Pessimistic Model-based Offline Reinforcement Learning under Partial Coverage

Masatoshi Uehara*1 and Wen Sun †1

1Department of Computer Science, Cornell University

Abstract

We study model-based offline Reinforcement Learning with general function approximation. We present an algorithm named Constrained Pessimistic Policy Optimization (CPPO) which leverages a general function class and uses a constraint to encode pessimism. Under the assumption that the ground truth model belongs to our function class, CPPO can learn with the offline data only providing partial coverage, i.e., it can learn a policy that competes against any policy that is covered by the offline data, in polynomial sample complexity with respect to the statistical complexity of the function class. We then demonstrate that this algorithmic framework can be applied to many specialized Markov Decision Processes and the additional structural assumptions can further refine the concept of partial coverage. One notable example is low-rank MDP with representation learning where the partial coverage is defined using the concept of relative condition number measured by the underlying unknown ground truth feature representation. Finally, we introduce and study the Bayesian setting in offline RL. The key benefit of Bayesian offline RL is that algorithmically, we do not need to explicitly construct pessimism or reward penalty which could be hard beyond models with linear structures. We present a posterior sampling based incremental policy optimization algorithm (PS-PO) which proceeds by iteratively sampling a model from the posterior distribution and performing one step incremental policy optimization inside the sampled model. Theoretically, in expectation with respect to the prior distribution, PS-PO can learn a near optimal policy under partial coverage with polynomial sample complexity. This work is a long version of the conference paper in https://openreview.net/pdf?id=tyrJsbKAe6.

1 Introduction

Offline Reinforcement Learning (RL) is one of the important areas of RL where the learner is presented with a static dataset consisting of transition-related information (state, action, reward, and next state) collected by some behavior policy, and needs to learn purely from the offline data without any future online interaction with the environment. Offline RL is used in a number of applications where online random experimentation is costly or dangerous such as health care (Kosorok and Laber, 2019), digital marketing (Chen et al., 2019) and robotics (Levine et al., 2020).

The performance guarantees of offline RL often rely on two quantities: the coverage of the offline data and the property of the function approximation used in the algorithms. For instance, for the classic Fitted-Q-iteration (FQI) algorithm (Ernst et al., 2005; Munos and Szepesvári, 2008), it requires (a) full coverage in the offline data, i.e., \( \max_{(s,a)} d^\pi(s,a)/\rho(s,a) < \infty \) for any stochastic policies \( \pi \) including history-dependent non-Markovian policies, where \( d^\pi(s,a) \) is a state-action occupancy distribution of a policy \( \pi \) and \( \rho(s,a) \) is an offline distribution, (b) realizability in a Q function class, i.e., the optimal Q function belongs to the function class, and (c) Bellman

---

*mu223@cornell.edu
†ws455@cornell.edu
completeness, i.e., applying the Bellman operator on any function in the function class results in a new function that also belongs to the function class (see the first row in Table 1). Among these three assumptions, the full coverage and the Bellman completeness are particularly strong. The full coverage means that the behavior policy needs to be exploratory enough, although figuring out an exploratory policy itself is an extremely hard problem for large-scale MDPs. The Bellman completeness assumption does not have a monotonic property, i.e., even starting with a function class that originally permits Bellman completeness, slightly increasing the capacity of the function class could result in a new class that does not have Bellman completeness anymore. Thus, we aim to relax the assumptions on the offline data and the function class. Particularly, we are interested in the following question:

Given a realizable function class and an offline distribution that only provides partial coverage, can we learn a policy that is able to compete with any policy that is covered by the offline distribution?

We study this question from a model-based learning perspective and provide an affirmative answer to the question. More specifically, different from FQI, we start with a realizable model class, i.e., the ground truth transition falls into the model class. We further abandon the strong full coverage assumption, and instead, assume partial coverage which means the offline data distribution only covers a state-action distribution of some high-quality comparator policy \( \pi^* \) (\( \pi^* \) is not necessarily the optimal policy, and \( \pi^* \) could be non-Markovian), i.e., \( \max_{s,a} d_{\pi^*}(s,a)/\rho(s,a) < \infty \).

We design an algorithm — Constrained Pessimistic Policy Optimization (CPPO), which can learn a policy that is as good as any comparator policy \( \pi^* \) that is covered by the offline data. The fact that CPPO can learn to compete against history-dependent policies is meaningful in offline RL when the offline data does not cover the optimal policy.

While one could assume density ratio based concentrability coefficient (\( \max_{s,a} d_{\pi^*}(s,a)/\rho(s,a) \)) to be under control for small size MDPs, in large-scale MDPs (e.g. continuous state space), the density ratio could quickly become an extremely large quantity which makes the performance guarantee vacuous. When applying CPPO to MDPs with additional structural assumptions, we can seamlessly refine the density ratio based concentrability coefficient to more natural and tighter quantities. Notably, we consider the offline representation learning setting where the underlying MDPs permit a low-rank structure (unlikely linear MDPs (Jin et al., 2020a; Yang and Wang, 2020), we do not assume the ground truth state-action feature representation \( \phi^* \) is known, and instead we need to learn \( \phi^* \)) and we show that we can refine the density ratio to a relative condition number that is defined using the unknown true state-action feature representation \( \phi^* \). Intuitively this means that as long as there exists a high-quality comparator policy that only visits the subspace (defined using the true representation \( \phi \)) that is covered by the offline data, CPPO can compete against such a policy, even without knowing the true \( \phi^* \). Such bounded relative condition number assumption is much weaker than the bounded density ratio assumption. While the concept of relative condition number was originally introduced in the online RL setting (e.g., Agarwal et al. (2020c,a) with a known linear feature \( \phi \)), and later was introduced in offline RL (Zhang et al. (2021b); Chang et al. (2021)), these prior works all rely on the fact that the feature representation \( \phi \) is known to the learner a priori (see Table 1 for the comparison). Another interesting example is factored MDPs (Kearns and Koller, 1999) where we show CPPO refines the density ratios to be density ratio associated with individual factors, which leverages the factored structure and is provably tighter. We also give examples on parametric linear MDPs (Yang and Wang, 2020), nonparametric linear MDPs (Jin et al., 2020a), linear mixture MDPs (Ayoub et al., 2020; Modi et al., 2020), kernelized nonlinear regulators (KNRs) and MDPs with Gaussian processes (GPs) (Kakade et al., 2020; Curi et al., 2020), where we again show that CPPO enjoys problem specific quantities for measuring the coverage.

Our contributions. Our contributions are three-folds, which we summarize below:

1. We show that in the model-based setting, realizability and partial coverage is enough to learn a high-quality comparator policy (Theorem 1 and Theorem 2). Notably, (1) this result holds for any MDPs with realizable model classes, (2) we can compete against even history-dependent policies. This is in sharp contrast to the
Table 1: Comparison among existing works regarding their type, coverage, and additional structural assumptions on the function class or MDPs. Type F means model-free and type B means model-based. Linear mixture MDPs, factored MDPs, and low-rank MDPs are models that our algorithm gives the partial coverage result for the first time. Partial coverage means that the offline distribution \( \rho \) covers a state-action distribution of a comparator policy \( \pi^* \). \dagger means it assumes an accurate density estimator for \( \rho(s,a) \). \dagger† means although the analysis in Jin et al. (2020b) is done under the full coverage for linear MDPs, based on the argument (Zhang et al., 2021b), we can show the algorithm has the PAC guarantee under partial coverage in terms of the relative condition number for linear MDPs. \dagger†† means that we can refine it to a more adaptive quantity using the model class (i.e., Definition 1). All the methods in the table require realizability in the function class.

1. state-of-art provable model-free offline RL results: see Table 1 on page 3 for detailed comparisons to prior works.

2. Under additional structural assumptions (e.g., KNRs, linear MDPs, linear mixture MDPs, low-rank MDPs, factored MDPs), we show that we can seamlessly refine the density ratio based concentrability coefficients to problem specific quantities. This flexibility to adapt to problem specific coverage measuring quantities is in sharp contrast to standard offline RL algorithms. Especially, two notable settings are low-rank MDPs (with unknown features) (Theorem 4) and factored MDPs (Theorem 5): (a) for offline representation learning in low-rank MDPs, the density ratio concentrability coefficient is refined to be a relative condition number under...
the true (but unknown) representation (Theorem 4); (b) for factored MDPs, the concentrability coefficient is refined using the density ratios associated to individual factors (Theorem 5).

3. For computational purpose, we develop incremental policy optimization and posterior sampling-based offline RL algorithms under Bayesian setting (Algorithm 8.1 and Theorem 8 in Section 8). While moving to the Bayesian setting, we sacrifice from a worst-case guarantee to a guarantee on the Bayesian suboptimality gap, we gain benefits in terms of no need to design pessimism inside the algorithms.

While we focus on the model-based setting and have demonstrated advantages of our approach over model-free ones (i.e., no more Bellman completeness assumption on function classes, being able to compete against a larger pool of policies, and the ability to seamlessly adapt to problem-dependent structures), it is worth noting that realizability in the model-based setting is usually considered stronger than the one in the model-free setting. On the empirical side, model-based offline RL algorithms are the state-of-art (e.g., Yu et al. (2020); Kidambi et al. (2020); Matsushima et al. (2020); Cang et al. (2021); Chang et al. (2021)). Our theoretical results provide a sharp contrast between model-based and model-free approaches in offline RL. For details, refer to Section 4.3.

The rest of the article is organized as follows. In Section 2, we discuss the related work. In Section 3, we introduce our setting and notation. In Section 4, we introduce two types of main algorithms, which we term Constrained Pessimistic Policy Optimization (CPPO). In Section 5, we instantiate our results in several models such as tabular MDPs, linear mixture MDPs, (parametric) linear MDPs, low-rank MDPs and factored MDPs. In Section 6, we continue this instantiation in KNRs. In Section 7, we modify CPPO to capture (nonparametric) linear MDPs. In Section 8, we introduce the posterior sampling-based offline RL algorithm under the Bayesian setting. In Section 9, we discuss our summary and future works.

2 Related work

We discuss two families of related works: offline RL and representation learning in RL.

Offline RL. Insufficient coverage of the dataset due to the lack of online exploration is known as the main challenge in offline RL (Wang et al., 2020). To deal with this problem, a number of methods have been recently proposed from both model-free (Wu et al., 2019; Touati et al., 2020; Kumar et al., 2020; Liu et al., 2020; Rezaeifar et al., 2021; Fujimoto et al., 2019; Fakoor et al., 2021; Ghasempipour et al., 2021; Buckman et al., 2020) and model-based perspectives (Yu et al., 2020; Kidambi et al., 2020; Matsushima et al., 2020; Yin et al., 2021). More or less, their methods rely on the idea of pessimism and its variants in the sense that the learned policy can avoid uncertain regions not covered by offline data. As a theoretical side, Munos and Szepesvári (2008); Duan et al. (2020, 2021); Fan et al. (2020) proved FQI has a PAC (probably approximately correct) guarantee under realizability, the global coverage, and Bellman completeness. Other offline model-free RL methods such as minimax offline RL methods also require realizability and the global coverage (Chen and Jiang, 2019; Antos et al., 2008; Uehara et al., 2021a; Duan et al., 2021; Zhang et al., 2020; Nachum et al., 2019). Recently, by being inspired by aforementioned the pessimism idea, Jin et al. (2020a); Rajaraman et al. (2020) showed that FQI with an additional pessimistic bonus (penalty) term can weaken the assumption from the global coverage to partial coverage. Comparing to their works, our analysis focuses on a model-based method. The offline model-based method is known to have a PAC guarantee under the realizability and the global coverage (Ross and Bagnell, 2012; Chen and Jiang, 2019). As the most closely related work, Chang et al. (2021) proved a model-based method with an additional penalty term can weaken the assumption from the global coverage to the partial coverage for structured MDPs such as KNRs and Gaussian Processes models (Deisenroth and Rasmussen, 2011). In this work, we consider arbitrary MDPs with a realizable model class and aim for PAC bounds under a partial coverage condition.
Representation learning. We discuss literature related to representation learning in RL. Representation learning for low-rank MDPs (ground truth feature representation is unknown) in online learning is studied from a model-based perspective (Agarwal et al., 2020b) and model-free perspective (Modi et al., 2021). In the online setting, Zhang et al. (2021a); Papini et al. (2021) also study representation learning under different model assumptions. Comparing with these works, since our setting is offline, the algorithm and analysis are totally different.

In the offline setting, Ni et al. (2021) study dimensionality reduction in a given kernel space, and Hao et al. (2021) study feature selection in sparse linear MDPs. Their focus is different as they do not study PAC guarantees (2021); Papini et al. (2021) also study representation learning under different model assumptions. Comparing with these works, since our setting is offline, the algorithm and analysis are totally different.

Throughout this work, we do not assume partial coverage. Hereafter, \(c,c_1,c_2,\cdots\) are always universal constants.

3 Preliminaries

We consider a Markov Decision process (MDP) \(\mathcal{M} = \{\mathcal{S}, \mathcal{A}, P, \gamma, r, d_0\}\) where \(P : \mathcal{S} \times \mathcal{A} \rightarrow \Delta(\mathcal{S})\) is the transition, \(r : \mathcal{S} \times \mathcal{A} \rightarrow [0,1]\) is the reward function, \(\gamma \in [0,1)\) is the discount factor, and \(d_0 \in \Delta(\mathcal{S})\) is the initial state distribution. With slight abuse of notation, we denote the Radon-nikodym derivative of \(P\) with respect to a baseline measure \(\iota\) by \(P\) as well, i.e., \(P\) is a probability mass function in the discrete case (\(\iota\) is the counting measure) and a probability density function in the continuous setting (\(\iota\) is the Lebesgue measure). A policy \(\pi\) maps from state (or history) to distribution over actions. Given a policy \(\pi\) and a transition distribution \(P\), \(V^\pi_P\) denotes the expected cumulative reward of \(\pi\) under \(P, d_0\) and \(r\). Similarly, \(Q^\pi_P : \mathcal{S} \times \mathcal{A} \rightarrow \mathbb{R}\) are a Q-function and advantage-function under \(P\) and \(\pi\). Given a transition \(P\), we denote \(\pi(P)\) as the optimal policy associated with model \(P\) under reward \(r\). We also denote \(d^\pi_P \in \Delta(\mathcal{S} \times \mathcal{A})\) as the average state-action distribution of \(\pi\) under the transition model \(P\), i.e., \(d^\pi_P = (1 - \gamma) \sum_{t=0}^{\infty} \gamma^t d^\pi_P,\) where \(d^\pi_P \in \Delta(\mathcal{S} \times \mathcal{A})\) is the distribution of \((s_t,a_t)\) under \(\pi\) and \(P\) at a time-step \(t\). We denote the true transition distribution as \(P^\star\), which we do not know in advance. For simplicity, we suppose \(r\) is known. The extension to the unknown reward is straightforward.

In the offline RL setting, we have an offline distribution \(\rho \in \Delta(\mathcal{S} \times \mathcal{A})\), and an offline dataset \(\mathcal{D} = \{s^{(i)}, a^{(i)}, r^{(i)}, s'^{(i)}\}_{i=1}^\gamma\) which is sampled in the following way: \(s,a \sim \rho, r = r(s,a), s' \sim P^\star(\cdot|s,a)\). We hope to obtain \(\pi(P^\star) = \arg \max_{\pi} V^\pi_P\) from this offline dataset without any further interaction with the environment. We often denote \(\mathbb{E}_{\mathcal{D}}[f(s,a,s')] = 1/\gamma \sum_{(s,a,s') \in \mathcal{D}} f(s,a,s')\). Our goal is to construct an offline RL algorithm Alg, which maps from \(\mathcal{D}\) to \(\pi\) so that the suboptimality gap \(V^\pi_P - V^{\pi_{Alg(\mathcal{D})}}_P\) for any comparator policy \(\pi^\star \in \Pi\) is minimized, where \(\Pi\) in this work can be an unrestricted policy class (e.g., including non-Markovian policies). Hereafter, \(c_1, c_2, \cdots\) are always universal constants.

Partial coverage. Throughout this work, we do not assume \(\rho\) has global coverage. The global coverage in this work means that the density ratio based concentrability coefficient \(d^\rho_P(s,a)/\rho(s,a)\) is upper-bounded by some constant \(C \in \mathbb{R^+}\) for all polices \(\pi \in \Pi\), or the feature covariance matrix corresponding to the offline distribution \(\mathbb{E}_{s,a \sim \rho} \phi(s,a)\phi(s,a)^\top\) (\(\phi \in \mathcal{S} \times \mathcal{A} \rightarrow \mathbb{R}\) is a feature representation) is full rank and has a non-zero minimum eigenvalue, which are commonly used assumptions in offline RL (Munos, 2005; Antos et al., 2008; Chen and Jiang, 2012).
4 Pessimistic Model-based Offline RL

We first introduce a general model-based algorithm that has a PAC guarantee of the suboptimality gap under partial coverage, where the first inequality uses \( \hat{P}_{\pi} \). Depending on the concentrability coefficient for the comparator policy, the final error only incurs the policy evaluation error for the comparator policy \( \pi^* \). We want to design an algorithm that can compete against any policy \( \pi^* \) that is covered by the offline data. This assumption is much weaker than the global coverage.

4.1 With Total Variation Constraints

Our algorithm, Constrained Pessimistic Policy Optimization with total variation constraints (CPPO-TV) (Algorithm 1), takes a realizable hypothesis class \( M \) (with \( P^* \in M \)) consisting of \( |M| \) candidate models as input, computes the maximum likelihood estimator (MLE) \( \hat{P}_{\text{MLE}} \) using the given offline data \( D = \{ s, a, s' \} \). It then forms a min-max objective subject to a constraint. The min-max objective introduces pessimism via searching for the least favorable model \( P \) (in terms of its policy’s value \( V^*_P \)) that is feasible with respect to the constraint. We can also express the constrained optimization procedure using a version space \( M_D \) and a policy optimization procedure defined below:

\[
\max_{\pi \in \Pi} \min_{P \in M_D} V^*_P, \quad \text{where } M_D = \left\{ P \mid P \in M, \mathbb{E}_D \left[ \text{TV}(\hat{P}_{\text{MLE}}(\cdot|s, a), P(\cdot|s, a))^2 \right] \leq \xi \right\},
\]

where \( TV(P_1, P_2) \) is a total variation (TV) distance between two distributions \( P_1 \) and \( P_2 \). The version space \( M_D \) contains models that are not far away from \( \hat{P}_{\text{MLE}} \) in terms of the average TV distance under \( D \). The version space is constructed such that with high probability \( P^* \in M_D \).

Below we state the algorithm’s performance guarantee. Assuming for now that \( P^* \in M_D \) holds with high probability, then, \( \hat{V}^\pi := \min_{P \in M_D} V^*_P \) is a pessimistic policy evaluation estimator, which satisfies \( \hat{V}^\pi \leq V^*_P \) for all \( \pi \in \Pi \). Using the idea of pessimism, we have the following observation:

\[
V^*_P - \hat{V}^*_P = V^*_P - \hat{V}^\pi + \hat{V}^\pi - V^*_P \leq V^*_P - \hat{V}^\pi + \hat{V}^\pi - V^*_P \leq V^*_P - \hat{V}^\pi,
\]

where the first inequality uses \( \hat{\pi} = \arg \max_{\pi \in \Pi} \hat{V}^\pi \) and the second inequality uses \( \hat{V}^\pi \leq V^*_P \) for all \( \pi \in \Pi \). Thus, the final error only incurs the policy evaluation error for the comparator policy \( \pi^* \), which leads to the error only depending on the concentrability coefficient for the comparator policy.

We define the following new concentrability coefficient that uses the model class \( M \):

**Definition 1** (Model-based Concentrability Coefficient). For a comparator policy \( \pi^* \), we define the concentrability coefficient \( C^\pi_{\pi^*} \) as follows:

\[
C^\pi_{\pi^*} = \sup_{P \in M} \frac{\mathbb{E}_{(s,a) \sim \hat{P}_{\pi}^*}[\text{TV}(P'(\cdot|s, a), P^*(\cdot|s, a))^2]}{\mathbb{E}_{(s,a) \sim \rho}[\text{TV}(P'(\cdot|s, a), P^*(\cdot|s, a))^2]}.
\]

The following theorem shows CPPO learns a policy that competes against \( \pi^* \) when \( C^\pi_{\pi^*} < \infty \).
Algorithm 1 Constrained Pessimistic Policy Optimization with Total Variation constraints (CPPO-TV)

1: **Require**: Models \( \mathcal{M} \), dataset \( \mathcal{D} \), parameter \( \xi \), policy class \( \Pi \) (note \( \Pi \) could be unrestricted)

2: Obtain the estimator \( \hat{P}_{MLE} \) by MLE: \( \hat{P}_{MLE} = \arg \max_{P \in \mathcal{M}} \mathbb{E}_D[\ln P(s' | s, a)] \).

3: Constrained policy optimization:

\[
\hat{\pi} = \arg \max_{\pi \in \Pi} \min_{P \in \mathcal{M}} V_{\hat{P}}(\pi), \text{ s.t., } \mathbb{E}_D[TV(\hat{P}_{MLE}(\cdot | s, a), P(\cdot | s, a))^2] \leq \xi.
\]

4: **Return** \( \hat{\pi} \)

**Theorem 1** (PAC Bound for CPPO-TV with general function class). Assume \( P^* \in \mathcal{M} \). We set \( \xi = c_1 \frac{\ln(c_2 |\mathcal{M}|/\delta)}{n} \).

Then, with probability \( 1 - \delta \), for any comparator policy \( \pi^* \in \Pi \) (\( \Pi \) can be the unrestricted policy class containing non-Markovian policies),

\[
V_{P^*} - V_{\hat{P}} \leq c_3 (1 - \gamma)^{-2} \sqrt{\frac{C^\dagger_{\pi^*} \ln(c_2 |\mathcal{M}|/\delta)}{n}}.
\]

To the best of our knowledge, this is the first algorithm that achieves a PAC guarantee for any MDPs under the partial coverage assumption \( C^\dagger_{\pi^*} < \infty \) with only a realizable hypothesis class. We emphasize that the inequality in the above uniformly holds for all policies with probability \( 1 - \delta \) including history-dependent non-Markovian policies.

Note that the ability to compete against non-Markovian policies in offline RL is meaningful when the offline data does not cover the optimal policy \( \pi^* \) (i.e., there could be a high-quality history-dependent policy that is covered by the offline data against which we want to compete). In model-free approaches, this type of result generally cannot be obtained. Indeed, the model-free approach from Xie et al. (2021) requires \( \Pi \) to be a restricted Markovian policy class, since their bound contains \( \text{poly}(\ln(|\Pi|)) \) dependence. For the detailed discussion, refer to Section 4.3.

The quantity \( C^\dagger_{\pi^*} \), adaptively captures the discrepancy between the offline data and the state-action occupancy measure under a comparator policy \( \pi^* \) depending on the model class \( \mathcal{M} \). For example, \( C^\dagger_{\pi^*} \) can be reduced to a relative condition number in KNRs. Besides, it is always upper bounded by the density ratio based concentrability coefficient:

\[
C_{\pi^*, \infty} := \sup_{(s, a)} \frac{d_{P^*}(s, a)}{\rho(s, a)}.
\]

Prior works that achieve PAC guarantees with only realizable model classes rely on much stronger global coverage \( \sup_{\pi} C_{\pi, \infty} < \infty \) (Chen and Jiang, 2019). Even when the comparator policy is the optimal policy \( \pi(P^*) \), the partial coverage condition \( C_{\pi(P^*), \infty} < \infty \) is weaker. Existing pessimistic model-based algorithms and their theoretical results (Chang et al., 2021) often assume that a point-wise model uncertainty measure is given as a by-product of model fitting, which limits the applicability to special linear models such as KNRs/GPs. CPPO-TV can work for any MDPs with the realizable function class having a valid statistical complexity such that the MLE properly works.

**Remark 1** (Variations of Concentrability Coefficients). With a slight modification of the proof, we can obtain the bound (2) where \( C^\dagger_{\pi^*} \) is replaced with

\[
C_{\pi^*, 2} := \mathbb{E}_{(s, a) \sim \rho} \left( \frac{d_{P^*}(s, a)}{\rho(s, a)} \right)^{2} \right)^{1/2}.
\]
Algorithm 2 Constrained Pessimistic Policy Optimization with Likelihood-Ratio based constraints (CPPO-LR)

1: **Require**: Models $\mathcal{M}$, dataset $D$, parameter $\zeta$, policy class $\Pi$ (note $\Pi$ could be unrestricted)
2: Constrained policy optimization:

$$\hat{\pi} = \arg\max_{\pi \in \Pi} \min_{P \in \mathcal{M}_D} V_P^\pi, \text{ s.t. }$$

$$\mathcal{M}_D = \{ P \in \mathcal{M} : \mathbb{E}_P[\ln P(s' | s, a)] \geq \max_{P \in \mathcal{M}} \mathbb{E}_P[\ln P(s' | s, a)] - \zeta \}. $$

3: **Return** $\hat{\pi}$

4.2 With Likelihood-ratio Based Constraints

In Algorithm 1, the constraint is given using the total variation distance. Here, we propose a similar contained pessimistic policy optimization algorithm in Algorithm 2. The only difference compared to Algorithm 1 is that the constraint is given based on the log likelihood-ratio. Since this new constraint is generally easier to calculate than the total variation distance, Algorithm 1 might be preferable compared to Algorithm 1.

CPPO-LR has the following same statistical guarantee as the one obtained in Theorem 1 for CPPO-TV.

**Theorem 2** (PAC Bound for CPPO-LR with general function class). Assume $P^* \in \mathcal{M}$. We set $\bar{\zeta} = c_1 \frac{\ln(\epsilon_{2} |\mathcal{M}| / \delta)}{n}$. Then, with probability $1 - \delta$, for any comparator policy $\pi^* \in \Pi$ ($\Pi$ can be the unrestricted policy class containing non-Markovian policies),

$$V_{P^*} - V_P^\pi \leq c_3 (1 - \gamma)^{-2} \sqrt{\frac{C_{\pi^*} \ln(\epsilon_{2} |\mathcal{M}| / \delta)}{n}}.$$

Next, we consider the case where the function class is infinite. To quantify statistical complexities for infinite function classes, we define bracketing numbers as follows (van de Geer, 2000).

**Definition 2** (Bracketing numbers). Consider a function class $\mathcal{F}$ that maps $X$ to $\mathbb{R}$. Given two functions $l(\cdot)$ and $u(\cdot)$, the bracket $[l, u]$ is the set of all functions $f \in \mathcal{F}$ with $l(x) \leq f(x) \leq u(x)$ for all $x \in X$. An $\epsilon$-bracket is a bracket $[l, u]$ with $\|l - u\| \leq \epsilon$. The bracketing number of $\mathcal{F}$ w.r.t. the metric $\|\cdot\|$ denoted by $N_{\|\cdot\|}(\epsilon, \mathcal{F}, \|\cdot\|)$ is the minimum number of $\epsilon$-brackets needed to cover $\mathcal{F}$.

Using bracketing numbers, we can obtain the guarantee when the function class is infinite. Note $\iota(S)$ is $|S|$ in the discrete state space, and the volume of $S$ in the continuous state space. Recall $\iota(\cdot)$ is a baseline measure.

**Theorem 3** (PAC Bound for CPPO-LR with general function class). Assume $P^* \in \mathcal{M}$. We set $\bar{\zeta} = c_1 \frac{\ln(\epsilon_{2} N_{\|\cdot\|}(\epsilon, \mathcal{M}, \|\cdot\|_{\infty}) / \delta)}{n}$ where $\epsilon = 1/(n \iota(S))$. Then, with probability $1 - \delta$, for any comparator policy $\pi^* \in \Pi$ ($\Pi$ can be the unrestricted policy class containing non-Markovian policies),

$$V_{P^*} - V_P^\pi \leq c_3 (1 - \gamma)^{-2} \sqrt{\frac{C_{\pi^*} \ln(\epsilon_{2} N_{\|\cdot\|}(\epsilon, \mathcal{M}, \|\cdot\|_{\infty}) / \delta)}{n}}.$$

**Remark 2** (Comparison between CPPO-TV and CPPO-LR). Theorem 1 consider the case where the hypothesis class $\mathcal{M}$ is finite in CPPO-TV. When the hypothesis class is infinite, we can still obtain the PAC guarantee of CPPO-TV by utilizing the generalized result for any realizable model class with valid statistical complexity. However, in this result, we still need certain non-trivial calculations for each model while Theorem 3 just requires the simple calculation of log bracketing numbers of models. For example, this benefit is later seen when we consider linear mixture MDPs. Refer to Remark 3.
4.3 Comparison to the model-free approach from Xie et al. (2021); Zanette et al. (2021)

Xie et al. (2021) study the model-free setting where the function class $Q$ models $Q$ functions assumed to be Bellman complete for any Markovian policy in $\Pi$. While directly comparing model-based approaches to model-free approaches is hard as they use different inductive biases in function classes, we can leverage the approach from Chen and Jiang (2019, Corollary 6) to convert a model class $M$ to a pair of $Q$ and $\Pi$ class. Specifically, we can convert a model class $M$ to a pair of $Q$ class and $\Pi$ class such that $Q$ will be realizable and also Bellman complete with respect to all $\pi \in \Pi$. After such conversion from the model-based setting to the model-free setting, running the algorithm from Xie et al. (2021) using $Q$ and $\Pi$ achieves $V_{P^*}^\pi - V_{\hat{P}^*}^\pi = \sqrt{C^\pi \ln(|M||\Pi|/n)}$, $\forall \pi^* \in \Pi$, where $C^\pi$ is some concentrability coefficient. For the detailed derivation, we refer readers to Appendix A. Since the suboptimality gap from such conversion incurs $\ln |\Pi|$, a policy class $\Pi$ cannot be too large. Especially, unlike our results, it cannot take the unrestricted policy class as $\Pi$. This restriction cannot be fixed even if we use natural policy gradient (NPG) algorithms unless models have special structures (Xie et al., 2021; Zanette et al., 2021). The details are given in Section A.

In summary, our theorem (Theorem 1 and Theorem 2) indicates two advantages of model-based approaches: (1) realizability in function class is enough to ensure a PAC guarantee under a partial coverage condition, (2) it can compete against a larger pool of candidate policies including history-dependent non-Markovian policies, which is a meaningful property when the offline data does not cover the globally optimal policy.

5 Examples with Refined Concentrability Coefficients

In the previous section, our results apply to any MDP as long as its true transition belongs to a function class $M$. In this section, we consider several concrete MDPs with additional structural conditions. We show that by leveraging the additional structural conditions, we can refine the model-based concentrability coefficient to more natural quantities. The examples that we discuss here are: (1) linear mixture MDPs which generalize linear MDPs from Yang and Wang (2020) and tabular MDPs, (3) low-rank MDPs, and (4) factored MDPs.

5.1 Tabular MDPs

Tabular MDPs are MDPs where the state and action spaces are finite. Although the corresponding hypothesis class for tabular MDPs is infinite, we can still run MLE, that is, estimating $P^*$ by the empirical distribution. Then, Algorithm 1 and Algorithm 2 has the following guarantee.

**Corollary 1** (PAC bound for tabular MDP). We set $\xi = c_1 [S]^{2} |A| \ln(n|S||A|c_2/A^2) / n$ and denote an output of CPPO-TV (Algorithm 1) by $\hat{\pi}$. Then with probability $1 - \delta$, for all $\pi^* \in \Pi$ ($\Pi$ is the unrestricted policy class),

$$V_{P^*}^\pi - V_{\hat{P}^*}^\pi \leq c_3(1 - \gamma)^{-2} \left\{ \sqrt{C^\pi_\infty |S|^2 |A| \ln(n|S||A|c_4/\delta)} / n \right\}.$$ 

The same statement holds when $\pi$ is an output of CPPO-LR (Algorithm 2) by setting $\tilde{\xi} = c_1 [S]^{2} |A| \ln(n|S||A|c_2/A^2) / n$.

Here, for tabular MDPs with $M = \{ P : P(s,a) \in \Delta(S), \forall s,a \}$, the model-based concentrability coefficient in Definition 1 is equal to the density ratio based concentrability coefficient $C^\pi_\infty$ which is the right quantity for small-size tabular MDPs.

5.2 Linear Mixture MDPs

We define linear mixture MDPs (Ayoub et al., 2020; Modi et al., 2020).
Definition 3 (Linear mixture MDPs). Given a feature vector $\psi : (S, A, S) \to \mathbb{R}^d$, a linear mixture MDP is an MDP where the ground truth transition is $P^*(s' | s, a) := \theta^* \top \psi(s, a, s')$, $\theta^* \in \mathbb{R}^d$.

By setting, $\psi(s, a, s') = \mu(s') \bigotimes \phi(s, a)$ ($\bigotimes$ denotes the Kronecker product), linear mixture MDPs include the following parametric linear MDPs (Yang and Wang, 2020):

Definition 4 (Parametric linear MDPs). Parametric linear MDP admits a decomposition:

$$P^*(s' | s, a) := \sum_{i=1}^{d_1} \sum_{j=1}^{d_2} M_{ij}^* \phi_j(s, a)$$

with $\mu : S \to \mathbb{R}^{d_1}$ and $\phi : S \times A \to \mathbb{R}^{d_2}$. Here, $\mu$ and $\phi$ are known features, and $M^* \in \mathbb{R}^{d_1 \times d_2}$ is unknown.

We use CPPO to learn on linear mixture MDPs. The corresponding $\mathcal{M}$ is

$$\mathcal{M}_{\text{Mix}} = \left\{ \theta^\top \psi(s, a, s') \mid \theta \in \Theta \subseteq \mathbb{R}^d, \int \theta^\top \psi(s, a, s') d\mu(s') = 1 \quad \forall (s, a) \right\}.$$

Given a function $V : S \to \mathbb{R}$, define the state-action feature indexed by $V$ as

$$\psi_V(s, a) := \int \psi(s, a, s') V(s') d\mu(s'),$$

we have the following PAC guarantee.

Corollary 2 (PAC bound for linear mixture MDPs). Suppose $\Theta = \{ \theta : ||\theta||_2 \leq R \}$, $||\psi_V(s, a)||_2 \leq 1$ for any $V \in \{ S \to [0, 1] \}$, and $P^* \in \mathcal{M}_{\text{Mix}}$. Let $\hat{\pi}$ be the output of CPPO-LR (Algorithm 2) when we set $\zeta = c_1 d \ln(c_2 n R_t(S)/\delta)/n$. Then, with probability $1 - \delta$, for any $\pi^*$ in $\Pi$ (again $\Pi$ can be the unrestricted policy class), CPPO outputs a policy $\hat{\pi}$ such that:

$$V_{\hat{\pi}}^* - V_{\pi^*}^* \leq c_3 (1 - \gamma)^{-2} \sqrt{\min \left( d C^\dagger_{\pi^*}, d^2 C_{\pi^*, \text{mix}}^\dagger \right) \ln \left( c_4 n R_t(S)/\delta \right) / n},$$

where the concentrability coefficient $C_{\pi^*, \text{mix}}$ is defined as:

$$C_{\pi^*, \text{mix}} := \sup_{P \in \mathbb{Z}_{\pi^*}} \sup_{x \in \mathbb{R}^d} \left( \frac{x^\top \Sigma_{\pi^*, \psi_{V_P^*}} x}{x^\top \Sigma_{P, \psi_{V_P^*}} x} \right)$$

with the localized class $\mathbb{Z}_{\pi^*} := \{ P \in \mathcal{M}_{\text{mix}} : \mathbb{E}_{(s,a) \sim \rho}[\text{TV}(P(\cdot | s, a), P^*(\cdot | s, a))^2] \leq \zeta \}$, $\Sigma_{P, \psi_{V_P^*}}$ $\psi_{V_P^*} = \mathbb{E}_{(s,a) \sim \rho} [\psi_{V_P^*}(s, a) \psi_{V_P^*}(s, a)^\top]$, and $\Sigma_{\pi^*, \psi_{V_P^*}} = \mathbb{E}_{s,a \sim d_{\pi^*}^P} [\psi_{V_P^*}(s, a) \psi_{V_P^*}(s, a)^\top]$.

When specializing to parametric linear MDPs, the above bound still holds with $C_{\pi^*, \text{mix}}$ being replaced by the relative condition number $C_{\pi^*, \phi}$:

$$C_{\pi^*, \phi} := \sup_{x \in \mathbb{R}^d} \frac{x^\top \Sigma_{\pi^*, \phi} x}{x^\top \Sigma_{\pi^*, \phi} x},$$

where $\Sigma_{\phi} = \mathbb{E}_{(s,a) \sim \rho}[\phi(s,a)\phi(s,a)^\top]$, $\Sigma_{\pi^*} = \mathbb{E}_{(s,a) \sim d_{\pi^*}^P} [\phi(s,a)\phi(s,a)^\top]$.

This is the first PAC guarantee result in the offline setting under partial coverage $C_{\pi^*, \text{mix}} < \infty$ for linear mixture MDPs. The quantity $C_{\pi^*, \text{mix}}$ is a newly-introduced concentrability coefficient for linear mixture MDPs. This coefficient is measured on the integrated feature vectors $\phi_V(s, a)$ for $V : S \to [0, 1]$. Note the class of $V$ is localized,
We consider the representation learning in offline RL. Following FLAMBE (Agarwal et al., 2020b), we study

\[ \hat{\pi} \]

for all \( \pi \) (see Lemma 14 in Section G).

Note that these relative condition number based quantifiers are always tighter than the density ratio based concentrability coefficients (i.e., \( \max\{\bar{C}_{\pi^*}, \bar{C}_{\pi^*, \text{mix}}\} \leq C_{\pi^*, \infty} \)). For the special case where \( \phi(s, a) \) is a one-hot encoding vector, then they are reduced to the density ratio based concentrability coefficient. In a non-tabular setting, even if when the density ratio is infinite, the relative condition number can still be finite. Intuitively, the bounded relative condition number implies that the offline data covers the subspace that the comparator policy \( \pi^* \) visits.

We finally remark the norm assumption \( \|\psi_V(s, a)\|_2 < 1 \) is commonly assumed in the online setting (Zhou et al., 2021).

**Remark 3 (Guarantee of CPPO-TV).** Corollary 2 is for CPPO-LR. Under \( \inf_{s, a, s'} P^*(s' \mid s, a) \geq c_3 > 0 \), we can ensure the similar guarantee for CPPO-TV. However, apparently, it is not obvious how to relax this assumption when we use CPPO-TV.

### 5.3 Low-rank MDPs with Representation Learning

We consider the representation learning in offline RL. Following FLAMBE (Agarwal et al., 2020b), we study low-rank MDPs but in the offline setting. Note that low-rank MDPs here are a more generalized model of the aforementioned parametric linear MDPs (Yang and Wang, 2020) since the true feature representation \( \phi^* \) in a low-rank MDP is unknown.

**Definition 5 (Low rank MDPs).** The ground-truth model \( P^* \) admits a low rank decomposition with a dimension \( d \) if there exists two embedding functions \( \mu^* : S \rightarrow \mathbb{R}^d, \phi^* : S \times A \rightarrow \mathbb{R}^d \) s.t. \( P^*(s' \mid s, a) = \mu^*(s')^\top \phi^*(s, a) \). Neither \( \mu^* \) nor \( \phi^* \) is known to the learner.

One interesting special case of a low-rank MDP is the following latent variable model (see Agarwal et al. (2020b) for more details).

**Definition 6 (Latent variable models).** There exists a latent space \( \mathcal{Z} \) along with functions \( \mu^* : \mathcal{Z} \rightarrow \Delta(S) \) and \( \phi^* : S \times A \rightarrow \Delta(\mathcal{Z}) \) s.t. \( P^*(\cdot \mid s, a) = \sum_{z \in \mathcal{Z}} \mu^*(\cdot \mid z) \phi^*(z \mid s, a) \).

To tackle representation learning under partial coverage on low-rank MDPs, we setup function classes as follows: given two function classes \( \Psi \subset S \rightarrow \mathbb{R}^d, \Phi \subset S \times A \rightarrow \mathbb{R}^d \) (both are realizable in the sense that \( \mu^* \in \Psi \) and \( \phi^* \in \Phi \)), we consider a hypothesis class \( \{\mu(s')^\top \phi(s, a) ; \mu \in \Psi, \phi \in \Phi\} \). Then, CPPO (Algorithm 1) and Theorem 1 still work under this setting. Note that this function class setup is exactly the same as the one from FLAMBE.

Here we show that by leveraging the low-rankness, we can refine the concentrability coefficient to a relative condition number defined by the unknown true representation \( \phi^* \). We emphasize that this does not depend on the other features. Particularly, given a comparator policy \( \pi^* \), we define \( \bar{C}_{\pi^*, \phi^*} \):

\[
\bar{C}_{\pi^*, \phi^*} = \sup_{x \in \mathbb{R}^d} \frac{x^\top \Sigma_{\pi^*, \phi^*} x}{\|x\|_2^2}, \quad \Sigma_{\pi^*, \phi^*} := \mathbb{E}_{s, a \sim P^{\pi^*}} \phi^*(s, a) \phi^*(s, a)^\top, \quad \Sigma_{\mu} := \mathbb{E}_{s, a \sim \rho} \phi^*(s, a) \phi^*(s, a)^\top.
\]

We can show CPPO learns a policy that can compete against \( \pi^* \) as long as \( \bar{C}_{\pi^*, \phi^*} < \infty \).

**Theorem 4 (PAC bound for low-rank MDP).** We set \( \xi = c_4 \frac{\ln(\|\Psi\|_{\text{size}})}{n} \). Suppose (a): \( \|\phi(s, a)\|_{L_2} \leq 1, \forall (s, a) \in S \times A \) for any \( \phi \in \Phi \), \( \int \mu(s')^\top \phi(s, a) d\mu(s') = 1 \) and \( \|\mu\|_{L_2} \leq \sqrt{d} \) for any \( \mu \in \Psi \), \( \phi \in \Phi \), (b) \( \rho(s, a) = d_{P^{\pi^*}}^\rho(s, a) \), (c) \( P^*(s' \mid s, a) = \mu(s')^\top \phi^*(s, a) \) for some \( \mu^* \in \Psi, \phi^* \in \Phi \). With probability at least \( 1 - \delta \), for all \( \pi^* \in \Pi \) (again \( \Pi \) can be an unrestricted policy class), CPPO-TV (Algorithm 1) and CPPO-LR (Algorithm 2) find \( \hat{\pi} \) such that:

\[
V_{P^{\pi^*}} - V_{P^{\hat{\pi}}} \leq c_5 \sqrt{\bar{C}_{\pi^*, \phi^*} \omega_{\pi^*} \rank(\Sigma_{\mu}) \ln(\|\Psi\|_{\text{size}} c_4/\delta)} (1 - \gamma)^{4n}, \quad \omega_{\pi^*} = \left( \max_{(s, a)} \pi^*(a \mid s) \right) / \left( \max_{(s, a)} \pi_{b}(a \mid s) \right).
\]
To the best of our knowledge, this is the first established PAC result under the partial coverage condition \( \hat{C}_{\pi^*, \phi^*} < \infty, \omega_{\pi^*} < \infty \) for low-rank MDPs in the offline setting. We also emphasize that our bound in Theorem 4 is distribution dependent, i.e., it depends on \( \text{rank}(\Sigma_\rho) \) rather than the exact rank \( d \). Note that \( \text{rank}(\Sigma_\rho) \leq d \), and \( \text{rank}(\Sigma_\rho) \) could be much smaller than \( d \) when the offline distribution only concentrates on a low-dimensional subspace (defined using \( \phi^* \)). Note that the assumption that \( \omega_{\pi^*} < \infty \) does not imply the state-action density ratio \( C_{\pi^*, \infty} \) is small. Indeed, \( \omega_{\pi^*} < \infty \) is much weaker than \( C_{\pi^*, \infty} < \infty \).

### 5.4 Factored MDPs

The last example we include is the factored MDP (Kearns and Koller, 1999) defined as follows:

**Definition 7 (Factored MDPs).** Let \( d \in \mathbb{N}^+ \) and \( O \) being a small finite set. The state space \( S = O^d \), and for each state \( s \), we denote \( s[i] \in O \) as the \( i \)-th variable of the state \( s \). For each \( i \in [1, \ldots, d] \), the parents of \( i \), \( \text{pa}_i \subset [1, \ldots, d] \), is the subset of state variables that directly influences \( i \), i.e., the transition is defined as follows:

\[
\forall s, a, s' : P^*(s'|s,a) = \prod_{i=1}^{d} P^*_i(s'_i|s[\text{pa}_i], a).
\]

We will denote \( S_i = O^{|	ext{pa}_i|} \), and given \( s \in S \), we will have \( s[\text{pa}_i] \in S_i \).

Due to the factorization, the transition operator \( P^* \) can be described with \( L := \sum_{i=1}^{d} |A||O|^{1+|\text{pa}_i|} \) many parameters. In contrast, the non-factored transition will need \( O(|O|^d) \) parameters. When \( |\text{pa}_i| \ll d \forall i \), it is expected that we can learn this model with lower sample complexity by leveraging the factorization which has been demonstrated in the online setting (Kearns and Koller, 1999). We remark a factored MDP is an example where model-based approaches are necessary as neither the optimal policy nor the Q functions are factored (Koller and Parr, 2000).

**Algorithm.** Next, we consider the algorithm. While Algorithm 1 (CPPO-TV) and Algorithm 2 (CPPO-LR) can ensure partial coverage results in terms of \( C_{\pi^*, \infty} \), we modify these algorithms to obtain more refined results so that we can take the factored structure into account.

We consider the modification of CPPO-TV. First, we perform MLE for model learning: each factor \( P^*_i \) is independently learned via MLE:

\[
\forall i \in [d], \hat{P}_{\text{MLE},i} = \arg \max_P \mathbb{E}_D[\ln P(s'[i]|s[\text{pa}_i], a)], \quad \hat{P} = \prod_i \hat{P}_{\text{MLE},i}.
\]

Next, the constrained policy optimization procedure is defined as

\[
\hat{\pi} = \arg \max \pi \min_{P:=\prod_i P_i} V^\pi_{\hat{P}}, \text{ s.t. } \mathbb{E}_D[\text{TV}(P_i(\cdot|s,a), \hat{P}_{\text{MLE},i}(\cdot|s,a))^2] \leq \xi_i (\forall i \in [1, \ldots, d]). \tag{5}
\]

Compared to the original CPPO-TV, we modify the constraint so that the constraint is factored as well. Note that in the above objective, there is no restriction on the policy, i.e., the \( \arg \max \) operator searches over all possible policies including non-Markovian ones.

Next, we consider the modification of CPPO-LR. The algorithm is given as follows:

\[
\hat{\pi} = \arg \max \pi \min_{P:=\prod_i P_i} V^\pi_{\hat{P}}, \text{ s.t. } \mathbb{E}_D[\log(\hat{P}_{\text{MLE},i}(\cdot|s,a)/P_i(\cdot|s,a))] \leq \bar{\xi}_i (\forall i \in [1, \ldots, d]). \tag{6}
\]

Compared to the original CPPO-LR, we modify the constraint so that the constraint is factored as well.
We consider the example of KNRs (Kakade et al., 2020; Curi et al., 2020) in this section. More specifically, we demonstrate the wide applicability of our constrained pessimistic model-based RL framework. We have already obtained in Chang et al. (2021) with bonus-based pessimistic policy optimization, we aim to tailor CPPO-TV and CPPO-LR to obtain tight guarantees on KNRs. Although the partial coverage results in KNRs have already been obtained in Chang et al. (2021) with bonus-based pessimistic policy optimization, we aim to demonstrate the wide applicability of our constrained pessimistic model-based RL framework.

**Lemma 1.** (Comparison of density-ratio based concentrability coefficients between factorized MDPs and non-factorized MDPs) We have \( \tilde{C}_{\pi^*, \infty} \leq C_{\pi^*, \infty} \)

With the new definition of the concentrability coefficients, now we are ready to state the PAC bound of CPPO for factorized MDPs. Recall \( L := \sum_{i=1}^{d} L_i \), \( L_i = |A||O|^{1+|pa_i|} \).

**Theorem 5** (PAC bound for factored MDP). We set \( \bar{\zeta}_i = c_1 L_i \ln(L_i c_2 d / \delta) \) and \( \bar{\zeta}_i = c_3 L_i \ln(L_i c_2 d / \delta) \). Then with probability \( 1 - \delta \), modified CPPO-TV (5) and modified CPPO-LR (6) find a policy \( \hat{\pi} \) such that for all comparator policy \( \pi^* \in \Pi \) (\( \Pi \) can be unrestricted),

\[
V_{\hat{\pi}} - V_{\pi^*} \leq c_3 (1 - \gamma)^{-2} \sqrt{\frac{d \tilde{C}_{\pi^*, \infty} L \cdot \ln(n L c_4 d / \delta)}{n}}.
\]

Note that our sub-optimality gap scales polynomially with respect to \( L \), i.e., the complexity of the factored MDP, rather than \( |S| \) which can be \( \Omega(\exp(d)) \). Importantly, the bound does not scale with \( C_{\pi^*, \infty} \), which will be obtained using the original CPPO-TV and CPPO-LR. Instead, it scales with \( \tilde{C}_{\pi^*, \infty} \), which is expected to be much smaller than \( C_{\pi^*, \infty} \) from Lemma 1.

**Remark 4** (Improved Concentrability Coefficients). For interpretability, in the above theorem, we use density ratio based concentrability coefficient. We remark that indeed \( \tilde{C}_{\pi^*, \infty} \) can be replaced with an \( L_2 \)-based concentrability coefficient

\[
\tilde{C}_{\pi^*, 2} = \max_{j \in [1, \ldots, d]} \mathbb{E}_{(s_j, a) \sim \rho} \left[ \left( \frac{d_{\pi^*, j}(s_j, a)}{\rho(s_j, a)} \right)^2 \right]^{1/2}.
\]

In this \( L_2 \)-form, we can still leverage the factorized structure of factored MDPs using the following lemma.

**Lemma 2.** (Comparison of density-ratio based concentrability coefficients between factorized MDPs and non-factorized MDPs)

\[ \tilde{C}_{\pi^*, 2} \leq C_{\pi^*, 2}. \]

6 Constrained Pessimistic Model-Based Policy Optimization for KNRs

We consider the example of KNRs (Kakade et al., 2020; Curi et al., 2020) in this section. More specifically, we tailor CPPO-TV and CPPO-LR to obtain tight guarantees on KNRs. Although the partial coverage results in KNRs have already been obtained in Chang et al. (2021) with bonus-based pessimistic policy optimization, we aim to demonstrate the wide applicability of our constrained pessimistic model-based RL framework.
6.1 Finite Dimensional Kernelized Nonlinear Regulators

A kernelized Nonlinear Regulator (KNR) (Kakade et al., 2020) is a model where the ground truth transition \( P^*(s'|s, a) \) is defined as \( s' = W^* \phi(s, a) + \epsilon, \epsilon \sim \mathcal{N}(0, \zeta^2 I) \), with \( \phi : \mathcal{S} \times \mathcal{A} \rightarrow \mathbb{R}^d \) being a possibly nonlinear feature mapping. We denote the corresponding model on \( W \) by \( P(W) \). We can apply Algorithm 1 and obtain its guarantee. Especially, since \( \text{TV}(P(W)(s, a), P(W^*)(s, a))^2 = \Theta((W - W^*)\phi(s, a))^2) \) (Devroye et al., 2018), \( C_{\pi^*} \) is upper-bounded by the relative condition number \( dC_{\pi^*,\phi} \) as follows.

**Lemma 3** (Model-based Concentrability Coefficient for KNRs). In KNRs, we have

\[
C_{\pi^*}^d \leq dC_{\pi^*,\phi}.
\]

We tailor Algorithm 1 to KNRs as follows to obtain a tighter guarantee. First, MLE procedure is replaced with \( \hat{W}_{\text{MLE}} \) by regularized MLE:

\[
\hat{W}_{\text{MLE}} = \arg \min_{W \in \mathbb{R}^{d_s \times d}} \mathbb{E}_D[\|W\phi(s, a) - s'\|_F^2 + \lambda \|W\|_F^2],
\]

where \( \| \cdot \|_F \) is a Frobenius norm. Then, the final policy optimization procedure is

\[
\hat{\pi} = \arg \max_{\pi \in \Pi} \min_{W \in W_D} V_{\hat{W}(W)}^\pi, \text{ s.t., } W_D = \{ W \in \mathbb{R}^{d_s \times d} : \|\hat{W}_{\text{MLE}} - W\)(\Sigma_n)^{1/2}\|_2 \leq \xi \}
\]

where \( \Sigma_n = \sum_{i=1}^n \phi(s, a_i)\phi^T(s_i, a_i) + \lambda I \). We state the theoretical guarantee for KNRs below.

**Corollary 3** (PAC bound for KNRs). Assume \( \|\phi(s, a)\|_2 \leq 1, \forall (s, a) \in \mathcal{S} \times \mathcal{A} \). We set

\[
\xi = \sqrt{2\lambda\|W^*\|_2^2 + 8\zeta^2 (d_s \ln(5) + \ln(1/\delta)) + \tilde{T}_n}, \quad \tilde{T}_n = \ln (\det(\Sigma_n)/\det(\lambda I)),
\]

Suppose the KNR model is well-specified. By letting \( \|W^*\|_2 = O(1), \zeta^2 = O(1), \lambda = O(1) \), with probability \( 1 - \delta \), for all \( \pi^* \in \Pi \), we have

\[
V_{\pi^*} - V_{\hat{\pi}} \leq c_1 (1 - \gamma)^{-2} \min(d^{1/2}, \check{R}) \sqrt{\frac{d_s C_{\pi^*\phi} \ln(c_2 n/\delta)}{n}}, \quad \text{where } \check{R} := \text{rank}[\Sigma_\rho]/\text{rank}[\Sigma_\rho] + \ln(c_2/\delta).
\]

This implies CPPO can learn a policy that can compete against \( \pi^* \) with partial coverage \( \hat{C}_{\pi^*} < \infty \). Then, we can also recover the result of Chang et al. (2021) which proposes a reward penalty-based pessimistic offline RL algorithm. Note that the condition \( \hat{C}_{\pi^*} < \infty \) does not require \( \Sigma_\rho \) to be full-rank. Also the bound uses \( \text{rank}[\Sigma_\rho] \) instead of \( d \), which means that our bound is distribution dependent and is still valid even when \( d = \infty \) as long as the offline data only concentrates on a low-dimensional subspace.

6.2 KNRs with RKHS (Gaussian Processes)

We consider the ground truth model \( P^*(s'|s, a) \) defined as \( s' = g^*(s, a) + \epsilon, \epsilon \sim \mathcal{N}(0, \sigma^2 I) \) where each component in \( g^* \) belongs to an RKHS \( \mathcal{H}_k \) with a kernel \( k(\cdot, \cdot) \) (Curi et al., 2020). We assume \( s \in \mathbb{R}^{d_s} \).

We denote a \( d_s \) dimensional RKHS as \( \bigoplus \mathcal{H}_k \). We also denote the corresponding model to \( g \) by \( P(g) \). We can learn \( g^* \) by regularized MLE (kernel ridge regression) using offline dataset \( D \). We tailor Algorithm 1 and Algorithm 2 as follows.

First, by letting \( x := (s, a), x_1 = (s_1, a_i) \), MLE procedure is replaced with \( g_{\text{MLE}} \) by regularized MLE:

\[
g_{\text{MLE}}(\cdot) = S(K_n + \zeta^2 I)^{-1}k_n(\cdot), \quad S = [s_1, \cdots, s_n] \in \mathbb{R}^{d_s \times n}, \quad k_n(x) = [k(x_1, x), \cdots, k(x_n, x)]^T, \quad \{k_n\}_{i,j} = k(x_i, x_j) \ (1 \leq i \leq n, 1 \leq j \leq n), \quad k_n(x, x') = k(x, x') - k_n(x)^T(K_n + \zeta^2 I)^{-1}k_n(x'),
\]

where \( K_n \) and \( k_n \) are the kernel matrix and feature mapping, respectively.
where the notation $\| \cdot \|_{k_n}$ is a norm associated with an RKHS with a kernel $k_n(\cdot, \cdot)$. The final optimization procedure is replaced with

$$
\hat{\pi} = \arg \max_{\pi \in \Pi} \min_{g \in \mathcal{G}_D} V_{\pi}^\pi(P(g), s.t., \mathcal{G}_D) = \{ g \in \bigoplus \mathcal{H}_k : \sum_{i=1}^{d_S} \| \hat{g}_i, \text{MLE} - g_i \|_{k_n}^2 \leq \xi^2 \}.
$$

We state the theoretical guarantee for KNRs with RKHS below. Before proceeding to the result, we prepare several notations and definitions. For simplicity, following Srinivas et al. (2010), we suppose as follows:

**Assumption 1.** $k(x, x) \leq 1, \forall x \in S \times A$ and there exists a set of pairs of eigenvalues and eigenfunctions $\{ \mu_i, \psi_i \}_{i=1}^{\infty}$, where $\int \rho(x) \psi_i(x) \psi_i(x) dx = 1$ for all $i$ and $\int \rho(x) \psi_i(x) \psi_j(x) dx = 0$ for $i \neq j$.

The above is ensured by Mercer’s theorem (Rasmussen and Williams, 2005). Eigenfunctions and eigenvalues essentially defines an infinite-dimensional feature mapping $\phi(x) := [\sqrt{\mu_1} \psi_1(x), \ldots, \sqrt{\mu_\infty} \psi_\infty(x)]^T$. By setting eigenvalues $\{ \mu_1, \ldots, \mu_\infty \}$ in non-increasing order, we define the effective dimension below:

**Definition 8 (Effective dimension).** $d^* = \min\{ j \in \mathbb{N} : j \geq B(j + 1)n/\xi^2 \}$, $B(j) = \sum_{k=j}^{\infty} \mu_k$.

The effective dimension $d^*$ is commonly used and calculated for many kernels (Zhang, 2005; Bach, 2017; Valko et al., 2013). In finite-dimensional linear kernels $\{ x \mapsto a^T \phi(x) : a \in \mathbb{R}^d \}$ $(k(x, x) = \phi^T(x) \phi(x))$, we have $d^* \leq \text{rank}[\Sigma_\rho]$. Thus, $d^*$ is regarded as a natural extension of $\text{rank}[\Sigma_\rho]$ to infinite-dimensional models. Note that $d^*$ itself is offline distribution dependent, i.e., the eigenvalues and eigenfunctions are defined using the offline distribution $\rho$.

With the above preparations in mind, we present the theoretical result below.

**Corollary 4 (PAC bound for RKHS models).** Let $\Sigma_{\pi^*} = \mathbb{E}_{(s,a) \sim d^*_{\pi^*}}[\phi(s, a) \phi(s, a)^T]$, $\Sigma_{\mu} = \mathbb{E}_{(s,a) \sim \rho}[\phi(s, a) \phi(s, a)^T]$. We set $\xi$:

$$
\xi = \sqrt{d_S \{ 2 + 150 \ln^3(d_S n/\delta) I_n \}}, \quad I_n = \ln(\text{det}(I + \zeta^{-2} K_n))
$$

and $\nu^2 = O(1)$. With probability at least $1 - \delta$, for all comparator policy $\pi^* \in \Pi$, we have:

$$
V_{\pi^*} - V_{\hat{\pi}} \leq c_1 (1 - \gamma)^{-2}\{ d^* + \ln(c_2/\delta) \} d^* \sqrt{d_S C_{\pi^*}\phi \ln^3(c_3 d_S n/\delta) \ln(n)/n},
$$

This implies the algorithm has a valid PAC guarantee under the partial coverage of MDPS with RKHS.

### 7 Constrained Pessimistic Model-based Policy Optimization for (nonparametric) linear MDPs

CPPO cannot directly capture (nonparametric) linear MDPS in Jin et al. (2020a), which is different from the one in Yang and Wang (2020) without any modification since MLE is no longer applicable to them. However, with slight modification, we can learn nonparametric linear MDPS from model-based viewpoints. Although the partial coverage results in linear MDPS have already been obtained in Xie et al. (2021); Zanette et al. (2021); Zhang et al. (2021b), in this section, we aim to demonstrate the wide applicability of the pessimistic model-based RL framework.

We first define (nonparametric) linear MDPS.

**Definition 9 (Nonparametric linear MDPS in Jin et al. (2020a)).** Linear MDPS admit the following decomposition:

$$
P^*(s' | s, a) = \langle \mu^*(s'), \phi(s, a) \rangle
$$

where $\phi : S \times A \to \mathbb{R}^d$ is a known feature. Parameters $\theta^* \in \mathbb{R}^d$ and $\mu^*(s') : S \to \mathbb{R}^d$ are unknown to learners.
Algorithm 3 Constrained Pessimistic Policy Optimization for Nonparametric linear MDPs

1: **Require:** Models $\mathcal{M}$, dataset $\mathcal{D}$, parameter $\xi$, policy class $\Pi$, $\mathcal{V} = \{\phi(\cdot, \pi); \pi \in \Pi\}$
2: Constrained policy optimization:

$$\hat{\pi} = \arg\max_{\pi \in \Pi} \min_{P \in \mathcal{M}_{\text{linear}, \mathcal{D}}} V_P^\pi,$$

$$\mathcal{M}_{\text{linear}, \mathcal{D}} = \left\{ P \in \mathcal{M} : \sup_{v \in \mathcal{V}} \mathbb{E}_{\mathcal{D}} \left[ \left| \int \{ \hat{P}(\tilde{s} \mid s, a) - P(\tilde{s} \mid s, a) \} v(\tilde{s}) d\xi(\tilde{s}) \right|^2 \right] \leq \zeta \right\}.$$

3: **Return** $\hat{\pi}$

In linear MDPs, the model $\mathcal{M}$ is

$$\mathcal{M} = \left\{ (\mu(s'), \phi(s, a)) : \left\langle \int \mu(s') d\xi(s'), \phi(s, a) \right\rangle = 1 (\forall (s, a)), \mu : S \rightarrow \mathbb{R}^d \right\}.$$

Since the restriction on $\mu(s)$ is nonparametric, it is difficult to perform standard MLE. However, following Lykouris et al. (2021); Neu and Pike-Burke (2020), we can still learn models using other objective functions.

As a first step, we introduce a witness function $v : S \rightarrow [0, 1]$ to facilitate the learning. Instead of directly estimating $\mu^*(\cdot)$, we aim to estimate $\int \mu^*(s) v(s) d\xi(s)$. Especially, in the tabular case, for $\tilde{s} \in S$, by taking $v(s) = I(s = \tilde{s})$, it amounts to estimate $\mu(\tilde{s})$. Informally, in the non-tabular case, by taking $v(s)$ as a Dirac delta at $\tilde{s}$, it amounts to estimate $\mu(\tilde{s})$ as well. Then, since

$$\int P^*(s' \mid s, a) v(s') d\xi(s') = \left\langle \phi(s, a), \int \mu^*(s') v(s') d\xi(s') \right\rangle$$

it is natural to perform regularized least squares:

$$\hat{\theta}_v = \arg\min_{\theta \in \mathbb{R}^d} \mathbb{E}_{\mathcal{D}} [\{ v(s') - \langle \phi(s, a), \theta \rangle \}^2] + \lambda \| \theta \|_2^2.$$

The analytical form of $\hat{\theta}_v$ is as follows:

$$\hat{\theta}_v = \langle \phi(s, a), (\Lambda_n / n)^{-1} \mathbb{E}_{\mathcal{D}} [\phi(s, a) v(s')] \rangle, \quad \Lambda_n = n \mathbb{E}_{\mathcal{D}} [\phi(s, a) \phi^\top(s, a)] + \lambda I.$$

Finally, after introducing certain function class $\mathcal{V} := \{ s \mapsto \phi(s, \pi); \pi \in \Pi \}$, the estimator $\hat{P}$ is the one satisfying (not needed to be unique nor in $\mathcal{M}$)

$$\int \hat{P}(s' \mid s, a) v(s') d\xi(s') = \langle \phi(s, a), \hat{\theta}_v \rangle$$

for any $v \in \mathcal{V}$ and $(s, a) \in S \times A$. This choice of $\mathcal{V}$ is determined so that it includes a set of state value functions for each model in $\mathcal{M}$. We remark the analog of MLE equipped with witness function classes is widely used, e.g., in Sun et al. (2019). Using this $\hat{P}$, we introduce constrained pessimistic policy optimization for linear MDPs in Algorithm 3. Note in Algorithm 3, what we need to know is not $\hat{P}$ itself but $\int \hat{P}(s' \mid s, a) v(\tilde{s}) d\xi(\tilde{s})$.

**Theorem 6** (PAC bound for linear MDPs). We assume the following assumptions regarding the norm: (1) $\sup_{(s, a)} \| \phi(s, a) \| \leq 1$, (2) $\| \int \mu^*(s) v(s) d\xi(s) \|_2 \leq \sqrt{d}$ for any $v : S \rightarrow \mathbb{R}$ such that $\| v \|_\infty \leq 1$ and (3) $\| \theta \|_2 \leq W$.

We set $\zeta = (1 - \gamma)^{-1} \sqrt{d^2 \ln(n |\Pi| W/\delta) / n}$. With probability at least $1 - \delta$, for all comparator policy $\pi^* \in \Pi$, we have

$$V_{\hat{P}}^{\pi^*} - V_{\hat{P}}^{\hat{\pi}} \leq c_1 (1 - \gamma)^{-2} \sqrt{C_{\pi^*, \phi, \xi} \text{rank}[\Sigma_{\phi}]^2 d \ln(c_2 n |\Pi| W/\delta) / n},$$

16
Algorithm 4 PS-PO: Policy Optimization with Posterior Sampling for Offline RL

1: Require: dataset $D$, prior distribution $\beta \in \Delta(M)$, learning rate $\eta$.
2: Bayesian update: Compute model posterior $\beta(\cdot|D) \in \Delta(M)$
3: Initialize policy $\pi_0$ where $\pi_0(\cdot|s) = \text{Uniform}(A)$
4: for $t = 0, \cdots, T - 1$ do
5:  Posterior sampling: $P_t \sim \beta(\cdot|D)$
6:  Policy update: $\pi_{t+1}(a|s) \propto \pi_t(a|s) \exp(\eta A_{P_t}^\pi(s, a))$
7: end for
8: Return $\pi_T$.

Compared to PAC bounds in other models in our article, Theorem 6 incurs $\ln(|\Pi|)$. Thus, it requires that $\Pi$ is restricted. It is known that this dependence can be removed by using pessimistic model-free algorithms with a natural policy gradient (Xie et al., 2021; Zanette et al., 2021). Hence, our bound might be worse than their results in nonparametric linear MDPs. However, as we mention in Section 4.3, their algorithm incurs $\ln(|\Pi|)$ in many other models such as finite models (finite $|M|$), KNRs, and linear mixture MDPs while CPPO does not incur $\ln(|\Pi|)$. This suggests that nonparametric linear MDPs are more amenable to model-free RL while KNRs and linear mixture MDPs are more amenable to model-based RL.

8 Bayesian Offline RL: Policy Optimization via Posterior Sampling

The mini-max constrained optimization step in Algorithm 1 is not computationally efficient as it is equivalent to a version space based algorithm shown in Eq. 1. In this section, we consider offline RL in the Bayesian setting, and study posterior sampling based offline RL algorithms. The goal here is to design offline RL algorithms that rely on posterior sampling rather than explicit pessimism. While as we will show, the benefit of leveraging posterior sampling is that we do not need to design pessimism or reward penalty, the downside is that we sacrifice from worst-case suboptimality gap to the Bayesian suboptimality gap.

8.1 Algorithm

We consider posterior sampling together with incremental policy optimization procedure. Algorithm 4 summarizes the posterior sampling based policy optimization algorithm PS-PO. The algorithm relies on two computational oracles, a posterior distribution update oracle, and a posterior sampling oracle. The algorithm consists of two procedures. The first procedure calls the posterior update oracle, i.e., given the prior distribution $\beta$, and given the offline dataset $D$, the posterior update gives the posterior distribution over models conditioned on the dataset $D$, i.e., we get $\beta(\cdot|D)$. Hereafter, We always assume that $\beta(\cdot|D)$ exists, i.e., the prior distribution $\beta$ is proper.

Once we have the posterior distribution $\beta(\cdot|D)$, the second procedure of our algorithm is to perform policy optimization with $\beta(\cdot|D)$. More specifically, at iteration $t$ with the latest learned policy $\pi_t$, we sample a model from $\beta(\cdot|D)$, i.e., $P_t \sim \beta(\cdot|D)$. We then update policy from $\pi_t$ to $\pi_{t+1}$ using incremental policy update, i.e., $\pi_{t+1}(a|s) \propto \pi_t(a|s) \exp(\eta A_{P_t}^\pi(s, a))$, $\forall s, a$, with $\eta \in \mathbb{R}^+$ being some learning rate. We emphasize that every iteration $t$, our algorithm samples a fresh model $P_t$ from $\beta(\cdot|D)$. Note that this new algorithm does not explicitly use any pessimism or reward penalty inside the algorithm.

What is the intuition behind this algorithm, and what is the benefit of this algorithm compared to a naïve model-based policy optimization approach (i.e., simply training a model from $D$ and using that model over and over again during the entire policy optimization procedure such as the offline version of natural policy gradient (Agarwal et al., 2020c))? The random sampling procedure prevents policy optimization from exploiting the error in a single model trained on $D$. A sample $P_t$ is an accurate model under the space that is well covered by the offline data $D$, but
can be inaccurate at the space that is not covered by the offline data \( \mathcal{D} \). Similarly, \( P_{t+1} \) is accurate under the covered space as well. However, \( P_t \) and \( P_{t+1} \) could disagree with each other on the space that is not covered by the offline data. Thus, the random sampling procedure makes PG algorithm hard to consistently exploit model errors inside a single model. Yet PG algorithm can make progress inside the region that is well covered by the offline data since models sampled from the posterior distribution are accurate and all agree with each other in the covered region.

### 8.2 Analysis

To analyze the Bayesian regret of PO-PS, we first introduce the concentrability coefficient and the relative condition number in the Bayesian setting. Recall that given a model \( P \), we denote \( \pi(P) = \arg\max_{\pi} V_\pi^P \) as the (global) optimal policy under model \( P \). We define the following quantities related to partial coverage:

\[
C_{\beta}^{\dagger, \text{Bayes}} = \mathbb{E}_{P^* \sim \beta} [C_{\pi(P^*)}^{\dagger}], \quad C_{\beta}^{\text{Bayes}} = \mathbb{E}_{P^* \sim \beta} [C_{\pi(P^*)}], \quad C_{\beta}^{\text{Bayes}} = \mathbb{E}_{P^* \sim \beta} [C_{\pi(P^*)}]\tag{7}
\]

where

\[
C_{\pi(P^*)}^{\dagger} = \sup_{P^* \in \mathcal{M}} \frac{\mathbb{E}_{(s,a) \sim d_{P^*}^{\pi}(s,a)} [\text{TV}(P'(|s,a), P^*|s,a)]^2}{\mathbb{E}_{(s,a) \sim \rho} [\text{TV}(P'(|s,a), P^*|s,a)]^2}
\]

\[
C_{\pi(P^*)} = \sup_{(s,a)} \frac{d_{P^*}^{\pi}(s,a)}{\rho(s,a)}
\]

\[
\bar{C}_{\pi(P^*)} = \sup_{x \in \mathbb{R}^d} \frac{x^T \Sigma_{\pi} x}{\Sigma_{\rho}}, \quad \Sigma_{\pi} = \mathbb{E}_{(s,a) \sim d_{P^*}^{\pi}} [\phi(s,a)\phi(s,a)^\top], \quad \Sigma_{\rho} = \mathbb{E}_{(s,a) \sim \rho} [\phi(s,a)\phi(s,a)^\top].
\]

Comparing to the frequentist quantities, the density ratio and relative condition number quantities are also averaged over the prior distribution. The partial coverage means these types of quantities are upper-bounded by some constants.

#### 8.2.1 The Implicit Pessimism in Posterior Sampling

Before diving into the analysis of PS-PO, we consider a simpler algorithm as a warm-up. This algorithm takes the model \( P \) sampled from the posterior \( \beta(\cdot|\mathcal{D}) \) and outputs the optimal policy for this model \( P \) (i.e., by using a planning oracle). Namely, the algorithm has the following two steps:

\[ P \sim \beta(\cdot|\mathcal{D}), \quad \pi(P) = \arg\max_{\pi} V_\pi^P. \]

To analyze the above two-step algorithm in the Bayesian setting, we first introduce some additional notations. We first define a function over the policy class depending on \( \mathcal{D} \), i.e., \( L(\pi; \mathcal{D}) : \Pi \to [0, (1-\gamma)^{-1}] \). This function \( L(\cdot; \mathcal{D}) \) is fully determined by the dataset \( \mathcal{D} \). Then, inspired by [Russo and Van Roy (2014)](https://doi.org/10.1162/NECO_a_00555), for the model \( P \) sampled from \( \beta(\cdot|\mathcal{D}) \), we have the following decomposition for Bayesian suboptimality gap:

\[
\mathbb{E} \left[ V_{P^*}^P - V_{\pi}^P \right] = \mathbb{E} \left[ V_{\pi}^{P^*} - L(\pi(P^*); \mathcal{D}) + L(\pi(P^*); \mathcal{D}) - V_{\pi}^P \right]
\]

\[
= \mathbb{E} \left[ V_{\pi}^{P^*} - L(\pi(P^*); \mathcal{D}) + \mathbb{E}[L(\pi(P^*); \mathcal{D}) | \mathcal{D}] - V_{\pi}^P \right]
\]

\[
= \mathbb{E} \left[ V_{\pi}^{P^*} - L(\pi(P^*); \mathcal{D}) + L(\pi(P); \mathcal{D}) - V_{\pi}^P \right].
\]

We use \( \mathbb{E} [L(\pi(P^*); \mathcal{D}) | \mathcal{D}] = \mathbb{E} [L(\pi(P); \mathcal{D}) | \mathcal{D}] \) as \( P \) and \( P^* \) are independently and identically distributed from \( \beta(\cdot|\mathcal{D}) \). Then, given \( P^* \) and \( \mathcal{D} \) generated based on \( P^* \) (i.e., \( P^* \sim \beta, (s,a) \sim \rho, s' \sim P^*(|s,a) \)), if \( L(\pi; \mathcal{D}) \) gives a
lower confidence bound of \( V_{π∗}^γ \), such that \( ∀π ∈ \Pi : V_{π∗}^γ ≥ L(π; D) \), we have
\[
E \left[ V_{π∗}^{γ(P∗)} - V_{π∗}^{P(P)} \right] ≤ E \left[ V_{π∗}^{γ(P∗)} - L(π(P∗); D) \right].
\] (8)

This is summarized in the following theorem with the formalized definition of \( L(π; D) \).

**Assumption 2.** Given a model \( P∗ \) on the support \( \{P∗ : β(P∗) > 0\} \), let \( D \) be the dataset generated following \( P∗ \). We have a function \( L(π; D) : Π → [0, (1 − γ)^−1] \) s.t. \( P(L(π; D) ≤ V_{π∗}^γ, ∀π ∈ Π | P∗) ≥ 1 − δ \). We denote \( L_\mathcal{D} \) as the set the contains all such functions \( L(\cdot; D) \).

In the above assumption, the randomness in the high probability statement is with respect to the dataset \( D \) conditioned on \( P∗ \).

**Theorem 7.** Suppose Assumption 2 holds.
\[
E \left[ V_{π∗}^{γ(P∗)} - V_{π∗}^{P(P)} \right] ≤ E \left[ V_{π∗}^{γ(P∗)} - L(π(P∗); D) \right] + 2(1 − γ)^−1δ.
\]

This result satisfies our desiderata, i.e., we can obtain the bound for Bayesian suboptimality gap under the partial coverage as we only need to be concern about the distribution \( d_{π∗}^{γ(P∗)} \) with \( P∗ \) being sampled from the prior \( β \), which allows us to use the quantities define in Eq. (7).

To obtain Bayesian suboptimality gap bounds from Theorem 7 under the partial coverage, we need to design \( L(π; D) \) on a case-by-case basis. The first choice is \( \min_M V_M^γ \) in Algorithm 1, which satisfies the condition \( \min_M V_M^γ \) \( ≤ \) \( V_{π∗}^γ \), \( ∀π ∈ Π \). Then, we can plug in the frequentist suboptimality gap result Theorem 1 into Theorem 7, which leads to the Bayesian suboptimality gap result under partial coverage. The second choice is \( \min_M V_M^γ \) in Algorithm 2. Then, we can plug in the frequentist suboptimality gap result Theorem 2 into Theorem 7, which again leads to the Bayesian suboptimality gap result under partial coverage. Another choice is a reward penalty (Chang et al., 2021). Given the dataset \( D \), we compute a model estimator \( P(\cdot|s, a) \) and a model uncertainty measure \( σ(s, a) \) s.t. \( ∀s, a : TV(P(\cdot|s, a), P(\cdot|s, a)) ≤ σ(s, a) \), then we can design a reward penalty \( b(s, a) = Hσ(s, a) \) so that \( V_{P∗}^γ \) satisfies the condition \( V_{P∗}^γ ≤ V_{P∗}^γ \), \( ∀π ∈ Π \), where \( V_{P∗}^γ \) is a policy value under a transition \( P∗ \), a reward \( r − b \) and a policy \( π \). Then, by translating the frequentist result of Chang et al. (2021) into the Bayesian setting, we can obtain the Bayesian suboptimality bound under the partial coverage. We will see more specific bounds in Section 8.2.3.

### 8.2.2 Analysis of PS-PO

Now we are ready to analyze PS-PO where we combine the analysis of NPG with the above Bayesian analysis. As in the previous section, we introduce \( L(π; D) : Π → [0, (1 − γ)^−1] \) and \( L(\cdot; D) \) is a mapping that is fully determined by the dataset \( D \).

We start by bounding the per-iteration regret:

**Lemma 4** (Per-iteration regret). Suppose Assumption 2 holds. For any iteration \( t \), we have
\[
E \left[ V_{π∗}^{γ(P∗)} - V_{π∗}^π \right] ≤ E \left[ V_{π∗}^{γ(P∗)} - L(π(P∗); D) \right] + E \left[ V_{π∗}^{γ(P∗)} - V_{π∗}^π \right] + 2(1 − γ)^−1δ.
\]

The proof is similarly done as the proof of Theorem 7. We use a key relation \( E[L(π(P∗); D) | D] = E[L(π(P_t); D) | D] \). The first term is upper-bounded under the partial coverage following the argument after Theorem 7. The third term is negligible by taking sufficiently small \( δ \). Thus, we analyze the second term of r.h.s in detail. The second term corresponds to the regret term for the model-based policy optimization procedure. Recall that we update policy as \( π_{t+1}(a|s) ∝ π_t(a|s) \exp(ηA_{π_t}^γ (s, a)) \).
Lemma 5. Consider a fixed iteration $t$. Suppose $\eta < 0.5(1 - \gamma)$. We have:

$$
E \left[ V_{\pi^*}^{(P^*)} - V_{\pi^*}^{(P^*)} \right] \leq E \left[ 4\eta(1 - \gamma)^{-3} + \frac{(1 - \gamma)^{-1}}{\eta} E_{s \sim d_{P^*}^+} \left[ D_{KL}(\pi(P^*))(\cdot|s), \pi_{t+1}(\cdot|s)) - D_{KL}(\pi(P^*))(\cdot|s), \pi_{t}(\cdot|s)) \right] \right]
$$

By combining the above two lemmas and considering all iterations, we conclude the following general theorem.

Theorem 8. Suppose Assumption 2. When $\eta < 0.5(1 - \gamma)$, then,

$$
E \left[ V_{\pi^*}^{(P^*)} - \max_{t \in [T]} V_{\pi^*}^{(P^*)} \right] \leq \min_{L \in L_D} E \left[ V_{\pi^*}^{(P^*)} - L(\pi(P^*); D) \right] + 4(1 - \gamma)^{-2} \sqrt{\frac{\ln(|A|)}{T}} + 2(1 - \gamma)^{-1}. \tag{S1}
$$

By taking sufficiently large $T$, the second term (S2) is negligible. Thus, the first term (S1) dominates the error which we will analyze in detail under the partial coverage. Note that the Bayesian result in Theorem 8 allows us to pick the tightest lower confidence bound among all possible valid LCBs that satisfy Assumption 2.

8.2.3 Detailed Bounds on the Bayesian suboptimality Gap

In this section, we specialize Theorem 8 to concrete examples. Here, we use Bayesian concentrability coefficients defined in Eq. (7). We start with the general realizable mode class $M$. Here, we set $L(\pi; D) := \min_{P \in M_D} V_{\pi}^\pi$. Note that we have proved that given $P^*$ and $D$ being generated based on $D$, $\min_{P \in M_D} V_{\pi}^\pi \leq V_{\pi}^\pi$, with high probability. By plugging $\min_{P \in M_D} V_{\pi}^\pi$ into Theorem 8, we arrive at the following corollary.

Corollary 5 (PS-PO with General Function Class). Suppose the partial coverage $C_{\beta}^{Bayes} < \infty$.

$$
E \left[ V_{\pi^*}^{(P^*)} - \max_{t \in [T]} V_{\pi^*}^{(P^*)} \right] \leq c_1(1 - \gamma)^{-2} \sqrt{C_{\beta}^{Bayes} \ln(|M|) n} + (1 - \gamma)^{-2} \sqrt{\frac{\ln(|A|)}{T}}.
$$

Corollary 6 (PS-PO for Tabular MDPs). Suppose the partial coverage $C_{\beta}^{Bayes} < \infty$.

$$
E \left[ V_{\pi^*}^{(P^*)} - \max_{t \in [T]} V_{\pi^*}^{(P^*)} \right] \leq c_1(1 - \gamma)^{-2} \sqrt{C_{\beta}^{Bayes} |S|^2 |A| \ln(|S|) ||A| c_2|} + (1 - \gamma)^{-2} \sqrt{\frac{\ln(|A|)}{T}}.
$$

Corollary 7 (PS-PO for Linear Mixture MDPs). Suppose $\|\theta^*\| \leq R$, $\sup_{(s,a)} \|\psi_V(s,a)\|_2 \leq 1$, $\forall V \in \{S \rightarrow [0,1]\}$. Then, we have

$$
E \left[ V_{\pi^*}^{(P^*)} - \max_{t \in [T]} V_{\pi^*}^{(P^*)} \right] \leq c_1(1 - \gamma)^{-2} \sqrt{dC_{\beta}^{Bayes} \ln(c_2n) S \ln(R) c_2} + (1 - \gamma)^{-2} \sqrt{\frac{\ln(|A|)}{T}}.
$$

For KNRs with the known feature $\phi$, we can use the Bayesian relative condition number. Here again we set $L(\pi; D) = \min_{W \in W_D} V_{\pi}^W$.

Corollary 8 (PS-PO for KNRs). Assume $\|\phi(s,a)\|_2 \leq 1$, $\forall (s,a) \in S \times A$. Suppose the partial coverage $C_{\beta}^{Bayes} < \infty$. By letting $\|W^*\|_2^2 = O(1)$, $\|u\| = O(1)$, we have

$$
E \left[ V_{\pi^*}^{(P^*)} - \max_{t \in [T]} V_{\pi^*}^{(P^*)} \right] \leq c_1(1 - \gamma)^{-2} \min\{d_{1 / 2}, R\} \sqrt{\frac{dS C_{\beta}^{Bayes} \ln(1 + n)}{n}} + (1 - \gamma)^{-2} \sqrt{\frac{\ln(|A|)}{T}},
$$

where $R = \text{rank}[\Sigma_{\delta}]\{\text{rank}[\Sigma_{\delta}] + \ln(c_2n)\}$.
Similarly, we can also extend the above result to KNRs with infinite-dimensional $\phi$ based on the result of Corollary 4 by using the effective dimension $d^*$.

Finally, for low-rank MDPs, we use $L(\pi; D) = \min_{P \in \mathcal{M}} V^\pi_P$.

**Corollary 9** (PS-PO for low-rank MDPs). Suppose (a): $\|\phi(s, a)\|_2 \leq 1, \forall (s, a) \in S \times A, \forall \phi \in \Phi, \int \mu(s')^T \phi(s, a) d\mu(s') = 1$ and $\int \|\mu(s)\|_2 d\mu(s) \leq \sqrt{d}, \forall \mu \in \Psi, \phi \in \Phi$, (b) $\rho(s, a) = d^\pi \pi^b P \star (s, a)$. We have

$$E \left[ V^\pi_{P^*} - \max_{t \in [T]} V^\pi_{P^*} \right] \leq c_3 \sqrt{C_{Bayes} \omega_{\pi^*} \ln(\frac{\|\Psi\| \|\phi\|_2}{\delta}) + (1 - \gamma)^{-2} \sqrt{\frac{\ln(|A|)}{T}}}, \omega_{\pi^*} = \left( \max_{(s, a)} \pi^*(a | s) \right).$$

(9)

## 9 Conclusion

We study model-based offline RL with function approximation under partial coverage. We show that for the model-based setting, realizability in function class and partial coverage together are enough to learn a policy that is comparable to any policies (including history-dependent policies) covered by the offline distribution. Our result demonstrates a sharp contrast to model-free offline RL approaches which often require additional structural conditions in the function class (e.g., Bellman completion) and have restrictions on the pool of candidate policies that they can compete against.

Some readers might wonder whether CPPO-TV and CPPO-LR is computationally efficient. The minimax optimization problem $\arg \max_{\pi \in \Pi} \min_{P \in \mathcal{M}} V^\pi_P$ fits into a framework of planning on robust MDPs (Nilim and El Ghaoui, 2005; Iyengar, 2005). By introducing a robust Bellman equation, they proposed value iteration and policy iteration algorithms and showed that algorithms are practically tractable in the tabular setting. In the non-tabular setting, Lim and Autef (2019); Tamar et al. (2014) propose the extension using function approximation. Thus, we can apply their methods to approximately solve the minimax optimization problem in a model-free fashion. We leave the formal theoretical justification when using these approximation planning algorithms as an important direction for future work. As a first step, we propose a natural policy gradient based policy optimization method based on posterior sampling in Section 8. In some models such as low-rank MDPs, follow-up works propose computationally efficient algorithms (Uehara et al., 2021b; Zhang et al., 2022; Qiu et al., 2022).

## Acknowledgement

The authors would like to thank Nan Jiang, Tengyang Xie, Audrey Huang, Jinglin Chen, Runzhe Wu for their valuable feedback.

Masatoshi Uehara was partially supported by Masason foundation.

## References

Alekh Agarwal, Nan Jiang, Sham M Kakade, and Wen Sun. Reinforcement learning: Theory and algorithms. CS Dept., UW Seattle, Seattle, WA, USA, Tech. Rep, 2019.

Alekh Agarwal, Mikael Henaff, Sham Kakade, and Wen Sun. Pc-pg: Policy cover directed exploration for provable policy gradient learning. In *Advances in Neural Information Processing Systems*, volume 33, pages 13399–13412, 2020a.
Alekh Agarwal, Sham Kakade, Akshay Krishnamurthy, and Wen Sun. Flambe: Structural complexity and representation learning of low rank mdps. In Advances in Neural Information Processing Systems, volume 33, pages 20095–20107, 2020b.

Alekh Agarwal, Sham M Kakade, Jason D Lee, and Gaurav Mahajan. Optimality and approximation with policy gradient methods in markov decision processes. In Proceedings of Thirty Third Conference on Learning Theory, volume 125 of Proceedings of Machine Learning Research, pages 64–66, 2020c.

András Antos, Csaba Szepesvári, and Rémi Munos. Learning near-optimal policies with bellman-residual minimization based fitted policy iteration and a single sample path. Machine Learning, 71:89–129, 2008.

Alex Ayoub, Zeyu Jia, Csaba Szepesvari, Mengdi Wang, and Lin Yang. Model-based reinforcement learning with value-targeted regression. In International Conference on Machine Learning, pages 463–474. PMLR, 2020.

Francis Bach. On the equivalence between kernel quadrature rules and random feature expansions. Journal of machine learning research, 18(21):1–38, 2017.

Jacob Buckman, Carles Gelada, and Marc G Bellemare. The importance of pessimism in fixed-dataset policy optimization. arXiv preprint arXiv:2009.06799, 2020.

Catherine Cang, Aravind Rajeswaran, Pieter Abbeel, and Michael Laskin. Behavioral priors and dynamics models: Improving performance and domain transfer in offline rl. arXiv preprint arXiv:2106.09119, 2021.

Jonathan D Chang, Masatoshi Uehara, Dhruv Sreenivas, Rahul Kidambi, and Wen Sun. Mitigating covariate shift in imitation learning via offline data without great coverage. 2021.

Jinglin Chen and Nan Jiang. Information-theoretic considerations in batch reinforcement learning. In Proceedings of the 36th International Conference on Machine Learning, volume 97, pages 1042–1051, 2019.

Minmin Chen, Alex Beutel, Paul Covington, Sagar Jain, Francois Belletti, and Ed Chi. Top-k off-policy correction for a reinforce recommender system. In Proceedings of the Twelfth ACM International Conference on web search and data mining, WSDM ’19, pages 456–464, 2019.

Sebastian Curi, Felix Berkenkamp, and Andreas Krause. Efficient model-based reinforcement learning through optimistic policy search and planning. 2020.

Marc Deisenroth and Carl E Rasmussen. Pilco: A model-based and data-efficient approach to policy search. In Proceedings of the 28th International Conference on machine learning (ICML-11), pages 465–472. Citeseer, 2011.

Luc Devroye, Abbas Mehrabian, and Tommy Reddad. The total variation distance between high-dimensional gaussians. arXiv preprint arXiv:1810.08693, 2018.

Yaqi Duan, Zeyu Jia, and Mengdi Wang. Minimax-optimal off-policy evaluation with linear function approximation. In Proceedings of the 37th International Conference on Machine Learning, volume 119 of Proceedings of Machine Learning Research, pages 2701–2709, 2020.

Yaqi Duan, Chi Jin, and Zhiyuan Li. Risk bounds and rademacher complexity in batch reinforcement learning. arXiv preprint arXiv:2103.13883, 2021.

Damien Ernst, Pierre Geurts, and Louis Wehenkel. Tree-based batch mode reinforcement learning. Journal of Machine Learning Research, 6:503–556, 2005.
Rasool Fakoor, Jonas Mueller, Pratik Chaudhari, and Alexander J Smola. Continuous doubly constrained batch reinforcement learning. arXiv preprint arXiv:2102.09225, 2021.

Jianqing Fan, Zhaoran Wang, Yuchen Xie, and Zhuoran Yang. A theoretical analysis of deep q-learning. In Proceedings of the 2nd Conference on Learning for Dynamics and Control, volume 120 of Proceedings of Machine Learning Research, pages 486–489, 2020.

Scott Fujimoto, David Meger, and Doina Precup. Off-policy deep reinforcement learning without exploration. In International Conference on Machine Learning, pages 2052–2062. PMLR, 2019.

Seyed Kamyar Seyed Ghasemipour, Dale Schuurmans, and Shixiang Shane Gu. Emaq: Expected-max q-learning operator for simple yet effective offline and online rl. In International Conference on Machine Learning, pages 3682–3691. PMLR, 2021.

Botao Hao, Yaqi Duan, Tor Lattimore, Csaba Szepesvári, and Mengdi Wang. Sparse feature selection makes batch reinforcement learning more sample efficient. In International Conference on Machine Learning, pages 4063–4073. PMLR, 2021.

Garud N Iyengar. Robust dynamic programming. Mathematics of Operations Research, 30(2):257–280, 2005.

Chi Jin, Zhuoran Yang, Zhaoran Wang, and Michael I Jordan. Provably efficient reinforcement learning with linear function approximation. In Proceedings of Thirty Third Conference on Learning Theory, volume 125 of Proceedings of Machine Learning Research, pages 2137–2143, 2020a.

Ying Jin, Zhuoran Yang, and Zhaoran Wang. Is pessimism provably efficient for offline rl? arXiv preprint arXiv:2012.15085, 2020b.

Sham Kakade, Akshay Krishnamurthy, Kendall Lowrey, Motoya Ohnishi, and Wen Sun. Information theoretic regret bounds for online nonlinear control. In Advances in Neural Information Processing Systems, volume 33, pages 15312–15325, 2020.

Michael Kearns and Daphne Koller. Efficient reinforcement learning in factored mdps. In IJCAI, volume 16, pages 740–747, 1999.

Rahul Kidambi, Aravind Rajeswaran, Praneeth Netrapalli, and Thorsten Joachims. Morel: Model-based offline reinforcement learning. In Advances in Neural Information Processing Systems, volume 33, pages 21810–21823. Curran Associates, Inc., 2020.

Daphne Koller and Ronald Parr. Policy iteration for factored mdps. In Proceedings of the Sixteenth conference on Uncertainty in artificial intelligence, pages 326–334, 2000.

Michael R. Kosorok and Eric B. Laber. Precision medicine. 6:263–286, 2019.

Aviral Kumar, Aurick Zhou, George Tucker, and Sergey Levine. Conservative q-learning for offline reinforcement learning. arXiv preprint arXiv:2006.04779, 2020.

Sergey Levine, Aviral Kumar, George Tucker, and Justin Fu. Offline reinforcement learning: Tutorial, review, and perspectives on open problems. arXiv preprint arXiv:2005.01643, 2020.

Shiau Hong Lim and Arnaud Autef. Kernel-based reinforcement learning in robust markov decision processes. In International Conference on Machine Learning, pages 3973–3981. PMLR, 2019.
Yao Liu, Adith Swaminathan, Alekh Agarwal, and Emma Brunskill. Provably good batch off-policy reinforcement learning without great exploration. In *Advances in Neural Information Processing Systems*, volume 33, pages 1264–1274, 2020.

Thodoris Lykouris, Max Simchowitz, Alex Slivkins, and Wen Sun. Corruption-robust exploration in episodic reinforcement learning. In *Conference on Learning Theory*, pages 3242–3245. PMLR, 2021.

Tatsuya Matsushima, Hiroki Furuta, Yutaka Matsuo, Ofir Nachum, and Shixiang Gu. Deployment-efficient reinforcement learning via model-based offline optimization. *ICLR*, 2020.

Aditya Modi, Nan Jiang, Ambuj Tewari, and Satinder Singh. Sample complexity of reinforcement learning using linearly combined model ensembles. In *International Conference on Artificial Intelligence and Statistics*, pages 2010–2020. PMLR, 2020.

Aditya Modi, Jinglin Chen, Akshay Krishnamurthy, Nan Jiang, and Alekh Agarwal. Model-free representation learning and exploration in low-rank mdps. *arXiv preprint arXiv:2102.07035*, 2021.

Rémi Munos. Error bounds for approximate value iteration. In *Proceedings of the National Conference on Artificial Intelligence*, volume 20, page 1006. Menlo Park, CA; Cambridge, MA; London; AAAI Press; MIT Press; 1999, 2005.

Rémi Munos and Csaba Szepesvári. Finite-time bounds for fitted value iteration. *Journal of Machine Learning Research*, 9(May):815–857, 2008.

Ofir Nachum, Bo Dai, Ilya Kostrikov, Yinlam Chow, Lihong Li, and Dale Schuurmans. Algaedice: Policy gradient from arbitrary experience. *arXiv preprint arXiv:1912.02074*, 2019.

Gergely Neu and Ciara Pike-Burke. A unifying view of optimism in episodic reinforcement learning. *arXiv preprint arXiv:2007.01891*, 2020.

Chengzhuo Ni, Anru Zhang, Yaqi Duan, and Mengdi Wang. Learning good state and action representations via tensor decomposition. *arXiv preprint arXiv:2105.01136*, 2021.

Arnab Nilim and Laurent El Ghaoui. Robust control of markov decision processes with uncertain transition matrices. *Operations Research*, 53(5):780–798, 2005.

Matteo Papini, Andrea Tirinzoni, Marcello Restelli, Alessandro Lazaric, and Matteo Pirotta. Leveraging good representations in linear contextual bandits. *arXiv preprint arXiv:2104.03781*, 2021.

Shuang Qiu, Lingxiao Wang, Chenjia Bai, Zhuoran Yang, and Zhaoran Wang. Contrastive ucb: Provably efficient contrastive self-supervised learning in online reinforcement learning. In *International Conference on Machine Learning*, pages 18168–18210. PMLR, 2022.

Nived Rajaraman, Lin F Yang, Jiantao Jiao, and Kannan Ramachandran. Toward the fundamental limits of imitation learning. *arXiv preprint arXiv:2009.05990*, 2020.

Paria Rashidinejad, Banghua Zhu, Cong Ma, Jiantao Jiao, and Stuart Russell. Bridging offline reinforcement learning and imitation learning: A tale of pessimism. *arXiv preprint arXiv:2103.12021*, 2021.

Carl Edward Rasmussen and Christopher K. I. Williams. *Gaussian Processes for Machine Learning (Adaptive Computation and Machine Learning)*. 2005.
Shideh Rezaeifar, Robert Dadashi, Nino Vieillard, Léonard Hussenot, Olivier Bachem, Olivier Pietquin, and Matthieu Geist. Offline reinforcement learning as anti-exploration. *arXiv preprint arXiv:2106.06431*, 2021.

Stéphane Ross and J Andrew Bagnell. Agnostic system identification for model-based reinforcement learning. In *Proceedings of the 29th International Coference on International Conference on Machine Learning*, pages 1905–1912, 2012.

Daniel Russo and Benjamin Van Roy. Learning to optimize via posterior sampling. *Mathematics of operations research*, 39(4):1221–1243, 2014.

Niranjan Srinivas, Andreas Krause, Sham Kakade, and Matthias Seeger. Gaussian process optimization in the bandit setting: No regret and experimental design. In *Proceedings of the 27th International Conference on International Conference on Machine Learning*, ICML’10, page 1015–1022, 2010.

Wen Sun, Nan Jiang, Akshay Krishnamurthy, Alekh Agarwal, and John Langford. Model-based rl in contextual decision processes: Pac bounds and exponential improvements over model-free approaches. In *Proceedings of the Thirty-Second Conference on Learning Theory*, volume 99 of *Proceedings of Machine Learning Research*, pages 2898–2933, 2019.

Aviv Tamar, Shie Mannor, and Huan Xu. Scaling up robust mdps using function approximation. In *International conference on machine learning*, pages 181–189. PMLR, 2014.

Ahmed Touati, Amy Zhang, Joelle Pineau, and Pascal Vincent. Stable policy optimization via off-policy divergence regularization. *arXiv preprint arXiv:2003.04108*, 2020.

Masatoshi Uehara, Jiawei Huang, and Nan Jiang. Minimax weight and q-function learning for off-policy evaluation. In *Proceedings of the 37th International Conference on Machine Learning*, pages 9659–9668, 2020.

Masatoshi Uehara, Masaaki Imaizumi, Nan Jiang, Nathan Kallus, Wen Sun, and Tengyang Xie. Finite sample analysis of minimax offline reinforcement learning: Completeness, fast rates and first-order efficiency. *arXiv preprint arXiv:2102.02981*, 2021a.

Masatoshi Uehara, Xuezhou Zhang, and Wen Sun. Representation learning for online and offline rl in low-rank mdps. *arXiv preprint arXiv:2110.04652*, 2021b.

Michal Valko, Nathan Korda, Rémi Munos, Ilias Flounas, and Nello Cristianini. Finite-time analysis of kernelised contextual bandits. In *Proceedings of the Twenty-Ninth Conference on Uncertainty in Artificial Intelligence*, UAI’13, page 654–663, Arlington, Virginia, USA, 2013. AUAI Press.

S van de Geer. *Empirical Processes in M-Estimation*. Cambridge Series in Statistical and Probabilistic Mathematics. Cambridge University Press, 2000.

Martin J Wainwright. *High-Dimensional Statistics : A Non-Asymptotic Viewpoint*. Cambridge University Press, New York, 2019.

Ruosong Wang, Dean P. Foster, and Sham M. Kakade. What are the statistical limits of offline rl with linear function approximation?. *arXiv preprint arXiv:2010.11895*, 2020.

Yifan Wu, George Tucker, and Ofir Nachum. Behavior regularized offline reinforcement learning. *arXiv preprint arXiv:1911.11361*, 2019.

Tengyang Xie and Nan Jiang. Batch value-function approximation with only realizability. *arXiv preprint arXiv:2008.04990*, 2020.
Tengyang Xie, Ching-An Cheng, Nan Jiang, Paul Mineiro, and Alekh Agarwal. Bellman-consistent pessimism for offline reinforcement learning. *arXiv preprint arXiv:2106.06926*, 2021.

Lin Yang and Mengdi Wang. Reinforcement learning in feature space: Matrix bandit, kernels, and regret bound. In *Proceedings of the 37th International Conference on Machine Learning*, pages 10746–10756, 2020.

Ming Yin, Yu Bai, and Yu-Xiang Wang. Near-optimal offline reinforcement learning via double variance reduction. *arXiv preprint arXiv:2102.01748*, 2021.

Tianhe Yu, Garrett Thomas, Lantao Yu, Stefano Ermon, James Y Zou, Sergey Levine, Chelsea Finn, and Tengyu Ma. Mopo: Model-based offline policy optimization. In *Advances in Neural Information Processing Systems*, volume 33, pages 14129–14142, 2020.

Andrea Zanette, Martin J Wainwright, and Emma Brunskill. Provable benefits of actor-critic methods for offline reinforcement learning. *arXiv preprint arXiv:2108.08812*, 2021.

Ruiyi Zhang, Bo Dai, Lihong Li, and Dale Schuurmans. Gendice: Generalized offline estimation of stationary values. In *International Conference on Learning Representations*, 2020.

Tianjun Zhang, Tongzheng Ren, Mengjiao Yang, Joseph Gonzalez, Dale Schuurmans, and Bo Dai. Making linear mdps practical via contrastive representation learning. In *International Conference on Machine Learning*, pages 26447–26466. PMLR, 2022.

Tong Zhang. Learning bounds for kernel regression using effective data dimensionality. *Neural computation*, 17(9):2077–2098, 2005.

Weitong Zhang, Jiafan He, Dongrui Zhou, Amy Zhang, and Quanquan Gu. Provably efficient representation learning in low-rank markov decision processes. *arXiv preprint arXiv:2106.11935*, 2021a.

Xuezhou Zhang, Yiding Chen, Jerry Zhu, and Wen Sun. Corruption-robust offline reinforcement learning. *arXiv preprint arXiv:2106.06630*, 2021b.

Dongrui Zhou, Quanquan Gu, and Csaba Szepesvari. Nearly minimax optimal reinforcement learning for linear mixture markov decision processes. In *Conference on Learning Theory*, pages 4532–4576. PMLR, 2021.
A Comparison to Xie et al. (2021)

We compare a result in (Xie et al., 2021) to our result in detail. Let $\mathcal{F}$ be a function class for $Q$-functions. Here, we consider a more general version of their algorithm by replacing the original $\mathcal{E}(f, \pi; \mathcal{D})$ in their algorithm with

$$E(f, \pi; \mathcal{D}) := L(f, f; \pi, \mathcal{D}) - \min_{g \in \mathcal{G}} L(g, f; \pi, \mathcal{D}).$$

In their original algorithm, they set $\mathcal{G} = \mathcal{F}$. Here, we consider the version such that a discriminator class $\mathcal{G}$ can be different from $\mathcal{F}$.

They show the PAC result under partial coverage as follows. Here, $T^\pi_{P^*}$ is a Bellman operator under $\pi$ and $P^*$:

$$T^\pi_{P^*} : \{S \times A \to \mathbb{R}\} \ni f \mapsto r(s, a) + \mathbb{E}_{P^*(s'|s, a)}[f(s', \pi)] \in \{S \times A \to \mathbb{R}\}.$$  

**Theorem 9** (Extension of Result in (Xie et al., 2021). Suppose realizability $Q^\pi_{P^*} \in \mathcal{F}$, $\forall \pi \in \Pi$ and closeness $\max_{f \in \mathcal{F}} \min_{g \in \mathcal{G}} \mathbb{E}_{s,a \sim \rho}[\|g - T^\pi_{P^*} f\|^2(s, a)] = 0$, $\forall \pi \in \Pi$. Then, with $1 - \delta$, for any $\pi^* \in \Pi$, we have

$$V^\pi_{P^*} - V^{\hat{\pi}}_{P^*} = O(\sqrt{C^\infty \ln(|\Pi| |\mathcal{F}| |\mathcal{G}| / \delta) / n}), \quad C^\infty = \sup_{f \in \mathcal{F}} \mathbb{E}_{s,a \sim \rho}[|f - T^\pi_{P^*} f|^2(s, a)].$$

By combining this result with the conversion from model-free results to model-based results in (Chen and Jiang, 2019, Corollary 6), we can obtain the following result under partial coverage.

**Theorem 10. (PAC guarantee from the direct application of (Xie et al., 2021) to mode-based RL.)** Assume $P^* \in \mathcal{M}$. Then, there exists an algorithm s.t. with $1 - \delta$, for any policy $\pi^* \in \Pi$,

$$V^\pi_{P^*} - V^{\hat{\pi}}_{P^*} = O(\sqrt{C^\infty \ln(|\Pi| |\mathcal{M}| / \delta) / n}).$$

**Proof of Theorem 10.** Given a model class $\mathcal{M}$, consider the following reduction. We define a $Q$-function class:

$$\mathcal{F} = \{q^\pi_P \mid \pi \in \Pi, P \in \mathcal{M}\}.$$  

Then, we define a discriminator class $\mathcal{G}$:

$$\mathcal{G} = \{T^\pi_{P'} q^\pi_P \mid \pi \in \Pi, \pi' \in \Pi, P \in \mathcal{M}, P' \in \mathcal{M}\}.$$  

The above satisfies the realizability $Q^\pi_{P'} \in \mathcal{F}$, $\forall \pi \in \Pi$ and the closedness $T^\pi_{P'} \mathcal{F} \subset \mathcal{G}$, $\forall \pi \in \Pi$. Thus, the assumptions in Theorem 9 are satisfied. Then, we have

$$V^\pi_{P^*} - V^{\hat{\pi}}_{P^*} = O(\sqrt{C^\infty \ln(|\Pi| |\mathcal{F}| |\mathcal{G}| / \delta) / n}) = O(\sqrt{C^\infty \ln(|\Pi| |\mathcal{M}| / \delta) / n}) ,$$

noting $|\mathcal{F}| = |\Pi| |\mathcal{M}|$ and $|\mathcal{G}| = |\Pi|^2 |\mathcal{M}|^2$.

As we mentioned, this is worse than our result since it includes $|\Pi|$. Besides, the algorithm can only compete against policies restricted in $\Pi$, while our algorithm works for the unrestricted policy class $\Pi$ which could even include history dependent policies. For completeness, we give the proof as follows.

We remark that their results (Theorem 4.1) with NPG that can possibly compete with any stochastic policies, are not applicable here. This is because they need an assumption that the comparator policy $\pi^*$ needs to satisfy $Q^\pi_{P^*} \in \mathcal{F}$ and $\max_{f \in \mathcal{F}} \min_{g \in \mathcal{G}} \mathbb{E}_{s,a \sim \rho}[\|g - T^\pi_{P^*} f\|^2(s, a)] = 0$, which does not hold for the corresponding Q-function class $\mathcal{F}$ after the conversion. As a notable exception, when the model is a linear Bellman-complete MDP (Zanette et al., 2021), any stochastic policies satisfy the Bellman completeness for the linear Q-function class; then, their algorithms can learn policies that can compete with any stochastic policies satisfying partial coverage.
B. Missing Proofs in Section 4

Below we use $c, c_1, c_2, \cdots$ to denote universal constants. For a $d$-dimensional vector $a$ and a matrix $A \in \mathbb{R}^{d \times d}$, we denote $\|a\|_A^2 = a^\top A a$. Here, $a \preceq B$ means $a \leq cB$ for some universal constant $c$.

B.1 Proofs for General Function Approximation for CPPO-TV (Proof of Theorem 1)

From Lemma 10, the MLE guarantee gives us the following generalization bound: with probability $1 - \delta$,

$$
\mathbb{E}_{s,a \sim \rho} [\text{TV}(\hat{P}_{\text{MLE}}(\cdot | s, a), P^*(\cdot | s, a))^2] \lesssim \frac{\ln(|\mathcal{M}|/\delta)}{n}.
$$

(10)

Letting

$$
A(P) := \mathbb{E}_{s,a \sim \rho} [\text{TV}(P(\cdot | s, a), P^*(\cdot | s, a))^2] - \mathbb{E}_D[\text{TV}(P(\cdot | s, a), P^*(\cdot | s, a))^2].
$$

with probability $1 - \delta$, from union bound and Bernstein’s inequality, we also have

$$
A(P) \leq \sqrt{\frac{c_1 \text{var}_{(s,a) \sim \rho} [\text{TV}(P(\cdot | s, a), P^*(\cdot | s, a))^2] \ln(|\mathcal{M}|/\delta)}{n} + \frac{c_2 \ln(|\mathcal{M}|/\delta)}{n}, \forall P \in \mathcal{M}.
$$

(11)

Hereafter, we condition on the above two events. Recall that we construct the version space using $D$ and $\hat{P}_{\text{MLE}}$ as follows:

$$
\mathcal{M}_D := \left\{ P \in \mathcal{M} : \mathbb{E}_D[\text{TV}(P(\cdot | s, a), \hat{P}_{\text{MLE}}(\cdot | s, a))^2] \leq \xi \right\}.
$$

First Step: Show $P^* \in \mathcal{M}_D$ in high-probability. We set $\xi = c \frac{\ln(|\mathcal{M}|/\delta)}{n}$. Conditioning on the above two events equations (10) and (11), we prove $P^* \in \mathcal{M}_D$. This is proved by

$$
\mathbb{E}_D[\text{TV}(\hat{P}_{\text{MLE}}(\cdot | s, a), P^*(\cdot | s, a))^2]
= \mathbb{E}_D[\text{TV}(\hat{P}_{\text{MLE}}(\cdot | s, a), P^*(\cdot | s, a))^2] - \mathbb{E}_{(s,a) \sim \rho}[\text{TV}(\hat{P}_{\text{MLE}}(\cdot | s, a), P^*(\cdot | s, a))^2]
+ \mathbb{E}_{(s,a) \sim \rho}[\text{TV}(\hat{P}_{\text{MLE}}(\cdot | s, a), P^*(\cdot | s, a))^2]
= \mathbb{E}_D[\text{TV}(\hat{P}_{\text{MLE}}(\cdot | s, a), P^*(\cdot | s, a))^2] - \mathbb{E}_{(s,a) \sim \rho}[\text{TV}(\hat{P}_{\text{MLE}}(\cdot | s, a), P^*(\cdot | s, a))^2] + \frac{c_1 \ln(|\mathcal{M}|/\delta)}{n}
\lesssim \sqrt{\frac{\text{var}_{(s,a) \sim \rho} [\text{TV}(\hat{P}_{\text{MLE}}(\cdot | s, a), P^*(\cdot | s, a))^2] \ln(|\mathcal{M}|/\delta)}{n} + \frac{\ln(|\mathcal{M}|/\delta)}{n}} (\text{From (11)})
\lesssim \sqrt{\frac{\mathbb{E}_{(s,a) \sim \rho}[\text{TV}(\hat{P}_{\text{MLE}}(\cdot | s, a), P^*(\cdot | s, a))^2] \ln(|\mathcal{M}|/\delta)}{n} + \frac{\ln(|\mathcal{M}|/\delta)}{n}}
\lesssim \frac{1}{n} \ln(|\mathcal{M}|/\delta).
$$

(Plug in MLE guarantee)

Second Step: Show $\mathbb{E}_{s,a \sim \rho}[\text{TV}(P(\cdot | s, a), P^*(\cdot | s, a))^2] \leq c_\xi$, $\forall P \in \mathcal{M}_D$ in high probability. We show for any $P \in \mathcal{M}_D$, the distance between $P^*$ is sufficiently controlled in terms of TV distance. More concretely (conditioning on the above two events (10) and (11)), we show

$$
\mathbb{E}_{s,a \sim \rho}[\text{TV}(P(\cdot | s, a), P^*(\cdot | s, a))^2] \lesssim \xi, \quad \forall P \in \mathcal{M}_D.
$$
In order to observe this, for any \( P \in \mathcal{M}_D \), we have
\[
\mathbb{E}_D[TV(P(\cdot | s, a), P^*(\cdot | s, a))^2] \\
\leq 2\mathbb{E}_D[TV(\hat{P}_{\text{MLE}}(\cdot | s, a), P(\cdot | s, a))^2] + 2\mathbb{E}_D[TV(\hat{P}_{\text{MLE}}(\cdot | s, a), P^*(\cdot | s, a))^2] \leq 4\xi
\]
(From \((a + b)^2 \leq 2a^2 + 2b^2\).)

Thus, we have:
\[
\mathbb{E}_{s,a \sim \rho}[TV(P(\cdot | s, a), P^*(\cdot | s, a))^2] \\
= \mathbb{E}_{s,a \sim \rho}[TV(P(\cdot | s, a), P^*(\cdot | s, a))^2] - \mathbb{E}_D[TV(P(\cdot | s, a), P^*(\cdot | s, a))^2] + \mathbb{E}_D[TV(P(\cdot | s, a), P^*(\cdot | s, a))^2] \\
\leq A(P) + c\xi.
\]
(12)

Here, from (11), we have
\[
A(P) \leq \sqrt{\frac{c_1 \text{var}(s,a) \sim \rho[TV(P(\cdot | s, a), P^*(\cdot | s, a))^2]}{n}} \ln(|\mathcal{M}|/\delta) + \frac{c_2 \ln(|\mathcal{M}|/\delta)}{n}, \forall P \in \mathcal{M}_D.
\]

Then, for any \( P \in \mathcal{M}_D \), we have
\[
A(P) \leq \sqrt{\frac{c_1 \mathbb{E}_{s,a \sim \rho}[TV(P(\cdot | s, a), P^*(\cdot | s, a))^2]}{n}} \ln(|\mathcal{M}|/\delta) + \frac{c_2 \ln(|\mathcal{M}|/\delta)}{n}
\]
\[
\leq \sqrt{\frac{4c_1 \mathbb{E}_{s,a \sim \rho}[TV(P(\cdot | s, a), P^*(\cdot | s, a))^2]}{n}} \ln(|\mathcal{M}|/\delta) + \frac{c_2 \ln(|\mathcal{M}|/\delta)}{n}
\]
\[
\leq \sqrt{\frac{4c_1 (A(P) + c\xi) \ln(|\mathcal{M}|/\delta)}{n}} + \frac{c_2 \ln(|\mathcal{M}|/\delta)}{n}.
\]

From \((a + b)^2 \leq 2a^2 + 2b^2\),
\[
A^2(P) \lesssim \left( \sqrt{\frac{c(A(P) + \xi) \ln(|\mathcal{M}|/\delta)}{n}} + \frac{c \ln(|\mathcal{M}|/\delta)}{n} \right)^2 \lesssim \left( \frac{A(P) + \xi}{n} + \frac{c \ln(|\mathcal{M}|/\delta)}{n} \right)^2
\]
\[
\lesssim \left( \frac{A(P) + \xi}{n} \ln(|\mathcal{M}|/\delta) \right)
\]
\[
\lesssim \left( \frac{A(P) + 1/n \ln(|\mathcal{M}|/\delta)}{n} \right) \ln(|\mathcal{M}|/\delta).
\]

Then, we have
\[
A^2(P) - B_1 A(P) - B_2 \leq 0, \quad B_1 = c \ln(|\mathcal{M}|/\delta)/n, \quad B_2 = c(1/n)^2 \ln(|\mathcal{M}|/\delta)^2.
\]

This concludes
\[
0 \leq A(P) \leq B_1 + \frac{\sqrt{B_1^2 + 4B_2}}{2} \leq c(B_1 + \sqrt{B_2}) \lesssim \frac{c \ln(|\mathcal{M}|/\delta)}{n} \lesssim \xi.
\]

Thus, by using the above \( A(P) \lesssim \xi (P \in \mathcal{M}_D) \) and (12), with probability \( 1 - \delta \), we have:
\[
\mathbb{E}_{s,a \sim \rho}[TV(P(\cdot | s, a), P^*(\cdot | s, a))^2] \leq A(P) + c\xi \lesssim \xi, \quad P \in \mathcal{M}_D.
\]
Third Step: Calculate the final error bound taking the distribution shift into account. For any \( P \in \mathcal{M}_D \), we prove

\[
V_P^\pi - V_P^\hat{\pi} \leq (1 - \gamma)^{-2} c \sqrt{C^*_{\pi}} \sqrt{\frac{\ln(|\mathcal{M}|/\delta)}{n}}.
\] (13)

For any \( P \in \mathcal{M}_D \), this is proved as follows:

\[
V_P^\pi - V_P^\hat{\pi} \leq (1 - \gamma)^{-2} \mathbb{E}_{(s,a) \sim d_P^\pi} [\text{TV}(P(\cdot | s, a), P^*(\cdot | s, a))] \quad \text{(Simulation lemma, Lemma 9)}
\]

\[
\leq (1 - \gamma)^{-2} \sqrt{\mathbb{E}_{(s,a) \sim d_P^\pi} [\text{TV}(P(\cdot | s, a), P^*(\cdot | s, a))^2]}
\]

\[
\leq (1 - \gamma)^{-2} \sqrt{C^\pi_{\pi} \mathbb{E}_{(s,a) \sim \rho} [\text{TV}(P(\cdot | s, a), P^*(\cdot | s, a))^2]}
\]

\[
\leq c(1 - \gamma)^{-2} \sqrt{C^\pi_{\pi} \sqrt{\frac{\ln(|\mathcal{M}|/\delta)}{n}}}. \quad \text{(Based on the consequence of the second step)}
\]

Combining all things together, with probability \( 1 - \delta \), for any \( \pi^* \in \Pi \), we have

\[
V_{P^*}^\pi - V_{P^*}^\hat{\pi} \leq V_{P^*}^\pi - \min_{P \in \mathcal{M}_D} V_P^\pi + \min_{P \in \mathcal{M}_D} V_P^\pi - V_P^\hat{\pi},
\]

\[
\leq V_{P^*}^\pi - \min_{P \in \mathcal{M}_D} V_P^\pi + \min_{P \in \mathcal{M}_D} V_P^\hat{\pi} - V_P^\pi, \quad \text{(definition of } \hat{\pi})
\]

\[
\leq V_{P^*}^\pi - \min_{P \in \mathcal{M}_D} V_P^\pi - \min_{P \in \mathcal{M}_D} V_P^\hat{\pi} \quad \text{(Fist step, } P^* \in \mathcal{M}_D)
\]

\[
\leq (1 - \gamma)^{-2} c_1 \sqrt{C^\pi_{\pi} \sqrt{\frac{\ln(|\mathcal{M}|/\delta)}{n}}}. \quad \text{(From (13))}
\]

**Remark 5** (To compete with all history-dependent polices). Consider the case where \( \Pi \) is all Markovian polices. We want to show we can compete with all history-dependent non-Markovian polices:

\[
\tilde{\Pi} = \left\{ \prod_{i=1}^{\infty} \pi_i \mid \pi_i \in \left[ \left( \prod_{k=1}^{i-1} S \times \mathcal{A} \right) \rightarrow \Delta(\mathcal{A}) \right] \right\}.
\]

We take an element \( \pi^* \) from \( \tilde{\Pi} \). Then, \( V_{P^*}^\pi \) and \( d_P^\pi \), are still well-defined. Then, every step in the proof still holds. The only step we need to check carefully is this line:

\[
V_{P^*}^\pi - V_{P^*}^\hat{\pi} \leq V_{P^*}^\pi - \min_{P \in \mathcal{M}_D} V_P^\pi + \min_{P \in \mathcal{M}_D} V_P^\pi - V_P^\hat{\pi}.
\]

\[
\leq V_{P^*}^\pi - \min_{P \in \mathcal{M}_D} V_P^\pi + \min_{P \in \mathcal{M}_D} V_P^\hat{\pi}.
\]

This is proved by \( \max_{\pi \in \tilde{\Pi}} V_P^\pi = \max_{\pi \in \Pi} V_P^\pi \) for any \( P \).

**B.2 Proofs for general function approximation for CPPO-LR with infinite hypothesis class (Proof of Theorem 3)**

We firsts show two lemmas as building blocks to prove the main statement.

**Lemma 6.** Set \( \epsilon = 1/(n_1(S)) \). With probability \( 1 - \delta \), for any \( P \in \mathcal{M} \),

\[
\mathbb{E}_{(s,a) \sim \rho} [\text{TV}(P(\cdot | s, a), P^*(\cdot | s, a))^2] \leq 2 \mathbb{E}_D [\log(P^*(s' | s, a)/P(s' | s, a))] + 4n^{-1} \log(c_1 N_{\mathcal{I}}(\epsilon, \mathcal{M}, \| \cdot \|_{\infty}/\delta)).
\]
Proof. Take a $\epsilon = 1/(n\lambda(S))$-bracket $\{[u_i, l_i]\}$ and denote the set of upper bounds $\{l_i\}$ by $\tilde{M}$. Using the proof of Agarwal et al. (2020b, Lemma 25 and Theorem 21), for any $\tilde{P} \in \tilde{M}$,

$$\mathbb{E}_{(s,a) \sim \rho}[\text{TV}(\tilde{P}(\cdot | s,a), P^*(\cdot | s,a))^2] \leq \mathbb{E}_D[\log(P^*(s' | s,a)/\tilde{P}(s' | s,a))] + 2n^{-1} \log(|\tilde{M}|/\delta).$$

Here, for any $P \in M$, we can take $\tilde{P} \in \tilde{M}$ such that

$$\mathbb{E}_D[\log(P^*(s' | s,a)/P(s' | s,a))] \leq \mathbb{E}_D[\log(P^*(s' | s,a)/\tilde{P}(s' | s,a))]. \quad (14)$$

Besides, it satisfies

$$\mathbb{E}_{(s,a) \sim \rho}[\text{TV}(P(\cdot | s,a), P^*(\cdot | s,a))^2] \leq 2\mathbb{E}_{(s,a) \sim \rho}[\text{TV}(\tilde{P}(\cdot | s,a), P^*(\cdot | s,a))^2] + 2\mathbb{E}_{(s,a) \sim \rho}[\text{TV}(P(\cdot | s,a), \tilde{P}(\cdot | s,a))^2] \leq 2\mathbb{E}_{(s,a) \sim \rho}[\text{TV}(\tilde{P}(\cdot | s,a), P^*(\cdot | s,a))^2] + 2n^{-2}.$$  

This concludes the statement. In the last line, we use

$$\text{TV}(\tilde{P}(\cdot | s,a), P^*(\cdot | s,a)) = 0.5 \int_{s' \in S} |\tilde{P}(s' | s,a) - P^*(s' | s,a)|d\lambda(s') \leq 0.5\lambda(S)/n \times \lambda(S) = 0.5/n.$$ 

Next, we show the following lemma.

**Lemma 7.** Set $\epsilon = 1/(n\lambda(S))$. With probability $1 - \delta$, for any $P \in M$, we have

$$\mathbb{E}_D[\log(P^*/P)(s' | s,a)] \geq -n^{-1} \log(N_{\parallel}([\epsilon, M, \parallel \cdot \parallel_\infty])\delta).$$

Proof. We use Cramér-Chernoff’s method. Take a $1/(n\lambda(S))$-bracket $\{[u_i, l_i]\}$ and denote the set of upper bounds $\{l_i\}$ by $\tilde{M}$ and denote it by $\tilde{M}$. For $\tilde{P} \in \tilde{M}$, we have

$$\mathbb{E}\left[ \exp\left( \sum_{i=1}^{n} \log \frac{\tilde{P}(s^{(i)} | s^{(i)}, a^{(i)})}{P^*(s^{(i)} | s^{(i)}, a^{(i)})} \right) \right] \leq \mathbb{E}\left[ \exp\left( \sum_{i=1}^{n-1} \log \frac{\tilde{P}(s^{(i)} | s^{(i)}, a^{(i)})}{P^*(s^{(i)} | s^{(i)}, a^{(i)})} \frac{\tilde{P}(s^{(n)} | s^{(n)}, a^{(n)})}{P^*(s^{(n)} | s^{(n)}, a^{(n)})} \right) \right] \leq \mathbb{E}\left[ \exp\left( \sum_{i=1}^{n-1} \log \frac{\tilde{P}(s^{(i)} | s^{(i)}, a^{(i)})}{P^*(s^{(i)} | s^{(i)}, a^{(i)})} \right) \right] \leq \mathbb{E}\left[ \exp\left( \sum_{i=1}^{n-1} \log \frac{\tilde{P}(s^{(i)} | s^{(i)}, a^{(i)})}{P^*(s^{(i)} | s^{(i)}, a^{(i)})} \right) \right] \{1 + 1/n\} \leq ... \leq (1 + 1/n)^n \leq \epsilon.$$ 

Hence by Markov’s inequality, we have

$$\mathbb{P}\left( \sum_{i=1}^{n} \log \frac{\tilde{P}(s^{(i)} | s^{(i)}, a^{(i)})}{P^*(s^{(i)} | s, a)} > \log(1/\delta) \right) \leq \epsilon \delta.$$
By taking a union bound, for any \( \tilde{P} \in \mathcal{M} \), we obtain

\[
\mathbb{P} \left( \sum_{i=1}^{n} \log \left[ \tilde{P}(s'(i) \mid s(i), a(i)) \bigg/ \mathcal{P}^\star(s'(i) \mid s(i), a(i)) \right] > \log(|\mathcal{M}|/\delta) \right) \leq \epsilon \delta.
\]

Finally, noting for any \( P \in \mathcal{M} \), there exists \( \tilde{P} \in \mathcal{M} \) s.t. \( P(s' \mid s, a) \leq \tilde{P}(s' \mid s, a) \), we have for any \( P \in \mathcal{M} \),

\[
\mathbb{P} \left( \sum_{i=1}^{n} \log \left[ \frac{P(s'(i) \mid s(i), a(i))}{\mathcal{P}^\star(s'(i) \mid s(i), a(i))} \right] > \log(|\mathcal{M}|/\delta) \right) \leq \epsilon \delta.
\]

We condition on events where Lemma 6 and Lemma 7 hold.

**First Step (pessimism).** Lemma 7 tells us that \( \mathcal{P}^\star \in \mathcal{M}_D \).

**Second Step.** Lemma 6 implies for any \( P \in \mathcal{M}_D \),

\[
\mathbb{E}_{(s,a) \sim \rho} [TV(P(\cdot \mid s, a), \mathcal{P}^\star(\cdot \mid s, a))^2] \leq n^{-1} \log(N_{\|\|}(\epsilon, \mathcal{M}, \cdot \|\|_\infty)/\delta)
\]

using the definition of \( P \in \mathcal{M}_D \).

**Third step: calculate the final bound taking the distribution shift into account.** For any \( P \in \mathcal{M}_D \), we prove

\[
V_P^\pi - V_P^\pi \leq (1 - \gamma)^{-2} c \sqrt{C_\pi^* \frac{\ln(N_{\|\|}(\epsilon, \mathcal{M}, \cdot \|\|_\infty)/\delta)}{n}}.
\]  

(16)

For any \( P \in \mathcal{M}_D \), this is proved as follows:

\[
V_P^\pi - V_P^\pi \leq (1 - \gamma)^{-2} \mathbb{E}_{(s,a) \sim \rho}[TV(P(\cdot \mid s, a), \mathcal{P}^\star(\cdot \mid s, a))] \quad \text{(Simulation lemma)}
\]

\[
\leq (1 - \gamma)^{-2} \sqrt{\mathbb{E}_{(s,a) \sim \rho}[TV(P(\cdot \mid s, a), \mathcal{P}^\star(\cdot \mid s, a))^2]}
\]

\[
\leq (1 - \gamma)^{-2} \sqrt{C_{\pi^*} \mathbb{E}_{(s,a) \sim \rho}[TV(P(\cdot \mid s, a), \mathcal{P}^\star(\cdot \mid s, a))^2]}
\]

\[
\leq c(1 - \gamma)^{-2} \sqrt{C_{\pi^*} \frac{\ln(N_{\|\|}(\epsilon, \mathcal{M}, \cdot \|\|_\infty)/\delta)}{n}}. \quad \text{(Based on the consequence of the second step)}
\]

Combining all things together, with probability \( 1 - \delta \), for any \( \pi^* \in \Pi \), we have

\[
V_P^\pi - V_P^\pi \leq V_P^\pi - \min_{P \in \mathcal{M}_D} V_P^\pi + \min_{P \in \mathcal{M}_D} V_P^\pi - V_P^\pi \leq V_P^\pi - \min_{P \in \mathcal{M}_D} V_P^\pi + \min_{P \in \mathcal{M}_D} V_P^\pi - V_P^\pi \leq V_P^\pi - \min_{P \in \mathcal{M}_D} V_P^\pi \leq (1 - \gamma)^{-2} c_1 \sqrt{C_{\pi^*} \frac{\ln(N_{\|\|}(\epsilon, \mathcal{M}, \cdot \|\|_\infty)/\delta)}{n}}.
\]

(From (16))

32
C Missing Proofs in Section 5

C.1 Proofs for Tabular MDPs (Proof of Corollary 1)

Here, we show the result for CPPO-TV. The result in CPPO-LR is obtained in the proof of Corollary 2. We prove in a similar way as Theorem 1.

First step. We set
\[ \xi = c \frac{|S|^2 |A| \ln(n|S| |A| c/\delta)}{n}. \]

Then, from Lemma 11, with probability \( 1 - \delta \), we can show
\[ P^* \in \mathcal{M} \] since
\[ \mathbb{E}_{s,a \sim \mathcal{D}} \left[ \text{TV}(\hat{P}_{\text{MLE}}(\cdot | s, a), P^*(\cdot | s, a))^2 \right] \leq \xi. \]

Hereafter, we condition on the above event.

Second step. Following the second step in the proof of Theorem 1 based on (12), for any \( P \in \mathcal{M} \), we have
\[ \mathbb{E}_{s,a \sim \rho} \left[ \text{TV}(P(\cdot | s, a), P^*(\cdot | s, a))^2 \right] \leq c \xi + A(P) \] (17)

where
\[ A(P) := |\mathbb{E}_{s,a \sim \rho}[\text{TV}(P(\cdot | s, a), P^*(\cdot | s, a))^2] - \mathbb{E}_{\mathcal{D}}[\text{TV}(P(\cdot | s, a), P^*(\cdot | s, a))^2]|. \]

Our goal here is showing with probability \( 1 - \delta \),
\[ A(P) \lesssim \xi, \forall P \in \mathcal{M}. \] (18)

To prove (18), consider an \( \epsilon \)-net \( \{P_1(s,a), \cdots, P_K(s,a)\} \) covering a simplex in terms of \( \| \cdot \|_1 \) \(^3\) for each fixed pair \( (s,a) \in S \times A \). We take \( \epsilon = 1/n \). Since the covering number \( K \) is upper-bounded by \( (c/\epsilon)^{|S|} \) (Wainwright, 2019, Lemma 5.7), we can obtain \( \bar{M} = \{P_1, \cdots, P_K|S| \times |A| \} \) s.t. for any possible \( P \subset S \times A \rightarrow \Delta(S) \), there exists \( P_i \) s.t.
\[ \text{TV}(P_1(\cdot | s, a), P(\cdot | s, a)) \leq \epsilon, \forall (s,a). \]

This implies for any \( P \subset S \times A \rightarrow \Delta(S) \), there exists \( P_i(\cdot | s, a) \) s.t. \( \forall (s,a), \)
\[ |\text{TV}(P(\cdot | s, a), P^*(\cdot | s, a))^2 - \text{TV}(P_i(\cdot | s, a), P^*(\cdot | s, a))^2| \]
\[ \leq 4|\text{TV}(P(\cdot | s, a), P^*(\cdot | s, a)) - \text{TV}(P_i(\cdot | s, a), P^*(\cdot | s, a))| \]
\[ \leq 4\text{TV}(P(\cdot | s, a), P_i(\cdot | s, a)) \]
\[ \leq 4\epsilon. \] (19)

We often use this property (19) hereafter.

Next, we define \( \mathcal{M}' \subset \mathcal{M} \) so that it covers \( \mathcal{M}_{\mathcal{D}} \). Concretely, we define \( \mathcal{M}' \):
\[ \mathcal{M}' = \{P \in \bar{M} : \exists P'' \in \mathcal{M}_{\mathcal{D}}, \text{TV}(P(\cdot | s, a), P''(\cdot | s, a)) \leq \epsilon \ \forall (s,a)\}. \] (20)

The construction is illustrated in Figure 1. Here, from the definition, for any \( P \in \mathcal{M}_{\mathcal{D}}, \) we can also find \( P' \in \mathcal{M}' \) s.t.
\[ \text{TV}(P(\cdot | s, a), P'(\cdot | s, a)) \leq \epsilon, \forall (s,a). \]

\(^3\)In the tabular setting, since the state space is countable, it is equivalent to L1 distance.
This is because from the definition of $\bar{M}$, we can always find $P \in \bar{M}$ satisfying the above. Such $P$ belongs to $M'$ from the definition of $M'$. We use this fact later.

Then, from (20) and recalling (17), we have

$$E_{s,a} \sim \rho \left[ TV(P(\cdot \mid s,a), P^*(\cdot \mid s,a))^2 \right] \lesssim \xi + A(P), \quad \forall P \in M'.$$

(21)

because

$$E_{s,a} \sim \rho \left[ TV(P(\cdot \mid s,a), P^*(\cdot \mid s,a))^2 \right] \leq E_{s,a} \sim \rho \left[ TV(P'(\cdot \mid s,a), P^*(\cdot \mid s,a))^2 \right] + \epsilon^2 \quad \text{(Take some } P'' \in M_D \text{ noting (20))}$$

$$\leq c \xi + A(P). \quad \text{(From (17))}$$

Then, with probability $1 - \delta$, from Bernstein’s inequality, we have

$$A(P) \leq \sqrt{c \var[TV(P(\cdot \mid s,a), P^*(\cdot \mid s,a))^2] \ln(K|S| \times |A| / \delta)} + \epsilon \ln(K|S| \times |A| / \delta), \forall P \in M.$$
Then, with probability $1 - \delta$, we have
\[ A(P) \leq \frac{\ln(K^{|S| \times |A|} / \delta)}{n} + \sqrt{\frac{\ln(K^{|S| \times |A|} / \delta)}{n}} \xi^{1/2} \lesssim \xi, \quad \forall P \in \mathcal{M}' . \tag{22} \]

This shows for any $P \in \mathcal{M}_D$, we have
\[ |\{E_D - E(s,a)\_\rho\}[TV(P(\cdot | s,a), P^*(\cdot | s,a)]| \]
\[ \leq |\{E_D - E(s,a)\_\rho\}[TV(P'(\cdot | s,a), P(\cdot | s,a)]^2 + TV(P'(\cdot | s,a), P^*(\cdot | s,a)]^2| \]
\[ \lesssim \xi, \quad \forall P' \in \mathcal{M}' \] (We take $P' \in \mathcal{M}'$ such that (20))
\[ \leq |\{E_D - E(s,a)\_\rho\}[TV(P'(\cdot | s,a), P^*(\cdot | s,a)]^2] + 8\epsilon \]
\[ \leq \xi. \quad \text{(From the definition of } \mathcal{M}') \]

Thus, (18) is proved.

**Third step.** We follow the third step of Theorem 1:
\[ V_{P^*} - V_{P^*} \lesssim (1 - \gamma)^{-2} \sqrt{C_{\pi^*} \xi}. \]

### C.2 Proofs for Linear Mixture MDPs (Proof of Corollary 2)

We follow the way in Theorem 2. Let $P(\theta) = \theta^T \psi(s, a, s')$.

We first calculate the bracketing number. By letting $\theta^{(1)}, \ldots, \theta^{(K)}$ be an $\epsilon$-cover of the $d$-dimensional ball with a radius $R$, i.e., $B_d(R)$, we have the brackets $\{[P(\theta^{(i)} - \epsilon, P(\theta^{(i)} + \epsilon)] \}_{i=1}^K$, which cover $\mathcal{M}_{mix}$. This is because for any $P(\theta) \in \mathcal{M}_{mix}$, we can take $\theta^{(i)}$ s.t. $\|\theta - \theta^{(i)}\|_2 \leq \epsilon$, then,
\[ P(\theta^{(i)}) - \epsilon < P(\theta) < P(\theta^{(i)}) + \epsilon, \quad \forall (s, a, s') \]
noting
\[ |P(\theta)(s, a, s') - P(\theta^{(i)})(s, a, s')| \leq \|\theta - \theta^{(i)}\|_2 \leq \epsilon, \quad \forall (s, a, s') \] (23)

The last equality is from Lemma 14.

The brackets above are size of $\epsilon$. Therefore, we have
\[ \mathcal{N}(\epsilon, \mathcal{M}_{mix}, \|\cdot\|_2) \leq \mathcal{N}(\epsilon, B_d(cR), \|\cdot\|_2), \]

where $\mathcal{N}(\epsilon, B_d(cR), \|\cdot\|_2)$ is a covering number of $B_d(cR)$ w.r.t $\|\cdot\|_2$. This is upper-bounded by $(cR/\epsilon)^d$ (Wainwright, 2019, Lemma 5.7).

**First Step (pessimism).** Lemma 2 tells us that $P(\theta^*) \in \mathcal{M}_D$.

**Second Step.** Lemma 1 implies for any $P(\theta) \in \mathcal{M}_D$,
\[ E(s,a)\_\rho[TV(P(\theta)(\cdot | s,a), P(\theta^*)(\cdot | s,a)]^2] \leq \beta. \]

using the definition of $P(\theta) \in \mathcal{M}_D$. 

35
Third step: distribution shift part. Here, for \( P \in \mathcal{M}_D \) we prove
\[
V_{P^*}^\pi - V_{P^*}^\pi \lesssim (1 - \gamma)^{-2} \sqrt{dC_{\pi^*}^{\pi^*, \text{mix} \beta}},
\]
(24)
\[
V_{P^*}^\pi - V_{P^*}^\pi \lesssim (1 - \gamma)^{-2} \sqrt{C_{\pi^*}^{\pi^*, \beta}}.
\]
(25)

Following the third step of the proof of Theorem 3, this immediately concludes the bound
\[
V_{P^*}^\pi - V_{P^*}^\pi \lesssim (1 - \gamma)^{-2} \sqrt{dC_{\pi^*}^{\pi^*, \text{mix} \beta}},
\]
\[
V_{P^*}^\pi - V_{P^*}^\pi \lesssim (1 - \gamma)^{-2} \sqrt{C_{\pi^*}^{\pi^*, \beta}}.
\]

Since (25) is obvious from simulation lemma, we only prove (24). To prove (24), we take a distribution \( P(\theta) \in \mathcal{M}_D \). First, recall for \( P(\theta) \in \mathcal{M}_D \), we have
\[
\mathbb{E}_{(s,a) \sim \rho} [\text{TV}(P(\theta) | \cdot, s, a), P(\theta) | \cdot, s, a)]^2 \lesssim \beta.
\]

From the third statement of Lemma 14, for any \( V: S \to [0, 1] \), we have
\[
\mathbb{E}_{(s,a) \sim \rho} [(\theta - \theta^*)^\top \psi_V(s, a)]^2 \lesssim \beta.
\]

Thus,
\[
\forall V: S \to [0, 1], \quad (\theta - \theta^*)^\top \Sigma_{\rho, V}(\theta - \theta^*) \lesssim \beta,
\]
\[
\Sigma_{\rho, V} = \mathbb{E}_{(s,a) \sim \rho} [\psi_V(s, a) \psi_V^\top(s, a)].
\]

Here, we have
\[
V_{P^*}^\pi - V_{P^*}^\pi \leq (1 - \gamma)^{-1} \left| \mathbb{E}_{(s,a) \sim d_{P^*}^\pi} \left[ \int \{ P(s' | s, a) - P^*(s' | s, a) \} V_{P^*}^\pi(s') \mathrm{d}(s') \right] \right|
\]

(Simulation lemma, Lemma 9)
\[
\leq (1 - \gamma)^{-1} \left| \mathbb{E}_{(s,a) \sim d_{P^*}^\pi} \left[ (\theta - \theta^*) \psi_{V^*}^\pi(s, a) \right] \right| \quad \text{(Recall } \psi_V = \int \psi(s, a, s') V_{P^*}^\pi(s') \mathrm{d}(s'))
\]
\[
\leq (1 - \gamma)^{-1} \left| \theta - \theta^* \right| \left| \lambda I + \Sigma_{\rho, V^*} \right| \mathbb{E}_{(s,a) \sim d_{P^*}^\pi} \left[ \left\| \psi_{V^*}^\pi(s, a) \right\|_{(\Sigma_{\rho, V^*} + \lambda I)}^{-1} \right] \quad \text{(CS inequality)}
\]

The first term (a) is upper-bounded by \( \sqrt{(1 - \gamma)^{-2} \beta + \lambda R^2} \) noting \( 0 \leq V_{P^*}^\pi \leq (1 - \gamma)^{-1} \). The term (b) is upper-bounded by
\[
\mathbb{E}_{(s,a) \sim d_{P^*}^\pi} \left[ \left\| \psi_{V^*}^\pi(s, a) \right\|_{(\Sigma_{\rho, V^*} + \lambda I)}^{-1} \right] \leq \mathbb{E}_{(s,a) \sim d_{P^*}^\pi} \left[ \left\| \psi_{V^*}^\pi(s, a) \right\|_{(\Sigma_{\rho, V^*} + \lambda I)}^{-1} \right]^{1/2} \quad \text{(Jensen’s inequality)}
\]

\[
= \sqrt{\text{Tr}(\Sigma_{d_{P^*}^\pi, V^*}^\pi \left( \lambda I + \Sigma_{\rho, V^*} \right)^{-1})}
\]
\[
\leq \sqrt{C_{\pi^*}^{\pi^*, \text{mix}} \text{Tr}(\Sigma_{\rho, V^*} \left( \lambda I + \Sigma_{\rho, V^*} \right)^{-1})} \quad \text{(From Lemma 15)}
\]
\[
\leq \sqrt{C_{\pi^*}^{\pi^*, \text{mix}} \text{rank}(\Sigma_{\rho, V^*})} \leq \sqrt{\bar{C}_{\pi^*}^{\pi^*, \text{mix} d}}.
\]

By taking \( \lambda \) s.t. \( \lambda R^2 \lesssim (1 - \gamma)^{-2} \beta \), (24) is proved.

For linear MDPs, from the fourth statement of Lemma 14, \( C_{\pi^*}^{\pi^*, \text{mix}} \leq \bar{C}_{\pi^*}^{\pi^*} \). Then, the statement is concluded.
C.3 Proofs for Low-rank MDPs (Proof of Theorem 4)

Until the second step, we can perform the same analysis as Theorem 1. More concretely, with probability $1 - \delta$, we have $P^* \in \mathcal{M}_D$ and

$$
E_{s,a \sim \rho}[TV(P(\cdot \mid s, a), P^*(\cdot \mid s, a))^2] \leq \xi, \quad \forall P \in \mathcal{M}_D, \xi := \frac{c \ln(|\mathcal{M}|/\delta)}{n}.
$$

(26)

Hereafter, we condition on the above event.

Letting $f(s, a) = TV(P(\cdot \mid s, a), P^*(\cdot \mid s, a))$, we use Lemma 8, which will be showed later. Then,

$$
\mathbb{E}_{(s, a) \sim d_{P^*}^\rho}[f(s, a)] \leq \mathbb{E}_{(s, a) \sim d_{P^*}^\rho}[\|\phi^*(s, a)\|_{\Sigma^{-1}}] \sqrt{n\omega_{\pi} E_{\rho}[f^2(s, a)] + 4\gamma^2 \lambda d + \sqrt{(1 - \gamma)\omega_{\pi} E_{\rho}[f^2(s, a)]}}
$$

where $\Sigma_{\rho, \phi^*} = n\mathbb{E}_{\rho}[\phi^* \phi^T] + \lambda I$. We consider how to bound $\mathbb{E}_{(s, a) \sim d_{P^*}^\rho}[\|\phi^*(s, a)\|_{\Sigma^{-1}}]$. This is upper-bounded by

$$
\mathbb{E}_{(s, a) \sim d_{P^*}^\rho}[\|\phi^*(s, a)\|_{\Sigma^{-1}}] \leq \sqrt{\text{tr}(\mathbb{E}_{(s, a) \sim d_{P^*}^\rho}[\phi^* \phi^T \Sigma_{\rho, \phi^*}^{-1}])}
$$

$$
\leq \sqrt{C_{\pi, \phi^*} \text{tr}(\mathbb{E}_{(s, a) \sim d_{P^*}^\rho}[\phi^* \phi^T \Sigma_{\rho, \phi^*}^{-1}])} \quad \text{(From Lemma 15)}
$$

$$
\leq \sqrt{C_{\pi, \phi^*} \text{rank}(\Sigma_{\rho})/n}.
$$

Here, in the last line, by letting the SVD of $\Sigma_{\rho} = \mathbb{E}_{\rho}[\phi \phi^T]$ be $U \tilde{\Sigma}_{\rho} U^T$ where $\tilde{\Sigma}_{\rho}$ is a $d \times d$ diagonal matrix and $U$ is a $d \times d$ orthogonal matrix, we use

$$
\text{tr} \left( \Sigma_{\rho} \Sigma_{\rho, \phi^*}^{-1} \right) = \text{tr} \left( (U \tilde{\Sigma}_{\rho} U^T \{nU \tilde{\Sigma}_{\rho} U^T + \lambda I\}^{-1}U \right) = \text{tr}(\tilde{\Sigma}_{\rho} U^T \{nU \tilde{\Sigma}_{\rho} U^T + \lambda I\}^{-1}U)
$$

$$
= \text{tr}(\tilde{\Sigma}_{\rho} U^T \{n\tilde{\Sigma}_{\rho} + \lambda I\} U^{-1}U)
$$

$$
= \text{tr}(\tilde{\Sigma}_{\rho} \{n\tilde{\Sigma}_{\rho} + \lambda I\})^{-1} \leq \text{rank}(\Sigma_{\rho})/n.
$$

Hence, when $P \in \mathcal{M}_D$, by setting $\lambda$ s.t. $\lambda d \lesssim \omega_{\pi} \xi$, we have

$$
\mathbb{E}_{(s, a) \sim d_{P^*}^\rho}[f(s, a)] \leq \frac{\gamma C_{\pi, \phi^*} \text{rank}(\Sigma_{\rho}) \omega_{\pi} \ln(|\mathcal{M}|/\delta)}{n} + \sqrt{\frac{(1 - \gamma)\omega_{\pi} \ln(|\mathcal{M}|/\delta)}{n}}.
$$

We use (26) here.

Finally,

$$
V_{P^*}^\pi - V_{P^*}^{\pi^*}
$$

$$
\leq V_{P^*}^\pi - \min_{P \in \mathcal{M}_D} V_{P}^\pi \quad \text{(Recall the proof of the third step in the proof of Theorem 1)}
$$

$$
\leq (1 - \gamma)^{-2} \mathbb{E}_{s, a \sim d_{P^*}^\rho} \text{TV}(P'(s, a), P^*(\cdot \mid s, a)) \quad (P' = \arg \min_{P \in \mathcal{M}_D} V_{P}^\pi)
$$

$$
\lesssim \sqrt{\frac{C_{\pi, \phi^*} \text{rank}(\Sigma_{\rho}) \omega_{\pi} \ln(|\mathcal{M}|/\delta)}{n(1 - \gamma)^4}}.
$$

The following inequality is an important lemma to connect $\mathbb{E}_{(s, a) \sim d_{P^*}^\rho}[f(s, a)]$ with an elliptical potential $\mathbb{E}_{(\tilde{s}, \tilde{a}) \sim d_{P^*}^\rho}[\|\phi^*(\tilde{s}, \tilde{a})\|_{\Sigma^{-1}}]$. 37
Lemma 8 (One-step back inequality). Take any $f \in S \times A \to \mathbb{R}$ s.t. $\|f\|_\infty \leq B$ and $0 < \lambda \in \mathbb{R}$. Letting $\omega = \max_{s,a}(\pi(a \mid s)/\pi_0(a \mid s))$, for any policy $\pi$, we have

$$\|E(s,a)\|_2 \leq \|\phi^* (\tilde{s}, \tilde{a})\|_{\Sigma^{-1}} \sqrt{n\omega \gamma \|E(s,a)\|} + \gamma^2 \lambda dB^2$$

$$+ \sqrt{(1-\gamma) \omega_n \|E(s,a)\|} / \pi$$

where $\Sigma = nE(s,a)\omega [\phi^* (s,a)\phi^* (s,a)] + \lambda I$.

Proof of Lemma 8. First, we have an equality:

$$E(s,a) = \gamma E(s,a) - d_{p,\gamma} \{ f(s,a) \} + (1-\gamma) E_{s-d_{p,\gamma}} \{ f(s,a) \} . \tag{27}$$

The second term in (27) is upper-bounded by

$$E_{s-d_{p,\gamma}} \{ f(s,a) \} \leq E_{s-d_{p,\gamma}} \{ f^2(s,a) \} ^{1/2} = \sqrt{\omega_n \{ f^2(s,a) \} } / (1-\gamma).$$

Next we consider the first term in (27). By CS inequality, we have

$$\|E_{(s,a)-d_{p,\gamma}} \{ f(s,a) \} \|_{\Sigma^{-1}} \leq \|\phi^* (\tilde{s}, \tilde{a})\|_{\Sigma^{-1}} \int \mu(s)\pi(a \mid s)f(s,a)d(s,a)$$

Then,

$$\|\int \mu(s)\pi(a \mid s)f(s,a)d(s,a)\|_{\Sigma^{-1}} \leq \left\{ n\|E(s,a)\| \right\} \left\{ \int \mu(s)\pi(a \mid s)f(s,a)d(s,a) \right\}$$

$$\leq n \left\{ E_{(s,a)-\rho} \left[ \int \mu(s)\phi^* (s,a) \pi(a \mid s)f(s,a)d(s,a) \right] \right\} ^2 + \lambda dB^2$$

(Use the assumption $\|f(s,a)\|_\infty \leq B$ and $\|\int \mu(s)d(s)\|_2 \leq \sqrt{d}$)

Finally, the first term in (27) is upper-bounded by

$$n \left\{ E_{(s,a)-\rho} \{ f^2(s,a) \} \right\} + \lambda dB^2$$

(Importance sampling)

The final statement is immediately concluded.
C.4 Proofs for Factored MDPs (Proof of Theorem 5)

We focus on the proof of modified CPPO-TV. The proof of CPPO-LR is similarly completed.

We denote the constrained set as $\mathcal{M}_D$:

$$\mathcal{M}_D = \left\{ P = \prod_i P_i \mid \mathbb{E}_D \left[ TV(\hat{P}_{MLE,i}(\cdot \mid s[pai], a), P_i(\cdot \mid s[pai], a))^2 \right] \leq \xi_i, \forall i \in [1, \cdots, d] \right\}.$$  

Following the first step in the proof of Corollary 1, with probability $1 - \delta$, the product $\prod_i P_i^*$ is in $\mathcal{M}_D$, i.e.,

$$\mathbb{E}_{s,a \sim D} \left[ TV(\hat{P}_{MLE,i}(\cdot \mid s[pai], a), P_i^*(\cdot \mid s[pai], a))^2 \right] \leq \xi_i, \forall i \in [1, \cdots, d], \quad \xi_i = \sqrt{\frac{L_d \log(L_d/d)}{n}}.$$  

Note $d$ comes from the union bound. Besides, following the second step in the proof of Corollary 1, for any $P \in \mathcal{M}_D$, with probability $1 - \delta$,

$$\mathbb{E}_{s,a \sim P} \left[ TV(\hat{P}_i(\cdot \mid s[pai], a), P_i^*(\cdot \mid s[pai], a))^2 \right] \leq \xi_i, \forall i \in [1, \cdots, d].$$

After conditioning on the above two events, then, for any $P \in \mathcal{M}_D$ and $\pi^* \in \Pi$, we have

$$V_{\hat{P}}^\pi - V_P^\pi \leq (1 - \gamma)^{-2} \mathbb{E}_{(s,a) \sim d_{\pi^*}^{\hat{P}}} [TV(P(\cdot \mid s, a), P^*(\cdot \mid s, a))]$$

$$\leq (1 - \gamma)^{-2} \mathbb{E}_{(s,a) \sim d_{\pi^*}^{P}} \sum_i TV(P_i(\cdot \mid s[pai], a), P_i^*(\cdot \mid s[pai], a))$$

$$\leq (1 - \gamma)^{-2} \sum_i \mathbb{E}_{(s,a) \sim \rho} \left[ \left( \frac{d_{\pi^*}^{P}(s[pai], a)}{\rho(s[pai], a)} \right)^2 \right] \mathbb{E}_{(s,a) \sim \rho} [TV(P_i(\cdot \mid s[pai], a), P_i^*(\cdot \mid s[pai], a))^2]$$

$$\leq (1 - \gamma)^{-2} \sum_i \sqrt{\hat{C}_{\pi^*, \infty} \mathbb{E}_{(s,a) \sim \rho} [TV(P_i(\cdot \mid s, a), P_i^*(\cdot \mid s, a))^2]} \leq (1 - \gamma)^{-2} \sum_i \sqrt{\hat{C}_{\pi^*, \infty} \xi_i}$$

$$\leq (1 - \gamma)^{-2} \sqrt{d \hat{C}_{\pi^*, \infty} \sum_i \xi_i}$$

$$\leq c(1 - \gamma)^{-2} \sqrt{d \hat{C}_{\pi^*, \infty} \frac{L \ln(\frac{Ld}{\delta})}{n}}.$$  

Here, recall

$$\hat{C}_{\pi^*, \infty} = \max_{s \in [1, \cdots, d]} \mathbb{E}_{(s,a) \sim \rho} \left[ \left( \frac{d_{\pi^*}^{P}(s[pai], a)}{\rho(s[pai], a)} \right)^2 \right].$$

Following the third step in the proof of Corollary 1, the statement is concluded.

Proof of Lemma 1. Next, we show that $\hat{C}_{\pi^*, \infty} \leq C_{\pi^*, \rho^*} = \max_{s,a} \frac{d_{\pi^*}^{P}(s,a)}{\rho(s,a)}$.

From now on, for any $i \in [1, \cdots, d]$, by defining $S'_i$ s.t. $S = S_1 \times S'_i$, we prove

$$\max_{s_i \in S_i, a \in A} \frac{d_{\pi^*}^{P}(s_i, a)}{\rho(s_i, a)} \leq \max_{s \in S_1, a \in A} \frac{d_{\pi^*}^{P}(s, s'_i, a)}{\rho(s, s'_i, a)} = C_{\pi^*, \infty}.$$
First, for any $s_i \in S_i$, $a \in A$, we have
\[
\max_{s_i} \frac{d^*_p(s_i, s_i', a)}{\rho(s_i, s_i', a)} = \max_{s_i} \frac{d^*_p(s_i, a)d^*_p(s_i' \mid s_i, a)}{\rho(s_i, a)\rho(s_i' \mid s_i, a)} = \frac{d^*_p(s_i, a)}{\rho(s_i, a)} \max_{s_i'} \frac{d^*_p(s_i') \mid s_i, a)}{\rho(s_i') \mid s_i, a)} = \frac{d^*_p(s_i, a)}{\rho(s_i, a)}. \tag{28}
\]
Here, we use
\[
1 \leq \max_{s_i'} \frac{d^*_p(s_i' \mid s_i, a)}{\rho(s_i' \mid s_i, a)},
\]
which is proved by the contradiction argument, that is, if $1 > \max_{s_i'} \frac{d^*_p(s_i' \mid s_i, a)}{\rho(s_i' \mid s_i, a)}$, both $\rho$ and $d^*_p$ cannot be probability mass functions since we would get
\[
1 = \sum_{s_i'} d^*_p(s_i' \mid s_i, a) \leq \max_{s_i'} \left( \frac{d^*_p(s_i' \mid s_i, a)}{\rho(s_i' \mid s_i, a)} \right) \sum_{s_i'} \rho(s_i' \mid s_i, a) < \sum_{s_i'} \rho(s_i' \mid s_i, a).
\]
Then, by taking the maximum over $s_i \in S_i$, $a \in A$ for both sides on (28), we have
\[
\max_{s_i, a} \frac{d^*_p(s_i, a)}{\rho(s_i, a)} \leq \max_{s_i', a} \frac{d^*_p(s_i, s_i', a)}{\rho(s_i, a)}.
\]

**Proof of Lemma 2.** By denoting $s_j = s[pa_i]$, we prove for any $i$,
\[
E_{(s,a) \sim \rho} \left[ \left( \frac{d^*_p(s_i, a)}{\rho(s_i, a)} \right)^2 \right] \leq C^*_{\pi^*}.2.
\]
Here, letting $s_i'$ be a value s.t. $s = (s_i, s_i')$, we have
\[
C^*_{\pi^*} = E_{(s,a) \sim \rho} \left[ \frac{d^*_p(s_i, a)}{\rho(s_i, a)} \right] = E_{(s_i,s_i') \sim d^*_p} \left[ \frac{d^*_p(s_i, s_i', a)}{\rho(s_i, a)} \right]
\]
\[
= E_{(s_i,a) \sim d^*_p} \left[ E_{s_i' \sim d^*_p\pi^*} (s_i,a) \frac{d^*_p(s_i, s_i', a)}{\rho(s_i, s_i', a)} \right]
\]
\[
= E_{(s_i,a) \sim d^*_p} \left[ \frac{d^*_p(s_i, a)}{\rho(s_i, a)} E_{s_i' \sim d^*_p\pi^*} (s_i,a) \frac{d^*_p(s_i' \mid s_i, a)}{\rho(s_i' \mid s_i, a)} \right]
\]
\[
\geq E_{(s_i,a) \sim d^*_p} \left[ \frac{d^*_p(s_i, a)}{\rho(s_i, a)} \right] = E_{(s,a) \sim \rho} \left[ \left( \frac{d^*_p(s_i, a)}{\rho(s_i, a)} \right)^2 \right].
\]
In the above inequality, we use
\[
E_{s_i' \sim d^*_p\pi^*} (s_i,a) \frac{d^*_p(s_i' \mid s_i, a)}{\rho(s_i' \mid s_i, a)} - 1 \geq 0, \forall s_i \in S_i, \forall a \in A
\]
as this is Chi-square divergence between two conditional distributions.

**D Missing Proofs in Section 6**

**D.1 Proofs for Finite-Dimensional KNRS (Proof of Corollary 3)**

We prove in a similar way as Theorem 1.
Thus, from Lemma 12, with probability $1 - \delta$, we can show $W^* \in \mathcal{W}_D$ since
\[
\left\| \left( \hat{W}_{MLE} - W^* \right) (\Sigma_n)^{1/2} \right\|_2 \leq \xi.
\]
Hereafter, we condition on this event.

**Second step.** For any $W \in \mathcal{W}_D$, with probability $1 - \delta$, we have
\[
\left\| (W - W^*) (\Sigma_n)^{1/2} \right\|_2 \leq \left\| (W - \hat{W}) (\Sigma_n)^{1/2} \right\|_2 + \left\| (W^* - \hat{W}) (\Sigma_n)^{1/2} \right\|_2 \leq \xi.
\]

**Third step.** Note $P^* = P(W^*)$. Then,
\[
V_{P^*} - \hat{V}_{P^*} \leq V_{P(W)} - \hat{V}_{P(W)} \leq \min_{W \in \mathcal{W}_D} V_{P(W)} - \hat{V}_{P(W)} \leq \hat{V}_{P(W)} - \hat{V}_{P(W)}.
\]

Then, by setting $W' = \arg \min_{W \in \mathcal{M}_D} V_{P(W)}^\pi$, we have
\[
V_{P(W)}^\pi - \hat{V}_{P(W)}^\pi \leq (1 - \gamma)^{-2} \mathbb{E}_{(s,a) \sim d_{p^*}^\pi} \left[ \| P'(s, a) - P^*(s, a) \|_{TV} \right]
\leq \frac{(1 - \gamma)^{-2}}{\zeta} \mathbb{E}_{(s,a) \sim d_{p^*}^\pi} \left[ \| (W' - W^*) \phi(s, a) \|_2 \right] \quad (\text{Lemma 13})
\leq \frac{(1 - \gamma)^{-2}}{\zeta} \mathbb{E}_{(s,a) \sim d_{p^*}^\pi} \left[ \left\| (W' - W^*) (\Sigma_n)^{1/2} \right\|_2 \| \phi(s, a) \|_{\Sigma_n^{-1}} \right] \quad (\text{CS inequality})
\leq \frac{(1 - \gamma)^{-2}}{\zeta} \mathbb{E}_{(s,a) \sim d_{p^*}^\pi} \left[ \| \phi(s, a) \|_{\Sigma_n^{-1}} \right] \quad (\text{Second step})
\]

From Chang et al. (2021, Theorem 20), with probability $1 - \delta$, we have
\[
\xi \leq c_1 \sqrt{\| W^* \|_2 + d_S \min \{ \text{rank}(\Sigma_\rho) \{ \text{rank}(\Sigma_\rho) + \ln(c_2/\delta) \}, d \} \ln(1 + n)}.
\]
In addition, from Chang et al. (2021, Theorem 21), with probability $1 - \delta$, we also have
\[
\mathbb{E}_{(s,a) \sim d_{p^*}^\pi} \left[ \| \phi(s, a) \|_{\Sigma_n^{-1}} \right] \leq c_1 \sqrt{\frac{C_{p^*,\phi} \text{rank}(\Sigma_\rho) \{ \text{rank}(\Sigma_\rho) + \ln(c_2/\delta) \}}{n}}.
\]
Finally, by combining all things, we have
\[
V_{P^*} - \hat{V}_{P^*} \leq c_1 (1 - \gamma)^{-2} \min(d^{1/2}, R) \sqrt{R} \frac{d_S C_{p^*,\phi} \ln(1 + n)}{n}, \quad R = \text{rank}(\Sigma_\rho) \{ \text{rank}(\Sigma_\rho) + \ln(c_2/\delta) \}.
\]

41
D.2 Proof of Lemma 3

Using $\text{TV}(P(W)(\cdot \mid s, a), P(W^*)(\cdot \mid s, a))^2 = \Theta(\|W - W^*\|_2^2)$ (Devroye et al., 2018), we have

$$C_{\pi^*}^\dagger \leq \sup_W \frac{\mathbb{E}_{(s,a) \sim d_{\pi^*}}[\|(W - W^*)\phi(s,a)\|_2^2]}{\mathbb{E}_{(s,a) \sim \rho}[\|(W - W^*)\phi(s,a)\|_2^2]}.$$ 

Here, we have

$$\mathbb{E}_{(s,a) \sim d_{\pi^*}}[\|(W - W^*)\phi(s,a)\|_2^2] = \text{tr}((W - W^*)^\top (W - W^*) \mathbb{E}_{(s,a) \sim d_{\pi^*}}[\phi(s,a)\phi(s,a)^\top]) = \sum_i a_i u_i^\top \mathbb{E}_{(s,a) \sim d_{\pi^*}}[\phi(s,a)\phi(s,a)^\top] u_i.$$ 

In the above derivation, we use SVD:

$$(W - W^*)^\top (W - W^*) = \sum_{i=1}^d a_i u_i^\top.$$

Hence,

$$C_{\pi^*}^\dagger \leq d C_{\pi^*, \phi}.$$ 

D.3 Proofs for Infinite-Dimensional KNRs (Proof of Corollary 4)

We prove in a similar way as Theorem 1.

First step. Recall

$$\xi = \sqrt{d_S \{2 + 150 \ln^3(d_S n/\delta)\mathcal{I}_n\}}, \quad \mathcal{I}_n = \ln(\det(I + \zeta^{-2}K_n)).$$

From Chang et al. (2021, Lemma 14), with probability $1 - \delta$, we can show $g^* \in \mathcal{G}_D$ since

$$\sum_{i=1}^{d_S} \|\hat{g}_i - g_i^*\|_{k_n}^2 \leq \xi^2.$$ 

Hereafter, we condition on this event.

Second step. For any $g \in \mathcal{G}_D$, with probability $1 - \delta$, we have

$$\sum_{i=1}^{d_S} \|g_i - g_i^*\|_{k_n}^2 \leq \sum_{i=1}^{d_S} \|g_i - \hat{g}_i\|_{k_n}^2 + \sum_{i=1}^{d_S} \|\hat{g}_i - g_i^*\|_{k_n}^2 \leq 2\xi.$$
Third step. Note $P^* = P(g^*)$. Then,
\[
V_{P^*}^\pi - V_{\hat{P}}^\pi \leq V_{P^*}^\pi - \min_{g \in \mathcal{D}} V_{P(g)}^\pi + \min_{g \in \mathcal{D}} V_{P(g)}^\hat{\pi} - V_{\hat{P}}^\pi
\]
\[
\leq V_{P^*}^\pi - \min_{g \in \mathcal{D}} V_{P(g)}^\pi + \min_{g \in \mathcal{D}} V_{P(g)}^\hat{\pi} - V_{\hat{P}}^\pi
\quad \text{(definition of $\hat{\pi}$)}
\]
\[
\leq V_{P^*}^\pi - \min_{g \in \mathcal{D}} V_{P(g)}^\pi.
\quad \text{(First step, $g^* \in \mathcal{D}$)}
\]

Then, by setting $g' = \arg \min_{g \in \mathcal{D}} V_{P(g)}^\pi$, we have
\[
V_{P^*}^\pi - V_{\hat{P}}^\pi \leq (1 - \gamma)^{-2} \mathbb{E}_{(s,a) \sim d_{P^*}^\pi} \left\| P'(s,a) - P^*(s,a) \right\|_{TV}
\]
\[
\leq \frac{(1 - \gamma)^{-2}}{\zeta} \mathbb{E}_{(s,a) \sim d_{P^*}^\pi} \left( \| g'(s,a) - g(s,a) \|_2 \right)
\quad \text{(Lemma 13)}
\]
\[
\leq \frac{(1 - \gamma)^{-2}}{\zeta} \mathbb{E}_{(s,a) \sim d_{P^*}^\pi} \left( \sqrt{k_n((s,a),(s,a))} \left( \sum_{i=1}^{d_S} \| g_i' - g_i \|_k \right)^2 \right)^{1/2}
\quad \text{(CS inequality)}
\]
\[
\leq \frac{(1 - \gamma)^{-2} \xi}{\zeta} \mathbb{E}_{(s,a) \sim d_{P^*}^\pi} \left( \sqrt{k_n((s,a),(s,a))} \right).
\quad \text{(Second step)}
\]

From Chang et al. (2021, Theorem 24), with probability $1 - \delta$, we have
\[
\xi \leq c_1 \sqrt{d_S \ln^3(c_2 d_S n/\delta) \{ d^* + \ln(c_2/\delta) \} d^* n \ln(1 + n)}
\]
In addition, from Chang et al. (2021, Theorem 25), with probability $1 - \delta$, we have
\[
\mathbb{E}_{x \sim d_{P^*}^\pi} \left( \sqrt{k_n(x,x)} \right) \leq c_1 \sqrt{\frac{C^* c \ln^3(c_2 d_S n/\delta)}}{n}
\]
Combining all things together, with probability $1 - \delta$, we have
\[
V_{P^*}^\pi - V_{\hat{P}}^\pi \leq c_1 (1 - \gamma)^{-2} \{ d^* + \ln(c_2/\delta) \} d^* \sqrt{\frac{d_S C^* c \ln^3(c_2 d_S n/\delta)}{n} \ln(1 + n)}
\]

E Missing Proofs in Section 7

The proof consists of three steps.

First step (pessimism). We set $\lambda = 1$. Using a result in Agarwal et al. (2019, Lemma 8.7), with probability $1 - \delta$,
\[
\mathbb{E}_{\mathcal{D}} \left[ \int \{ \hat{P}(s' | s,a) - P^*(s' | s,a) \} v(s') \mathrm{d}s' \right]^2 \leq (1 - \gamma)^{-2} \mathbb{E}_{\mathcal{D}} \left[ \| \phi(s,a) \|^2 \right] d \ln(n) \Pi W/\delta
\]
for all $(s,a) \in \mathcal{V}$. Hereafter, we condition on this event. Then,
\[
\mathbb{E}_{\mathcal{D}} \left[ \int \{ \hat{P}(s' | s,a) - P^*(s' | s,a) \} v(s') \mathrm{d}s' \right]^2 \leq (1 - \gamma)^{-2} \mathbb{E}_{\mathcal{D}} \left[ \| \phi(s,a) \|^2 \right] d \ln(n) \Pi W/\delta
\]
\[
\leq (1 - \gamma)^{-2} \frac{d^2 \ln(n) \Pi W/\delta}{n}
\]
for any $v \in \mathcal{V}$.
Second step. From the construction of the algorithm, for any $P \in \mathcal{M}_D$, we have
\[
\mathbb{E}_D \left[ \left( \int \{P(s' | s, a) - P^*(s' | s, a)\} v(s') \text{d}t(s') \right)^2 \right]^{1/2} \lesssim (1 - \gamma)^{-1} \sqrt{\frac{d^2 \ln(n \| \| W/\delta)}{n}}.
\]

Third step: distribution shift part. Here, for any $P \in \mathcal{M}_D$, we will prove
\[
V_{P^*} - V_{P^*} \leq c_1 (1 - \gamma)^{-2} \sqrt{\frac{C_{\pi^*, \rho, \text{rank}[\Sigma]}^2 d \ln(c_2 n \| \| W/\delta)}{n}}.
\]

Following the third step of the proof of Theorem 1, this immediately concludes the bound:
\[
V_{P^*} - V_{P^*} \lesssim (1 - \gamma)^{-2} \sqrt{\frac{C_{\pi^*, \rho, \text{rank}[\Sigma]}^2 d \ln(c_2 n \| \| W/\delta)}{n}}.
\]

From now on, we focus on the proof of (29). Here, we have
\[
V_{P^*} - V_{P^*} \leq (1 - \gamma)^{-1} \mathbb{E}_{(s, a) \sim d_{P^*}} \left[ \int \{P(s' | s, a) - P^*(s' | s, a)\} V_{P^*} (s') \text{d}t(s') \right]
\]

(Simulation lemma, Lemma 9)

\[
\leq (1 - \gamma)^{-1} \mathbb{E}_{(s, a) \sim d_{P^*}} \left[ \left\| \phi(s, a) \right\|_{\Sigma_n^{-1}} \right] \times \left\| \int \{\mu(s') - \mu^*(s')\} V_{P^*} (s') \text{d}t(s') \right\|_{\Sigma_n}.
\]

Recall from Chang et al. (2021, Theorem 21), with probability $1 - \delta$, we also have
\[
\mathbb{E}_{(s, a) \sim d_{P^*}} \left[ \left\| \phi(s, a) \right\|_{\Sigma_n^{-1}} \right] \leq c_1 \sqrt{\frac{C_{\pi^*, \rho, \text{rank}[\Sigma]} \{\text{rank}[\Sigma] + \ln(c_2/\delta)\}}{n}}.
\]

Furthermore,
\[
\left\| \int \{\mu(s') - \mu^*(s')\} V_{P^*} (s') \text{d}t(s') \right\|_{\Sigma_n}
\]
\[
\leq 2\sqrt{n} \mathbb{E}_D \left[ \left( \int \{P(s' | s, a) - P^*(s' | s, a)\} V_{P^*} (s') \text{d}t(s') \right)^2 \right]^{1/2} + 2\lambda \left\| \int \mu(s') V_{P^*} (s') \text{d}t(s') \right\|_2
\]
\[
\lesssim 2\sqrt{n} \times (1 - \gamma)^{-1} \sqrt{\frac{d^2 \ln(n \| \| W/\delta)}{n}} + 2\lambda (1 - \gamma)^{-1} \left\| \int \mu(s') \text{d}t(s') \right\|_2
\]
\[
\lesssim (1 - \gamma)^{-1} \sqrt{\frac{d^2 \ln(n \| \| W/\delta)}{n}}.
\]

Hence,
\[
V_{P^*} - V_{P^*} \leq c_1 (1 - \gamma)^{-2} \sqrt{\frac{C_{\pi^*, \rho, \text{rank}[\Sigma]}^2 d \ln(c_2 n \| \| W/\delta)}{n}}.
\]
F Missing Proofs in Section 8

Here, \( P^* \sim \beta(\cdot), \mathcal{D} \sim d(\cdot \mid P^*) \). Then, by denoting the posterior distribution of \( P^* \) given \( \mathcal{D} \) as \( \beta(\cdot \mid \cdot) \), then \( P_t \sim \beta(\cdot \mid \mathcal{D}) \).

We start with the proof of Lemma 4.

F.1 Proof of Lemma 4

\[
\mathbb{E} \left[ V_{P^*}^{\pi(P^*)} - V_{P^*}^{\pi_t} \right] = \mathbb{E} \left[ V_{P^*}^{\pi(P^*)} - L(\pi(P^*); \mathcal{D}) + L(\pi(P^*); \mathcal{D}) - V_{P^*}^{\pi_t} \right] \\
= \mathbb{E} \left[ V_{P^*}^{\pi(P^*)} - L(\pi(P^*); \mathcal{D}) + \mathbb{E}[L(\pi(P^*); \mathcal{D}) \mid \mathcal{D}] - V_{P^*}^{\pi_t} \right] \\
= \mathbb{E} \left[ V_{P^*}^{\pi(P^*)} - L(\pi(P^*); \mathcal{D}) + \mathbb{E}[L(\pi(P_t); \mathcal{D}) \mid \mathcal{D}] - V_{P^*}^{\pi_t} \right] \\
= \mathbb{E} \left[ V_{P^*}^{\pi(P^*)} - L(\pi(P^*); \mathcal{D}) + L(\pi(P_t); \mathcal{D}) - V_{P^*}^{\pi_t} \right].
\]

From the second line to the third line, we use \( \Pr(P^* \mid \mathcal{D}) = \beta'(P^* \mid \mathcal{D}), \Pr(P_t \mid \mathcal{D}) = \beta'(P_t \mid \mathcal{D}) \).

Besides, by denoting the event \( Z = \{ L(\pi; \mathcal{D}) \leq V_{P^*}^{\pi_t}, \forall \pi \in \Pi \} \) from the assumption,

\[
\mathbb{E} \left[ L(\pi(P_t); \mathcal{D}) \right] = \mathbb{E} \left[ \mathbb{E} \left[ L(\pi(P_t); \mathcal{D}) \mid Z, P^* \right] P(Z \mid P^*) \right] + \mathbb{E}[2(1 - \gamma)^{-1}(1 - P(Z \mid P^*))]
\]

\[
\leq \mathbb{E} \left[ \mathbb{E} \left[ V_{P^*}^{\pi(P_t)} \mid Z, P^* \right] \right] + 2(1 - \gamma)^{-1} \delta
\]

\[
\leq \mathbb{E} \left[ \mathbb{E} \left[ V_{P^*}^{\pi(P^*)} \mid Z, P^* \right] \right] + 2(1 - \gamma)^{-1} \delta
\]

\[
= \mathbb{E} \left[ V_{P^*}^{\pi(P^*)} \right] \mathbb{E} \left[ 1 \mid Z, P^* \right] + 2(1 - \gamma)^{-1} \delta = \mathbb{E} \left[ V_{P^*}^{\pi(P^*)} \right] + 2(1 - \gamma)^{-1} \delta.
\]

Thus,

\[
\mathbb{E} \left[ V_{P^*}^{\pi(P^*)} - V_{P^*}^{\pi_t} \right] \leq \mathbb{E} \left[ V_{P^*}^{\pi(P^*)} - L(\pi(P^*); \mathcal{D}) + V_{P^*}^{\pi(P^*)} - V_{P^*}^{\pi_t} \right] + 2(1 - \gamma)^{-1} \delta.
\]

Next, we prove Lemma 5.

F.2 Proof of Lemma 5

\[
\mathbb{E} \left[ V_{P^*}^{\pi(P^*)} - V_{P^*}^{\pi_t} \right] = H \mathbb{E}_{(s,a) \sim d_{P^*}^{\pi'(P^*)}} \left[ A_{P^*}^{\pi_t}(s,a) \right]. \quad \text{(Performance difference lemma)}
\]

Here, we have

\[
\mathbb{E}_{(s) \sim d_{P^*}^{\pi(P^*)}} \left[ \frac{D_{KL}(\pi(P^*) \mid \cdot \mid s, \pi_{t+1} \mid \cdot, s)) - D_{KL}(\pi(P^*) \mid \cdot \mid s, \pi_t \mid \cdot, s))}{\eta} \right] \\
= \mathbb{E}_{(s) \sim d_{P^*}^{\pi(P^*)}, a \sim \pi(P^*)(s)} \left[ \ln \frac{\pi_{t+1}(a \mid s)}{\pi_t(a \mid s)} \right] \\
= \mathbb{E}_{(s) \sim d_{P^*}^{\pi(P^*)}, a \sim \pi(P^*)(s)} \left[ A_{P^*}^{\pi_t}(s,a) - \frac{1}{\eta} \ln \mathbb{E}_{a \sim \pi^t} \left[ \exp(\eta A_{P^*}^{\pi_t}(s,a)) \right] \right] \\
\geq \mathbb{E}_{(s) \sim d_{P^*}^{\pi(P^*)}, a \sim \pi(P^*)(s)} \left[ A_{P^*}^{\pi_t}(s,a) - 4\eta(1 - \gamma)^{-2} \right].
\]
From the second line to third line, we use the following
\[
\ln \mathbb{E}_{\alpha \sim \pi_t(s)}[\exp(\eta A^\pi_{P^*}(s, a))] \leq \ln \{\mathbb{E}_{\alpha \sim \pi_t(s)}[1 + \eta A^\pi_{P^*}(s, a)] + \{\eta A^\pi_{P^*}(s, a)\}^2]\]
\[
(\eta \leq 2(1 - \gamma), \exp(x) \leq 1 + x + x^2(x \leq 1))
\]
\[
\leq \ln \{\mathbb{E}_{\alpha \sim \pi_t(s)}[1 + 4\eta^2(1 - \gamma)^{-2}]\}
\]
\[
(\log(1 + x) \leq x)
\]
\[
\leq 4\eta^2(1 - \gamma)^{-2}.
\]

Then,
\[
\mathbb{E}\left[V^\pi(P^*) - V^\pi_{P^*}\right]
= H\mathbb{E}[E_{(s, a) \sim d^\pi_{P^*}}[E[A^\pi_{P^*}(s, a)]]]
\leq H\mathbb{E}\left[E_{(s, a) \sim d^\pi_{P^*}}\left[4\eta(1 - \gamma)^{-2} + \frac{D_{KL}(\pi(P^*)|\pi(s), \pi_{t+1}(\cdot|s)) - D_{KL}(\pi(P^*)|\pi(s), \pi_t(\cdot|s))}{\eta}\right]\right].
\]

**F.3 Proof of Theorem 8**

Finally,
\[
\min_{t \leq T} \mathbb{E}\left[V^\pi_{P^*}(P^*) - V^\pi_{P^*}\right]
\leq \left\{\mathbb{E}[V^\pi_{P^*}(P^*) - L(\pi(P^*); D)]\right\} + \frac{1}{T} \sum_{t=1}^{T} \mathbb{E}\left[V^\pi_{P^*}(P^*) - V^\pi_{P^*}\right] + 2(1 - \gamma)^{-1}\delta
\]
\[
\leq \left\{\mathbb{E}[V^\pi_{P^*}(P^*) - L(\pi(P^*); D)]\right\}
\]
\[
+ H\left\{4\eta(1 - \gamma)^{-2} + \frac{1}{T} \mathbb{E}\left[E_{(s, a) \sim d^\pi_{P^*}}\left[\frac{D_{KL}(\pi(P^*)|\pi(s), \pi_{t+1}(\cdot|s)) - D_{KL}(\pi(P^*)|\pi(s), \pi_t(\cdot|s))}{\eta}\right]\right]\right\}
\]
\[
+ 2(1 - \gamma)^{-1}\delta
\]
\[
\leq \left\{\mathbb{E}[V^\pi_{P^*}(P^*) - L(\pi(P^*); D)]\right\}
\]
\[
+ H\left\{4\eta(1 - \gamma)^{-2} + \frac{\ln |A|}{\eta T}\right\} + 2(1 - \gamma)^{-1}\delta
\]
\[
\leq \left\{\mathbb{E}[V^\pi_{P^*}(P^*) - L(\pi(P^*); D)]\right\}
\]
\[
+ 4(1 - \gamma)^{-2} \sqrt{\frac{\ln |A|}{T}} + 2(1 - \gamma)^{-1}\delta.
\]

Thus,
\[
\min_{t \leq T} \mathbb{E}\left[V^\pi_{P^*}(P^*) - V^\pi_{P^*}\right] \leq \left\{\min_{L \in \mathcal{L}_D} \mathbb{E}[V^\pi_{P^*}(P^*) - L(\pi(P^*); D)]\right\}
\]
\[
+ 4(1 - \gamma)^{-2} \sqrt{\frac{\ln |A|}{T}} + 2(1 - \gamma)^{-1}\delta.
\]

**F.4 Proof of Corollary 5**

We take \(L(\pi; D)\) as \(\max(\min_{M \in \mathcal{M}_D} V^\pi_{M}, H), 0\) in Theorem 1. Then, from the first step in the proof of Theorem 1, conditional on \(P^*\), with probability \(1 - \delta\), \(L(\pi; D)\) satisfies
\[
L(\pi; D) \leq V^\pi_{P^*}, \forall \pi \in \Pi.
\]

and
\[
\mathbb{E}_{(s, a) \sim p}[\text{TV}(P^*(\cdot | s, a), P^*(\cdot | s, a))] \leq \xi.
\]
where \( P' = \arg \min_{M \in \mathcal{M}_D} V_M^{\pi(P')} \). We denote the above event as \( \mathcal{Z} \). We have \( P(\mathcal{Z} \mid P^*) \geq 1 - \delta \). In addition, from the third step in the proof of Theorem 1,

\[
\mathbb{E}[V_{P^*}^{\pi(P^*)} - L(\pi(P^*); \mathcal{D})] \leq \mathbb{E}[V_{P^*}^{\pi(P^*)} - V_{P'}^{\pi(P^*)}]
\]

(The third step in the proof of Theorem 1)

\[
\leq (1 - \gamma)^{-2} \mathbb{E}_{P^* \sim \beta}[\mathbb{E}_{(s,a) \sim d^{(P^*)}_{P^*}}[TV(\pi' \mid s, a), P^*(\cdot \mid s, a)) \mid \mathcal{Z}, P^*] P(\mathcal{Z} \mid P^*)]
\]

(Simulation lemma, Lemma 9)

\[
\leq (1 - \gamma)^{-2} \mathbb{E}_{P^* \sim \beta} \left[ \mathbb{E}_{(s,a) \sim d^{(P^*)}_{P^*}}[TV(\pi' \mid s, a), P^*(\cdot \mid s, a)) \mid \mathcal{Z}, P^*] + 2(1 - \gamma)^{-1} \delta \right]
\]

\[
\leq (1 - \gamma)^{-2} \mathbb{E}_{P^* \sim \beta} \left[ \mathbb{E}_{(s,a) \sim d^{(P^*)}_{P^*}}[TV(\pi' \mid s, a), P^*(\cdot \mid s, a))^{2} \mid \mathcal{Z}, P^*] + 2(1 - \gamma)^{-1} \delta \right]
\]

\[
\leq (1 - \gamma)^{-2} \mathbb{E}_{P^* \sim \beta} \left[ \mathbb{E}_{(s,a) \sim d^{(P^*)}_{P^*}}[TV(\pi' \mid s, a), P^*(\cdot \mid s, a))^{2} \mid \mathcal{Z}, P^*] + 2(1 - \gamma)^{-1} \delta \right]
\]

\[
= (1 - \gamma)^{-2} \sqrt{\xi} \mathbb{E}_{P^* \sim \beta} \left[ C_{\pi(P^*), P^*} \mathbb{E}[1 \mid \mathcal{Z}, P^*] + 2(1 - \gamma)^{-1} \delta \right].
\]

By taking \( \delta = 1/n \), the statement is concluded.

### F.5 Proof of Corollary 6

The proof is done as in the proof of Corollary 5. We omit the proof.

### F.6 Proof of Corollary 7

The proof is done as in the proof of Corollary 5. We omit the proof.

### F.7 Proof of Corollary 8

We take \( L(\pi; \mathcal{D}) \) as \( \max(\min_{W \in \mathcal{W}_D} V_{P(W)}^{\pi}, 0) \) in Theorem 1. Then, from the first and second step in the proof of Corollary 3, conditioning on \( P^* \), with probability \( 1 - \delta \), \( L(\pi; \mathcal{D}) \) satisfies

\[
L(\pi; \mathcal{D}) \leq V_{P^*}^{\pi}, \forall \pi \in \Pi.
\]

and

\[
\left\| (W' - W^*) (\Sigma_n)^{1/2} \right\|_2 \leq \xi,
\]

where \( W' = \arg \min_{W \in \mathcal{W}_D} V_{P(W)}^{\pi(P^*)} \). Besides, from Chang et al. (2021, Theorem 20), with probability \( 1 - \delta \), we have

\[
\xi \leq c_1 \sqrt{1 + d_\Sigma \min(\text{rank}(\Sigma), (\text{rank}(\Sigma) + \ln(c_2/\delta)), d)} \ln(1 + n).
\]

47
We take \( L(\pi; D) \) as \( \max(\min_{M \in M_D} V_M^\pi, H) \) in Theorem 1. Then, from the first step in the proof of Theorem 1, conditional on \( P^* \), with probability \( 1 - \delta \), \( L(\pi; D) \) satisfies
\[
L(\pi; D) \leq V_{P^*}^\pi, \forall \pi \in \Pi.
\]
and
\[
\mathbb{E}_{(s,a) \sim \rho} [\text{TV}(P'(\cdot | s, a), P^*(\cdot | s, a))^2] \lesssim \zeta.
\]
where \( P' = \arg \min_{M \in M_D} V_M^{\pi(P^*)} \). We denote the above event as \( Z \). We have \( P(Z | P^*) \geq 1 - \delta \). In addition, from the third step in the proof of Theorem 1,
\[ \mathbb{E}[V_{\pi}(P^*) - L(\pi(P^*); D)] \leq \mathbb{E}[V_{\pi}(P^*) - V_{\pi}(P^*)] \]  
(The third step in the proof of Theorem 1)

\[ \leq (1 - \gamma)^{-2} \mathbb{E}_{P^{*}\sim\beta}[\mathbb{E}_{(s,a)\sim d_{\pi}(P^*)}[TV(P' | s, a, P^{*}(s, a))]] \]  
(Simulation lemma, Lemma 9)

\[ \leq (1 - \gamma)^{-2} \mathbb{E}_{P^{*}\sim\beta}[\mathbb{E}_{(s,a)\sim d_{\pi}(P^*)}[TV(P'(s, a, P^{*}(s, a)) | Z, P^*)]P(Z | P^*)] \]

\[ + \mathbb{E}_{P^{*}\sim\beta}[2(1 - \gamma)^{-1}(1 - P(Z | P^*))] \leq (1 - \gamma)^{-2} \mathbb{E}_{P^{*}\sim\beta}[\mathbb{E}_{(s,a)\sim d_{\pi}(P^*)}[TV(P'(s, a, P^{*}(s, a)) | Z, P^*)]] + 2(1 - \gamma)^{-1}\delta. \]

The final statement is immediately concluded.

### G Auxiliary Lemmas

**Lemma 9** (Simulation Lemma). Consider any two transitions \( P \) and \( \hat{P} \), and any policy \( \pi : S \rightarrow \Delta(A) \). We have:

\[ |V_{\pi} - V_{\hat{\pi}}| \leq |(1 - \gamma)^{-1}\mathbb{E}_{s,a \sim \hat{P},(s,a) \sim d_{\pi}(P)}[V_{\pi}(s')] - E_{s,a \sim P}(V_{\pi}(s'))]\]

\[ \leq (1 - \gamma)^{-2}\mathbb{E}_{s,a \sim \hat{P},(s,a) \sim d_{\pi}(P)}[TV(P(|s,a), \hat{P}(|s,a))]. \]

**Proof.** Such simulation lemma is standard in model-based RL literature and the derivation can be found, for instance, in the proof of Lemma 10 from Sun et al. (2019).

**Lemma 10** (MLE guarantee). Given a set of models \( \mathcal{M} = \{P : S \times A \rightarrow \Delta(S)\} \) with \( P^* \in \mathcal{M} \), and a dataset \( D = \{(s_i, a_i, s_i')\}_{i=1}^n \) with \( s_i, a_i \sim \rho \), and \( s_i' \sim P^*(s_i, a_i) \), let \( \hat{P}_{M} \) be

\[ \hat{P}_{M} = \arg\min_{P \in \mathcal{M}} \sum_{i=1}^n -\ln P(s_i|s_i, a_i). \]

With probability at least \( 1 - \delta \), we have:

\[ \mathbb{E}_{s,a \sim \rho}TV(\hat{P}_{M}(|s,a), P^{*}(|s,a))^2 \leq \frac{\ln(|\mathcal{M}|/\delta)}{n}. \]

**Proof.** Refer to (Agarwal et al., 2020b, Section E).

**Lemma 11** (MLE guarantee for tabular models).

\[ \mathbb{E}_D \left[ TV(P(|s,a), \hat{P}_{M}(|s,a))^2 \right] \leq \frac{|S||A|\{\ln(2 + \ln(2|S||A|/\delta))\}}{2n}. \]

**Proof.** From Chang et al. (2021, Lemma 12), with probability \( 1 - \delta \),

\[ TV(P(|s,a), \hat{P}_{M}(|s,a))^2 \leq \frac{|S|\ln(2 + \ln(2|S||A|/\delta))}{2N(s,a)} \quad \forall (s,a) \in S \times A, \]

where \( N(s,a) \) is the number of visiting times for \((s,a)\). Then,

\[ \mathbb{E}_D \left[ TV(P(|s,a), \hat{P}_{M}(|s,a))^2 \right] \leq \mathbb{E}_D \left[ TV(P(|s,a), \hat{P}_{M}(|s,a))^2 \right] \leq \frac{|S|\ln(2 + \ln(2|S||A|/\delta))}{2N(s,a)} \]

\[ \leq \sum_{(s,a)} \frac{|S|\ln(2 + \ln(2|S||A|/\delta))}{2n} = \frac{|S||A|\{\ln(2 + \ln(2|S||A|/\delta))\}}{2n}. \]

49
Lemma 12 (MLE guarantee for KNRs).
\[
\left\| \left( \hat{W}_{\text{MLE}} - W^* \right) \left( \Sigma_n \right)^{1/2} \right\|_2 \leq \beta_n.
\]

Proof. The proof directly follows the confidence ball construction and proof from (Kakade et al., 2020).

Lemma 13 ($\ell_1$ Distance between two Gaussians). Consider two Gaussian distributions $P_1 := \mathcal{N}(\mu_1, \sigma_1^2 \mathbf{I})$ and $P_2 := \mathcal{N}(\mu_2, \sigma_2^2 \mathbf{I})$. We have:
\[
\text{TV}(P_1, P_2) \leq \frac{1}{\zeta} \| \mu_1 - \mu_2 \|_2.
\]

Proof. This lemma is proved by Pinsker’s inequality and the closed-form of the KL divergence between $P_1$ and $P_2$. Refer to (Kakade et al., 2020).

Lemma 14 (Property of linear mixture MDPs). Let $P(\theta) = \theta^\top \psi(s, a, s')$. Suppose $P(\theta) \in S \times A \rightarrow \Delta(S)$. For any function $V \in S \rightarrow [0, 1]$, letting $\psi(s, a) = \int \psi(s, a, s')V(s')d(s')$, we suppose $\|\psi(s, a)\|_2 \leq 1$. The following theorems hold:

1. For any $(s, a, s')$, we have $|P(\theta)(s, a, s') - P(\theta')(s, a, s')| \leq \|\theta - \theta'\|_2$.

2. For any $(s, a)$, we have $\text{TV}(P(\theta)(s, a, \cdot), P(\theta')(s, a, \cdot)) \leq \|\theta - \theta'\|_2$. Besides, for any $V : S \rightarrow [0, 1]$, we have
\[
|\theta - \theta'|\psi_V(s, a) | \leq \text{TV}(P(\theta)(s, a, \cdot), P(\theta')(s, a, \cdot)).
\]

3. $C^\dagger_{\pi^*, P^*} = \sup_x x^\top \mathbb{E}_{(s, a) \sim d^*_P}[\psi_V(s, a)] x$.
\[
V(s, a, x) = \arg \max_{V : S \rightarrow [0, 1]} \left| x^\top \int \phi(s, a, s')V(s')d(s') \right|.
\]

4. In linear MDPs (i.e., $\psi(s, a, s') = \phi(s, a) \otimes \mu(s')$), we have
\[
\sup_{V \in (S \rightarrow [0, 1])} \sup_x \frac{x^\top \mathbb{E}_{(s, a) \sim d^*_P}[\psi_V(s, a)] x}{x^\top \mathbb{E}_{(s, a) \sim \mu}[\psi_V(s, a)] x} = \sup_x \frac{x^\top \mathbb{E}_{d^*_P}[\phi(s, a) \phi(s, a)^\top] x}{x^\top \mathbb{E}_{\mu}[\phi(s, a) \phi(s, a)^\top] x}.
\]

Proof. We prove the first statement. This is proved by
\[
|P(\theta) - P(\theta')| = |(\theta - \theta')\psi(s, a, s')| \leq \|\theta - \theta'\|_2 \|\psi(s, a, s')\|_2 \leq \|\theta - \theta'\|_2,
\]
Here, we use $\|\psi(s, a, s')\|_2 \leq 1$ which is proved by the assumption by setting $V(s) = I(s' = s)$ for any $s'$. Next, we prove the second statement. For fixed $\theta \in \mathbb{R}^d$ and $(s, a) \in S \times A$, we have
\[
\text{TV}(P(\theta)(s, a, \cdot), P(\theta^*)(s, a, \cdot)) = \sup_{V : S \rightarrow [0, 1]} |(\theta - \theta^*)^\top \psi(s, a, s')V(s')d(s')|
\]
\[
= \sup_{V : S \rightarrow [0, 1]} |(\theta - \theta^*)^\top \psi(s, a, s')V(s')d(s')|
\]
\[
= |(\theta - \theta^*)^\top \psi_V(s, a) s'|d(s')|
\]
\[
= |(\theta - \theta^*)^\top \psi_V(s, a) (s')|.n
In the third line, we define $TV(P(\theta)(s, a, \cdot), P(\theta^*)(s, a, \cdot)) = \|(\theta - \theta^*)\|_2 \|\psi_V(s, a, \theta)\|_2 \leq \|\theta - \theta^*\|_2$.

The third statement is immediately concluded by

$$\frac{\mathbb{E}_{(s, a) \sim \rho}[TV(P(\theta)(s, a, \cdot), P(\theta^*)(s, a, \cdot))]}{\mathbb{E}_{(s, a) \sim \rho}[(\theta - \theta^*)\|\psi_V(s, a, \theta)\|_2]} = \frac{\mathbb{E}_{(s, a) \sim \rho}[(\theta - \theta^*)\|\psi_V(s, a, \theta)\|_2]}{\mathbb{E}_{(s, a) \sim \rho}[(\theta - \theta^*)\|\psi_V(s, a, \theta)\|_2]}.$$ (30)

Finally, we prove the fourth statement. Suppose $\psi(s, a, s') = \phi(s, a) \otimes \mu(s')$ ($\otimes$ denotes kronerker product). Then, $\phi_V(s, a, s') = \phi(s, a) \otimes \int \mu(s')V(s')d(s')$. Then, by defining a vector $\mu(V) = \int \mu(s')V(s')d(s')$, we immediately have

$$\frac{x^\top \mathbb{E}_{(s, a) \sim \rho}[\psi_V(s, a, \psi_V(s, a))]x}{x^\top \mathbb{E}_{(s, a) \sim \rho}[(\phi(s, a) \otimes \mu(V))(\phi(s, a) \otimes \mu(V))]x} = \sup_x \frac{x^\top \mathbb{E}_{(s, a) \sim \rho}[\phi(s, a) \otimes \mu(V))]x}{x^\top \mathbb{E}_{(s, a) \sim \rho}[(\phi(s, a) \otimes \mu(V))]x}.$$ (31)

Here, we have

$$\mathbb{E}_\rho[(\phi(s, a) \otimes \mu(V))(\phi(s, a) \otimes \mu(V))] = \mathbb{E}_\rho[(\phi(s, a) \otimes \mu(V))(\phi(s, a) \otimes \mu(V))\text{]} = \mathbb{E}_\rho[(\phi(s, a)\phi(s, a)^\top) \otimes (\mu(V)\mu(V)^\top)].$$

We notice

$$\{\mathbb{E}_\rho[(\phi(s, a)\phi(s, a)^\top)] \otimes (\mu(V)\mu(V)^\top)\}^{1/2} = \mathbb{E}_\rho[(\phi(s, a)\phi(s, a)^\top)^{1/2} \otimes (\mu(V)\mu(V)^\top)^{1/2}].$$

This is because the square root of a matrix is unique and we have $(A^{1/2} \otimes B^{1/2})(A^{1/2} \otimes B^{1/2}) = AB$ for symmetric matrices $A$ and $B$. Then, by denoting $F_{\rho} = \mathbb{E}_{\rho}[\phi(s, a)\phi(s, a)^\top], F_{\rho}^{*} = \mathbb{E}_{\rho}[\phi(s, a)\phi(s, a)^\top]$ and denoting the pseudo inverse of $F$ as $F^+$, we can see (31) is equal to

$$\{F_{\rho}^{1/2} \otimes (\mu(V)\mu(V)^\top)^{1/2}\}^{+}\{F_{\rho}^{*} \otimes (\mu(V)\mu(V)^\top)^{1/2}\} = \{F_{\rho}^{1/2} \otimes (\mu(V)\mu(V)^\top)^{-1/2}\}^{+}\{F_{\rho}^{*} \otimes (\mu(V)\mu(V)^\top)^{-1/2}\} = \{F_{\rho}^{1/2}F_{\rho}^{*}F_{\rho}^{-1/2}\} \otimes \{(\mu(V)\mu(V)^\top)^{-1/2}(\mu(V)\mu(V)^\top)^{-1/2}\} = \{F_{\rho}^{1/2}F_{\rho}^{*}F_{\rho}^{-1/2}\} \otimes I_k (k = \text{rank}(\mu(V)\mu(V)^\top)).$$

Here, $I_k$ is a diagonal matrix s.t. $k \in \mathbb{N}^+$ values in the diagonal entries are 1 and the rest of values are 0. Then, the maximum singular value of $\{F_{\rho}^{1/2}F_{\rho}^{*}F_{\rho}^{-1/2}\} \otimes I_k$ is equal to the one of $\{F_{\rho}^{1/2}F_{\rho}^{*}F_{\rho}^{-1/2}\}$. This is equal to

$$\sup_x \frac{x^\top F_{\rho}^{*}F_{\rho}^{-1/2}x}{x^\top F_{\rho}x}$$

Hence, the fourth statement is concluded.
Lemma 15 (Distribution shift lemma). Suppose $A_1, A_2, A_3$ are semipositive definite matrices:

$$\text{Tr}(A_1 A_2) \leq \sigma_{\text{max}}(A_3^{-1/2} A_1 A_3^{-1/2}) \text{Tr}(A_3 A_2).$$

Note

$$\sigma_{\text{max}}(A_3^{-1/2} A_1 A_3^{-1/2}) = \sup_{x \in \mathbb{R}^d} x^\top A_1 x.$$ 

Proof.

$$\text{Tr}(A_1 A_2) = \text{Tr}(A_1^{1/2} A_2 A_1^{1/2}) = \text{Tr}(A_1^{1/2} A_3^{-1/2} A_3 A_3^{-1/2} A_2 A_3^{1/2} A_3^{-1/2} A_1^{1/2})$$

$$= \text{Tr}(A_3^{-1/2} A_1 A_3^{-1/2} A_3 A_3^{-1/2} A_2 A_3^{1/2}).$$

In addition, for any semipositive definite matrices $A, B$ we have

$$\text{Tr}(AB) = \text{Tr}(UAU^\top B) = \text{Tr}(AU^\top BU) \leq \sigma_{\text{max}}(A) \text{Tr}(U^\top BU) = \sigma_{\text{max}}(A) \text{Tr}(B),$$

where $UAU^\top$ is the SVD decomposition of $A$. This concludes that

$$\text{Tr}(A_1 A_2) \leq \sigma_{\text{max}}(A_3^{-1/2} A_1 A_3^{-1/2}) \text{Tr}(A_3 A_2).$$

The following lemma is useful to obtain the generalized result of Theorem 1. The proof is given in Wainwright (2019, Theorem 3.27). We first define

$$Z = \sup_{f \in \mathcal{F}} |\mathbb{E}_D - \mathbb{E}_\rho[f]|$$

$$\Sigma^2 = \sup_{f \in \mathcal{F}} \mathbb{E}_D \left[ \{f(s, a) - \mathbb{E}_\rho[f(s, a)]\}^2 \right], \quad \sigma^2 = \sup_{f \in \mathcal{F}} \text{var}[f(s, a)].$$

Lemma 16 (Functional Bernstein’s inequality). Suppose $\|f\|_\infty \leq B$. With probability $1 - \delta$,

$$|Z - \mathbb{E}[Z]| \leq \Sigma^2 \sqrt{\frac{\log(c/\delta)}{n}} + \frac{B \log(c/\delta)}{n}.$$ 

As an immediate corollary,

$$|Z - \mathbb{E}[Z]| \leq \{\sigma^2 + B \mathbb{E}[Z]\} \sqrt{\frac{\log(c/\delta)}{n}} + \frac{B \log(c/\delta)}{n}.$$