^*}^2$. Here $f_p(o | a_1) = \int_i dF(o | a_1, i)dP(i)$ and is assumed known in the planning stage.

Besides, other assumptions on the ill-posed condition and completeness of function class $F$ are also almost the same with Assumptions 5.2 and 5.3 by treating $(o, a_2)$ as the covariate and $a_1$ as the instrumental variable. In specific, we let $\tau_1$ be the associated ill-posed coefficient such that

$$\sup_{R \in \mathbb{R}_1 - R^*} \frac{\mathbb{E}_p[R^2(o_1, a_{2t})]}{\mathbb{E}_p[|R(o_1, a_{2t}) | a_{1t}|^2]} \leq \tau_1^2.$$
Combining these assumptions, we provide an upper bound on the suboptimality of \( \hat{\pi} \) constructed by \textsc{plan} in the following proposition.

**Proposition 6.2.** Under Assumption 6.1, Assumptions 5.2 and 5.3 (treating \((o, a_2)\) as the covariate and \(a_1\) as the instrumental variable), with probability \(1 - \delta - 1/K\), we obtain

\[
\text{SubOpt}(\hat{\pi}) \lesssim C_\pi \tau_1 \delta_{R, \delta},
\]

where \(\delta_{R, \delta} = \delta_R + \sqrt{\log(c_0/\delta)/K}\) with \(\delta_R\) being the upper bound of the critical radii of \(F\) and \(R^* := \{(a_{2t}, o_t, a_{1t}) \rightarrow c(R(a_{2t}, o_t) - R^*(a_{2t}, o_t)) \cdot E[R(a_{2t}, o_t) - R^*(a_{2t}, o_t) | a_{1t}], \forall R \in \mathbb{R}_1, \forall c \in [0, 1]\}\).

In addition to strategic regression and bandits, our algorithm \textsc{plan} also works for the principal when noncompliant agents exist in the recommendation system, as discussed in Example 3.1. We present the corresponding paragraph in the Appendix §F.3.

### 7 Conclusion

In this paper, we study multi-agent reinforcement learning with information asymmetry and propose a general framework named strategic MDP to model the interaction between the principal and strategic agents. We design a provably efficient algorithm \textsc{plan} using instrumental variable regression and pessimism principal with general function approximation to handle the challenges of studying the strategic MDP, including the existence of unobserved confounders and distribution shift. We prove that \textsc{plan} outputs near optimal policy under mild conditions. Our framework also admits several real-world examples such as strategic regression, strategic bandits, and non-compliance agents in recommendation systems as exceptional cases.

There are a few future directions that are worth exploring. First, it would be interesting to study the online setting of strategic MDP. In addition, we consider the interaction between one principal with multiple agents. It will be appealing to extend strategic MDP to the setting with multiple principals that are either cooperative or competitive.
A Additional Related Works

Our work is also related to the literature on offline RL in stochastic games. Most of the existing works focus on two-player zero-sum stochastic games. See, e.g., Lagoudakis and Parr (2012); Perolat et al. (2015); Pérolat et al. (2016b); Fan et al. (2019); Zhao et al. (2021); Pérolat et al. (2016a); Alacaoglu et al. (2022); Cui and Du (2022b); Zhong et al. (2022); Xiong et al. (2022); Yan et al. (2022b); Cui and Du (2022a) and the references therein. In addition, Pérolat et al. (2017); Cui and Du (2022a) study offline RL for general-sum stochastic games and Zhong et al. (2021) study Stackelberg equilibria in stochastic games with myopic followers via offline RL. All of these works consider the settings where the learner has complete information, and thus do not face the issue of unobserved confounders. Furthermore, there is a recent line of research that develops decentralized online reinforcement learning algorithms for stochastic games, where the goal is to learn the optimal policy from the perspective of a single player based on its local information (Wei et al., 2017; Xie et al., 2020; Tian et al., 2021; Song et al., 2021; Jin et al., 2021a; Sayin et al., 2021; Liu et al., 2022b; Zhan et al., 2022; Kao et al., 2022; Mao et al., 2022). In such a decentralized setting, it shown in Liu et al. (2022b) that, when the actions of the opponent are hidden, learning the optimal policy in hindsight against an arbitrarily adversarial opponent is statistically intractable. Thus, existing works mainly focus on either learning the value of the game (Wei et al., 2017; Xie et al., 2020; Tian et al., 2021), or the optimal policy based on some side information (Liu et al., 2022b; Zhan et al., 2022), or finding Nash or correlated equilibria in the tabular setting (Song et al., 2021; Jin et al., 2021a; Sayin et al., 2021; Kao et al., 2022; Mao et al., 2022). Compare to these works, we also design a learning algorithm for a single player, namely the principal, who is unaware of the private information of the agents. However, we focus on the offline setting where the private information brings the challenge of confounding. Thus, our work is not directly comparable to these works.

Meanwhile, our work adds to the rapidly growing literature on strategic classification. See, e.g., Dalvi et al. (2004); Brückner and Scheffer (2011); Alacaoglu et al. (2022); Brückner et al. (2012); Hardt et al. (2016); Dong et al. (2018); Hu et al. (2019); Milli et al. (2019); Miller et al. (2020); Ghalme et al. (2021); Ahmadi et al. (2021); Levanon and Rosenfeld (2021); Zrnic et al. (2021); Nair et al. (2022) and the references therein. In addition to classification, various works study regression and ranking models under strategic manipulations (Liu and Chen, 2016; Shavit et al., 2020; Bechavod et al., 2020; Gast et al., 2020; Harris et al., 2021b,a; Liu et al., 2022a). Moreover, there is a line of research on performative prediction, which is a general framework of machine learning models with strategic data (Perdomo et al., 2020; Mendler-Dünner et al., 2020; Miller et al., 2021; Narang et al., 2022; Brown et al., 2022; Li and Wai, 2022; Jagadeesan et al., 2022). These works can all be formulated as a stackelberg game between the machine learning model and an agent, where the machine learning models performs certain prediction about the agent, while the agent strategically manipulates its feature in order to maximize its own reward. Among these works, our work is particularly related to Miller et al. (2020); Harris et al. (2021b); Shavit et al. (2020), which study strategic classification and regression from a causal inference perspective. In particular, under the setting of strategic regression, Harris et al. (2021b) show that the announced regression model serves as a valid instrument. Our work generalize such a key observation to the dynamic setting with sequential interactions.
B Proof of Results in §4

In this section, we provide the proof of Lemma 4.1.

B.1 Proof of Lemma 4.1

Proof of Lemma 4.1. We prove that for any given \( h \in [H] \), \((s_h, a_h)\) serves as an instrumental variable for \((\phi_x(s_h, a_h, o_h), r_h)\) and \((\phi_x(s_h, a_h, o_h), s_{h+1})\). We see that \( Z_h := (s_h, a_h) \) affects \( X_h := \phi_x(s_h, a_h, o_h) \) by the definition of \( o_h \), which justifies the first point of Definition 4.2. To demonstrate the second point, we observe that \( Z_h := (s_h, a_h) \) is independent with \( g_h, \xi_h \) by our Definition 3.1 and Assumption 4.1 and thus affects \((r_h, s_{h+1})\) only through \( X_h \). Thus, the second point of Definition 4.2 is also satisfied. Combining the arguments given above, we conclude our proof of Lemma 4.1.

C Proof of Theorem 5.1

In this section, we will prove Theorem 5.1, which establishes the suboptimality of \( \hat{\pi} \) returned by PLAN.

Proof of Theorem 5.1. First, we prove that for any \( h \in [H] \), \( R_h^* (\cdot) \), \( G_h^* (\cdot) \) belong to the confidence sets \( R_h, G_h \) with high probability, respectively. We summarize the results in the following lemma.

Lemma C.1. Given the confidence sets \( R_h, G_h, \forall h \in [H], j \in [d_1] \) constructed in (4.8) and (4.9), for any \( h \in [H] \), with probability \( 1 - \delta - 1/(d_1 K)^\beta \), we have

\[
R_h^* \in R_h = \left\{ R_h \in \mathbb{R}_+ : L_n(R_h) - L_n(\hat{R}_h) \lesssim L_{K,\beta,1}^2 \delta_{R_h,\delta} \right\},
\]

\[
G_h^* \in G_h = \left\{ G_h \in (G_{h,1}, G_{h,2}, \ldots, G_{h,d_1}) : \right\},
\]

where \( G_h, \forall h \in [H] \), with probability \( 1 - \delta - 1/(d_1 K)^\beta \), we have

\[
G_h, G_h^* \in G_h = \left\{ G_h \in \mathbb{R}_+ : L_n(G_h) - L_n(\hat{G}_h) \lesssim L_{K,\beta,1}^2 \delta_{G_h,\delta} \right\}.
\]

Here we let \( \delta_{R_h,\delta} = \delta_{R_h} + c_1 \sqrt{\log(c_0 / \delta) / K}, \delta_{G_h,\delta} = \delta_{G_h} + c_2 \sqrt{\log(c_0 d_1 / \delta) / K} \) and \( L_{K,\beta,1} := L + \sigma \sqrt{\beta} / K d_1 \) with \( c_0, c_1, c_2 \) being absolute constants. Moreover, \( \delta_{R_h} \) is an upper bound of the maximum critical radius of \( F, G_h, G_h^* \forall j \in [d_1] \) (defined in (5.2)) and \( \delta_{R_h} \) is an upper bound of the maximum radius of \( F, R_h^* \) (defined in (5.1)).

Proof. See §C.1 for a detailed proof.

After proving that the true model lies in the confidence sets with high probability, we next show that the suboptimality given in (6.2) is bounded by the estimation errors of the pessimistic models. We summarize these results in the following Lemma C.2.
Lemma C.2. We let $\bar{M} := \{(\bar{R}_h, \bar{P}_h)\}_{h=1}^H = \text{argmin}_{M \in \mathcal{M}} V_M^\pi$, where $\mathcal{M}$ is the confidence set defined in (4.7). Then we have

$$J(M^*, \pi) - J(M^*, \hat{\pi}) \leq H \sum_{h=1}^H \mathbb{E}_{a_h \sim \pi^*(\cdot | s_h), s_h \sim d_h^{\pi^*}} \left[ \left\| (\bar{P}_h - \bar{P}_h^\pi)(\cdot | s_h, a_h) \right\|_1 \right]$$

$$+ \sum_{h=1}^H \mathbb{E}_{a_h \sim \pi^*(\cdot | s_h), s_h \sim d_h^{\pi^*}} \left[ \left\| \bar{R}_h(s_h, a_h) - \bar{R}_h^*(s_h, a_h) \right\| \right], \quad (C.1)$$

where $d_h^{\pi^*}$ represents the distribution of state $s_h$, which is generated by following policy $\pi^*$ and the true transition functions $\{\bar{P}_h\}_{j=1}^H$ defined in (3.6).

Proof. See §C.2 for a detailed proof. \qed

Next, we prove that for all functions in the confidence sets $\mathcal{R}_h, \mathcal{G}_h, \forall h \in [H]$, their projected MSEs are small. We summarize this property in the following lemma.

Lemma C.3. For all $R_h, G_h$ given in $\mathcal{R}_h, \mathcal{G}_h$, with probability $1 - H \delta - H/(Kd_1)^{\beta}$, we have

$$\mathbb{E}_\rho \left[ \mathbb{E}_\rho \left[ R_h(s_h, a_h, o_h) - R_h^*(s_h, a_h, o_h) | s_h, a_h \right]^2 \right] \leq L^2_{K, \beta, 1} \delta^2_{R,h, \delta}, \quad (C.2)$$

$$\mathbb{E}_\rho \left[ \mathbb{E}_\rho \left[ G_h(s_h, a_h, o_h) - G_h^*(s_h, a_h, o_h) | s_h, a_h \right]^2 \right] \leq d_1 L^2_{K, \beta, d_1} \delta^2_{G,h, \delta}. \quad (C.3)$$

Proof. See §C.3 for a detailed proof. \qed

Finally, we utilize conclusions from Lemma C.1, Lemma C.2 and Lemma C.3 to prove Theorem 5.1. Specifically, by Lemma C.2, we have

$$(I) := \mathbb{E}_{a_h \sim \pi^*(\cdot | s_h), s_h \sim d_h^{\pi^*}} \left[ \left\| (\bar{P}_h - \bar{P}_h^\pi)(\cdot | s_h, a_h) \right\|_1 \right]$$

$$= \mathbb{E}_{a_h \sim \pi^*(\cdot | x_h), s_h \sim d_h^{\pi^*}} \left[ \int_{i_h, o_h} \bar{P}(\cdot | s_h, a_h, o_h, i_h) - \bar{P}^*(\cdot | s_h, a_h, o_h, i_h) dF_h(o_h | s_h, a_h, i_h) dP_h(i_h) \right]$$

$$\leq \mathbb{E}_{a_h \sim \pi^*(\cdot | s_h), s_h \sim d_h^{\pi^*}} \left[ \int_{i_h, o_h} \bar{P}(\cdot | s_h, a_h, o_h, i_h) - \bar{P}^*(\cdot | s_h, a_h, o_h, i_h) dF_h(o_h | s_h, a_h, i_h) dP_h(i_h) \right]$$

$$\leq \mathbb{E}_{a_h \sim \pi^*(\cdot | x_h), s_h \sim d_h^{\pi^*}, i_h \sim P_h(\cdot | s_h, a_h), o_h \sim F_h(\cdot | s_h, a_h, i_h)} \left[ \text{TV}(\bar{P}_h(\cdot | s_h, a_h, o_h, i_h), \bar{P}_h^\pi(\cdot | s_h, a_h, o_h, i_h)) \right]^2$$

Here the first inequality follows from Jensen’s inequality. In addition, the second inequality follows from Cauchy-Schwartz inequality and the relation between total variation distance and $\ell_1$-distance, namely, $\text{TV}(P, Q) = \|P - Q\|_1/2$ for any two probability measures $P, Q$ (Levin and Peres, 2017). Next, we leverage our assumption on Gaussian transition in §3 to derive an upper bound for $(I)$. 31
To be more specific, we have

$$\mathbb{E}_{a_h \sim \pi^* \cdot \mid s_h), s_h \sim d^*_h, o_h \sim P_h \cdot \mid s_h, a_h) \left[ \left\| \tilde{G}_h(s_h, a_h, o_h) - G^*_h(s_h, a_h, o_h) \right\|^2 \right] \leq C_{\pi^*} \left( \mathbb{E}_{\rho(s_h, a_h, o_h)} \left[ \left\| \tilde{G}_h(s_h, a_h, o_h) - G^*_h(s_h, a_h, o_h) \right\|^2 \right] \right) \leq C_{\pi^*} \tau_{K,G,h} \sqrt{d_1 L_{K,\beta,d_1} \delta_h, \rho, \delta}. \quad (C.4)$$

Here $P_h(\cdot \mid s_h, a_h) = \int_{i_h} F_h(\cdot \mid s_h, a_h, i_h) dP_h(i_h)$ denotes the conditional distribution of $o_h$ given state and action $(s_h, a_h)$ in the planning stage. Here, the first inequality follows from our model assumption on Gaussian transition given $(s_h, a_h, o_h, i_h)$ by Theorem 1.2 of Devroye et al. (2018). The second inequality follows from our Assumption 5.1, where we shift the probability measure to our sample distribution $\rho$. The third inequality follows from the ill-posed condition in Assumption 5.2. Finally, the last inequality follows from (C.3). Similarly, to bound the second term of suboptimality (differences between reward functions) given in (C.1), we obtain

$$\mathbb{E}_{a_h \sim \pi^* \cdot \mid s_h), s_h \sim d^*_h, o_h \sim P_h(\cdot \mid s_h, a_h) \left[ \left\| \tilde{R}_h(s_h, a_h) - \tilde{R}^*_h(s_h, a_h) \right\| \right] \leq \mathbb{E}_{a_h \sim \pi^* \cdot \mid s_h), s_h \sim d^*_h, o_h \sim P_h(\cdot \mid s_h, a_h) \left[ \left\| \tilde{R}_h(s_h, a_h, o_h) - \tilde{R}^*_h(s_h, a_h, o_h) \right\|^2 \right] \leq C_{\pi^*} \mathbb{E}_{\rho(s_h, a_h, o_h)} \left[ \left\| \tilde{R}_h(s_h, a_h, o_h) - \tilde{R}^*_h(s_h, a_h, o_h) \right\|^2 \right] \leq C_{\pi^*} \tau_{K,r,h} L_{K,\beta,1} \delta_h, \rho, \delta. \quad (C.5)$$

The first and second inequalities follow from the Jensen’s and Cauchy Schwartz inequalities, respectively. The third inequality follows from our Assumption 5.1. Moreover, the last but one inequality holds by the ill-posed condition in Assumption 5.2. Finally, the last one holds by Lemma C.3.

Finally, leveraging our conclusions obtained from Lemma C.2, we have

$$\text{SubOpt}(\hat{\pi}) \leq C_{\pi^*} \left[ H \sum_{h=1}^{H} \tau_{K,G,h} \sqrt{d_1 L_{K,\beta,d_1} \delta_h, \rho, \delta} + \sum_{h=1}^{H} \tau_{K,r,h} L_{K,\beta,1} \delta_h, \rho, \delta \right],$$

with probability $1 - H \delta - H/(K d_1)^\beta$. By utilizing the union bound and taking $\delta' = \delta/H$ and $\beta = \log H$, we conclude the proof of Theorem 5.1. \qed

In the following subsections, we provide detailed proofs of Lemma C.1, Lemma C.2 and Lemma C.3, respectively.
C.1 Proof of Lemma C.1

In this subsection, we will prove Lemma C.1 by demonstrating that the true model \( \{ R_h^*, \mathbb{P}_h \}_{h=1}^H \) lies in our constructed confidence sets with high probability. Here, without loss of generality, we assume \( G_h(\cdot), R_h(\cdot), \forall h \in [H] \) are functions that maps \( \mathcal{X} \) to \( \mathbb{R}^d_1 \) with \( d_1 = 1 \). Otherwise we can construct confidence sets for every dimension of \( G_h(\cdot) \) and \( R_h(\cdot) \) following the similar proof.

**Proof.** Here we only prove that \( R_h^*(\cdot) \) falls in \( \mathcal{R}_h \). One can derive the corresponding proof for every coordinate of \( G_h^*(\cdot) \) similarly. To simplify the notation, we use \( x_h^{(k)} = (s_h^{(k)}, a_h^{(k)}, o_h^{(k)}) \) and let \( z_h^{(k)} = (s_h^{(k)}, a_h^{(k)}) \) in the following proof. It is worth noting that here we omit the embedding functions \( \phi_x(\cdot), \psi_z(\cdot) \) to simply the notation.

First, by the definition of \( \mathcal{L}_K \), we have

\[
\mathcal{L}_K(R_h^*) - \mathcal{L}_K(\hat{R}_h) = \sup_{f \in \mathcal{F}} \left\{ \frac{1}{K} \sum_{k=1}^{K} \left( R_h^*(x_h^{(k)}) - R_h(x_h^{(k)}) \right) f(z_h^{(k)}) - \frac{1}{2K} \sum_{k=1}^{K} f^2(z_h^{(k)}) \right\}
- \sup_{f \in \mathcal{F}} \left\{ \frac{1}{K} \sum_{k=1}^{K} \left( \hat{R}_h(x_h^{(k)}) - R_h(x_h^{(k)}) \right) f(z_h^{(k)}) - \frac{1}{2K} \sum_{i=1}^{K} f^2(z_h^{(k)}) \right\}
:= (I) - (II).
\]

In order to obtain an upper bound of \( \mathcal{L}_K(R_h^*) - \mathcal{L}_K(\hat{R}_h) \), we establish an upper bound of (I) and a lower bound of (II).

We first establish an upper bound for (I). To simplify the notation, we define

\[
\Phi_K(R_h, f) := \frac{1}{K} \sum_{k=1}^{K} \left( R_h(x_h^{(k)}) - R_h(x_h^{(k)}) \right) f(z_h^{(k)}) , \quad \text{and} \quad \Phi(R_h, f) := \mathbb{E}[(R_h(x_h) - R_h)f(z_h)].
\]

We then have

\[
(I) = \sup_{f \in \mathcal{F}} \left\{ \Phi_K(R_h^*, f) - \frac{1}{2K} \sum_{k=1}^{K} f^2(z_h^{(k)}) \right\}.
\]

In the following Lemma, we derive a concentration inequality for \( \Phi_K(R_h^*, f) \).

**Lemma C.4.** If \( \mathcal{F} \) is a star-shaped, \( b \)-uniformly bounded function class and for all \( k \in [K] \) and the loss function \( \ell(R_h, f) = (R_h(x_h^{(k)}) - R_h(x_h^{(k)}))f(z_h^{(k)}) \) is \( L_{K, \beta, d_1} := L + \sigma\sqrt{(\beta + 1)\log K d_1} \)-Lipschitz in \( f, \forall f \in \mathcal{F} \), with high-probability, then with probability \( 1 - \delta - 1/K^\beta \), \( \forall f \in \mathcal{F} \), we have

\[
|\Phi_K(R_h^*, f) - \Phi(R_h, f)| \lesssim \left( L_{K, \beta, 1} \delta_{\mathcal{R}, h, \delta} \| f \|_2 + L_{K, \beta, 1} \delta_{\mathcal{R}, h, \delta}^2 \right).
\]

Here \( \delta_{\mathcal{R}, h, \delta} = \delta_{\mathcal{R}, h} + c_0 \sqrt{\log(c_1/\delta)/n} \) with \( \delta_{\mathcal{R}, h} \) being an upper bound of the critical radius of the function classes \( \mathcal{F} \) and \( \mathcal{R}_h^* \). A similar inequality also holds for \( G_j^*, \forall j \in [d_1] \) with probability \( 1 - \delta - 1/(d_1 K)^\beta \) by replacing \( L_{K, \beta, 1}, \delta_{\mathcal{R}, h, \delta} \) with \( L_{K, \beta, d_1}, \delta_{\mathcal{G}, h, \delta} \).
Thus, we have
\[ (2019), \text{with probability } 1 - \delta - 1/K^\beta, \] we have
\[ \| \cdot \| \quad \text{with probability } 1 - \delta - 1/K^\beta, \]
\begin{align*}
\| f \|_{2,K}^2 & = \mathbb{E} [ f(z_h)^2 ] \leq 0.5 \mathbb{E} [ f(z_h)^2 ] + 0.5 \delta_{R,h,\delta}^2.
\end{align*}

Thus, we have
\[ \frac{1}{4} \mathbb{E} [ f^2(z_h) ] - \frac{1}{4} \delta_{R,h,\delta}^2 \leq \frac{1}{2K} \sum_{k=1}^{K} f^2(z_h^{(k)}) \leq \frac{3}{4} \mathbb{E} [ f^2(z_h) ] + \frac{1}{4} \delta_{R,h,\delta}^2. \]

Combining (C.7) with (C.9), with probability \( 1 - \delta - 1/K^\beta \), we have
\[ (I) \leq \sup_{f \in \mathcal{F}} \left\{ \Phi(R^*_h, f) - \frac{1}{4} \mathbb{E} [ f(z_h)^2 ] + \frac{1}{4} \delta_{R,h,\delta}^2 + L_{K,\beta,1} C_1 \left( \delta_{R,h,\delta} \sqrt{\mathbb{E} [ f(z_h)^2 ] + \delta_{R,h,\delta}^2} \right) \right\}. \]

Next, we use a general inequality to obtain an upper bound for the right hand side of (C.10). For all \( a, b > 0 \), by simple calculation, we have
\[ \sup_{f \in \mathcal{F}} (a\|f\| - b\|f\|^2) \leq \frac{a^2}{4b}. \]

Here \( \| \cdot \| \) can represent any norm. Moreover, we also have \( \Phi(R^*_h, f) = 0 \) by the identifiability condition in (4.1). Thus, we finally have
\[ (I) \lesssim L_{K,\beta,1}^2 \delta_{R,h,\delta}^2, \]

Next, we aim at getting a lower bound for (II). Recall that the (II) given in (C.6). We have
\begin{align*}
(II) = & \sup_{f \in \mathcal{F}} \left\{ \frac{1}{K} \sum_{k=1}^{K} \left( \hat{R}_h(x_h^{(k)}) - r_h^{(k)} \right) f(z_h^{(k)}) - \frac{1}{K} \sum_{k=1}^{K} \left( R^*_h (x_h^{(k)}) - r_h^{(k)} \right) f(z_h^{(k)}) ight. \\
& + \left. \frac{1}{K} \sum_{k=1}^{K} \left( \hat{R}_h(x_h^{(k)}) - r_h^{(k)} \right) f(z_h^{(k)}) - \frac{1}{2K} \sum_{k=1}^{K} f(z_h^{(k)})^2 \right\} \\
& \geq \sup_{f \in \mathcal{F}} \left\{ \Phi_K(\hat{R}_h, f) - \Phi_K(R^*_h, f) - \| f \|^2_{2,K} \right\} + \inf_{f \in \mathcal{F}} \left\{ \Phi_K(R^*_h, f) + \frac{1}{2} \| f \|^2_{2,K} \right\} \\
& = \sup_{f \in \mathcal{F}} \left\{ \Phi_K(\hat{R}_h, f) - \Phi_K(R^*_h, f) - \| f \|^2_{2,K} \right\} - \sup_{f \in \mathcal{F}} \left\{ \Phi_K(R^*_h, f) - \frac{1}{2} \| f \|^2_{2,K} \right\} \quad \text{(C.13)}
\end{align*}
Here, the second equality holds since we assume \( \mathcal{F} \) is symmetric in Assumption 5.3. The last inequality follows from the obtained upper bound for (I) in (C.12) and \( C \) is an absolute constant.

Next we will state the following Lemma C.5 which is crucial in providing a lower bound for
\[
\sup_{f \in \mathcal{F}} \{ \Phi_K(\widetilde{R}_h, f) - \Phi_K(R^*_h, f) - \|f\|_{2,K}^2 \}.
\]

**Lemma C.5.** We let
\[
f_{\widetilde{R}_h}(z_h) := \mathbb{T}(R_h - R^*_h) = \mathbb{E}[R_h(x_h) - R^*_h(x_h) | z_h].
\]
As \( \mathcal{R}^*_h \) is star-shaped, then with probability \( 1 - \delta \), we have
\[
\left| \Phi_K(R_h, f_{\widetilde{R}_h}) - \Phi_K(R^*_h, f_{\widetilde{R}_h}) - \left[ \Phi(R_h, f_{\widetilde{R}_h}) - \Phi(R^*_h, f_{\widetilde{R}_h}) \right] \right| 
\lesssim \delta_{\mathcal{R},h,\delta} \sqrt{\mathbb{E} \left\{ \left[ (R_h - R^*_h)(x_h)f_{\widetilde{R}_h}(z_h) \right]^2 \right\}} + \delta_{\mathcal{R},h,\delta}^2, \forall R_h \in \mathbb{R}_h.
\]
Here \( \delta_{\mathcal{R},h,\delta} \) is an upper bound of the critical radius of \( \mathcal{R}^*_h \).

**Proof.** See §G for a detailed proof. \( \square \)

Next, we use the conclusion of Lemma C.5 to derive a lower bound for \( \sup_{f \in \mathcal{F}} \{ \Phi_K(\widetilde{R}_h, f) - \Phi_K(R^*_h, f) - \|f\|_{2,K}^2 \} \). Here we recall that we denote \( f_{\widetilde{R}_h} = \mathbb{T}(\widetilde{R}_h - R^*_h) = \mathbb{E}[(R_h(x_h) - R^*_h(x_h) | z_h)] \) in (C.14). By our Assumption 5.3, we assume for all \( R_h \in \mathbb{R}_h, \mathbb{T}(R_h - R^*_h) \in \mathcal{F} \). We next divide our analysis into two cases.

When \( \|f_{\widetilde{R}_h}\|_2 \leq \delta_{\mathcal{R},h,\delta} \), we have
\[
\sup_{f \in \mathcal{F}} \left\{ \Phi_K(\widetilde{R}_h, f) - \Phi_K(R^*_h, f) - \|f\|_{2,K}^2 \right\} \geq \Phi_K(\widetilde{R}_h, f_{\widetilde{R}_h}) - \Phi_K(R^*_h, f_{\widetilde{R}_h}) - \|f_{\widetilde{R}_h}\|_{2,K}^2,
\]
since \( f_{\widetilde{R}_h} \) belongs to \( \mathcal{F} \). By Lemma C.5, with probability \( 1 - \delta \), we further have
\[
\Phi_K(\widetilde{R}_h, f_{\widetilde{R}_h}) - \Phi_K(R^*_h, f_{\widetilde{R}_h}) - \|f_{\widetilde{R}_h}\|_{2,K}^2 \geq \Phi(\widetilde{R}_h, f_{\widetilde{R}_h}) - \Phi(R^*_h, f_{\widetilde{R}_h}) - \delta_{\mathcal{R},h,\delta}\|f_{\widetilde{R}_h}\|_2 - \delta_{\mathcal{R},h,\delta}^2 - \|f_{\widetilde{R}_h}\|_{2,K}^2
\]
\[
\geq \mathbb{E}[(\widetilde{R}_h(x_h) - R^*_h(x_h))\mathbb{E}[R_h(x_h) - R^*_h(x_h) | z_h)] - C_3\delta_{\mathcal{R},h,\delta}^2
\]
\[
\geq 0 - C_3\delta_{\mathcal{R},h,\delta}^2.
\]
Here \( C_3 \) is an absolute constant. The second inequality holds since we assume \( \|f_{\widetilde{R}_h}\|_2 \leq \delta_{\mathcal{R},h,\delta} \), and the fact that \( \|f_{\widetilde{R}_h}\|_{2,K}^2 \leq 1.5\|f_{\widetilde{R}_h}\|_2^2 + \delta_{\mathcal{R},h,\delta}^2 \) according to (C.8).

When \( \|f_{\widetilde{R}_h}\|_2 \geq \delta_{\mathcal{R},h,\delta} \), we let \( \kappa = \xi_{\mathcal{R},h,\delta}/(2\|f_{\widetilde{R}_h}\|_2) \in [0,0.5] \). We have \( \kappa f_{\widetilde{R}_h} \in \mathcal{F} \) as \( \mathcal{F} \) is assumed to be star-shaped in Assumption 5.3. In this case, we have
\[
\sup_{f \in \mathcal{F}} \left\{ \Phi_K(\widetilde{R}_h, f) - \Phi_K(R^*_h, f) - \|f\|_{2,K}^2 \right\} \geq \kappa \left[ \Phi_K(\widetilde{R}_h, f_{\widetilde{R}_h}) - \Phi_K(R^*_h, f_{\widetilde{R}_h}) \right] - \kappa^2\|f_{\widetilde{R}_h}\|_{2,K}^2.
\]
\[
\geq \kappa \left[ \Phi(\widetilde{R}_h, f_{\widetilde{R}_h}) - \Phi(R^*_h, f_{\widetilde{R}_h}) \right]
\]
\[
- \kappa(\delta_{\mathcal{R},h,\delta}\|f_{\widetilde{R}_h}\|_2 + \delta_{\mathcal{R},h,\delta}^2) - \kappa^2\|f_{\widetilde{R}_h}\|_{2,K}^2
\]
\[
\geq 0 - C_4\delta_{\mathcal{R},h,\delta}^2.
\]
\[\text{(C.15)}\]
Here $C_4$ is an absolute constant. The second inequality holds by Lemma C.5. The last inequality follows from several facts. First, we have $\kappa \delta_{R,h} \| f_{\hat{R}_h} \|_2 \lesssim \delta_{R,h}^2$, by the definition of $\kappa = \delta_{R,h}/\sqrt{\| f_{\hat{R}_h} \|_2}$. Next, we obtain $\delta_{R,h}^2$, since $\kappa \in [0, 0.5]$. Moreover, we obtain $\kappa^2 \| f_{\hat{R}_h} \|_{2,K} \leq \kappa^2 (1.5 \| f_{\hat{R}_h} \|_2^2 + \delta_{R,h}^2) \lesssim \delta_{R,h}^2$. Combining these together, we obtain (C.15).

Finally, combining the upper bound for (I) and lower bound for (II), we have

$$\mathcal{L}_K(R^*_h) - \mathcal{L}_K(\hat{R}_h) \lesssim L_{K,\beta,1}^2 \delta_{R,h}. $$

Thus, we conclude our proof of Lemma C.1. \hfill \qed

### C.2 Proof of Lemma C.2

In this subsection, we will prove Lemma C.2, which provides an upper bound of the suboptimality.

**Proof.** We let $\mathcal{M}$ be the product of the confidence sets $\{(\hat{R}_h, \hat{G}_h)^H\}_{h=1}$. We have $M^* = \{(\hat{R}_h^*, \hat{P}_h^*)\}_{h=1} \in \mathcal{M}$ with high probability, i.e. the true model lies in the confidence set with high probability by Lemma C.1.

For any given policy $\pi$, we denote $\tilde{J}(\pi) = \min_{M \in \mathcal{M}} J(M, \pi)$. We have

$$J(M^*, \pi^*) - J(M^*, \tilde{\pi}) = J(M^*, \pi^*) - \tilde{J}(\pi^*) - J(M^*, \tilde{\pi})$$

$$= J(M^*, \pi^*) - \tilde{J}(\pi^*) + \tilde{J}(\pi^*) - J(M^*, \tilde{\pi})$$

$$\leq J(M^*, \pi^*) - \tilde{J}(\pi^*) + \tilde{J}(\tilde{\pi}) - J(M^*, \tilde{\pi})$$

$$\leq J(M^*, \pi^*) - \tilde{J}(\pi^*).$$

The first inequality follows from the fact that $\min_{M \in \mathcal{M}} J(M, \pi^*) \leq \min_{M \in \mathcal{M}} J(M, \tilde{\pi})$ according to our selection of $\tilde{\pi}$ given in (4.7). The second inequality holds by pessimism, namely, $M^* \in \mathcal{M}$ and $\tilde{J}(\tilde{\pi}) = \min_{M \in \mathcal{M}} J(M, \tilde{\pi}) \leq J(M^*, \tilde{\pi})$. Thus, we have

$$\text{SubOpt}(\tilde{\pi}) \leq J(M^*, \pi^*) - \min_{M \in \mathcal{M}} J(M, \pi^*).$$

We next let $\tilde{M} := \{(\hat{R}_h, \hat{P}_h)^H\}_{h=1} = \text{argmin}_{M \in \mathcal{M}} J(M, \pi^*)$. In addition, we let $\tilde{M}_h = \{(\tilde{R}_j, \tilde{P}_j)^H\}_{j=h}$ and $M^*_h = \{(\hat{R}_j^*, \hat{P}_j^*)\}_{j=h}$ are models starting from stage $h$. Moreover, we define $\tilde{V}^*_M(s)$ as the total value function evaluated by policy $\pi$ on model $M_h$.

Next, we expand the expression of $J(M^*, \pi^*) - J(\tilde{M}, \pi^*)$. The intuition is similar with the simulation lemma given in Sun et al. (2019) and we deduce this in our own setting. By definition of the value function, we have

$$J(M^*, \pi^*) - J(\tilde{M}, \pi^*)$$

$$= - \left\{ \mathbb{E}_{a_1 \sim \pi^*_1(s_1, s_1) \sim \nu_0} \left[ \mathbb{E}_{s_2 \sim \tilde{P}_1(s_1, a_1)} \tilde{R}_1(s_1, a_1) + \tilde{V}^*_M(s_2) \right] 
- \mathbb{E}_{s_2 \sim \tilde{P}_1(s_1, a_1)} \tilde{R}_1(s_1, a_1) + \tilde{V}^*_M(s_2) 
- \mathbb{E}_{s_2 \sim \tilde{P}_1(s_1, a_1)} \tilde{R}_1(s_1, a_1) + \tilde{V}^*_M(s_2) \right\}. $$

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After a direct calculation, we have
\[
J(M^*, \pi^*) - J(\tilde{M}, \pi^*) = -\mathbb{E}_{a_1 \sim \pi_1^*(\cdot|s_1), s_1 \sim \rho_0} \left\{ \int \tilde{V}_{M_2}^\pi(\cdot) \left[ \tilde{d}\tilde{P}_1(\cdot|s_1, a_1) - \tilde{d}\tilde{P}_1^*(\cdot|s_1, a_1) \right] \right\} + \left[ (\tilde{R}_1 - \tilde{R}_1^*)(s_1, a_1) \right] + \mathbb{E}_{s_2 \sim \tilde{P}_1^*(\cdot|s_1, a_1)} \left[ \tilde{V}_{M_2}^\pi(s_2) - \tilde{V}_{M_2}^\pi(s_2^*) \right].
\]

After expanding $\tilde{V}_{M_h}^\pi(s_h) - \tilde{V}_{M_h}^\pi(s_h), h \geq 2$ in the same way as above, we obtain
\[
J(M^*, \pi^*) - J(\tilde{M}, \pi^*) = -\sum_{h=1}^H \mathbb{E}_{a_h \sim \pi_h^*(\cdot|s_h), s_h \sim \pi_{h-1}^*} \left\{ \int \tilde{V}_{M_{h+1}}^\pi(\cdot) \left[ \tilde{d}\tilde{P}_h - \tilde{d}\tilde{P}_h^*(\cdot|s_h, a_h) \right] \right\} - \sum_{h=1}^H \mathbb{E}_{a_h \sim \pi_h^*(\cdot|s_h), s_h \sim \pi_{h-1}^*} \left[ (\tilde{R}_h - \tilde{R}_h^*)(s_h, a_h) \right],
\]
where $\pi_{h-1}^*$ represents the distribution of state $s_h$, which is generated by following policy $\pi^*$ and the true transition functions $\left( \tilde{P}_j^\pi \right)_{j=1}^{h-1}$ defined in (3.6).

As we only consider bounded functions in our defined function classes, thus $H$ is an upper bound for our value functions under all policy $\pi$ and model all $M \in \mathcal{M}$. Finally, according the decomposition given above, we have
\[
J(M^*, \pi^*) - J(\tilde{M}, \pi^*) \leq \sum_{h=1}^H \mathbb{E}_{a_h \sim \pi_h^*(\cdot|s_h), s_h \sim \pi_{h-1}^*} \left[ 2H \cdot \left\| (\tilde{P}_h - \tilde{P}_h^*)(\cdot|s_h, a_h) \right\|_1 + \left| (\tilde{R}_h - \tilde{R}_h^*)(s_h, a_h) \right| \right].
\]

Thus, we finish our proof of Lemma C.2.

C.3 Proof of Lemma C.3

In this subsection, for any given $h \in [H]$, we will prove that for all $R_h \in \mathcal{R}_h, G_h \in \mathcal{G}_h$,
\[
\mathbb{E}_\rho \left[ \mathbb{E}_\rho \left[ R_h(s_h, a_h, o_h) - R_h^*(s_h, a_h, o_h) | s_h, a_h \right] \right]^2 \text{ and }
\mathbb{E}_\rho \left[ \mathbb{E}_\rho \left[ G_h(s_h, a_h, o_h) - G_h^*(s_h, a_h, o_h) | s_h, a_h \right] \right]^2
\]
are small with high probability. Here the distribution $\rho$ denotes the sampling distribution. Similar to the proof of Lemma C.1, here we also only prove the case for $R_h$, as the proof for every coordinate of $G_h$ is almost the same.

Proof. For all $R_h \in \mathcal{R}_h$, we have
\[
\sup_{f \in \mathcal{F}} \left\{ \Phi_K(R_h, f) - \frac{1}{2} \| f \|_{2, K}^2 \right\} \geq \sup_{f \in \mathcal{F}} \left\{ \Phi_K(R_h, f) - \Phi_K(R_h^*, f) - \| f \|_{2, K}^2 \right\} - \sup_{f \in \mathcal{F}} \left\{ \Phi_K(R_h^*, f) - \frac{1}{2} \| f \|_{2, K}^2 \right\},
\]
(C.16)
by using similar argument of (C.13). By the definition of $L_K(\cdot)$ in §3.3, \(\forall R_h \in \mathcal{R}_h\), with probability \(1 - \delta - 1/K^\beta\), we have

\[
\sup_{f \in \mathcal{F}} \left\{ \Phi_K(R_h, f) - \Phi_K(R_h^*, f) - \|f\|_{2,K}^2 \right\} \leq L_K(R_h) + L_K(R_h^*)
\]

\[
\leq L_K(\tilde{R}_h) + C_5 L_{K,\beta,1}^2 \delta_{R,h,\delta}^2 + L_K(R_h^*)
\]

\[
\leq 2L_K(R_h^*) + C_5 L_{K,\beta,1}^2 \delta_{R,h,\delta}^2
\]

\[
\leq L_{K,\beta,1}^2 \delta_{R,h,\delta}^2. \tag{C.17}
\]

Here the first inequality follows from (C.16). The second inequality holds since \(R_h \in \mathcal{R}_h\) and \(L_K(R_h) \lesssim L_K(R_h^*) + C_5 L_{K,\beta,1}^2 \delta_{R,h,\delta}^2\) by the definition of \(\mathcal{R}_h\). The third inequality holds by the definition of \(\tilde{R}_h\). The last inequality follows from (C.12).

Next, we prove that \(\mathbb{E}_p\left[\mathbb{E}_p[ R_h(s_h, a_h, o_h) - R_h^*(s_h, a_h, o_h) | s_h, a_h]^2]\right]\) is small. We assume there exists \(R_h \in \mathcal{R}_h\) such that \(\|R_h\|_2 = \sqrt{\mathbb{E}_p[T(R_h - R_h^*)^2]} \geq L_{K,\beta,1} \delta_{R,h,\delta}\), otherwise we obtain our conclusion directly. For such a \(R_h\), we let \(\kappa_{R_h} = L_{K,\beta,1} \delta_{R,h,\delta}/(2\|R_h\|_2)\), and we have \(\kappa_{R_h} \in [0, 0.5]\). Thus, \(\forall R_h \in \mathcal{R}_h\), when \(\|R_h\|_2 = \sqrt{\mathbb{E}_p[T(R_h - R_h^*)^2]} \geq L_{K,\beta,1} \delta_{R,h,\delta}\), with probability \(1 - \delta\), we obtain

\[
\sup_{f \in \mathcal{F}} \left\{ \Phi_K(R_h, f) - \Phi_K(R_h^*, f) - \|f\|_{2,K}^2 \right\} \geq \kappa_{R_h} \left\{ \Phi_K(R_h, f_{R_h}) - \Phi_K(R_h^*, f_{R_h}) \right\} - \kappa_{R_h}^2 \|f_{R_h}\|_{2,K}^2
\]

\[
\geq \kappa_{R_h} \left[ \Phi(R_h, f_{R_h}) - \Phi(R_h^*, f_{R_h}) \right] - \kappa_{R_h}^2 \|f_{R_h}\|_{2,K}^2
\]

\[
= \frac{L_{k,\beta,1} \delta_{R,h,\delta}}{2} \sqrt{\mathbb{E}_p[T(R_h - R_h^*)^2]} - C_6 L_{k,\beta,1}^2 \delta_{R,h,\delta}^2. \tag{C.18}
\]

The first inequality holds since \(\mathcal{F}\) is star-shaped and thus \(\kappa_{R_h} f_{R_h} \in \mathcal{F}\), when

\[
\|f_{R_h}\|_2 = \sqrt{\mathbb{E}_p[T(R_h - R_h^*)^2]} \geq L_{K,\beta,1} \delta_{R,h,\delta}.
\]

The second inequality holds uniformly for all \(R_h\) with high probability by Lemma C.5. The third inequality follows by several facts. First, we obtain \(\kappa_{R_h} \delta_{R,h,\delta} \|f_{R_h}\|_2 \leq L_{K,\beta,1} \delta_{R,h,\delta} \delta_{R,h,\delta}^2\), by the definition that \(\kappa_{R_h} = L_{K,\beta,1} \delta_{R,h,\delta}/(2\|f_{R_h}\|_2)\). Second, it holds that \(\kappa_{R_h} \delta_{R,h,\delta}^2 \lesssim \delta_{R,h,\delta}^2\), since \(\kappa_{R_h} \in [0, 0.5]\). Third, we obtain \(\kappa_{R_h}^2 \|f_{R_h}\|_{2,K}^2 \leq \kappa_{R_h}^2 (1.5 \|f_{R_h}\|_2^2 + \delta_{R,h,\delta}^2) \lesssim L_{K,\beta,1}^2 \delta_{R,h,\delta}^2\). Combining these together, we obtain (C.18).

Finally, combining our results obtained in (C.17) and (C.18), with probability \(1 - \delta - 1/K^\beta\), we have

\[
\sqrt{\mathbb{E}_p\left[\mathbb{E}_p\left[ R_h(s_h, a_h, o_h) - R_h^*(s_h, a_h, o_h) | s_h, a_h \right]^2\right]} \lesssim L_{K,\beta,1} \delta_{R,h,\delta}.
\]

Similarly, we are also able to obtain (C.3) with probability \(1 - \delta - 1/(d_1 K)^\beta\) by following the similar proof. To be more specific, one only needs to replace \(R_h(\cdot), R_h^{(k)}(\cdot), G_{h,j}(\cdot), s_{h+1,j}\) for each \(j \in [d_1]\) and obtain the upper bounds for \(\sqrt{\mathbb{E}_p[T(G_{h,j} - G_{h,j}^*)^2]}\) for all \(j\). Putting all pieces together, we conclude our proof of Lemma C.3. □
D Proof of Theorem 5.2

Proof of Theorem 5.2. In this section, we will provide theoretical proof for Theorem 5.2. Recall that we let \( \mathbb{R}_h \) and \( \mathcal{G}_{h,j} \) be the true function classes for \( R^*_h(\cdot) \) and \( G^*_h(\cdot) \), for all \( j \in [d_1], h \in [H] \). However, we use misspecified function classes \( \mathcal{R}_h, \mathcal{G}_{h,j} \) to estimate our model. In addition, for all \( h \in [H], j \in [d_1] \), we let \( R^0_h := \arg\min_{R_h \in \mathcal{R}_h} ||R_h - R^*_h||_\infty, G^0_{h,j} := \arg\min_{G_{h,j} \in \mathcal{G}_{h,j}} ||G_{h,j} - G^*_h||_\infty \).

First, we prove \( R^0_h, G^0_{h,j} \) belongs to the confidence sets defined in (4.8) and (4.9) (by replacing \( \mathcal{R}_h \) and \( \mathcal{G}_{h,j} \) with \( \mathcal{R}_h, \mathcal{G}_{h,j} \), respectively). We summarize the conclusion in the following Lemma D.1.

Lemma D.1. For any \( h \in [H] \), with probability \( 1 - \delta - 1/(d_1 K)^\beta \), we have
\[
R^0_h \in \mathcal{R}^M_h = \left\{ R_h \in \mathcal{R}_h : \mathcal{L}_n(R_h) - \mathcal{L}_n(\hat{R}_h) \leq L^2_{K,\beta,1}\delta^2_{R,h,\delta} + \eta^2_{K,G,h} \right\},
\]
\[
G^0_{h,j} \in \mathcal{G}^M_{h,j} = (\mathcal{G}_{h,1}^M, \mathcal{G}_{h,2}^M, \ldots, \mathcal{G}_{h,d_1}^M), \text{ where we define}
\]
\[
\mathcal{G}_{h,j} = \left\{ G_{h,j} \in \mathcal{G}_{h,j} : \mathcal{L}_n(G_{h,j}) - \mathcal{L}_n(\hat{G}_{h,j}) \leq L^2_{K,\beta,1}\delta^2_{G,h,\delta} + \eta^2_{K,G,h} \right\}.
\]
Here we have \( \delta_{R,h,\delta} = \delta_{R,h} + c_1 \sqrt{\log(c_0/\delta)/K}, \delta_{G,h,\delta} = \delta_{G,h} + c_2 \sqrt{\log(c_0 d_1/\delta)/K} \) with \( c_0, c_1, c_2 \) being absolute constants. Moreover, \( \delta_{G,h} \) is an upper bound of the maximum critical radius of \( \mathcal{F}, \mathcal{G}^M_{h,j} \), for all \( j \in [d_1] \) (given in (5.13)) and \( \delta_{R,h} \) is an upper bound of the maximum radius of \( \mathcal{F}, \mathcal{R}^M_h \) (given in (5.12)). Meanwhile, we define \( L_{K,\beta,d_1} := L + \sigma \sqrt{(\beta + 1) \log K d_1} \).

Proof. See §D.1 for a detailed proof.

Next, we prove that, for any given \( h \in [H] \), for all \( R_h \in \mathcal{R}_h, G_h \in \mathcal{G}_h \),
\[
\mathbb{E}\left[ \left( \mathbb{E}\left[ R_h(s_h, a_h, o_h) - R^0_h(s_h, a_h, o_h) \mid s_h, a_h \right] \right)^2 \right], \text{ and}
\]
\[
\mathbb{E}\left[ \left\| \mathbb{E}\left[ G_h(s_h, a_h, o_h) - G^0_h(s_h, a_h, o_h) \mid s_h, a_h \right] \right\|_2^2 \right]
\]
are small with high probability. We summarize this property in the following Lemma D.2.

Lemma D.2. For all \( R_h, G_h \) given in \( \mathcal{R}_h, \mathcal{G}_h \), with probability \( 1 - H\delta - H/(K d_1)^\beta \), we have
\[
\sqrt{\mathbb{E}_\rho\left[ \left( \mathbb{E}_\rho\left[ R_h(s_h, a_h, o_h) - R^0_h(s_h, a_h, o_h) \mid s_h, a_h \right] \right)^2 \right]} \leq L_{K,\beta,1}\delta_{R,h,\delta} + \xi_{K,R,h} + \frac{\eta^2_{K,R,h}}{\delta_{R,h,\delta}}, \tag{D.1}
\]
\[
\sqrt{\mathbb{E}_\rho\left[ \left\| \mathbb{E}_\rho\left[ G_h(s_h, a_h, o_h) - G^0_h(s_h, a_h, o_h) \mid s_h, a_h \right] \right\|_2^2 \right]} \leq d_1 L_{K,\beta,1}\delta_{G,h,\delta} + \xi_{K,G,h} + \frac{\eta^2_{K,G,h}}{\delta_{G,h,\delta}}, \tag{D.2}
\]
where \( \xi_{K,R,h}, \xi_{K,G,h}, \eta_{K,R,h}, \eta_{K,G,h} \) are approximation errors defined in §5.2.

Proof. See §D.2 for a detailed proof.

Finally we will provide an upper bound for the suboptimality of \( \tilde{\pi}^M \) given in (5.11).

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Recall that for all $h \in [H], j \in [d_1]$, we let

\[ R^0_h := \arg\min_{R_h \in \bar{R}_h} \| R_h - R_h^* \|_\infty, \quad G^0_{h,j} := \arg\min_{G_{h,j} \in G_{h,j}} \| G_{h,j} - G^*_h \|_\infty \]

in Assumption 5.7. In the following, we denote

\[ \tilde{R}^0_h = \int_{o_h, i_h} [R^0_h(s_h, a_h, o_h) + f_{1h}(i_h)]dF_h(o_h | s_h, a_h, i_h)dP_h(i_h). \]

In addition, we also define $\tilde{P}^0_h$ in the same way as in (3.6) using $G^0_h = \{ G^0_{h,j} \}_{j=1}^{d_1}$. Moreover, we let $\tilde{M}^* := \{(\tilde{R}^0_h, \tilde{P}^0_h)\}_{h=1}^H$.

The suboptimality is able to be written as:

\[ J(M^*, \pi^*) - J(M^*, \tilde{\pi}^M) = \left[ J(M^*, \pi^*) - J(M^*, \tilde{\pi}^M) \right] + \left[ J(M^*, \tilde{\pi}^M) - J(M^*, \pi^*) \right] \]

\[ = (i) + (ii) + (iii). \]

Next, we provide an upper bound for (ii). The way of controlling (ii) is almost the same as controlling the suboptimality without misspecification. To be more specific, we also define $\tilde{J}(\pi) = \min_{M \in \mathcal{M}^M} J(M, \pi)$, where $\mathcal{M}^M := \{(\tilde{G}^0_h, \tilde{R}^0_h)\}_{h=1}^H$ is defined in §5.2. We have

\[ J(M^*, \pi^*) - J(M^*, \tilde{\pi}^M) = \tilde{J}(\pi^*) + \tilde{J}(\pi^*) - J(M^*, \pi^*) \leq J(M^*, \pi^*) - J(M^*, \pi^*) \leq J(M^*, \pi^*) - J(M^*, \pi^*). \]

The first inequality follows from our definition of $\tilde{\pi}^M$. The second inequality follows from and pessimism and Lemma D.1 since $M^*$ is defined in §5.2. We next let $\widetilde{M} = \arg\min_{M \in \mathcal{M}^M} J(M, \pi^*)$, with $\widetilde{M} := \{ (\widetilde{P}_h, \widetilde{R}_h) \}_{h=1}^H$. Following similar arguments given in Lemma C.2 or the simulation lemma in Sun et al. (2019), we obtain

\[ (ii) = \left[ J(M^*, \pi^*) - J(M^*, \tilde{\pi}^M) \right] \]

\[ \leq H \sum_{h=1}^H \mathbb{E}_{a_h \sim \pi^* \cdot | s_h), s_h \sim d_{a_h}^*} \left[ \left\| (\widetilde{P}_h - \tilde{P}^0_h)(\cdot | s_h, a_h) \right\|_1 \right] \]

\[ + \sum_{h=1}^H \mathbb{E}_{a_h \sim \pi^* \cdot | s_h), s_h \sim d_{a_h}^*} \left[ \left\| \tilde{R}_h(s_h, a_h) - \tilde{R}^0_h(s_h, a_h) \right\|_1 \right]. \]

Combining Lemma D.2 and following the similar to the derivations of (C.4) and (C.5), we obtain

\[ (ii) \lesssim H \sum_{h=1}^H \tau_{K,G,h} \sqrt{d_1} \left( L_{K,G,h} \delta_{h,G,\delta} + \frac{\eta_{K,G,h}^2}{\delta_{h,G,\delta}} \right) \]

\[ + \sum_{h=1}^H \tau_{K,R,h} \left( L_{K,R,h} \delta_{R,h,\delta} + \frac{\eta_{K,R,h}^2}{\delta_{R,h,\delta}} \right). \]
Next, we will prove an upper bound for (i), and (iii) can be bounded in the same way. Following similar arguments in Lemma C.2, we obtain

\[
(i) \lesssim H \sum_{h=1}^{H} \mathbb{E}_{a_h \sim \pi^*(\cdot | s_h), s_h \sim d_{h-1}^{s_h}} \left[ \left\| \left( \frac{\mathbb{P}^{0}_{h} - \mathbb{P}^{*}_{h}}{\mathbb{E}_{h}} \right)(\cdot | s_h, a_h) \right\|_1 \right]
\]

\[ + \sum_{h=1}^{H} \mathbb{E}_{a_h \sim \pi^*(\cdot | s_h), s_h \sim d_{h-1}^{s_h}} \left[ \left| R_{h}^{0}(s_h, a_h) - R_{h}^{*}(s_h, a_h) \right| \right] = (iv) + (v). \tag{D.3}
\]

We next provide an upper bound for (iv) by following the similar idea of proving (C.4). In specific, we have

\[
(iv) = H \sum_{h=1}^{H} \mathbb{E}_{a_h \sim \pi^*(\cdot | s_h), s_h \sim d_{h-1}^{s_h}} \left[ \left| \int_{s_h, o_h} \mathbb{P}^{0}(\cdot | s_h, a_h, o_h, i_h) - \mathbb{P}^{*}(\cdot | s_h, a_h, o_h, i_h) \right| dF_{h}(o_h | s_h, a_h, i_h) dP_{h}(i_h) \right]
\]

\[ \leq H \sum_{h=1}^{H} \mathbb{E}_{a_h \sim \pi^*(\cdot | s_h), s_h \sim d_{h-1}^{s_h}} \left[ \int_{s_h, o_h} \left| \mathbb{P}^{0}(\cdot | s_h, a_h, o_h, i_h) - \mathbb{P}^{*}(\cdot | s_h, a_h, o_h, i_h) \right| dF_{h}(o_h | s_h, a_h, i_h) dP_{h}(i_h) \right]
\]

\[ \leq H \sum_{h=1}^{H} \sqrt{\mathbb{E}_{a_h \sim \pi^*(\cdot | s_h), s_h \sim d_{h-1}^{s_h}, o_h \sim \rho_{\pi}(\cdot | s_h, a_h)} \left[ TV \left( \mathbb{P}_{h}^{0}(\cdot | s_h, a_h, o_h, i_h), \mathbb{P}_{h}^{*}(\cdot | s_h, a_h, o_h, i_h) \right) \right]^{2}}
\]

\[ \lesssim H \sum_{h=1}^{H} \sqrt{\mathbb{E}_{a_h \sim \pi^*(\cdot | s_h), s_h \sim d_{h-1}^{s_h}, o_h \sim \rho_{\pi}(\cdot | s_h, a_h)} \left[ \left| G_{h}^{0}(s_h, a_h, o_h) - G_{h}^{*}(s_h, a_h, o_h) \right| \right]^{2}]. \tag{D.4}
\]

The first inequality follows from Jensen’s inequality and the second follows from Cauchy-Schwartz inequality. In addition, the third inequality follows from our assumption on Gaussian transition. Moreover, by our assumption on the approximation error in \(\ell_{\infty}\)-norm given in Assumption 5.7, we obtain

\[
(D.4) \lesssim H \sum_{h=1}^{H} \sqrt{d_{i} \max_{j \in [d_{i}]} \left\| G_{h,j}^{0} - G_{h,j}^{*} \right\|_{\infty}} \leq H \sum_{h=1}^{H} \sqrt{d_{i} \eta_{K,G,h}}
\]

For (v), following similar proof procedure, we have

\[
(v) \leq \sum_{h=1}^{H} \eta_{K,r,h}. \tag{D.5}
\]

In terms of upper bounding the term (iii), we only need to replace \(\pi^*\) by \(\tilde{\pi}\) and the other procedures will remain as the same. The reason is that we have obtained the upper bound of the difference between \(G_{h,j}^{0}\) and \(G_{h,j}^{*}\) (also \(R_{h}^{0}\) and \(R_{h}^{*}\)) in \(\ell_{\infty}\)-norm and it is robust to all probability measures including \(\pi^*\) and \(\tilde{\pi}\). Thus, the proof of bounding (iii) is the same with the proof of (i).
Combining all results for (i), (ii) and (iii), we have
\[
V_{M^*}^\pi - V_{\hat M^*}^\pi \leq H \sum_{h=1}^H C_{\pi^*} \tau_{K,G,h} \sqrt{d_1 \left( L_{K,\beta,1} \delta_{h,G,\delta} + \xi_{K,G,h} + \frac{\eta_{K,G,h}^2}{\delta_{h,G,\delta}} \right)} + \sum_{h=1}^H C_{\pi^*} \tau_{K,R,h} \left( L_{K,\beta,1} \delta_{R,h,\delta} + \xi_{K,R,h} + \frac{\eta_{K,R,h}^2}{\delta_{R,h,\delta}} \right) + H \sum_{h=1}^H \sqrt{d_1 \eta_{K,G,h}} + \sum_{h=1}^H \eta_{K,R,h}.
\]

We then conclude the proof of Theorem 5.2.

\[\square\]

D.1 Proof of Lemma D.1

Proof. Here we will prove that \( R_h^0 \) falls in \( R_h^M \), and one is able to derive the corresponding proof for every coordinate of \( G_h^0 \) in a similar way. To simplify our notation, we use \( x_h^{(k)} = (s_h^{(k)}, a_h^{(k)}, o_h^{(k)}) \) and \( z_h^{(k)} = (s_h^{(k)}, a_h^{(k)}) \) and in the following proof. We note that here we omit the embedding functions \( \phi_x(\cdot), \psi_z(\cdot) \) as we mentioned in the main body of this paper.

First, we have
\[
\mathcal{L}_K(R_h^0) - \mathcal{L}_K(\hat R_h) = \sup_{f \in \mathcal{F}} \left\{ \frac{1}{K} \sum_{k=1}^K \left( R_h^0 \left( x_h^{(k)} \right) - R_h^0 \left( \hat x_h^{(k)} \right) \right) f \left( z_h^{(k)} \right) - \frac{1}{2K} \sum_{k=1}^K f^2 \left( z_h^{(k)} \right) \right\} - \sup_{f \in \mathcal{F}} \left\{ \frac{1}{K} \sum_{k=1}^K \left( \hat R_h \left( x_h^{(k)} \right) - R_h^0 \left( \hat x_h^{(k)} \right) \right) f \left( z_h^{(k)} \right) - \frac{1}{2K} \sum_{k=1}^K f^2 \left( z_h^{(k)} \right) \right\}
:= (I) - (II).
\]

Next, we aim at obtaining an upper bound for (I). Similarly, we define
\[
\Phi_K(r, f) = \frac{1}{K} \sum_{k=1}^K \left( R_h \left( x_h^{(k)} \right) - R_h^0 \left( \hat x_h^{(k)} \right) \right) f \left( z_h^{(k)} \right), \quad \text{and} \quad \Phi(r, f) = \mathbb{E}[(r(x_h) - r_h)f(z_h)].
\]

We have
\[
(I) = \sup_{f \in \mathcal{F}} \left\{ \Phi_K(R_h^0, f) - \frac{1}{2K} \sum_{k=1}^K f^2 \left( z_h^{(k)} \right) \right\}.
\]

Next, according the conclusion from Lemma C.4, with probability \( 1 - \delta - 1/K^\beta \), we have
\[
(I) \leq \sup_{f \in \mathcal{F}} \left\{ \Phi(R_h^0, f) - \frac{1}{2K} \sum_{k=1}^K f^2 \left( z_h^{(k)} \right) + C_1 L_{K,\beta,1} \delta_{R,h,\delta} \norm{f(z)}_2 + \delta_{R,h,\delta}^2 \right\}. \quad (D.6)
\]
According to the expression of \( \Phi(R_0^0, f) = \mathbb{E}[(R_h^0(x_h) - R_h)f(z_h)], \forall f \in \mathcal{F}, \) we have
\[
\left| \Phi(R_h^0, f) - \Phi(R_n^*, f) \right| \leq \|(R_h^0 - R_n^*)(x_h)\|_\infty \|f(z_h)\|_2 \leq \eta_{K,r,h} \|f(z_h)\|_2.
\]

Combining this inequality with (D.6), we obtain
\[
\text{(D.6)} \leq \sup_{f \in \mathcal{F}} \left\{ \Phi(R_h^*, f) - \frac{1}{2K} \sum_{k=1}^K f^2(z_h^{(k)}) + (C_1 L_{K,\beta}^2 \delta_{R,h,\delta} + \eta_{K,r,h}) \|f(z_h)\|_2 + C_1 L_{K,\beta,1} \delta_{R,h,\delta} \right\}.
\]

Similar to the derivations of (C.9), (C.10) and (C.11), we have
\[
\text{(I)} \lesssim L_{K,\beta,1}^2 \delta_{R,h,\delta} + \eta_{K,r,h}^2.
\]

We have (II) \( \geq 0 \) as \( f = 0 \) is contained in the function class \( \mathcal{F} \). Thus, we have \( R_0 \) lies in the constructed level set. Similarly, we are also able to prove that \( G_{h,j}^0 \) lies in the level set given in (??) for any \( j \in [d_1], h \in [H] \).

**D.2 Proof of Lemma D.2**

**Proof.** Here we only prove the case for \( R_h(\cdot) \), since the case for \( G_{h,j}(\cdot) \) follows in the same way.

For all \( R_h \in \mathcal{R}_h \), we have
\[
\sup_{f \in \mathcal{F}} \left\{ \Phi_K(R_h, f) - \frac{1}{2} \|f\|_{2,K}^2 \right\} \geq \sup_{f \in \mathcal{F}} \left\{ \Phi_K(R_h, f) - \Phi_K(R_h^0, f) - \|f\|_{2,K}^2 \right\} - \sup_{f \in \mathcal{F}} \left\{ \Phi_K(R_h^0, f) - \frac{1}{2} \|f\|_{2,K}^2 \right\},
\]
by using similar argument as in (C.13). Similarly, by Lemma D.1 and our definition of \( L_K(\cdot) \) given in §5.2, we have
\[
\sup_{f \in \mathcal{F}} \left\{ \Phi_K(R_h, f) - \Phi_K(R_h^0, f) - \|f\|_{2,K}^2 \right\} \lesssim L_{K,\beta,1}^2 \delta_{R,h,\delta} + \eta_{K,r,h}^2. \tag{D.7}
\]

Recall that we define \( f_{R_h} = \arg\min_{f \in \mathcal{F}} \|f(z_h) - T(R_h - R_h^0)(z_h)\|_2 = \sqrt{\mathbb{E}_{z_h}[(f(z_h) - T(R_h - R_h^0)(z_h))^2]} \).

Without loss of generality, we assume there exist some \( R_h \in \mathcal{R}_h \) such that \( \|f_{R_h}\|_2 \geq L_{K,\beta,1} \delta_{R,h,\delta} + \xi_{K,r,h} + \eta_{K,r,h}^2 \delta_{R,h,\delta} \), otherwise, we obtain \( \|T(R_h - R_h^0)\|_2 \lesssim L_{K,\beta,1} \delta_{R,h,\delta} + \xi_{K,r,h} + \eta_{K,r,h}^2 \delta_{R,h,\delta} \) for all \( R_h \in \mathcal{R}_h \), directly by Assumption 5.7 and triangle inequality. For those \( R_h(\cdot) \), we let \( \kappa_{R_h} = L_{K,\beta,1} \delta_{R,h,\delta}/2 \|f_{R_h}\|_2 \) and we have \( \kappa_{R_h} \in [0,0.5] \). We then obtain
\[
\sup_{f \in \mathcal{F}} \left\{ \Phi_K(R_h, f) - \Phi_K(R_h^0, f) - \|f\|_{2,K}^2 \right\}
\geq \kappa_{R_h} \left( \Phi_K(R_h, f_{R_h}) - \Phi_K(R_h^0, f_{R_h}) \right) - \kappa_{R_h}^2 \|f_{R_h}\|_{2,K}
\geq \kappa_{R_h} \left[ \Phi(R_h, f_{R_h}) - \Phi(R_h^0, f_{R_h}) \right] - \kappa_{R_h}^2 \|f_{R_h}\|_{2,K}
\geq L_{K,\beta,1} \delta_{R,h,\delta} \|f_{R_h}\|_{2,K}^2 + \kappa_{R_h} \delta_{R,h,\delta}
\geq L_{K,\beta,1} \delta_{R,h,\delta} \|T(R_h - R_h^0)\|_2 \|f_{R_h}\|_{2,K}^2 - CL_{K,\beta,1} \delta_{R,h,\delta}^3.
\]

The first inequality holds since \( \mathcal{F} \) is star-shaped and \( \kappa_{R_h} f_{R_h} \in \mathcal{F} \). The second inequality holds uniformly for all \( R_h \) by a similar argument of Lemma C.5, where we only need to replace the
Finally, we claim our proof of Lemma D.2.

of the function class \( H \) follows by several facts. First, we have
\[ \kappa_{R,h} \delta_{R,h,\delta} \|f_{R,h}\|_2 \leq L_{K,\beta,1} \delta_{R,h,\delta} \] by the definition of \( \kappa_{R,h} = L_{K,\beta,1} \delta_{R,h,\delta} / (2\|f_{R,h}\|_2) \). Second, we obtain \( \kappa_{R,h} \delta_{R,h,\delta} \leq \delta_{R,h,\delta}^{2}, \) since \( \kappa_{R,h} \in [0,0.5] \). Last, we obtain
\[ \kappa_{R,h}^{2} \|f_{R,h}\|_{2,K}^{2} \leq \kappa_{R,h}^{2} (1.5\|f_{R,h}\|_{2}^{2} + \delta_{R,h,\delta}^{2}) \leq L_{K,\beta,1}^{2} \delta_{R,h,\delta}^{2}. \] Combining these together, we conclude the last inequality.

In addition, Combining the conclusions given above with (D.7), we have
\[ L_{K,\beta,1} \delta_{R,h,\delta} \|\mathbb{T}(R_{h} - R_{h}^{0})\|_2 \leq L_{K,\beta,1}^{2} \delta_{R,h,\delta}^{2} + L_{K,\beta,1} \delta_{R,h,\delta} \xi_{K,r,h} + \eta_{K,r,h}^{2}. \]

We finally obtain
\[ \|\mathbb{T}(R_{h} - R_{h}^{0})\|_2 \leq L_{K,\beta,1} \delta_{R,h,\delta} + \xi_{K,r,h} + \frac{\eta_{K,r,h}^{2}}{\delta_{R,h,\delta}}. \]

Similarly, we are also able to obtain an upper bound for \( \mathbb{E}[\mathbb{E}[G_{h}(s_{h}, a_{h}, o_{h}) - G_{h}^{0}(s_{h}, a_{h}, o_{h}) \mid s_{h}, a_{h}]^{2}] \).

Finally, we claim our proof of Lemma D.2. \( \square \)

E Proof of Examples in §5

In this section, we will provide theoretical proofs for our examples given in §5. We will give upper bounds for the suboptimality of our constructed policy under different function classes. To be more specific, we will prove our cases under linear function classes, RKHS and neural networks in §E.1, §E.2 and §E.3, respectively.

E.1 Proof of Corollary 5.1

The proof of Corollary 5.1 mainly requires computing the critical radius of (5.3), (5.5) and (5.6). We next aim at obtaining upper bounds for these critical radius mentioned above.

First, we will introduce some basic terminologies. An empirical \( \epsilon \)-cover of a function class \( \mathcal{H} \) is any function class \( \mathcal{H}_{\epsilon} \) such that for all \( f \in \mathcal{H} \), \( \inf_{f_{\epsilon} \in \mathcal{H}_{\epsilon}} \|f_{\epsilon} - f\|_{2,K} \leq \epsilon \). For any given function class \( \mathcal{H} \), we denote \( N(\epsilon, \mathcal{H}, S) \) as the smallest size of \( \epsilon \)-cover of \( \mathcal{H} \). An empirical \( \delta \)-slice of \( \mathcal{H} \) is defined as \( \mathcal{H}_{S,\delta} = \{ f \in \mathcal{H} : \|f\|_{2,K} \leq \delta \} \). By Corollary 14.3 of Wainwright (2019), the empirical critical radius of the function class \( \mathcal{H} \) is upper bounded by any solution of

\[ \int_{\delta^{2}/8}^{\delta} \sqrt{\log N(\epsilon, \mathcal{H}_{S,\delta}, S)} \frac{d\epsilon}{K} \leq \frac{\delta^{2}}{20}. \]  

(E.1)

We next make a relaxation by replacing \( \mathcal{H}_{S,\delta} \) by \( \mathcal{H} \), in order to obtain an upper bound of the solution to (E.1). When \( \mathcal{F} \) defined in (5.3) only contains linear functions, by setting \( \mathcal{H} \) as \( \mathcal{F} \) and solving this (E.1) for \( \mathcal{F} \), we obtain that the empirical critical radius of \( \mathcal{F} \) is upper bounded by \( O(\sqrt{m \log K / K}) \).

Next, we aim at getting an upper bound of the empirical critical radius of \( \mathcal{R}_{h}^{*} \). Since both \( \mathcal{R}_{h} \) and \( \mathcal{F} \) only contain uniformly bounded functions, then if \( \mathcal{R}_{h,\epsilon} \) is an empirical \( \epsilon \)-cover of \( \mathcal{R}_{h} \) and \( \mathcal{F}_{\epsilon} \) is an empirical \( \epsilon \)-cover of \( \mathcal{F} \), we have \{ \((R_{h,\epsilon} - R_{h}^{*})f_{\epsilon} : R_{h,\epsilon} \in \mathcal{R}_{h,\epsilon}, f_{\epsilon} \in \mathcal{F}_{\epsilon} \} \) acts as an empirical \( C-\epsilon \)
cover of the function class $\mathcal{R}^*_h$ with $C$ being an absolute constant. Similar situation also holds for $\mathcal{G}^*_{h,j}$. Thus, we have the empirical critical radius of $\mathcal{R}^*_h$ is upper bounded by any solution to the following inequality

$$
\int_{\delta^2/8}^{\delta} \sqrt{\frac{\log N(\epsilon, \mathcal{F}, S)}{K}} + \frac{\log N(\epsilon, \mathcal{R}_h, S)}{K} d\epsilon \leq \frac{\delta^2}{20}.
$$

(E.2)

Since $\mathcal{F}, \mathcal{R}_h$ are linear function classes that only have finite dimensions, we have the solution to inequality (E.2) is $\hat{\delta} = O\left(\sqrt{\max\{m, n_h\}} \log K/K\right)$. Moreover, as the function class $\mathcal{F}, \mathcal{R}_h$ only contain bounded functions, we have

$$
\delta_{h, \mathcal{R}_h} = O\left(\frac{\log(1/\delta)}{K}\right),
$$

with probability $1 - \delta$ with $\delta_{h, \mathcal{R}_h}$ and $\hat{\delta}_K$ being the maximal critical radius and maximal empirical critical radius of $\mathcal{F}, \mathcal{R}^*_h, \forall h \in [H]$, respectively, by Corollary 5 of Dikkala et al. (2020). In addition, we are also able to determine the value for $\delta_{h, \mathcal{G}_h}$ by following similar proof procedure. We finally claim our proof of Corollary 5.1 by plugging in values of $\delta_{h, \mathcal{R}_h}$ and $\delta_{h, \mathcal{G}_h}$ in Theorem 5.1.

### E.2 Proof of Corollary 5.2

In this subsection, we provide a proof for Corollary 5.2. We are interested in the local Rademacher complexity and those corresponding critical radius of function classes $\mathcal{F}, \mathcal{R}^*_h, \mathcal{G}^*_{h,j}, \forall j \in [d_1].$ Let $\{\lambda^\mathcal{F}_i\}_{i=1}^\infty$ be the eigenvalues of $K_{\mathcal{F}}$, we have

$$
\mathcal{R}_K(\delta, \mathcal{F}) \leq \sqrt{\frac{2}{K} \sum_{i=1}^{\infty} \min\{\delta^2, 4C_1 \lambda^\mathcal{F}_i\}},
$$

where $C_1$ is an absolute constant by following Corollary 14.5 of Wainwright (2019) stated in §H. Then the upper bound of the solution of $\mathcal{R}_K(\delta, \mathcal{F}) \leq \delta^2$ is given by

$$
\delta_{\mathcal{F}} = 2 \min_{j \in \mathbb{N}} \left\{ \frac{j}{K} + \sqrt{\frac{2C_1}{K} \sum_{i=j+1}^{\infty} \lambda^\mathcal{F}_i} \right\}.
$$

Similar situation also holds for function classes $\mathcal{R}^*_h, \mathcal{G}^*_{h,j}, \forall j \in [d_1]$.

Thus, when the eigenvalues of $K_{\mathcal{F}}, K_{\mathcal{R}^*_h}, \forall h \in [H], \forall j \in [d_1]$ decay exponentially, we have $\|T(R_h - R^*_h)\|_2 \lesssim L_{K, d_1} \sqrt{\log K/K} + \sqrt{\log(d_1/\delta)/K}$. The same situation also applies to $K_{\mathcal{G}^*_{h,j}}$ and $\|T(G_{h,j} - G^*_{h,j})\|_2$. The same proof procedure also applies to the setting when eigenvalues of aforementioned kernels decay in polynomial speed.

Thus, by plugging these values into Theorem 5.1, we conclude our proof of Corollary 5.2.
E.2.1 Example: Neural Network

In this subsection, we provide an example for Theorem 5.2, where we use the class neural network to approximate the underlying reward and transition functions. We let $x_h := \phi_x(s_h, a_h, o_h)$ with some bounded $\phi_x(\cdot)$ and $z_h := \psi_z(s_h, a_h)$ with some embedding functions $\psi_z(\cdot)$. In addition, for all $h \in [H]$, we assume $R_h(x_h) \in \mathbb{R}_h$, and $G_{h,j}(x_h) \in \mathbb{G}_{h,j}$, where $\mathbb{R}_h$ and $\mathbb{G}_{h,j}$ are true function classes that contain $R_h^*, G_{h,j}^*$. We next pose several needed assumptions on these function classes which build blocks for our theory.

**Assumption E.1.** We assume true functions (reward and transition) fall in $\mathbb{R}$ classes that contain $h$ for all $\phi$ some bounded Sobolev function class, by Theorem 1 of Yarotsky (2017) given in $\mathcal{P}$ distribution by Theorem 1 of Yarotsky (2017). Here the associated this probability measure is the sample $\xi$ with a smooth one. Moreover, under Assumption E.2, the upper bound of the approximation errors $\mathbb{R}$ We assume the minimizers exist and are defined as $R_h, G_{h,j}^*$.

**Example: Neural Network**

When we consider using aforementioned neural networks to approximate the true functions in Sobolev function class, by Theorem 1 of Yarotsky (2017) given in §H, we obtain for all $h \in [H], \forall j \in [d_1],$

$$\eta^N_{K,r,h} := \min_{R_h \in \mathbb{R}_h} \| (R_h - R_h^*)(\cdot) \|_{\infty} = \mathcal{O}(K^{-\frac{\alpha}{2d+\alpha}}),$$

$$\eta^N_{K,G,h} := \max_{j \in [d_1]} \min_{G_{h,j} \in \mathbb{G}_{h,j}} \| (G_{h,j} - G_{h,j}^*)(\cdot) \|_{\infty} = \mathcal{O}(K^{-\frac{\alpha}{2d+\alpha}}).$$

We assume the minimizers exist and are defined as $R_h^0, G_{h,j}^0, \forall h \in [H], j \in [d_1].$

Next, we put assumptions on $\mathcal{F}$ and projected function classes $\{T(R_h - R_h^0)(\cdot) := \mathbb{E}[(R_h - R_h^0)(x_h) | z_h = \cdot], R_h \in \mathbb{R}_h\}$ and $\{T(G_{h,j} - G_{h,j}^0)(\cdot) := \mathbb{E}[(G_{h,j} - G_{h,j}^0)(x_h) | z_h = \cdot], G_{h,j} \in \mathbb{G}_{h,j}\}$ as follows.

**Assumption E.2.** We assume $T(R_h - R_h^0)(\cdot)$, for all $R_h \in \mathbb{R}_h$ and $T(G_{h,j} - G_{h,j}^0)(\cdot)$, for all $G_{h,j} \in \mathbb{G}_{h,j}$ fall in the Sobolev ball with order $\alpha$ and input dimension $d$. In addition, we assume $\mathcal{F}$ is the star hull (with center 0) of a class of ReLU neural network with at most $\mathcal{O}(\log K)$ layers, $\mathcal{O}(K^\frac{d}{2d+\alpha})$ bounded weights. See Yarotsky (2017) for a detailed introduction to Sobolev ball and ReLU neural networks.

Assumption E.2 holds when the density of $\rho(x_h | z_h)$ is smooth enough. For example, when $x_h | z_h \sim \mathcal{N}(\phi(z_h), \sigma^2 \mathbb{I})$, we have $\rho(x_h | z_h) = \tilde{\rho}(x_h - \phi(z_h))$. In this case, the conditional expectation $T(R_h - R_h^0)(z_h) = \mathbb{E}[(R_h - R_h^0)(x_h) | z_h]$ is smooth as it is a convolution of a non-smooth function with a smooth one. Moreover, under Assumption E.2, the upper bound of the approximation errors $\xi_{r,h,K}, \xi_{G,h,K}$ involved in Assumption 5.7 are given below:

$$\forall R_h \in \mathbb{R}_h, \min_{f \in \mathcal{F}} \| f(z_h) - T(R_h - R_h^0)(z_h) \|_2 \leq \xi_{r,h,K} = \mathcal{O}(K^{-\frac{\alpha}{2d+\alpha}}),$$

$$\forall j \in [d_1], \forall G_{h,j} \in \mathbb{G}_{h,j}, \min_{f \in \mathcal{F}} \| f(z_h) - T(G_{h,j} - G_{h,j}^0)(z_h) \|_2 \leq \xi_{G,h,K} = \mathcal{O}(K^{-\frac{\alpha}{2d+\alpha}}),$$

by Theorem 1 of Yarotsky (2017). Here the associated this probability measure is the sample distribution $\rho$. 

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Putting all pieces into Theorem 5.2, we have the following Corollary E.1, which quantifies the suboptimality under misspecified function classes of neural networks.

**Corollary E.1.** Under Assumptions 5.1, 5.2 (with replacing \( R^*_h, G^*_h,j \) by \( R^0_h \) and \( G^0_h,j, \forall h \in [H], j \in [d_1] \)), E.1 and E.2. By constructing our policy \( \hat{\pi} \) by PLAN, with probability \( 1 - \delta - 1/K \), we obtain

\[
\text{SubOpt}(\hat{\pi}) \lesssim C_{\pi^*} \left[ \left( H \sum_{h=1}^{H} \tau_{G,h,K} \sqrt{d_1 L_{K,d_1}} + \sum_{h=1}^{H} \tau_{r,h,K} L_{K,1} \right) \cdot \left( K^{-\frac{\alpha}{2\alpha+\bar{d}}} + \sqrt{\frac{\log(d_1/\delta)}{K}} \right) \right].
\]

**E.3 Proof of Corollary E.1**

By Theorem 5.2, we observe that the upper bound only involves approximation errors \( \xi_{r,h,K}, \eta_{r,h,K}, \xi_{G,h,K}, \eta_{G,h,K} \) and critical radii \( \delta_{G,h}, \delta_{R,h} \). Next, we will specify these terms under the setting of §E.2.1.

The approximation error of ReLU neural networks with \( O(\log K) \) layers and \( O(K^{\frac{d_2}{2\alpha+\bar{d}}}) \) parameters to Sobolev ball with order \( \alpha \) in \( \ell_{\infty} \)-norm is \( O(K^{-\frac{\alpha}{2\alpha+\bar{d}}}) \). This conclusion follows directly from Theorem 1 of Yarotsky (2017).

We next provide an upper bound for the critical radii of \( F, \widetilde{\mathcal{G}}_{h,j}^*, \widetilde{\mathcal{R}}_{h,j}^* \). Note that \( \widetilde{\mathcal{R}}_{h,j}^* \) is contained by \( \{ c(R_h - R^0_h) \cdot f_h, R_h \in \widetilde{\mathcal{R}}_h, f_h \in F, c \in [0,1] \} \). Thus, the critical radii of \( \widetilde{\mathcal{R}}_{h,j}^* \) will give an upper bound of the critical radii of \( \widetilde{\mathcal{R}}_{h,j}^* \). We next use CR(\( \mathcal{H} \)) to represent the critical radius of a function class \( \mathcal{H} \). Following the same way of deriving (E.2), we have the \( \text{CR}(\widetilde{\mathcal{R}}_{h,j}^*) \leq \max\{\text{CR}(F), \text{CR}(\widetilde{\mathcal{R}}_h)\} \) in the sense that it is upper bounded by the maximum critical radii of \( F \) and \( \widetilde{\mathcal{R}}_h \). Similar situation also applies to \( \widetilde{\mathcal{G}}_{h,j}^* \), i.e., \( \text{CR}(\widetilde{\mathcal{G}}_{h,j}^*) \leq \max\{\text{CR}(F), \text{CR}(\widetilde{\mathcal{G}}_{h,j})\} \). In addition, the critical radii of function classes \( F, \widetilde{\mathcal{R}}_h, \widetilde{\mathcal{G}}_{h,j} \) which are defined in §E.2.1, are of order \( O(K^{-\frac{\alpha}{2\alpha+\bar{d}}}) \) by the proof of Corollary 6.6 in Uehara et al. (2021).

Finally, plugging in these values into the upper bound of Theorem 5.2, we conclude our proof of Corollary E.1.

**F Proof of Applications in §6**

**F.1 Proof of Proposition 6.1**

*Proof.* The proof of Proposition 6.1 is a special case of the proof of Corollary 5.1. Here we only consider strategic regression problem with time horizon \( H = 1 \) and no state transition. Thus, we only need to replace plug in \( m_h, n = d \) into the critical radii of linear function classes set \( H = 1 \) in Corollary 5.1. Putting all pieces together, we then finally conclude our proof of Proposition 6.1.

**F.2 Proof of Proposition 6.2**

*Proof.* In this subsection, we will provide our proof for Proposition 6.2. First, with high probability, we have \( r^* \in \mathcal{R} \) by following a similar proof of Lemma C.1. By our construction of \( \hat{\pi} \) using
pessimism, we further have
\[
\text{SubOpt}(\tilde{\pi}) = J(R^*, \pi^*) - J(R^*, \tilde{\pi}) \\
\leq J(R^*, \pi^*) - \min_{R \in \mathcal{R}} J(R, \pi^*) + \min_{R \in \mathcal{R}} J(R, \tilde{\pi}) - J(R^*, \tilde{\pi}) \\
\leq J(R^*, \pi^*) - \min_{R \in \mathcal{R}} J(R, \pi^*) =: (i).
\]

Here the first inequality holds by the definition of \(\tilde{\pi}\). The second inequality holds by pessimism. We denote \(\tilde{R} = \arg\min_{R \in \mathcal{R}} J(R, \pi^*)\). We next provide an upper bound for \((i)\).

\[
(i) = \int R^*(a_t, a_{2t}) - \tilde{R}(o_t, a_{2t}) d\pi^*(a_{2t} | a_t) dF(o_t | a_{1t}) d\pi^*(a_{1t}).
\]

Here \(F(o_t | a_{1t}) = \int_{i_t} P(o_t | a_{1t}, i_t) dP(i_t)\) is the conditional distribution of \(o_t\) given \(a_{1t}\). According to Cauchy-Schwartz inequality, we next have

\[
(i) \leq \left( \int [R^*(a_t, a_{2t}) - \tilde{R}(o_t, a_{2t})]^2 d\pi^*(a_{2t} | a_t) dF(o_t | a_{1t}) d\pi^*(a_{1t}) \right)^{1/2} \\
\leq C_{\pi^*} \left( \int [R^*(a_t, a_{2t}) - \tilde{R}(o_t, a_{2t})]^2 d\rho(a_{1t}, a_t, a_{2t}) \right)^{1/2} \\
\leq C_{\pi^*} \tau_1 \left( \int \left( \int [R^*(o_t, a_{2t}) - \tilde{R}(o_t, a_{2t})] d\rho(o_t, a_{2t} | a_{1t}) \right)^2 d\rho(a_{1t}) \right)^{1/2} \\
= C_{\pi^*} \tau_1 \|T(\tilde{R} - R^*)\|_2 \leq C_{\pi^*} \tau_1 L_{K, 1} \delta_{R, \delta}.
\]

The second inequality follows from the concentrability in Assumption 6.1 and the third inequality follows from the ill-posed condition in §6.2. Moreover, the last inequality follows by using similar proof procedure of Lemma C.3, so we omit the details here. It is worth to note that here \(L_{K} = L + \sigma \sqrt{\log(K)}\) with \(L\) being the upper bound of all functions in \(\mathbb{R}_1\). Moreover, we have \(\delta_{R, \delta} = \delta_{\mathcal{R}} + \frac{c_1 \sqrt{\log(c_0/\delta)}/K}{\tilde{C}}\) with \(\delta_{\mathcal{R}}\) being the upper bound of the critical radii of \(\mathcal{F}\) and \(\mathcal{R}^* := \{c(R(a_2, o) - R^*(a_2, o)) \cdot \mathbb{E}[R(a_2, o) - R^*(a_2, o) | z = a_1], \forall r \in \mathbb{R}_1, \forall c \in [0, 1] \}\).

\[\square\]

\section*{F.3 Noncompliant Agents in Recommendation System}

This subsection discusses our application to the recommendation system with noncompliant agents, which is the example we describe in §3. To avoid redundancy, in this section, we only introduce the mathematical formulation of this model.

- At stage \(h \in [H]\), the principal first announces a recommendation \(a_h\).

- The (noncompliant) myopic agent with private type \(i_h \sim P_h(\cdot)\) takes an action \(b\) that maximizes its immediate reward (utility) \(R^*_{a_h}(\cdot)\) given the suggested recommendation \(a_h\), state variable \(s_h\) and its private type \(i_h\), namely,

\[
b_h = \arg\max_b R^*_{a_h}(a_h, s_h, i_h, b).
\]
• The principal finally observes the $o_h = b_h$, which is the agent’s actual choice.

• The principal receives a reward $r_h = R_h^*(s_h, b_h) + g_h$, where $g_h = f_{1h}(i_h) + \epsilon_h$ with $\epsilon_h$ being subGaussian and independent of all other random variables.

• The system transits to next state variable $s_{h+1} \sim G_h(s_h, b_h) + \xi_h$. We assume $\xi_h = f_{2h}(i_h) + \eta_h$, where $\eta_h \sim N(0, \sigma^2 I)$ and is independent of all other random variables.

We observe that such a setting is a special case of strategic MDP defined in §3.1 with $o_h = b_h$, for all $h \in [H]$. Likewise, we focus on a target population of agents and for any given $h \in [H]$, we define a new MDP which marginalizes the effect of strategic agents. In this scenario, we assume the marginal distribution of $i_h \sim P_h(\cdot)$, $R_{ah}^*(\cdot)$ and $f_{1h}(i_h), f_{2h}(i_h)$ are known in the planning stage.

We then define the new (marginalized) true reward function and transition distribution as follows:

$$\bar{r}_h^*(s_h, a_h) = \int_{i_h} \left[ R_h^*(s_h, b_h) + f_{1h}(i_h) \right] dP_h(i_h),$$

$$\bar{P}_h^*(\cdot | s_h, a_h) = \int_{i_h} P_h(\cdot | s_h, b_h, i_h) dP(i_h),$$

where $b_h = \text{argmax}_b R_{ah}^*(a_h, s_h, i_h, b)$ and $\bar{P}_h^*(\cdot | s_h, b_h, i_h)$ is $N(G_h(s_h, b_h) + f_{2h}(i_h), \sigma^2 I)$. Thus, the true model is given as $\{\bar{R}_h^*(s_h, a_h), \bar{P}_h^*(\cdot | s_h, a_h)\}_h=1^H$, in the planning stage. Based on the defined reward and transition functions, we can determine our value function, Q-function, and Bellman equation in the same way as in §3.3.

Next, we discuss the data collecting process. We sample $K$ trajectories $\{(s_h^{(k)}, a_h^{(k)}, b_h^{(k)}, i_h^{(k)})\}_{h=1}^{H,K}$ independently of $\{(s_h^{(k)}, a_h^{(k)}, b_h^{(k)})\}_{h=1}^{H}$ following a joint distribution $\rho : \{(S_h \times A_h \times B_h)\}_{h=1}^{H} \rightarrow \mathbb{R}$. We then optimize the policy based on our collected dataset using PLAN. In specific, we obtain

$$\hat{\pi} = \arg \max_{\pi \in \Pi} \min_{M = \{(\bar{P}_h, \bar{R}_h)\}_{h=1}^{H}} J(M, \pi). \quad (F.1)$$

Here $\bar{G}_h$ and $\bar{R}_h$, $\forall h \in [H]$ are confidence sets that contain $\bar{P}_h^*$, $\bar{R}_h^*$, $\forall h \in [H]$ constructed via our offline dataset $\{(s_h^{(k)}, a_h^{(k)}, b_h^{(k)}, i_h^{(k)})\}_{k=1}^{K}$. The procedure is almost the same with that in §4.3.2, the only difference is to replace $\hat{a}_h^{(k)}, \hat{o}_h^{(k)}$ by $b_h^{(k)}$. Thus, we omit the details here.

Meanwhile, those needed assumptions are also similar with those in §5.1. Therefore, we finally summarize the suboptimality of $\hat{\pi}$ in this application in the following Proposition F.1.

**Proposition F.1.** Under Assumptions 5.1, 5.2 and 5.3 (only replacing $(a_h, o_h)$ by $b_h$), with probability $1 - \delta - 1/K$, the suboptimality is upper bounded by

$$\text{SubOpt}(\hat{\pi}) \leq C_{\pi^*} \left[ H \sum_{h=1}^{H} \tau_{G,h,K} \sqrt{\frac{d_1}{L_{K,d_1}}} \delta_{\bar{G},h,\delta} + \sum_{h=1}^{H} \tau_{\bar{R},h,K} L_{K,1} \delta_{\bar{R},h,\delta} \right],$$

where $L_{K,d_1} = L + \sigma \sqrt{\log H + 1} \log(Kd_1)$, $\delta_{\bar{G},h,\delta} = \delta_{\bar{G},h} + c_1 \sqrt{\log(c_0 H/\delta)/K}$, $\delta_{\bar{R},h,\delta} = \delta_{\bar{R},h} + c_2 \sqrt{\log(c_0 H_1/\delta)/K}$ with $c_0, c_1, c_2$ being absolute constants. Here we let $\delta_{\bar{G},h}$ and $\delta_{\bar{R},h}$ be the upper bounds of the maximum critical radii of $\mathcal{F}, \mathcal{G}_h^*$ and $\mathcal{F}, \mathcal{R}_h^*$, (with $\mathcal{F}, \mathcal{G}_h^*, \mathcal{R}_h^*$ being defined in §5.1 by replacing $(a_h, o_h)$ with $b_h$).
F.4 Proof of Proposition F.1

In this subsection, we provide our proof of Proposition F.1. Like our proof for Theorem 5.1, we are also able to prove Lemma C.1, C.2, C.3, only by replacing \((s_h, a_h, a_h)\) by \((s_h, b_h)\). We let \(\tilde{M} := \{ (\tilde{R}_h, \tilde{P}_h) \}_{h=1}^H\). Leveraging these conclusions, we have

\[
\begin{align*}
E_{h \sim \pi^*(\cdot | s_h), s_h \sim d_h^*} \left[ \left\| \left( \tilde{P}_h - P_h^* \right)(\cdot | s_h, a_h) \right\|_1 \right] \\
= E_{h \sim \pi^*(\cdot | s_h), s_h \sim d_h^*} \left[ \left\| \int \tilde{P}(\cdot | s_h, b_h, i_h) - P^*(\cdot | s_h, b_h, i_h) dP_h(i_h) \right\|_1 \right] \\
\leq E_{h \sim \pi^*(\cdot | s_h), s_h \sim d_h^*} \left[ \int \left\| \tilde{P}(\cdot | s_h, b_h, i_h) - P^*(\cdot | s_h, b_h, i_h) \right\|_1 dP_h(i_h) \right] \\
\leq \sqrt{E_{h \sim \pi^*(\cdot | s_h), i_h \sim P_h(\cdot), s_h \sim d_h^*} \left[ \text{TV}\left( \tilde{P}(\cdot | s_h, b_h, i_h), P^*(\cdot | s_h, b_h, i_h) \right)^2 \right]}
\end{align*}
\]

(F.2)

The first inequality follows form Jensen’s inequality. The second inequality follows from Cauchy-Schwarz inequality. Furthermore, we obtain

\[
\begin{align*}
(F.3) & \lesssim \sqrt{E_{h \sim \pi^*(\cdot | s_h), b_h \sim P_h(\cdot | s_h, a_h), s_h \sim d_h^*} \left[ \left\| \tilde{G}_h(s_h, b_h) - G_h^*(s_h, b_h) \right\|_2^2 \right]}
\\
& \lesssim C \pi^* \sqrt{E_{h \sim \pi^*(\cdot | s_h, b_h)} \left[ \left\| \tilde{G}_h(s_h, b_h) - G_h^*(s_h, b_h) \right\|_2 \right]}
\\
& \lesssim C \pi^* \tau_{K,G,h} \sqrt{d_1 L_{K,\beta,d_1} \delta_{h,G,\delta}}
\end{align*}
\]

(F.3)

Here \(P_h(\cdot | s_h, a_h)\) is the distribution of \(b_h = \arg\max R_{ah}(s_h, a_h, i_h)\) given \(s_h, a_h, R_{ah}(\cdot)\) and the distribution of \(i_h \sim P_h(\cdot)\). The first inequality follows from our model assumption on Gaussian transition given \((s_h, b_h, i_h)\). Moreover, the second inequality follows from our Assumption 5.1. Meanwhile, the third inequality follows from ill-posed condition in Assumption 5.2. Finally, similar
to the derivation of (C.3), we obtain last inequality. Likewise, we also obtain
\[
E_{a_h \sim \pi^*(\cdot | s_h), s_h \sim d_{\pi^*}^{h-1}} \left[ \left| \tilde{R}_h(s_h, a_h) - \tilde{R}^*_h(s_h, a_h) \right| \right]
\leq E_{a_h \sim \pi^*(\cdot | s_h), s_h \sim d_{\pi^*}^{h-1}, b_h \sim \mathcal{D}(\cdot | s_h, a_h)} \left[ \left| \tilde{R}_h(s_h, b_h) - R^*_h(s_h, b_h) \right| \right]^2
\leq C_{\pi^*} \sqrt{E_{\rho(s_h, b_h)} \left[ \left| (\tilde{R}_h(s_h, b_h) - R^*_h(s_h, b_h)) \right| \right]^2]
\leq C_{\pi^*} \tau_{K, r, h} \sqrt{E_{\rho(s_h, a_h)} \left[ \left( \mathbb{E} \left[ \tilde{R}_h(s_h, b_h) - R^*_h(s_h, b_h) | s_h, a_h \right] \right) \right]^2]
\leq C_{\pi^*} \tau_{K, r, h} L_{K, \beta, 1} \delta_{h, \mathcal{R}, \delta}.
\]

Here, the first and second inequalities follow from Jensen’s inequality and Cauchy-Schwartz inequalities, respectively. The third and fourth inequalities follow from Assumptions 5.1 and 5.2, respectively. The last inequality holds by a similar derivation of (C.2). Finally, we have
\[
\text{SubOpt}(\hat{\pi}) \leq C_{\pi^*} \left[ \sum_{h=1}^{H} \tau_{K, G, h} \sqrt{d_{1}} L_{K, \beta, d_{1}} \delta_{h, G, \delta} + \sum_{h=1}^{H} \tau_{K, r, h} L_{K, \beta, 1} \delta_{h, \mathcal{R}, \delta} \right].
\]

Thus, we conclude our proof for Proposition F.1.

G Proof of Technical Lemmas

In this subsection, we will prove some technical Lemmas which are used by us in proving our main theorems. First, we prove Lemma C.4.

G.1 Proof of Lemma C.4

First, we prove \( \ell(R_h, f) = (R_h(x_h^{(k)}) - R^*_h(x_h^{(k)}) + g_h^{(k)}) f(z_h^{(k)}) \) is \( L_{K, \beta, 1} \)-Lipschitz in \( f, \forall f \in \mathcal{F} \), with probability \( 1 - 1/K^\beta \). Here we define \( L_{K, \beta, d_1} := L + \sigma \sqrt{(\beta + 1) \log K d_1} \).

First, we have \( R_h(\cdot), R^*_h(\cdot) \) are bounded functions with upper bound \( L \). Since we assume \( g_h \) is a subGaussian random variable with variance proxy \( \sigma \). Then we have \( \max_{k \in [K]} |g_h^{(k)}| \leq \sigma \sqrt{(\beta + 1) \log(K)} \) with probability \( 1 - 1/K^\beta \) by union bound of subGaussian variables (Vershynin, 2011).
we have \( \ell \) functions. Then the conclusion of Lemma C.5 follows directly from Lemma 11 of Foster and Syrgkanis (2018). We next provide a upper bound for \(|\frac{1}{K} \sum_{k=1}^{K} g_h^{(k)} f(z_h^{(k)})|\). For any \( t_f \geq 0 \), we obtain

\[
\mathbb{P}\left( \exists f \in F, \left| \frac{1}{K} \sum_{k=1}^{K} g_h^{(k)} f(z_h^{(k)}) - 0 \right| \geq t_f \right) 
\leq \mathbb{P}\left( \exists f \in F, \left| \frac{1}{K} \sum_{k=1}^{K} g_h^{(k)} \mathbb{I}_{\{|g_h^{(k)}| \leq \sigma \sqrt{(\beta + 1) \log(K)} \}} f(z_h^{(k)}) - \mathbb{E}[g_h f(z_h) \mathbb{I}_{\{|g_h| \leq \sigma \sqrt{(\beta + 1) \log(K)} \}}] \right| \geq t_f / 2 \right) 
+ \mathbb{P}\left( \frac{1}{K} \sum_{k=1}^{K} g_h^{(k)} \mathbb{I}_{\{|g_h^{(k)}| \leq \sigma \sqrt{(\beta + 1) \log(K)} \}} f(z_h^{(k)}) \neq \frac{1}{K} \sum_{k=1}^{K} g_h^{(k)} f(z_h^{(k)}) \right) 
+ \mathbb{P}\left( \exists f \in F, \left| \mathbb{E}[g_h f(z_h) \mathbb{I}_{\{|g_h| \geq \sigma \sqrt{(\beta + 1) \log(K)} \}}] \right| \geq t_f / 2 \right) = (I) + (II) + (III).
\]

We have (II) \( \leq 1 / K^{\beta} \). For term (III), by Cauchy-Schartz inequality, we have

\[
\left| \mathbb{E}[g_h f(z_h) \mathbb{I}_{\{|g_h| \geq \sigma \sqrt{(\beta + 1) \log(K)} \}}] \right| \leq \sigma \|f\|_2 \sqrt{\mathbb{P}(\{|g_h| \geq \sigma \sqrt{(\beta + 1) \log(K)} \})} = \sigma \|f\|_2 / K^{\beta + 1}.
\]

Thus, when we choose \( t_f = 2C_1 \sigma \sqrt{(\beta + 1) \log K} (\delta_{R,h,\delta} \|f\|_2 + \delta_{R,h,\delta}^2) \), we have (III) = 0 when we choose \( \beta > 0 \) properly such that \( 1 / K^{\beta} = o(\delta_{R,h,\delta}^2) \).

Finally, by Lemma 11 in Foster and Syrgkanis (2019), we have (I) \( \leq \delta \) for such \( t_f \). Thus, with probability \( 1 - \delta - 1 / K^{\beta} \), we have

\[
\forall f \in F, \left| \frac{1}{K} \sum_{k=1}^{K} g_h^{(k)} f(z_h^{(k)}) \right| \lesssim \sigma \sqrt{(\beta + 1) \log K} (\delta_{R,h,\delta} \|f\|_2 + \delta_{R,h,\delta}^2). \quad (G.1)
\]

Here \( \delta_{R,h,\delta} = \delta_{R,h} + c_1 \sqrt{\log(c_0 / \delta)} / K \), with \( c_0, c_1 \) being absolute constants and \( \delta_{R,h} \) being an upper bound of the maximum critical radii of \( F \). Next, we provide an upper bound In addition, since \( R_h, R_h^{*} \) are bounded functions, we obtain with probability \( 1 - \delta \),

\[
\forall f \in F, \left| \frac{1}{K} \sum_{k=1}^{K} \left( R_h(x_h^{(k)}) - R_h^{*}(x_h^{(k)}) \right) f(z_h^{(k)}) - \Phi(R_h^{*}, f) \right| \lesssim L(\delta_{R,h,\delta} \|f\|_2 + \delta_{R,h,\delta}^2). \quad (G.2)
\]

following Lemma 11 in Foster and Syrgkanis (2019).

Combining (G.1) and (G.2), we conclude our proof of Lemma C.4.

### G.2 Proof of Lemma C.5

Here our loss function \( \ell(a, b) = a \), with \( a = (R_h - R_h^{*})(x) \mathbb{I}(R_h - R_h^{*})(z) \in R_h^{*} \). In this scenario, we have \( \ell(a, b) \) is Lipschitz continuous in \( a \). In addition, \( R_h^{*} \) is star-shaped and contains bounded functions. Then the conclusion of Lemma C.5 follows directly from Lemma 11 of Foster and Syrgkanis (2019).
**Auxiliary Lemma**

**Lemma H.1** (Corollary 14.5 of Wainwright (2019)). Let $H = \{ h \in \mathcal{H} : \|f\|_{\mathcal{H}} \leq C \}$ be a bounded ball of an RKHS with eigenvalues $\{\lambda_i\}_{i=1}^{\infty}$. Then the localized population Rademacher complexity $\mathcal{R}_K(\delta, H)$ is bounded as

$$\mathcal{R}_K(\delta, H) \leq \sqrt{\frac{2}{K} \cdot \sum_{j=1}^{\infty} \min\{\lambda_j, C^2\delta^2\}}.$$ 

Here $C$ is an absolute constant.

*Proof.* See the proof of Corollary 14.5 in Wainwright (2019) for more details.

**Lemma H.2** (Theorem 1 of Yarotsky (2017)). There exist a class of ReLU neural networks with depth at most $O(\ln(1/\epsilon))$ and $O(\epsilon^{-d/\alpha}\ln(1/\epsilon))$ weights and computation units, that approximate all $f$ in Sobolev ball with order $\alpha$ and input dimension $d$ in $\ell_\infty$-norm within error $\epsilon$.

*Proof.* See the proof of Theorem 1 in Yarotsky (2017) for more details.

**Lemma H.3** (Lemma 11 in Foster and Syrgkanis (2019)). Assume $\sup_{f \in \mathcal{F}} \|f\|_\infty \leq c$ for a constant $c$ and for any $f^* \in \mathcal{F}$. We define $\delta_K$ as the solution to

$$\mathcal{R}_K(\delta, \text{star}(\mathcal{F} - f^*)) \leq \delta^2/c.$$ 

Here the star($\cdot$) denotes the star-hull of a function class. Moreover, we assume the loss function $\ell(\cdot, \cdot)$ is $L$-Lipschitz in the first argument. The with probability $1 - x$, for all $f \in \mathcal{F}$, we have

$$\left| \frac{1}{K} \sum_{k=1}^{K} \ell(f(x_k), z_k) - \frac{1}{K} \sum_{k=1}^{K} \ell(f^*(x_k), z_k) - (\mathbb{E}[\ell(f(x), z)] - \mathbb{E}[\ell(f^*(x), z)]) \right| \leq L\delta_{K,x}(\|f - f^*\|_2 + \delta_{K,x}).$$

Here $\delta_{K,x} = \delta_K + \sqrt{\log(1/x)/K}$.

*Proof.* See the proof of Lemma 11 in Foster and Syrgkanis (2019) for more details.
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