PC-PG: Policy Cover Directed Exploration for Provable Policy Gradient Learning

Alekh Agarwal\textsuperscript{1}, Mikael Henaff\textsuperscript{2}, Sham Kakade\textsuperscript{3,1}, and Wen Sun\textsuperscript{*4}

\textsuperscript{1}Microsoft Research
\textsuperscript{2}Facebook AI Research
\textsuperscript{3}University of Washington
\textsuperscript{4}Cornell University

August 14, 2020

Abstract

Direct policy gradient methods for reinforcement learning are a successful approach for a variety of reasons: they are model free, they directly optimize the performance metric of interest, and they allow for richly parameterized policies. Their primary drawback is that, by being local in nature, they fail to adequately explore the environment. In contrast, while model-based approaches and Q-learning directly handle exploration through the use of optimism, their ability to handle model misspecification and function approximation is far less evident. This work introduces the the Policy Cover-Policy Gradient (PC-PG) algorithm, which provably balances the exploration vs. exploitation tradeoff using an ensemble of learned policies (the policy cover). PC-PG enjoys polynomial sample complexity and run time for both tabular MDPs and, more generally, linear MDPs in an infinite dimensional RKHS. Furthermore, PC-PG also has strong guarantees under model misspecification that go beyond the standard worst case $\ell_\infty$ assumptions; this includes approximation guarantees for state aggregation under an average case error assumption, along with guarantees under a more general assumption where the approximation error under distribution shift is controlled. We complement the theory with empirical evaluation across a variety of domains in both reward-free and reward-driven settings.

1 Introduction

Policy gradient methods are a successful class of Reinforcement Learning (RL) methods, as they are amenable to parametric policy classes, including neural policies [Schulman et al. [2015],[2017]], and

\textsuperscript{*}Work done while MH and WS were at Microsoft Research
they directly optimizing the cost function of interest. While these methods have a long history in the RL literature [Williams, 1992, Sutton et al., 1999, Konda and Tsitsiklis, 2000, Kakade, 2001], only recently have their theoretical convergence properties been established: roughly when the objective function has wide coverage over the state space, global convergence is possible [Agarwal et al., 2019, Geist et al., 2019, Bhandari and Russo, 2019, Abbasi-Yadkori et al., 2019a]. In other words, the assumptions in these works imply that the state space is already well-explored. Conversely, without such coverage (and, say, with sparse rewards), policy gradients often suffer from the vanishing gradient problem.

With regards to exploration, at least in the tabular setting, there is an established body of results which provably explore in order to achieve sample efficient reinforcement learning, including model based methods [Kearns and Singh, 2002, Brafman and Tennenholtz, 2002, Kakade, 2003, Jaksch et al., 2010, Azar et al., 2017, Dann and Brunskill, 2015], model free approaches such as Q-learning [Strehl et al., 2006, Li, 2009, Jin et al., 2018, Dong et al., 2019], thompson sampling [Osband et al., 2014, Agrawal and Jia, 2017, Russo, 2019], and, more recently, policy optimization approaches [Efroni et al., 2020, Cai et al., 2020]. In fact, more recently, there are number of provable reinforcement learning algorithms, balancing exploration and exploitation, for MDPs with linearly parameterized dynamics, including Jiang et al. [2017], Yang and Wang [2019b], Jin et al. [2019], Zanette et al. [2020], Ayoub et al. [2020], Zhou et al. [2020], Cai et al. [2020].

The motivation for our work is to develop algorithms and guarantees which are more robust to violations in the underlying modeling assumptions; indeed, the primary practical motivation for policy gradient methods is that the overall methodology is disentangled from modeling (and Markovian) assumptions, since they are an “end-to-end” approach, directly optimizing the cost function of interest. Furthermore, in support of these empirical findings, there is a body of theoretical results, both on direct policy optimization approaches [Kakade and Langford, 2002, Bagnell et al., 2004, Scherrer, 2014, Scherrer and Geist, 2014] and more recently on policy gradient approaches [Agarwal et al., 2019], which show that such incremental policy improvement approaches are amenable to function approximation and violations of modeling assumptions, under certain coverage assumptions over the state space.

This work focuses on how policy gradient methods can be extended to handle exploration, while also retaining their favorable properties with regards to how they handle function approximation and model misspecification. The practical relevance of answering these questions is evident by the growing body of empirical techniques for exploration in policy gradient methods such as pseudocounts [Bellemare et al., 2016], dynamics model errors [Pathak et al., 2017], or random network distillation (RND) [Burda et al., 2019].

1.1 Our Contributions

This work introduces the Policy Cover-Policy Gradient algorithm (PC-PG), a direct, model-free, policy optimization approach which addresses exploration through the use of a learned ensemble of policies, the latter provides a policy cover over the state space. The use of a learned policy cover addresses exploration, and also addresses what is the “catastrophic forgetting” problem in policy gradient approaches (which use reward bonuses); while the on-policy nature avoids the “delusional
Table 1: Comparison of algorithms in tabular (and state-aggregation) settings. For the last column, state-aggregation provides a means to compare tabular approaches when the aggregated MDP may only approximately be an MDP (i.e. when there is a model misspecification). We assume the agent starts at a fixed starting state \( s_0 \) and only has the ability to do rollouts from the state \( s_0 \). Sample complexity is for the number of samples required to learn an \( \epsilon \)-optimal policy. \( Q \)-learning and standard policy optimization have an exponential sample complexity in \( H := 1/(1 - \gamma) \) due to that they do not actively explore. If the starting state distribution had coverage (as opposed to starting at a single state \( s_0 \)), then stronger guarantees exist for policy optimization methods [Kakade and Langford, 2002, Agarwal et al., 2019], both with regards to sample complexity and state-aggregation. The optimistic policy optimization approaches of [Cai et al., 2020, Efroni et al., 2020] build an empirical model of the transition dynamics and do optimistic policy updates in this empirical model; as such, the can also viewed as being model based, unlike \( Q \)-learning and PC-PG which do not store and use prior data. PC-PG removes the initial state distribution assumptions [Kakade and Langford, 2002, Agarwal et al., 2019] from prior policy gradient results through incorporating strategic exploration; this is done via learning an ensemble of policies, the policy cover. PC-PG extends to linear MDPs with linear function approximation as well, and it also works under a weaker error condition when state aggregation is performed as the type of function approximation.
bias” inherent to Bellman backup-based approaches, where approximation errors due to model misspecification amplify (see [Lu et al., 2018] for discussion).

It is a conceptually different approach from the predominant prior (and provable) RL algorithms, which are either model-based — variants of UCB [Kearns and Singh, 2002], [Brafman and Tennenholtz, 2002], [Jaksch et al., 2010], [Azar et al., 2017] or based on Thompson sampling [Agrawal and Jia, 2017], [Russo, 2019] — or model-free and value based, such as Q-learning [Jin et al., 2018], [Strehl et al., 2006]. Our work adds policy optimization methods to this list, as a direct alternative: the use of learned covers permits a model-free approach by allowing the algorithm to plan in the real world, using the cover for initializing the underlying policy optimizer. We remark that only a handful of prior (provable) exploration algorithms [Jin et al., 2018], [Strehl et al., 2006] are model-free in the tabular setting, and these are largely value based.

Table 1 shows the relative landscape of results for the tabular case. Here, we can compare tabular approaches when the MDP may only approximately be an MDP. For the latter, we consider the question of state-aggregation, where states are aggregated into “meta-states” due to some given state-aggregation function [Li et al., 2006]. The hope is that the aggregated MDP is also approximately an MDP (with a smaller number of aggregated state). Table 1 compares the effectiveness of tabular algorithms in this case, where the state-aggregation function introduces model misspecification. Importantly, PC-PG provides a local guarantee, in a more model agnostic sense, unlike model-based and Bellman-backup based methods.

Our main results show that PC-PG is provably sample and computationally efficient for both tabular and linear MDPs, where PC-PG finds a near optimal policy with a polynomial sample complexity in all the relevant parameters in the (linear) MDP. Furthermore, we give theoretical support that the direct approach is particularly favorable with regards to function approximation and model misspecification. Highlights are as follows:

**RKHS in Linear MDPs:** For the linear MDPs proposed by [Jin et al., 2019], our results hold when the linear MDP features live in an infinite dimensional Reproducing Kernel Hilbert Space (RKHS). It is not immediately evident how to extend the prior work on linear MDPs (e.g. [Jin et al., 2019]) to this setting (due to concentration issues with data re-use). The following informal theorem summarizes this contribution.

**Theorem 1.1** (Informal theorem for PC-PG on linear MDPs). With high probability, PC-PG finds an $\epsilon$ near optimal policy with number of samples $\tilde{O}(\text{poly}(1/(1-\gamma), \mathcal{I}_N, 1/\epsilon, W))$, where $W$ is related to the maximum RKHS norm of any policy’s Q function and $\mathcal{I}_N$ is the maximum information gain defined with respect to the kernel. Here, $\mathcal{I}_N$ implicitly measures the effective dimensionality of the problem, and $\mathcal{I}_N = \tilde{O}(d)$ for a linear kernel with d-dimensional features.

**Bounded transfer error and state aggregation:** When specialized to a state aggregation setting, we show that PC-PG provides a different approximation guarantee in comparison to prior works. In particular, the aggregation need only be good locally, under the visitations of the comparison policy. This means that quality of the aggregation need only be good in the regions where a high value policy tends to visit. More generally, we analyze PC-PG under a notion of a small transfer error in critic fitting [Agarwal et al., 2019]—a condition on the error of a best on-policy critic under a
comparison policy’s state distribution—which generalizes the special case of state aggregation, and show that PC-PG enjoys a favorable sample complexity whenever this transfer error is small. We also instantiate the general result with other concrete examples where PC-PG is effective, and where we argue prior approaches will not be provably accurate. The following is an informal statement for the special case of state-aggregation with model-misspecification.

**Theorem 1.2** (Informal theorem for state aggregation). With high probability, PC-PG finds an $\epsilon + \epsilon_{\text{misspec}}$ near optimal policy with $O(\max(|Z|, 1/(1 - \gamma), 1/\epsilon))$ many samples, where $Z$ is the set of abstracted states; $\epsilon_{\text{misspec}} = O(\max_a \epsilon_{\text{misspec}}(s, a)/(1 - \gamma)^3)$ where $d^*$ is the state visitation distribution of an optimal policy (the distribution of which states an optimal policy tends to visit), and $\epsilon_{\text{misspec}}(s, a)$ is a measure of the model-misspecification error at state action $s, a$ (a disagreement measure between dynamics and rewards of state-action pairs aggregated to the same abstract state as $s, a$).

**Empirical evaluation:** We provide experiments showing the viability of PC-PG in settings where prior bonus based approaches such as Random Network Distillation [Burda et al., 2019] do not recover optimal policies with high probability. Our experiments show our basic approach complements and leverages existing deep learning approaches, implicitly also verifying the robustness of PC-PG outside the regime where the sample complexity bounds provably hold.

### 1.2 Related Work

We first discuss work with regards to policy gradient methods and incremental policy optimization; we then discuss work with regards to exploration in the context of explicit (or implicit) assumptions on the MDP (which permit sample complexity that does not explicitly depend on the number of states); and then “on-policy” exploration methods. Finally, we discuss the recent and concurrent work of Cai et al. [2020], Efroni et al. [2020], which provide an optimistic policy optimization approach which uses off-policy data.

Our line of work seeks to extend the recent line of provably correct policy gradient methods [Agarwal et al., 2019], Fazel et al. [2018], Bhandari and Russo [2019], Liu et al. [2019], Even-Dar et al. [2009], Neu et al. [2017], Azar et al. [2012], Abbasi-Yadkori et al. [2019a] to incorporate exploration. As discussed in the intro, our focus is that policy gradient methods, and more broadly “incremental” methods — those methods which make gradual policy changes such as Conservative Policy Iteration (CPI) [Kakade and Langford, 2002], Scherrer and Geist, 2014, Scherrer [2014], Policy Search by Dynamic Programming (PSDP) [Bagnell et al., 2004], and MD-MPI [Geist et al., 2019] — have guarantees with function approximation that are stronger than the more abrupt approximate dynamic programming methods, which rely on the boundedness of the more stringent concentrability coefficients [Munos 2005], Szepesvári and Munos [2005], Antos et al. [2008]; see Scherrer [2014], Agarwal et al. [2019], Geist et al. [2019], Chen and Jiang [2019], Shani et al. [2019] for further discussion. Our main agnostic result shows how PC-PG is more robust than all extant bounds with function approximation in terms of both concentrability coefficients and distribution mismatch coefficients; as such, our results require substantially weaker assumptions, building on the recent work of Agarwal et al. [2019] who develop a similar notion of robustness.
in the policy optimization setting without exploration. Specifically, when specializing to linear
MDPs and tabular MDPs, our algorithm is PAC while algorithms such as CPI and NPG are not PAC
without further assumption on the reset distribution [Agarwal et al. 2019].

We now discuss results with regards to exploration in the context of explicit (or implicit)
assumptions on the underlying MDP. To our knowledge, all prior works only provide provable
algorithms, under either realizability assumptions or under well specified modelling assumptions;
the violations tolerated in these settings are, at best, in an $\ell_\infty$-bounded, worst case sense. The most
general set of results are those in [Jiang et al. 2017], which proposed the concept of Bellman Rank to
characterize the sample complexity of value-based learning methods and gave an algorithm that has
polynomial sample complexity in terms of the Bellman Rank, though the proposed algorithm is not
computationally efficient. Bellman rank is bounded for a wide range of problems, including MDPs
with small number of hidden states, linear MDPs, LQRs, etc. Later work gave computationally
efficient algorithms for certain special cases [Dann et al. 2018, Du et al. 2019, Yang and Wang,
2019a, Jin et al. 2019, Misra et al. 2020]. Recently, Witness rank, a generalization of Bellman rank
to model-based methods, was proposed by [Sun et al. 2019] and was later extended to model-based
reward-free exploration by [Henaff 2019]. We focus on the linear MDP model, studied in [Yang
and Wang 2019a, Jin et al. 2019]. We note that Yang and Wang 2019a also prove a result for a
type of linear MDPs, though their model is significantly more restrictive than the model in [Jin et al.
2019]. Another notable result is due to Wen and Van Roy [2013], who showed that in deterministic
systems, if the optimal $Q$-function is within a pre-specified function class which has bounded Eluder
dimension (for which the class of linear functions is a special case), then the agent can learn the
optimal policy using a polynomial number of samples; this result has been generalized by [Du et al.
2019] to deal with stochastic rewards, using further assumptions such as low variance transitions
and strictly positive optimality gap.

With regards to “on-policy” exploration methods, to our knowledge, there are relatively few
provable results which are limited to the tabular case. These are all based on Q-learning with
uncertainty bonuses in the tabular setting, including the works in [Strehl et al. 2006, Jin et al.
2018]. More generally, there are a host of results in the tabular MDP setting that handle exploration,
which are either model-based or which re-use data (the re-use of data is often simply planning in the
empirical model), which include [Brafman and Tennenholtz 2003, Kearns and Singh 2002, Azar
et al. 2017, Kakade 2003, Jaksch et al. 2010, Agrawal and Jia 2017, Lattimore and Hutter
2014a, b, Dann and Brunskill 2015, Szita and Szepesvári 2010].

Cai et al. 2020, Efroni et al. 2020 recently study algorithms based on exponential gradient
updates for tabular MDPs, utilizing the mirror descent analysis first developed in [Even-Dar et al.
2009] along with idea of optimism in the face of uncertainty. Both approaches use a critic computed
from off-policy data and can be viewed as model-based, since the algorithm stores all previous
off-policy data and plans in what is effectively the empirically estimated model (with appropriately
chosen uncertainty bonuses); in constrast, the model-free approaches such as $Q$-learning do not
store the empirical model and have a substantially lower memory footprint (see [Jin et al. 2018]
for discussion on this latter point). Cai et al. 2020 further analyze their algorithm in the linear
kernel MDP model [Zhou et al. 2020], which is a different model from what is referred to as the
linear MDP model [Jin et al. 2019]. Notably, neither model is a special case of the other. It is
worth observing that the linear kernel MDP model of [Zhou et al., 2020] is characterized by at most \(d\) parameters, where \(d\) is the feature dimensionality, so that model-based learning is feasible; in contrast, the linear MDP model of [Jin et al., 2019] requires a number of parameter that is \(S \cdot d\) and so it is not describable using a small number of parameters (and yet, sample efficient RL is still possible). See [Jin et al., 2019] for further discussion.

2 Setting

A Markov Decision Process (MDP) \(\mathcal{M} = (S, A, P, r, \gamma, s_0)\) is specified by a state space \(S\); an action space \(A\); a transition model \(P : S \times A \to \Delta(S)\) (where \(\Delta(S)\) denotes a distribution over states), a reward function \(r : S \times A \to [0, 1]\), a discount factor \(\gamma \in [0, 1]\), and a starting state \(s_0\). We assume \(A\) is discrete and denote \(A = |A|\). Our results generalize to a starting state distribution \(\mu_0 \in \Delta(S)\) but we use a single starting state \(s_0\) to emphasize the need to perform exploration. A policy \(\pi : S \to \Delta(A)\) specifies a decision-making strategy in which the agent chooses actions based on the current state, i.e., \(a \sim \pi(.|s)\).

The value function \(V^\pi(\cdot, r) : S \to \mathbb{R}\) is defined as the expected discounted sum of future rewards, under reward function \(r\), starting at state \(s\) and executing \(\pi\), i.e.

\[
V^\pi(s; r) := \mathbb{E} \left[ \sum_{t=0}^{\infty} \gamma^t r(s_t, a_t) \mid \pi, s_0 = s \right],
\]

where the expectation is taken with respect to the randomness of the policy and environment \(\mathcal{M}\). The state-action value function \(Q^\pi(\cdot, \cdot; r) : S \times A \to \mathbb{R}\) is defined as

\[
Q^\pi(s, a; r) := \mathbb{E} \left[ \sum_{t=0}^{\infty} \gamma^t r(s_t, a_t) \mid \pi, s_0 = s, a_0 = a \right].
\]

We define the discounted state-action distribution \(d^\pi_s\) of a policy \(\pi\):

\[
d^\pi_s(s, a) := (1 - \gamma) \sum_{t=0}^{\infty} \gamma^t \Pr^\pi(s_t = s, a_t = a | s_0 = s'),
\]

where \(\Pr^\pi(s_t = s, a_t = a | s_0 = s')\) is the probability that \(s_t = s\) and \(a_t = a\), after we execute \(\pi\) from \(t = 0\) onwards starting at state \(s'\) in model \(\mathcal{M}\). Similarly, we define \(d^\pi_{s', a'}(s, a)\) as:

\[
d^\pi_{s', a'}(s, a) := (1 - \gamma) \sum_{t=0}^{\infty} \gamma^t \Pr^\pi(s_t = s, a_t = a | s_0 = s', a_0 = a').
\]

For any state-action distribution \(\nu\), we write \(d^\nu_{s, a} := \sum_{(s', a') \in S \times A} \nu(s', a') d^\nu_{s', a'}(s, a)\). For ease of presentation, we assume that the agent can reset to \(s_0\) at any point in the trajectory.\[\]\[\]

We denote \(d^\nu_s(s) = \sum_a d^\nu_{s, a}(s, a)\).

The goal of the agent is to find a policy \(\pi\) that maximizes the expected value from the starting state \(s_0\), i.e. the optimization problem is: \(\max_\pi V^\pi(s_0)\), where the max is over some policy class.

\[\]

\[\text{This can be replaced with a termination at each step with probability } 1 - \gamma.\]
Algorithm 1 \(d^\pi\) sampler and \(Q^\pi\) estimator

1: \textbf{function} \(d^\pi_\nu\)-SAMPLER
2: \textbf{Input}: \(\nu \in \Delta(S \times A), \pi, r(s, a)\)
3: Sample \(s_0, a_0 \sim \nu\)
4: Execute \(\pi\) from \((s_0, a_0)\); at any step \(t\) with \((s_t, a_t)\), terminate the episode with probability \(1 - \gamma\)
5: \textbf{Return}: \(s_t, a_t\)
6: \textbf{end function}

7: \textbf{function} \(Q^\pi\)-ESTIMATOR
8: \textbf{Input}: current state-action \((s, a)\), reward \(r(s, a)\)
9: Execute \(\pi\) from \((s_0, a_0) = (s, a)\); at step \(t\) with \((s_t, a_t)\), terminate with probability \(1 - \gamma\)
10: \textbf{Return}: \(\hat{Q}^\pi(s, a) = \sum_{i=0}^t r(s_i, a_i)\) where \((s_0, a_0) = (s, a)\)
11: \textbf{end function}

For completeness, we specify a \(d^\pi_\nu\)-sampler and an unbiased estimator of \(Q^\pi(s, a; r)\) in Algorithm 1 which are standard in discounted MDPs. The \(d^\pi_\nu\) sampler samples \((s, a)\) i.i.d from \(d^\pi_\nu\), and the \(Q^\pi\) sampler returns an unbiased estimate of \(Q^\pi(s, a; r)\) for a given triple \((s, a, r)\) by a single roll-out from \((s, a)\).

\textbf{Notation.} When clear from context, we write \(d^\pi(s, a)\) and \(d^\pi(s)\) to denote \(d^\pi_{s_0}(s, a)\) and \(d^\pi_{s_0}(s)\) respectively, where \(s_0\) is the starting state in our MDP. For iterative algorithms which obtain policies at each episode, we let \(V^n, Q^n\) and \(A^n\) denote the corresponding quantities associated with episode \(n\). For a vector \(v\), we denote \(\|v\|_2 = \sqrt{\sum_i v_i^2}, \|v\|_1 = \sum_i |v_i|,\) and \(\|v\|_\infty = \max_i |v_i|\). For a matrix \(V\), we define \(\|V\|_2 = \sup_{\|x\|_2 \leq 1} \|Vx\|_2,\) and \(\det(V)\) as the determinant of \(V\). We use Uniform(A) (in short Unif\(_A\)) to represent a uniform distribution over the set \(A\).

3 \textbf{The Policy Cover-Policy Gradient (PC-PG) Algorithm}

To motivate the algorithm, first consider the original objective function:

\[
\text{Original objective: } \max_{\pi \in \Pi} V^\pi(s_0; r) \quad (1)
\]

where \(r\) is the true cost function. Simply doing policy gradient ascent on this objective function may easily lead to poor stationary points due to lack of coverage (i.e. lack of exploration). For example, if the initial visitation measure \(d^\pi_0\) has poor coverage over the state space (say \(\pi^0\) is a random initial policy), then \(\pi^0\) may already being a stationary point of poor quality (e.g see Lemma 4.3 in Agarwal et al. [2019]).

In such cases, a more desirable objective function is of the form:

\[
\text{A wide coverage objective: } \max_{\pi \in \Pi} \mathbb{E}_{s_0, a_0 \sim \rho_{\text{cov}}} [Q^\pi(s_0, a_0; r)] \quad (2)
\]

where \(\rho_{\text{cov}}\) is some initial state-action distribution which has wider coverage over the state space. As argued in Agarwal et al. [2019] Kakade and Langford [2002], Scherrer and Geist [2014], Scherrer.
Algorithm 2 Policy Cover-Policy Gradient (PC-PG)

1: **Input**: iterations $N$, threshold $\beta$, regularizer $\lambda$
2: Initialize $\pi^0(s|a)$ to be uniform
3: for episode $n = 0, \ldots, N - 1$ do
4: Estimate the covariance of $\pi^n$ as $\hat{\Sigma}^n = \sum_{i=1}^{K} \phi(s_i, a_i)^T \phi(s_i, a_i) / K$ with $\{s_i, a_i\}_{i=1}^{K} \sim d^n$
5: Estimate the covariance of the policy cover as $\hat{\Sigma}_{cov}^n := \sum_{n=0}^{N} \hat{\Sigma}^n + \lambda I$
6: Set the exploration bonus $b^n$ to reward infrequently visited state-action under $\rho_{cov}^n$ (3)
7: Update $\pi^{n+1} = \text{NPG-Update}(\rho_{cov}^n, b^n)$ (Algorithm 3)
8: end for

[2014], wide coverage initial distributions $\rho_{cov}$ are critical to the success of policy optimization methods. However, in the RL setting, our agent can only start from $s_0$.

The idea of our iterative algorithm, PC-PG (Algorithm 2), is to successively improve both the current policy $\pi$ and the coverage distribution $\rho_{cov}$. The algorithm starts with some policy $\pi^0$ (say random), and works in episodes. At episode $n$, we have $n+1$ previous policies $\pi^0, \ldots, \pi^n$. Each of these policies $\pi^i$ induces a distribution $d^i := d^{\pi^i}$ over the state space. Let us consider the average state-action visitation measure over all of these previous policies:

$$\rho_{cov}^n(s, a) = \frac{\sum_{i=0}^{n} d^i(s, a)}{(n + 1)} \quad (3)$$

Intuitively, $\rho_{cov}^n$ reflects the coverage the algorithm has over the state-action space at the start of the $n$-th episode. PC-PG then uses $\rho_{cov}^n$ in the previous objective (2) with two modifications: PC-PG modifies the instantaneous reward function $r$ with a bonus $b^n$ in order to encourage the algorithm to find a policy $\pi^{n+1}$ which covers a novel part of the state-action space. It also modifies the policy class from $\Pi$ to $\Pi_{\text{bonus}}$, where all policies $\pi \in \Pi_{\text{bonus}}$ are constrained to simply take a random rewarding action for those states where the bonus is already large (random exploration is reasonable when the exploration bonus is already large, see Eq 5 in Alg. 3). With this, PC-PG’s objective at the $n$-th episode is:

PC-PG’s objective: $\max_{\pi \in \Pi_{\text{bonus}}} \mathbb{E}_{s_0, a_0 \sim \rho_{cov}^n} [Q^\pi(s_0, a_0; r + b^n)] \quad (4)$

The idea is that PC-PG can effectively optimize over the region where $\rho_{cov}^n$ has coverage. Furthermore, by construction of the bonus, the algorithm is encouraged to escape the current region of coverage to discover novel parts of the state-action space. We now describe the bonus and optimization steps in more detail.

**Reward bonus construction.** At each episode $n$, PC-PG maintains an estimate of feature covariance of the policy cover $\rho_{cov}^n$ (Line 5 of Algorithm 2). Next we use this covariance matrix to identify
Algorithm 3 Natural Policy Gradient (NPG) Update

1: **Input** $\rho_{\text{cov}}^n$, $b^n$, learning rate $\eta$, sample size $M$ for critic fitting, iterations $T$
2: Define $\mathcal{K}^n = \{ s : \forall a \in \mathcal{A}, b^n(s, a) = 0 \}$
3: Initialize policy $\pi^0 : \mathcal{S} \rightarrow \Delta(\mathcal{A})$, such that

$$
\pi^0(\cdot|s) = \begin{cases} 
\text{Uniform}(\mathcal{A}) & s \in \mathcal{K}^n \\
\text{Uniform}([0, \ldots, \mathcal{A}]) & s \notin \mathcal{K}^n.
\end{cases}
$$

4: **for** $t = 0 \rightarrow T - 1$ **do**
5: Draw $M$ i.i.d samples $\{s_i, a_i, \tilde{Q}^\pi(s_i, a_i; r + b^n)\}_{i=1}^M$ with $s_i, a_i \sim \rho_{\text{cov}}^n$ (see Alg 1)
6: **Critic** fit:

$$
\theta^t = \underset{||\theta|| \leq W}{\arg\min} \sum_{i=1}^M \left( \theta \cdot \phi(s_i, a_i) - \left( \tilde{Q}^\pi(s_i, a_i; r + b^n) - b^n(s_i, a_i) \right) \right)^2
$$

7: **Actor** update

$$
\pi^{t+1}(\cdot|s) \propto \pi^t(\cdot|s) \exp \left( \eta \left( b^n(s, \cdot) + \theta^t \cdot \phi(s, \cdot) \right) \mathbf{1}\{s \in \mathcal{K}^n\} \right)
$$

8: **end for**
9: **return** $\pi := \arg\max_{\pi \in \{\pi^0, \ldots, \pi^{T-1}\}} V^\pi(s_0; r + b^n)$

state-action pairs which are adequately covered by $\rho_{\text{cov}}^n$. The goal of the reward bonus is to identify state, action pairs whose features are less explored by $\rho_{\text{cov}}^n$ and incentivize visiting them. The bonus $b^n(s, a)$ defined in Line 6 achieves this. If $\Sigma_{\text{cov}}^n$ has a small eigenvalue along $\phi(s, a)$, then we assign the largest possible reward-to-go (i.e., $1/(1 - \gamma)$) for this $(s, a)$ pair to encourage exploration.\footnote{For an infinite dimensional RKHS, the bonus can be computed in the dual using the kernel trick (e.g., Valko et al. [2013]).}

**Policy Optimization.** With the bonus, we update the policy via $T$ steps of natural policy gradient (Algorithm 3). In the NPG update, we first approximate the value function $Q^\pi(s, a; r + b^n)$ under the policy cover $\rho_{\text{cov}}^n$ (line 6). Specifically, we use linear function approximator to approximate $Q^\pi(s, a; r + b^n) - b^n(s, a)$ via constrained linear regression (line 6), and then approximate $Q^\pi(s, a; r + b^n)$ by adding bonus back:

$$
\tilde{Q}^\pi_{b^n}(s, a) := b^n(s, a) + \theta^t \cdot \phi(s, a),
$$

Note that the error of $\tilde{Q}^\pi_{b^n}(s, a)$ to $Q^\pi(s, a; r + b^n)$ is simply the prediction error of $\theta^t \cdot \phi(s, a)$ to the regression target $Q^\pi(s, a; r + b^n) - b^n$. The purpose of structuring the value function estimation this way, instead of directly approximating $Q^\pi(s, a; r + b^n)$ with a linear function, for instance, is that the regression problem defined in line 6 will have a good linear solution for the special case...
linear MDPs, while we cannot guarantee the same for \( Q_t(s, a; r + b^n) \) due to the non-linearity of the bonus.

We then use the critic \( \bar{Q}_b^n \) for updating policy (Eq. (5)). These are the exponential gradient updates (as in [Kakade 2001], [Agarwal et al. 2019]), but are constrained for \( s \in \mathcal{K}_n \) (see line 2 for the definition of \( \mathcal{K}_n \)). The initialization and the update ensure that \( \pi_t \) chooses actions uniformly from \( \{ a : b^n(s, a) > 0 \} \subseteq A \) at any state \( s \) with \( \{ a : b^n(s, a) > 0 \} \) > 0 (the policy is restricted to act uniformly among positive bonus actions).

**Intuition for tabular setting.** In tabular MDPs (with “one-hot” features for each state-action pair), \((\hat{\Sigma}_n^{\text{cov}})^{-1}\) is a diagonal matrix with entries proportional to \( 1/n_{s,a} \), where \( n_{s,a} \) is the number of times \((s, a)\) is observed in the data collected to form the matrix \( \hat{\Sigma}_n^{\text{cov}} \). Hence the bonus simply rewards infrequently visited state-action pairs, and thus encourages reaching new state-action pairs.

## 4 Theory and Examples

For the analysis, we first state sample complexity results for linear MDPs. Specifically, we focus on analyzing linear MDPs with infinite dimensional features (i.e., the transition and reward live in an RKHS) and show that PC-PG’s sample complexity scales polynomially with respect to the maximum information gain [Srinivas et al., 2010].

We then demonstrate the robustness of PC-PG to model misspecification in two concrete ways. We first provide a result for state aggregation, showing that error incurred is only an average model error from aggregation averaged over the fixed comparator’s abstracted state distribution, as opposed to an \( \ell_\infty \) model error (i.e., the maximum possible model error over the entire state-action space due to state aggregation). We then move to a more general agnostic setting and show that our algorithm is robust to model-misspecification which is measured in a new concept of *transfer error* introduced by [Agarwal et al. 2019] recently. Compared to the Q-NPG analysis from Agarwal et al. [2019], we show that PC-PG eliminates the assumption of having access to a well conditioned initial distribution (recall in our setting agent can only reset to a fixed initial state \( s_0 \)), as our algorithm actively maintains a policy cover.

We also provide other examples where the linear MDP assumption is only valid for a sub-part of the MDP, and the algorithm competes with the best policy on this sub-part, while most prior approaches fail due to the delusional bias of Bellman backups under function approximation and model misspecification [Lu et al., 2018].

### 4.1 Well specified case: Linear MDPs

Let us define linear MDPs first [Jin et al., 2019]. Rather than focusing on finite feature dimension as [Jin et al., 2019] did, we directly work on linear MDPs in a general Reproducing Kernel Hilbert space (RKHS).

**Definition 4.1 (Linear MDP).** Let \( \mathcal{H} \) be a Reproducing Kernel Hilbert Space (RKHS), and define a feature mapping \( \phi : \mathcal{S} \times \mathcal{A} \rightarrow \mathcal{H} \). An MDP \((\mathcal{S}, \mathcal{A}, P, r, \gamma, s_0)\) is called a linear MDP if the reward
function lives in $\mathcal{H}$: $r(s, a) = \langle \theta, \phi(s, a) \rangle_\mathcal{H}$, and the transition operator $P(s'|s, a)$ also lives in $\mathcal{H}$: $P(s'|s, a) = \langle \mu(s'), \phi(s, a) \rangle_\mathcal{H}$ for all $(s, a, s')$. Denote $\mu$ as a matrix whose each row corresponds to $\mu(s)$. We assume the parameter norms\footnote{The norms are induced by the inner product in the Hilbert space $\mathcal{H}$, unless stated otherwise.} are bounded as $\|\theta\| \leq \omega, \|v^T \mu\| \leq \xi$ for all $v \in \mathbb{R}^{|S|}$ with $\|v\|_\infty \leq 1$.

As our feature vector $\phi$ could be infinite dimensional, to measure the sample complexity, we define the maximum information gain of the underlying MDP $\mathcal{M}$. First, denote the covariance matrix of any policy $\pi$ as $\Sigma^\pi = \mathbb{E}_{(s, a) \sim d^n} \left[ \phi(s, a) \phi(s, a)^\top \right]$. We define the maximum information gain below:

**Definition 4.2 (Maximum Information Gain $\mathcal{I}_N(\lambda)$).** We define the maximum information gain as:

$$\mathcal{I}_N(\lambda) := \max_{\{\pi^i\}_{i=1}^{N-1}} \log \det \left( \frac{1}{\lambda} \sum_{i=0}^{N-1} \Sigma^\pi_i + I \right),$$

where $\lambda \in \mathbb{R}^+$.\footnote{The norms are induced by the inner product in the Hilbert space $\mathcal{H}$, unless stated otherwise.}

**Remark 4.1.** This quantity is identical to the maximum information gain in Gaussian Process bandits [Srinivas et al., 2010] from a Bayesian perspective. A related quantity occurs in a more restricted linear MDP model, in Yang and Wang [2019a]. Note that when $\phi(s, a) \in \mathbb{R}^d$, we have that $\log \det \left( \sum_{i=1}^{n} \Sigma^\pi_i + I \right) \leq d \log(nB^2/\lambda + 1)$ assuming $\|\phi(s, a)\|_2 \leq B$, which means that the information gain is always at most $\tilde{O}(d)$. Note that $\mathcal{I}_N(\lambda) \ll d$ if the covariance matrices from a sequence of policies are concentrated in a low-dimensional subspace (e.g., $\phi$ is infinite dimensional while all policies only visits a two dimensional subspace).

For linear MDPs, we leverage the following key observation: we have that $Q^\pi(s, a; r + b^n) - b^n(s, a)$ is linear with respect to $\phi(s, a)$ for any possible bonus function $b^n$ and policy $\pi$, which we prove in [Claim D.1]. The intuition is that the transition dynamics are still linear (as we do not modify the underlying transitions) with respect to $\phi$, so a Bellman backup $r(s, a) + \mathbb{E}_{s' \sim P(s,a)} V^\pi(s'; r + b^n)$ is still linear with respect to $\phi(s, a)$ (recall that linear MDP has the property that a Bellman backup on any function $f(s')$ yields a linear function in features $\phi(s, a)$). This means that we can successfully find a linear critic to approximate $Q^\pi(s, a; r + b^n) - b^n(s, a)$ under $\rho^n_{\text{cov}}$ up to a statistical error, i.e.,

$$\mathbb{E}_{(s,a) \sim \rho^n_{\text{cov}}} \left( \theta^\top \cdot \phi(s, a) - \left( Q^\pi(s, a; r + b^n) - b^n(s, a) \right) \right)^2 = O \left( 1/\sqrt{M} \right),$$

where $M$ is number of samples used for constrained linear regression (line 6). This further implies that $\theta^\top \cdot \phi(s, a) + b^n(s, a)$ approximates $Q^\pi(s, a; r + b^n)$ up to the same statistical error.

With this intuition, the following theorem states the sample complexity of PC-PG under the linear MDP assumption.

**Theorem 4.1 (Sample Complexity of PC-PG for Linear MDPs).** Fix $\epsilon, \delta \in (0, 1)$ and an arbitrary comparator policy $\pi^*$ (not necessarily an optimal policy). Suppose that $\mathcal{M}$ is a linear MDP
There exists a setting of the parameters such that PC-PG uses a number of samples at most \( \text{poly}\left( \frac{1}{1-\gamma}, \log(A), \frac{1}{\epsilon}, I_N(1), \omega, \xi, \ln \left( \frac{1}{\delta} \right) \right) \) and, with probability greater than \( 1 - \delta \), returns a policy \( \tilde{\pi} \) such that:

\[
V^\tilde{\pi}(s_0) \geq V^{\pi^*}(s_0) - \epsilon.
\]

A few remarks are in order:

**Remark 4.2.** For tabular MDPs, as \( \phi \) is a \(|\mathcal{S}|\cdot|\mathcal{A}|\) indicator vector, the theorem above immediately extends to tabular MDPs with \( I_N(1) \) being replaced by \(|\mathcal{S}|\cdot|\mathcal{A}| \log(N+1)\).

**Remark 4.3.** In contrast with LSVI-UCB [Jin et al., 2019], PC-PG works for infinite dimensional \( \phi \) with a polynomial dependency on the maximum information gain \( I_N(1) \). To the best of our knowledge, this is the first efficient model-free on-policy policy gradient result for linear MDPs and also the first infinite dimensional result for the linear MDP model proposed by Jin et al. [2019].

Instead of proving [Theorem 4.1] directly, we will state and prove a general theorem of PC-PG for general MDPs with model-misspecification measured in a new concept transfer error (Assumption 4.1) introduced by Agarwal et al. [2019] in Section 4.3. Theorem 4.1 can be understood as a corollary of a more general agnostic theorem (Theorem 4.3). Detailed proof of [Theorem 4.1] is included in [Appendix D].

### 4.2 State-Aggregation under Model Misspecification

Consider a simple model-misspecified setting where the model error is introduced due to state action aggregation. Suppose we have an aggregation function \( \phi : \mathcal{S} \times \mathcal{A} \to \mathcal{Z} \), where \( \mathcal{Z} \) is a finite categorical set, the “state abstractions”, which we typically think of as being much smaller than the (possibly infinite) number of state-action pairs. Intuitively, we aggregate state-action pairs that have similar transitions and rewards to an abstracted state \( z \). This aggregation introduces model-misspecification, defined below.

**Definition 4.3 (State-Action Aggregation Model-Misspecification).** We define model-misspecification \( \epsilon_{\text{misspec}}(z) \) for any \( z \in \mathcal{Z} \) as

\[
\epsilon_{\text{misspec}}(z) := \max_{(s,a),(s',a') \text{ s.t. } \phi(s,a)=\phi(s',a')=z} \left\{ \| P(\cdot|s,a) - P(\cdot|s',a') \|_1, |r(s,a) - r(s',a')| \right\}.
\]

The model-misspecification measures the maximum possible disagreement in terms of transition and rewards of two state-action pairs which are mapped to the same abstracted state.

We now argue that PC-PG provides a unique and stronger guarantee in the case of error in our state aggregation. The folklore result is that with the definition \( \| \epsilon_{\text{misspec}} \|_\infty = \max_{z \in \mathcal{Z}} \epsilon_{\text{misspec}}(z) \), algorithms such as UCB and Q-learning succeed with an additional additive error of \( \| \epsilon_{\text{misspec}} \|_\infty / (1 - \gamma)^2 \), and will have sample complexity guarantees that are polynomial in only \(|\mathcal{Z}|\). Interestingly, see
Li [2009], Dong et al. [2019] for conditions which are limited to only $Q^*$, but which are still global in nature. The following theorem shows that PC-PG only requires a more local guarantee where our aggregation needs to be only good under the distribution of abstracted states where an optimal policy tends to visit.

**Theorem 4.2 (Misspecified, State-Aggregation Bound).** Fix $\epsilon, \delta \in (0, 1)$. Let $\pi^*$ be an arbitrary comparator policy. There exists a setting of the parameters such that PC-PG (Algorithm 2) uses a total number of samples at most \( \text{poly} \left( |Z|, \log(A), \frac{1}{1-\gamma}, \frac{1}{\epsilon}, \ln \left( \frac{1}{\delta} \right) \right) \) and, with probability greater than $1 - \delta$, returns a policy $\hat{\pi}$ such that,

$$V^{\hat{\pi}}(s_0) \geq V^{\pi^*}(s_0) - \epsilon - \frac{2\mathbb{E}_{s \sim d^{\pi^*}} \max_a [\epsilon_{\text{misspec}}(\phi(s, a))]}{(1 - \gamma)^3}.$$

Here, it could be that $\mathbb{E}_{s \sim d^{\pi^*}} \max_a [\epsilon_{\text{misspec}}(\phi(s, a))] \ll \|\epsilon_{\text{misspec}}\|_\infty$ due to that our error notion is an average case one under the comparator. We refer readers to Appendix E for detailed proof of the above theorem which can also be regarded as a corollary of a more general agnostic theorem (Theorem 4.3) that we present in the next section. Note that here we pay an additional $1/(1 - \gamma)$ factor in the approximation error due to the fact that after reward bonus, we have $r(s, a) + b^n(s, a) \in [0, 1/(1 - \gamma)]$.\(^4\)

One point worth reflecting on is how few guarantees there are in the more general RL setting (beyond dynamic programming), which address model-misspecification in a manner that goes beyond global $\ell_\infty$ bounds. Our conjecture is that this is not merely an analysis issue but an algorithmic one, where incremental algorithms such as PC-PG are required for strong misspecified algorithmic guarantees. We return to this point in Section 4.4 with an example showing why this might be the case.

### 4.3 Agnostic Guarantees with Bounded Transfer Error

We now consider a general MDP in this section, where we do not assume the linear MDP modeling assumptions hold. As $Q - b^n$ may not be linear with respect to the given feature $\phi$, we need to consider model misspecification due to the linear function approximation with features $\phi$. We use the new concept of transfer error from Agarwal et al. [2019] below. We use the shorthand notation:

$$Q^{t,b^n}_\pi(s, a) = Q^{t^\pi}(s, a; r + b^n)$$

below. We capture model misspecification using the following assumption.

**Assumption 4.1 (Bounded Transfer Error).** With respect to a target function $f : S \times A \rightarrow \mathbb{R}$, define the critic loss function $L(\theta; d, f)$ with $d \in \Delta(S \times A)$ as:

$$L(\theta; d, f) := \mathbb{E}_{(s, a) \sim d} (\theta \cdot \phi(s, a) - f)^2,$$

\(^4\)We note that instead of using reward bonus, we could construct absorbing MDPs to make rewards scale $[0, 1]$. This way we will pay $1/(1 - \gamma)^2$ in the approximation error instead.
which is the square loss of using the critic $\theta \cdot \phi$ to predict a given target function $f$, under distribution $d$. Consider an arbitrary comparator policy $\pi^*$ (not necessarily an optimal policy) and denote the state-action distribution $d^*(s, a) := d^\pi(s) \circ \text{Unif}_A(a)$. For all episode $n$ and all iteration $t$ inside episode $n$, define:

$$\theta^t_\ast \in \arg\min_{\|\theta\| \leq W} L(\theta; \rho_{\text{cov}}^n, Q^t_{\text{b}n} - b^n)$$

Then we assume that (when running Algorithm 2), $\theta^t_\ast$ has a bounded prediction error when transferred to $d^*$ from $\rho_{\text{cov}}^n$; more formally:

$$L(\theta^t_\ast; d^*, Q^t_{\text{b}n} - b^n) \leq \epsilon_{\text{bias}}$$

Note that the transfer error $\epsilon_{\text{bias}}$ measures the prediction error, at episode $n$ and iteration $t$, of a best on-policy fit $\overline{Q}^t_{\text{b}n}(s, a) := b^n(s, a) + \theta^t_\ast \cdot \phi(s, a)$ measured under a fixed distribution $d^*$ from the fixed comparator (note $d^*$ is different from the training distribution $\rho_{\text{cov}}^n$ hence the name transfer).

This assumption first appears in the recent work of Agarwal et al. [2019] in order to analyze policy optimization methods under linear function approximation. As our subsequent examples illustrate in the following section, this is a milder notion of model misspecification than $\ell_\infty$-variants more prevalent in the literature, as it is an average-case quantity which can be significantly smaller in favorable cases. We also refer the reader to Agarwal et al. [2019] for further discussion on this assumption.

With the above assumption on the transfer error, the next theorem states an agnostic result for the sample complexity of PC-PG:

**Theorem 4.3 (Agnostic Guarantee of PC-PG).** Fix $\epsilon, \delta \in (0, 1)$ and consider an arbitrary comparator policy $\pi^*$ (not necessarily an optimal policy). Assume Assumption 4.1 holds. There exists a setting of the parameters $(\beta, \lambda, K, M, \eta, N, T)$ such that PC-PG uses a number of samples at most

$$\text{poly}\left(\frac{1}{1-\gamma}, \log(A), \frac{1}{\epsilon}, \mathcal{I}_N(1), W, \ln\left(\frac{1}{\delta}\right)\right)$$

and, with probability greater than $1 - \delta$, returns a policy $\pi^*$ such that:

$$V_{\pi^*}^N(s_0) \geq V_{\pi^*}^N(s_0) - \epsilon - \frac{\sqrt{2A\epsilon_{\text{bias}}}}{1-\gamma}.$$
target $Q^π(\cdot, \cdot; r + b^n) - b^n$ function is always a linear function with respect to the features, one can easily show that $e_{bias} = 0$ (which we show in Appendix D), as one can pick the best on-policy fit $θ^*_t$ to be the exact linear representation of $Q^π(s, a; r + b^n) - b^n(s, a)$. Further, in the state-aggregation example, we can show that $e_{bias}$ is upper bounded by the expected model-misspecification with respect to the comparator policy’s distribution (Appendix E).

A few remarks are in order to illustrate how the notion of transfer error compares to prior work.

**Remark 4.4** (Comparison with concentrability assumptions [Kakade and Langford, 2002, Scherrer, 2014, Agarwal et al., 2019]). In the theory for policy gradient methods without explicit exploration, a standard device to obtain global optimality guarantees for the learned policies is through the use of some exploratory distribution $ν_0$ over initial states and actions in the optimization algorithm. Given such a distribution, a key quantity that has been used in prior analysis is the maximal density ratio to a comparator policy’s state distribution [Kakade and Langford, 2002, Scherrer, 2014]: $\max_{s \in S} d^*(s) ν_0(s)$, where we use $d^*(s)$ to refer to the probability of state $s$ under the comparator $π^*$. It is easily seen that if PC-PG is run with a similar exploratory initial distribution, then the transfer error is always bounded as well:

$$e_{bias} \leq \left\langle d^* \right\rangle_{ν_0} L(θ^*_t; ν_0, Q^t_{b^n} - b^n).$$

In this work, we do not assume access to a such an exploratory measure (with coverage); our goal is finding a policy with only access to rollouts from $s_0$. This makes this concetrability-style analysis inapplicable in general as the starting measure $ν_0$ for the algorithm is potentially the delta measure over the initial state $s_0$, which can induce an arbitrarily large density ratio. In contrast, the transfer error is always bounded and is zero in well-specified cases such as tabular MDPs and linear MDPs which we show in Appendix D.

**Remark 4.5** (Comparison with the NPG guarantees in Agarwal et al. [2019]). The bounded transfer error assumption (Assumption 4.1) stated here is developed in the recent work of Agarwal et al. [2019]. Their work focuses on understanding the global convergence properties of policy gradient methods, including the specific NPG algorithm used here; it does not consider the design of exploration strategies. Consequently, Assumption 4.1 alone is not sufficient to guarantee convergence in their setting; Agarwal et al. [2019] make an additional assumption on a relative condition number between the covariance matrices of the comparator distribution $d^*$ and the initial exploratory distribution $ν_0$:

$$κ = \sup_{w ∈ \mathbb{R}^d} \frac{w^T Σ w}{w^T Σ w}, \quad \text{where} \quad Σ = \mathbb{E}_{s,a∼ν}[φ(s, a)φ(s, a)^T].$$

Note that we consider a finite $d$-dimensional feature space for this discussion to be consistent with the prior results. Under the assumption that $κ < ∞$, Agarwal et al. [2019] provide a bound on the iteration complexity of NPG-style updates with an explicit dependence on $\sqrt{κ}$. Related (stronger) assumptions on the relative condition numbers for all possible policies or the initial distribution $ν_0$ also appear in the recent works [Abbasi-Yadkori et al., 2019a] and [Abbasi-Yadkori et al., 2019b] respectively (the latter work still assumes access to an exploratory initial policy). Our result does.
Figure 1: The binary tree example. Note that here $s_0$ and $s_1$ have features only span in the first three standard basis, and the features for states inside the binary tree (dashed) contains features in the null space of the first three standard bases. Note that the features inside the binary tree could be arbitrary complicated. Unless the feature dimension scales $\exp(H)$ with $H$ being the depth of the tree, we cannot represent this problem in linear MDPs. The on-policy nature of PC-PG ensures that it succeeds in this example. Due to the complex features and large $\ell_\infty$ model-misspecification inside the binary tree, Bellman-backup based approaches (e.g., Q-learning) cannot guarantee successes.

not have any such dependence. In contrast, the distribution $\rho_{\text{cov}}^n$ designed by the algorithm, serves as the initial distribution at episode $n+1$, and the reward bonus explicitly encourages our algorithm to visit places where the relative condition number with the current distribution $\rho_{\text{cov}}^n$ is large.

4.4 Robustness to “Delusional Bias” with Partially Well-specified Models

In this section, we provide an additional example of model misspecification where we show that PC-PG succeeds while Bellman backup based algorithms do not. The basic spirit of the example is that if our modeling assumption holds for a sub-part of the MDP, then PC-PG can compete with the best policy that only visits states in this sub-part with some additional assumptions. In contrast, prior model-based and $Q$-learning based approaches heavily rely on the modeling assumptions being globally correct, and bootstrapping-based methods fail in particular due to their susceptibility to the delusional bias problem [Lu et al., 2018].

We emphasize that this constructed MDP and class of features have the following properties:

- It is not a linear MDP; we would need the dimension to be exponential in the depth $H$, i.e. $d = \Omega(2^H)$, in order to even approximate the MDP as a linear MDP.

- We have no reason to believe that value based methods (that rely on Bellman backups, e.g., Q learning) or model based algorithms will provably succeed for this example (or simple variants of it).
• Our example will have large worst case function approximation error, i.e. the $\ell_\infty$ error in approximating $Q^*$ will be (arbitrarily) large.

• The example can be easily modified so that the concentrability coefficient (and the distribution mismatch coefficient) of the starting distribution (or a random initial policy) will be $\Omega(2^H)$.

Furthermore, we will see that PC-PG succeeds on this example, provably.

We describe the construction below (see Figure 1 for an example). There are two actions, denoted by $L$ and $R$. At initial state $s_0$, we have $P(s_1|s_0, L) = 1; P(s_1|s_1, a) = 1$ for any $a \in \{L, R\}$. We set the reward of taking the left action at $s_0$ to be $1/2$, i.e. $r(s_0, L) = 1/2$. This implies that there exists a policy which is guaranteed to obtain at least reward $1/2$. When taking action $a = R$ at $s_0$, we deterministically transition into a depth-$H$ completely balanced binary tree. We can further constrain the MDP so that the optimal value is $1/2$ (coming from left most branch), though, as we see later, this is not needed.

The feature construction of $\phi \in \mathbb{R}^d$ is as follows: For $s_0, L$, we have $\phi(s_0, L) = e_1$ and $\phi(s_0, R) = e_2$, and $\phi(s_1, a) = e_3$ for any $a \in \{L, R\}$, where $e_1, e_2, e_3$ are the standard basis vectors. For all other states $s \notin \{s_0, s_1\}$, we have that $\phi(s, a)$ is constrained to be orthogonal to $e_1, e_2,$ and $e_3$, but otherwise arbitrary. In other words, $\phi(s, a)$ has the first three coordinates equal to zero for any $s \notin \{s_0, s_1\}$ but can otherwise be pathological.

The intuition behind this construction is that the features $\phi$ are allowed to be arbitrary complicated for states inside the depth-$H$ binary tree, but are uncoupled with the features on the left path. This implies that both PC-PG and any other algorithm do not have access to a good global function approximator.

Furthermore, as discussed in the following remark, these features do not provide a good approximation of the true dynamics as a linear MDP.

Remark 4.6. (Linear-MDP approximation failure). As the MDP is deterministic, we would need dimension $d = \Omega(2^H)$ in order to approximate the MDP as a linear MDP (in the sense required in Jin et al. [2019]). This is due to that the rank of the transition matrix is $O(2^H)$.

However the on-policy nature of PC-PG ensures that there always exists a best linear predictor that can predict $Q^*$ well under the optimal trajectory (the left most path) due to the fact that the features on $s_0$ and $s_1$ are decoupled from the features in the rest of the states inside the binary tree. Thus it means that the transfer error is always zero. This is formally stated in the following lemma.

Corollary 4.1 (Corollary of Theorem 4.3). PC-PG is guaranteed to find a policy with value greater than $1/2 - \epsilon$ with probability greater than $1 - \delta$, using a number of samples that is $O(\text{poly}(H, d, 1/\epsilon, \log(1/\delta)))$. This is due to the transfer error being zero.

We provide a proof of the corollary in Appendix F.

Intuition for the success of PC-PG. Since the corresponding features of the binary subtree have no guarantees in the worst-case, PC-PG may not successfully find the best global policy in general. However, it does succeed in finding a policy competitive with the best policy that remains in the
favorable sub-part of the MDP satisfying the modeling assumptions (e.g., the leftmost trajectory in Figure 1). We do note that the feature orthogonality is important (at least for a provably guarantee), otherwise the errors in fitting value functions on the binary subtree can damage our value estimates on the favorable parts as well; this behavior effect may be less mild in practice.

Delusional bias and challenges with Bellman backup (and Model-based) approaches. While we do not explicitly construct algorithm dependent lower bounds in our construction, we now discuss why obtaining guarantees similar to ours with Bellman backup-based (or even model-based) approaches may be challenging with the current approaches in the literature. We are not assuming any guarantees about the quality of the features in the right subtree (beyond the aforementioned orthogonality). Specifically, for Bellman backup-based approaches, the following two observations (similar to those stressed in Lu et al. [2018]), when taken together, suggest difficulties for algorithms which enforce consistency by assuming the Markov property holds:

- (Bellman Consistency) The algorithm does value based backups, with the property that it does an exact backup if this is possible. Note that due to our construction, such algorithms will seek to do an exact backup for \( Q(s_0, R) \), where they estimate \( Q(s_0, R) \) to be their value estimate on the right subtree. This is due to that the feature \( \phi(s_0, R) \) is orthogonal to all other features, so a 0 error, Bellman backup is possible, without altering estimation in any other part of the tree.

- (One Sided Errors) Suppose the true value of the subtree is less than \( 1/2 - \Delta \), and suppose that there exists a set of features where the algorithm approximates the value of the subtree to be larger than \( 1/2 \). Current algorithms are not guaranteed to return values with one side error; with an arbitrary featurization, it is not evident why such a property would hold.

More generally, what is interesting about the state aggregation featurization is that it permits us to run any tabular RL learning algorithm. Here, it is not evident that any other current tabular RL algorithm, including model-based approaches, can achieve guarantees similar to our average-case guarantees, due to their strong reliance on how they use the Markov property. In this sense, our work provides a unique guarantee with respect to model misspecification in the RL setting.

Failure of concentrability-based approaches Some of the prior results on policy optimization algorithms, starting from the Conservative Policy Iteration algorithm [Kakade and Langford 2002] and further studied in a series of subsequent papers [Scherrer 2014, Geist et al. 2019, Agarwal et al. 2019] provide the strongest guarantees in settings without exploration, but considering function approximation. As remarked in Section 4.1, most works in this literature make assumptions on the maximal density ratio between the initial state distribution and comparator policy to be bounded. In the MDP of Figure 1, this quantity seems fine since the ratio is at most \( H \) for the comparator policy that goes on the left path (by acting randomly in the initial state). However, we can easily change the left path into a fully balanced binary tree as well, with \( O(H) \) additional features that let us realize the values on the leftmost path (where the comparator goes) exactly, while keeping all the other features orthogonal to these. It is unclear how to design an initial distribution to have a good
concentrability coefficient, but PC-PG still competes with the comparator following the leftmost path since it can realize the value functions on that path exactly and the remaining parts of the MDP do not interfere with this estimation.

5 Experiments

We provide experiments illustrating PC-PG’s performance on problems requiring exploration, and focus on showing the algorithm’s flexibility to leverage existing policy gradient algorithms with neural networks (e.g., PPO \cite{Schulman2017}). Specifically, we show that for challenging exploration tasks, our algorithm combined with PPO significantly outperforms both vanilla PPO as well as PPO augmented with the popular RND exploration bonus \cite{Burda2019}.

Specifically, we aim to show the following two properties of PC-PG:

1. PC-PG can build a policy cover that explores the state space widely; hence PC-PG is able to find near optimal policies even in tasks that have obvious local minimas and sparse rewards.

2. the policy cover in PC-PG avoids catastrophic forgetting issue one can experience in policy gradient methods due to the possibility that the policy can become deterministic quickly.

For all experiments, we use policies parameterized by fully-connected or convolutional neural networks. We use a kernel $\phi(s, a)$ to compute bonus as $b(s, a) = \phi(s, a)^\top \hat{\Sigma}_{\text{cov}}^{-1} \phi(s, a)$, where $\hat{\Sigma}_{\text{cov}}$ is the empirical covariance matrix of the policy cover. In order to prune any redundant policies from the cover, we use a rebalancing scheme to select a policy cover which induces maximal coverage over the state space. This is done by finding weights $\alpha^{(n)} = (\alpha_1^{(n)}, ..., \alpha_n^{(n)})$ on the simplex at each episode which solve the optimization problem: $\alpha^{(n)} = \operatorname{argmax}_\alpha \log \det \left[ \sum_{i=1}^n \alpha_i \hat{\Sigma}_i \right]$ where $\hat{\Sigma}_i$ is the empirical covariance matrix of $\pi_i$. Details of the implemented algorithm, network architectures and kernels can be found in Appendix \[H\].

5.1 Bidirectional Diabolical Combination Lock

We first provide experiments on an exploration problem designed to be particularly difficult: the Bidirectional Diabolical Combination Lock (a harder version of the problem in \cite{Misra2020}).

| Algorithm   | Horizon |
|-------------|---------|
| PPO         | 2.0     |
| PPO+RND    | 0.75   |
| PC-PG       | 1.0     |
see Figure [2]. In this problem, the agent starts at an initial state \( s_0 \) (left most state), and based on its first action, transitions to one of two combination locks of length \( H \). Each combination lock consists of a chain of length \( H \), at the end of which are two states with high reward. At each level in the chain, 9 out of 10 actions lead the agent to a dead state (black) from which it cannot recover and lead to zero reward. The problem is challenging for exploration for several reasons: (1) *Sparse positive rewards*: Uniform exploration has a \( 10^{-H} \) chance of reaching a high reward state; (2) *Dense antishaped rewards*: The agent receives a reward of \( -1/H \) for transitioning to a good state and 0 to a dead state. A locally optimal policy is to transition to a dead state quickly; (3) *Forgetting*: At the end of one of the locks, the agent receives a maximal reward of +5, and at the end of the other lock it receives a reward of +2. Since there is no indication which lock has the optimal reward, if the agent does not explore to the end of both locks it will only have a 50% chance of encountering the globally optimal reward. If it makes it to the end of one lock, it must remember to still visit the other one.

![RND trace during training](image1)

![PC-PG final trace](image2)

Figure 3: (a) shows the state visitation frequencies (brighter color depicts higher visitation frequency) when the RND bonus [Burda et al., 2019] is applied to a policy gradient method throughout training on the above problem. 'Ep' denotes epoch number showing the progress during a single training run. Although the agent manages to explore to the end of one chain (chain 2 in this case), its policy quickly becomes deterministic and it “forgets” to explore the remaining chain, missing the optimal reward. RND obtains the optimal reward on roughly half of the initial seeds. (b) panel shows the traces of policies in the policy cover of PC-PG. Together the policy cover provides a near uniform coverage over both chains.

For both the policy network input and the kernel we used a binary vector encoding the current lock, state and time step as one-hot components. We compared to two other methods: a PPO agent, and a PPO agent with a RND exploration bonus, all of which used the same representation as input.
Performance for the different methods is shown in Figure 2 (left). The PPO agent succeeds for the shortest problem of horizon $H = 2$, but fails for longer horizons due to the antishaped reward leading it to the dead states. The PPO+RND agent succeeds roughly 50% of the time: due to its exploration bonus, it avoids the local minimum and explores to the end of one of the chains. However, as shown in Figure 3(a), the agent’s policy quickly becomes deterministic and the agent forgets to go back and explore the other chain after it has reached the reward at the end of the first. PC-PG succeeds over all seeds and horizon lengths. We found that the policy cover provides near uniform coverage over both chains. In Figure 3(b) we demonstrate the traces of some individual policies in the policy cover and the trace of the policy cover itself as a whole.

5.2 Reward-free Exploration in Mazes

We next evaluated PC-PG in a reward-free exploration setting using maze environments adapted from [Oh et al., 2017]. At each step, the agent’s observation consists of an RGB-image of the maze with the red channel representing the walls and the green channel representing the location of the agent (an example is shown in Figure 4).

We compare PC-PG, PPO and PPO+RND in the reward-free setting where the agent receives a constant environment reward of 0 (note that PPO receives zero gradient; PC-PG and PPO+RND learn from their reward bonus). Figure 5 (left) shows the percentage of locations in the maze visited by each of the agents over the course of 10 million steps. The proportion of states visited by the PPO agent stays relatively constant, while the PPO+RND agent is able to explore to some degree. PC-PG quickly visits a significantly higher proportion of locations than the other two methods. Visualizations of traces from different policies in the policy cover can be seen in Figure 4 where we observe the diverse coverage of the policies in the policy cover.

5.3 Continuous Control

We further evaluated PC-PG on a continuous control task which requires exploration: continuous control MountainCar from OpenAI Gym [Brockman et al., 2016]. Note here actions are continuous in $[-1, 1]$ and incur a small negative reward. Since the agent only receives a large reward (+100) if it reaches the top of the hill, a locally optimal policy is to do nothing and avoid the action cost (e.g., PPO never escapes this local optimality in our experiments). Results for PPO, PPO+RND and PC-PG are shown in Figure 5 (right). The PPO agent quickly learns the locally optimal policy of
Figure 5: Results for maze (left) & control (right). Solid line is mean and shaded region is standard deviation over 5 seeds.

Figure 6: State visitations of different policies in PC-PG’s policy cover on MountainCar.

doing nothing. The PPO+RND agent exhibits wide variability across seeds: some seeds solve the task while others not. The PC-PG agent consistently discovers a good policy across all seeds. In Figure 6, we show the traces of policies in the policy cover constructed by PC-PG.

6 Discussion

This work proposes a new policy gradient algorithm for balancing the exploration-exploitation tradeoff in RL, which enjoys provable sample efficiency guarantees in the linear and kernelized settings. Our experiments provide evidence that the algorithm can be combined with neural policy optimization methods and be effective in practice. An interesting direction for future work would be to combine our approach with unsupervised feature learning methods such as autoencoders Jarrett et al. [2009], Vincent et al. [2010] or noise-contrastive estimation Gutmann and Hyvärinen [2010].
van den Oord et al. [2018] in rich observation settings to learn a good feature representation.

Acknowledgement

The authors would like to thank Andrea Zanette and Ching-An Cheng for carefully reviewing the proofs, and Akshay Krishnamurthy for helpful discussions.

References

Yasin Abbasi-Yadkori, Peter Bartlett, Kush Bhatia, Nevena Lazic, Csaba Szepesvari, and Gellért Weisz. Politex: Regret bounds for policy iteration using expert prediction. In International Conference on Machine Learning, pages 3692–3702, 2019a.

Yasin Abbasi-Yadkori, Nevena Lazic, Csaba Szepesvari, and Gellert Weisz. Exploration-enhanced politex. arXiv preprint arXiv:1908.10479, 2019b.

Alekh Agarwal, Sham M. Kakade, Jason D. Lee, and Gaurav Mahajan. On the theory of policy gradient methods: Optimality, approximation, and distribution shift, 2019.

Shipra Agrawal and Randy Jia. Optimistic posterior sampling for reinforcement learning: worst-case regret bounds. In Advances in Neural Information Processing Systems, pages 1184–1194, 2017.

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(1):89–129, 2008.

Alex Ayoub, Zeyu Jia, Csaba Szepesvári, Mengdi Wang, and Lin F. Yang. Model-based reinforcement learning with value-targeted regression. abs/2006.01107, 2020. URL https://arxiv.org/abs/2006.01107.

Mohammad Gheshlaghi Azar, Vicenc Gómez, and Hilbert J. Kappen. Dynamic policy programming. J. Mach. Learn. Res., 13(1), November 2012. ISSN 1532-4435.

Mohammad Gheshlaghi Azar, Ian Osband, and Rémi Munos. Minimax regret bounds for reinforcement learning. In Proceedings of the 34th International Conference on Machine Learning-Volume 70, pages 263–272. JMLR. org, 2017.

J. A. Bagnell, Sham M Kakade, Jeff G. Schneider, and Andrew Y. Ng. Policy search by dynamic programming. In S. Thrun, L. K. Saul, and B. Schölkopf, editors, Advances in Neural Information Processing Systems 16, pages 831–838. MIT Press, 2004.

Marc Bellemare, Sriram Srinivasan, Georg Ostrovski, Tom Schaul, David Saxton, and Remi Munos. Unifying count-based exploration and intrinsic motivation. In D. D. Lee, M. Sugiyama, U. V. Luxburg, I. Guyon, and R. Garnett, editors, Advances in Neural Information Processing Systems 29, pages 1471–1479. Curran Associates, Inc., 2016.
Jalaj Bhandari and Daniel Russo. Global optimality guarantees for policy gradient methods. *CoRR*, abs/1906.01786, 2019. URL [http://arxiv.org/abs/1906.01786](http://arxiv.org/abs/1906.01786).

Ronen I Brafman and Moshe Tennenholtz. R-max-a general polynomial time algorithm for near-optimal reinforcement learning. *Journal of Machine Learning Research*, 3(Oct):213–231, 2002.

Ronen I Brafman and Moshe Tennenholtz. R-max-a general polynomial time algorithm for near-optimal reinforcement learning. *The Journal of Machine Learning Research*, 3:213–231, 2003.

Greg Brockman, Vicki Cheung, Ludwig Pettersson, Jonas Schneider, John Schulman, Jie Tang, and Wojciech Zaremba. OpenAI gym. *arXiv preprint arXiv:1606.01540*, 2016.

Yuri Burda, Harrison Edwards, Amos Storkey, and Oleg Klimov. Exploration by random network distillation. In *International Conference on Learning Representations*, 2019. URL [https://openreview.net/forum?id=H1lJJnR5Ym](https://openreview.net/forum?id=H1lJJnR5Ym).

Qi Cai, Zhuoran Yang, Chi Jin, and Zhaoran Wang. Provably efficient exploration in policy optimization. *arXiv preprint arXiv:1912.05830*, 2020.

Jinglin Chen and Nan Jiang. Information-theoretic considerations in batch reinforcement learning. In *International Conference on Machine Learning*, pages 1042–1051, 2019.

Varsha Dani, Thomas P Hayes, and Sham M Kakade. Stochastic linear optimization under bandit feedback. In *COLT*, pages 355–366, 2008.

Christoph Dann and Emma Brunskill. Sample complexity of episodic fixed-horizon reinforcement learning. In *Advances in Neural Information Processing Systems*, pages 2818–2826, 2015.

Christoph Dann, Nan Jiang, Akshay Krishnamurthy, Alekh Agarwal, John Langford, and Robert E Schapire. On polynomial time PAC reinforcement learning with rich observations. *arXiv preprint arXiv:1803.00606*, 2018.

Shi Dong, Benjamin Van Roy, and Zhengyuan Zhou. Provably efficient reinforcement learning with aggregated states. *arXiv preprint arXiv:1912.06366*, 2019.

Simon S Du, Yuping Luo, Ruosong Wang, and Hanrui Zhang. Provably efficient q-learning with function approximation via distribution shift error checking oracle. *arXiv preprint arXiv:1906.06321*, 2019.

Yonathan Efroni, Lior Shani, Aviv Rosenberg, and Shie Mannor. Optimistic policy optimization with bandit feedback. *arXiv preprint arXiv:2002.08243*, 2020.

Eyal Even-Dar, Sham M Kakade, and Yishay Mansour. Online Markov decision processes. *Mathematics of Operations Research*, 34(3):726–736, 2009.

Maryam Fazel, Rong Ge, Sham M Kakade, and Mehran Mesbahi. Global convergence of policy gradient methods for the linear quadratic regulator. *arXiv preprint arXiv:1801.05039*, 2018.
Matthieu Geist, Bruno Scherrer, and Olivier Pietquin. A theory of regularized markov decision processes. *arXiv preprint arXiv:1901.11275*, 2019.

Michael Gutmann and Aapo Hyvärinen. Noise-contrastive estimation: A new estimation principle for unnormalized statistical models. In Yee Whye Teh and Mike Titterington, editors, *Proceedings of the Thirteenth International Conference on Artificial Intelligence and Statistics*, volume 9 of *Proceedings of Machine Learning Research*, pages 297–304, Chia Laguna Resort, Sardinia, Italy, 13–15 May 2010. PMLR. URL [http://proceedings.mlr.press/v9/gutmann10a.html](http://proceedings.mlr.press/v9/gutmann10a.html).

Mikael Henaff. Explicit explore-exploit algorithms in continuous state spaces. In *Advances in Neural Information Processing Systems*, pages 9377–9387, 2019.

Thomas Jaksch, Ronald Ortner, and Peter Auer. Near-optimal regret bounds for reinforcement learning. *Journal of Machine Learning Research*, 11(Apr):1563–1600, 2010.

Kevin Jarrett, Koray Kavukcuoglu, Marc’Aurelio Ranzato, and Yann LeCun. What is the best multi-stage architecture for object recognition? In *ICCV*, pages 2146–2153. IEEE Computer Society, 2009. ISBN 978-1-4244-4419-9. URL [http://dblp.uni-trier.de/db/conf/iccv/iccv2009.html#JarrettKRL09](http://dblp.uni-trier.de/db/conf/iccv/iccv2009.html#JarrettKRL09).

Nan Jiang, Akshay Krishnamurthy, Alekh Agarwal, John Langford, and Robert E. Schapire. Contextual decision processes with low Bellman rank are PAC-learnable. In *International Conference on Machine Learning*, 2017.

Chi Jin, Zeyuan Allen-Zhu, Sebastien Bubeck, and Michael I Jordan. Is q-learning provably efficient? In *Advances in Neural Information Processing Systems*, pages 4863–4873, 2018.

Chi Jin, Zhuoran Yang, Zhaoran Wang, and Michael I Jordan. Provably efficient reinforcement learning with linear function approximation. *arXiv preprint arXiv:1907.05388*, 2019.

S. Kakade. A natural policy gradient. In *NIPS*, 2001.

Sham Kakade and John Langford. Approximately Optimal Approximate Reinforcement Learning. In *Proceedings of the 19th International Conference on Machine Learning*, volume 2, pages 267–274, 2002.

Sham Machandranath Kakade. *On the sample complexity of reinforcement learning*. PhD thesis, University of College London, 2003.

Michael Kearns and Satinder Singh. Near-optimal reinforcement learning in polynomial time. *Machine Learning*, 49(2-3):209–232, 2002.

Vijay R Konda and John N Tsitsiklis. Actor-critic algorithms. In *Advances in neural information processing systems*, pages 1008–1014, 2000.
Tor Lattimore and Marcus Hutter. Near-optimal pac bounds for discounted mdp's. volume 558, pages 125–143. Elsevier, 2014a.

Tor Lattimore and Marcus Hutter. Near-optimal pac bounds for discounted mdp's. *Theoretical Computer Science*, 558:125–143, 2014b.

Lihong Li. *A unifying framework for computational reinforcement learning theory*. PhD thesis, Rutgers, The State University of New Jersey, 2009.

Lihong Li, Thomas J Walsh, and Michael L Littman. Towards a unified theory of state abstraction for MDPs. In *Proceedings of the 9th International Symposium on Artificial Intelligence and Mathematics*, pages 531–539, 2006.

Boyi Liu, Qi Cai, Zhuoran Yang, and Zhaoran Wang. Neural proximal/trust region policy optimization attains globally optimal policy. *CoRR*, abs/1906.10306, 2019. URL http://arxiv.org/abs/1906.10306.

Tyler Lu, Dale Schuurmans, and Craig Boutilier. Non-delusional q-learning and value-iteration. In *Advances in neural information processing systems*, pages 9949–9959, 2018.

Dipendra Misra, Mikael Henaff, Akshay Krishnamurthy, and John Langford. Kinematic state abstraction and provably efficient rich-observation reinforcement learning. In *International conference on machine learning*, 2020.

Rémi Munos. Error bounds for approximate value iteration. 2005.

Gergely Neu, Anders Jonsson, and Vicenç Gómez. A unified view of entropy-regularized markov decision processes. *CoRR*, abs/1705.07798, 2017.

Junhyuk Oh, Satinder Singh, and Honglak Lee. Value prediction network. In I. Guyon, U. V. Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett, editors, *Advances in Neural Information Processing Systems 30*, pages 6118–6128. Curran Associates, Inc., 2017. URL http://papers.nips.cc/paper/7192-value-prediction-network.pdf.

Ian Osband, Benjamin Van Roy, and Zheng Wen. Generalization and exploration via randomized value functions. *arXiv preprint arXiv:1402.0635*, 2014.

Adam Paszke, Sam Gross, Francisco Massa, Adam Lerer, James Bradbury, Gregory Chanan, Trevor Killeen, Zeming Lin, Natalia Gimelshein, Luca Antiga, Alban Desmaison, Andreas Kopf, Edward Yang, Zachary DeVito, Martin Raison, Alykhan Tejani, Sasank Chilamkurthy, Benoit Steiner, Lu Fang, Junjie Bai, and Soumith Chintala. Pytorch: An imperative style, high-performance deep learning library. In H. Wallach, H. Larochelle, A. Beygelzimer, F. d'Alché-Buc, E. Fox, and R. Garnett, editors, *Advances in Neural Information Processing Systems 32*, pages 8024–8035. Curran Associates, Inc., 2019.

Deepak Pathak, Pulkit Agrawal, Alexei A. Efros, and Trevor Darrell. Curiosity-driven exploration by self-supervised prediction. In *ICML*, 2017.
Ali Rahimi and Benjamin Recht. Weighted sums of random kitchen sinks: Replacing minimization with randomization in learning. In D. Koller, D. Schuurmans, Y. Bengio, and L. Bottou, editors, Advances in Neural Information Processing Systems 21, pages 1313–1320. Curran Associates, Inc., 2009. URL http://papers.nips.cc/paper/3495-weighted-sums-of-random-kitchen-sinks-replacing-minimization-with-randomization.pdf.

Daniel Russo. Worst-case regret bounds for exploration via randomized value functions. In Advances in Neural Information Processing Systems, pages 14410–14420, 2019.

Bruno Scherrer. Approximate policy iteration schemes: A comparison. In Proceedings of the 31st International Conference on International Conference on Machine Learning - Volume 32, ICML’14. JMLR.org, 2014.

Bruno Scherrer and Matthieu Geist. Local policy search in a convex space and conservative policy iteration as boosted policy search. In Joint European Conference on Machine Learning and Knowledge Discovery in Databases, pages 35–50. Springer, 2014.

John Schulman, Sergey Levine, Pieter Abbeel, Michael Jordan, and Philipp Moritz. Trust region policy optimization. In International Conference on Machine Learning, pages 1889–1897, 2015.

John Schulman, Filip Wolski, Prafulla Dhariwal, Alec Radford, and Oleg Klimov. Proximal policy optimization algorithms. arXiv preprint arXiv:1707.06347, 2017.

Zhang Shangtong. Modularized implementation of deep rl algorithms in pytorch. https://github.com/ShangtongZhang/DeepRL, 2018.

Lior Shani, Yonathan Efroni, and Shie Mannor. Adaptive trust region policy optimization: Global convergence and faster rates for regularized mdps, 2019.

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, pages 1015–1022, 2010.

Alexander L Strehl, Lihong Li, Eric Wiewiora, John Langford, and Michael L Littman. PAC model-free reinforcement learning. In Proceedings of the 23rd international conference on Machine learning, pages 881–888. ACM, 2006.

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 Conference on Learning Theory, pages 2898–2933, 2019.

Richard S Sutton, David A McAllester, Satinder P Singh, and Yishay Mansour. Policy gradient methods for reinforcement learning with function approximation. In Advances in Neural Information Processing Systems, volume 99, pages 1057–1063, 1999.
Csaba Szepesvári and Rémi Munos. Finite time bounds for sampling based fitted value iteration. In Proceedings of the 22nd international conference on Machine learning, pages 880–887. ACM, 2005.

István Szita and Csaba Szepesvári. Model-based reinforcement learning with nearly tight exploration complexity bounds. In Proceedings of the 27th International Conference on Machine Learning (ICML-10), pages 1031–1038, 2010.

Joel A Tropp et al. An introduction to matrix concentration inequalities. Foundations and Trends® in Machine Learning, 8(1-2):1–230, 2015.

Michal Valko, Nathaniel Korda, Rémi Munos, Ilias Flaounas, and Nelo Cristianini. Finite-time analysis of kernelised contextual bandits. arXiv preprint arXiv:1309.6869, 2013.

Aäron van den Oord, Yazhe Li, and Oriol Vinyals. Representation learning with contrastive predictive coding. CoRR, abs/1807.03748, 2018. URL http://arxiv.org/abs/1807.03748.

Pascal Vincent, Hugo Larochelle, Isabelle Lajoie, Yoshua Bengio, and Pierre-Antoine Manzagol. Stacked denoising autoencoders: Learning useful representations in a deep network with a local denoising criterion. J. Mach. Learn. Res., 11:33713408, December 2010. ISSN 1532-4435.

Zheng Wen and Benjamin Van Roy. Efficient exploration and value function generalization in deterministic systems. In Advances in Neural Information Processing Systems, pages 3021–3029, 2013.

Ronald J Williams. Simple statistical gradient-following algorithms for connectionist reinforcement learning. Machine learning, 8(3-4):229–256, 1992.

Lin F Yang and Mengdi Wang. Reinforcement leaning in feature space: Matrix bandit, kernels, and regret bound. arXiv preprint arXiv:1905.10389, 2019a.

Lin F. Yang and Mengdi Wang. Sample-optimal parametric q-learning using linearly additive features. In International Conference on Machine Learning, pages 6995–7004, 2019b.

Andrea Zanette, David Brandfonbrener, Emma Brunskill, Matteo Pirotta, and Alessandro Lazaric. Frequentist regret bounds for randomized least-squares value iteration. In Silvia Chiappa and Roberto Calandra, editors, Proceedings of the Twenty Third International Conference on Artificial Intelligence and Statistics, volume 108 of Proceedings of Machine Learning Research, pages 1954–1964, Online, 26–28 Aug 2020. PMLR.

Dongruo Zhou, Jiafan He, and Quanquan Gu. Provably efficient reinforcement learning for discounted mdps with feature mapping. arXiv preprint arXiv:2006.13165, 2020.

Martin Zinkevich. Online convex programming and generalized infinitesimal gradient ascent. In Proceedings of the 20th International Conference on Machine Learning (ICML-03), pages 928–936, 2003.
A  NPG Analysis (Algorithm 3)

In this section, we analyze Algorithm 3 for a particular episode $n$.

In order to carry out our analysis, we first set up some auxiliary MDPs which are needed in our analysis. Throughout this section, we focus on episode $n$.

A.1  Set up of Augmented MDPs

Denote

$$\mathcal{K}^n := \{(s, a) : \phi(s, a)^\top (\Sigma_{\text{cov}})^{-1} \phi(s, a) \leq \beta\}. \tag{6}$$

That is, $\mathcal{K}^n$ contains state-action pairs that obtain positive reward bonuses. We abuse notation a bit by denoting $s \in \mathcal{K}^n$ if and only if $(s, a) \in \mathcal{K}^n$ for all $a \in \mathcal{A}$.

We also add an extra action denoted as $a^\dagger$ in $\mathcal{M}^n$. For any $s \notin \mathcal{K}^n$, we add $a^\dagger$ to the set of available actions one could take at $s$. We set rewards and transitions as follows:

$$r^n(s, a) = r(s, a) + b^n(s, a) + 1\{a = a^\dagger\}; \quad P^n(\cdot|s, a) = P(\cdot|s, a), \forall (s, a), \quad P^n(s|s, a^\dagger) = 1, \tag{7}$$

where $r(s, a^\dagger) = b^n(s, a^\dagger) = 0$ for any $s$.

Note that at this point, we have three different kinds of MDPs that we will cross during the analysis:

1. the original MDP $\mathcal{M}$—the one that PC-PG is ultimately optimizing;

2. the MDP with reward bonus $b^n(s, a)$—the one is optimized by NPG in each episode $n$ in the algorithm, which we denote as $\mathcal{M}_{b^n} = \{P, r(s, a) + b^n(s, a)\}$ with $P$ and $r$ being the transition and reward from $\mathcal{M}$;

3. the MDP $\mathcal{M}^n$ that is constructed in Eq. (7) which is only used in analysis but not in algorithm.

The relationship between $\mathcal{M}_{b^n}$ (item 2) and $\mathcal{M}^n$ (item 3) is that NPG Algorithm 3 runs on $\mathcal{M}_{b^n}$ (NPG is not even aware of the existence of $\mathcal{M}^n$) but we use $\mathcal{M}^n$ to analyze the performance of NPG below.

Additional Notations.  We are going to focus on a fixed comparator policy $\tilde{\pi} \in \Pi$. We denote $\tilde{\pi}^n$ as the policy such that $\pi(\cdot|s) = \tilde{\pi}^n(\cdot|s)$ for $s \in \mathcal{K}^n$, and $\tilde{\pi}^n(a^\dagger|s) = 1$ for $s \notin \mathcal{K}^n$. This means that the comparator policy $\tilde{\pi}^n$ will self-loop in a state $s \notin \mathcal{K}^n$ and collect maximum rewards. We denote $\bar{d}_{\mathcal{M}^n}$ as the state-action distribution of $\tilde{\pi}^n$ under $\mathcal{M}^n$, and $V_{\mathcal{M}^n}^\pi, Q_{\mathcal{M}^n}^\pi, A_{\mathcal{M}^n}^\pi$ as the value, Q, and advantage functions of $\pi$ under $\mathcal{M}^n$. We also denote $Q_{b^n}^\pi(s, a)$ in short of $Q^n(s, a; r + b^n)$, similarly $A_{b^n}^\pi(s, a)$ in short of $A^n(s, a; r + b^n)$, and $V_{b^n}^\pi(s)$ in short of $V^n(s; r + b^n)$.

Remark A.1. Note that policies used in the algorithm do not pick $a^\dagger$ (i.e., algorithms does not even aware of $\mathcal{M}^n$). Hence for any policy $\pi$ that we would encounter during learning, we have $V_{\mathcal{M}^n}^\pi(s) = V_{b^n}^\pi(s)$ for all $s$, $Q_{\mathcal{M}^n}^\pi(s, a) = Q_{b^n}^\pi(s, a)$ and $A_{\mathcal{M}^n}^\pi(s, a) = A_{b^n}^\pi(s, a)$ for all $s$ with $a \neq a^\dagger$. This fact is important as our algorithm is running on $\mathcal{M}_{b^n}$ while the performance progress of the algorithm is tracked under $\mathcal{M}^n$. 

32
A.2 Performance of NPG (Algorithm 3) on the Augmented MDP $\mathcal{M}^n$

In this section, we focus on analyzing the performance of NPG (Algorithm 3) on a specific episode $n$. Specifically we leverage the Mirror Descent analysis similar to Agarwal et al. [2019] to show that regret between the sequence of learned policies $\{\pi_t^\pi\}_{t=1}^T$ and the comparator $\tilde{\pi}^n$ on the constructed MDP $\mathcal{M}^n$.

Via performance difference lemma Kakade [2003], we immediately have:

$$V_{\mathcal{M}^n} - V_{\mathcal{M}^n} = \frac{1}{1 - \gamma} E_{(s,a) \sim \tilde{\pi}^n} [A_{\mathcal{M}^n}^\pi(s, a)].$$

For notation simplicity below, given a policy $\pi$ and state $s$, we denote $\pi_s$ in short of $\pi(\cdot|s)$.

Lemma A.1 (NPG Convergence). Consider any episode $n$. Setting $\eta = \sqrt{\frac{\log(A)}{W^2 T}}$, assume NPG updates policy as:

$$\pi_{t+1}(\cdot|s) \propto \begin{cases} \pi_t(\cdot|s) \exp \left( \eta \hat{A}_t^b(s, a) \right), & s \in \mathcal{K}^n, \\ \pi_t(\cdot|s), & \text{else}, \end{cases}$$

with $\pi^0$ initialized as:

$$\pi^0(\cdot|s) = \begin{cases} \text{Uniform}(\mathcal{A}) & s \in \mathcal{K}^n, \\ \text{Uniform}\{a \in \mathcal{A} : (s, a) \notin \mathcal{K}^n\} & \text{else}. \end{cases}$$

Assume that $\sup_{s,a} |\hat{A}^b_t(s, a)| \leq W$ and $E_{a' \sim \pi_t^\pi} \hat{A}^b_t(s, a') = 0$ for all $t$. Then the NPG outputs a sequence of policies $\{\pi_t^\pi\}_{t=1}^T$ such that on $\mathcal{M}^n$, when comparing to $\tilde{\pi}^n$:

$$\frac{1}{T} \sum_{t=1}^T (V_{\mathcal{M}^n} - V_{\mathcal{M}^n}^t) = \frac{1}{T} \sum_{t=1}^T (V_{\mathcal{M}^n} - V_{\mathcal{M}^n}^t) 
\leq \frac{1}{1 - \gamma} \left( 2W \sqrt{\frac{\log(A)}{T}} + \frac{1}{T} \sum_{t=1}^T \left( E_{(s,a) \sim \tilde{\pi}^n} (A_{\mathcal{M}^n}^\pi(s, a) - \hat{A}_t^b(s, a)) 1\{s \in \mathcal{K}^n\} \right) \right),$$

Proof. First consider any policy $\pi$ which uniformly picks actions among $\{a \in \mathcal{A} : (s, a) \notin \mathcal{K}^n\}$ at any $s \notin \mathcal{K}^n$. Via performance difference lemma, we have:

$$V_{\mathcal{M}^n} - V_{\mathcal{M}^n} = \frac{1}{1 - \gamma} \sum_{(s,a)} \tilde{d}_{\mathcal{M}^n}(s, a) A_{\mathcal{M}^n}^\pi(s, a) \leq \frac{1}{1 - \gamma} \sum_{(s,a)} \tilde{d}_{\mathcal{M}^n}(s, a) A_{\mathcal{M}^n}^\pi(s, a) 1\{s \in \mathcal{K}^n\},$$

where the last inequality comes from the fact that $A_{\mathcal{M}^n}^\pi(s, a) 1\{s \notin \mathcal{K}^n\} \leq 0$. To see this, first note that for any $s \notin \mathcal{K}^n$, $\tilde{\pi}^n$ will deterministically pick $a^\dagger$, and $Q_{\mathcal{M}^n}^\pi(s, a^\dagger) = 1 + \gamma V_{\mathcal{M}^n}^\pi(s)$ as taking
where the centered feature is defined as
\[
\phi(s, a) = \sum_{(s, a)} \exp(\eta \hat{A}_b^n(s, a)) - \sum_{(s, a) \in \mathcal{K}} \phi(s, a)
\]
and the fact that for \(s \in \mathcal{K}^n\), \(\tilde{\pi}^n\) never picks \(a^\dagger\) (i.e., \(d_{\mathcal{M}^n}(s, a^\dagger) = 0\) for \(s \in \mathcal{K}^n\)).

Recall the update rule of NPG,
\[
\pi^{t+1}(\cdot|s) \propto \pi^t(\cdot|s) \exp\left(\eta \left(\hat{A}_b^n(s, \cdot)\right)\right) \mathbb{1}\{s \in \mathcal{K}^n\},
\]
where the centered feature is defined as \(\bar{\phi}(s, a) = \phi(s, a) - \mathbb{E}_{a' \sim \pi^t(s)} \phi(s, a')\). This is equivalent to updating \(s \in \mathcal{K}^n\) while holding \(\pi(\cdot|s)\) fixed for \(s \notin \mathcal{K}^n\), i.e.,
\[
\pi^{t+1}(\cdot|s) \propto \begin{cases} 
\pi^t(\cdot|s) \exp\left(\eta \hat{A}_b^n(s, \cdot)\right), & s \in \mathcal{K}^n, \\
\pi^t(\cdot|s), & \text{else}.
\end{cases}
\]

Now let us focus on any \(s \in \mathcal{K}^n\). Denote the normalizer \(z^t = \sum_a \pi^t(a|s) \exp\left(\eta \hat{A}_b^n(s, a)\right)\).

We have that:
\[
\text{KL}(\tilde{\pi}_s^n, \pi^{t+1}_s) - \text{KL}(\tilde{\pi}_s^n, \pi^t_s) = \mathbb{E}_{a \sim \mathcal{P}} \left[-\eta \hat{A}_b^n(s, a) + \log(z^t)\right],
\]
where we use \(\pi_s\) as a shorthand for the vector of probabilities \(\pi(\cdot|s)\) over actions, given the state \(s\).

For \(\log(z^t)\), using the assumption that \(\eta \leq 1/W\), we have that \(\eta \hat{A}_b^n(s, a) \leq 1\), which allows us to use the inequality \(\exp(x) \leq 1 + x + x^2\) for any \(x \leq 1\) and leads to the following inequality:
\[
\log(z^t) = \log\left(\sum_a \pi^t(a|s) \exp(\eta \hat{A}_b^n(s, a))\right) \leq \log\left(\sum_a \pi^t(a|s) \left(1 + \eta \hat{A}_b^n(s, a) + \eta^2 \left(\hat{A}_b^n(s, a)\right)^2\right)\right) = \log\left(1 + \eta^2 W^2\right) \leq \eta^2 W^2,
\]
where we use the fact that \(\sum_a \pi^t(a|s) \hat{A}_b^n(s, a) = 0\).

Hence, for \(s \in \mathcal{K}^n\) we have:
\[
\text{KL}(\tilde{\pi}_s^n, \pi^{t+1}_s) - \text{KL}(\tilde{\pi}_s^n, \pi^t_s) \leq -\eta \mathbb{E}_{a \sim \mathcal{P}} \hat{A}_b^n + \eta^2 W^2.
\]

34
Adding terms across rounds, and using the telescoping sum, we get:

$$\sum_{t=1}^{T} \mathbb{E}_{a \sim \tilde{\pi}_n} \hat{A}_b^t(s, a) \leq \frac{1}{\eta} \text{KL}(\tilde{\pi}_n, \pi_1) + \eta T W^2 \leq \frac{\log(A)}{\eta} + \eta T W^2, \quad \forall s \in \mathcal{K}^n.$$ 

Add $\mathbb{E}_{s \sim \tilde{d}_{M^n}}$, we have:

$$\sum_{t=1}^{T} \mathbb{E}_{(s,a) \sim \tilde{d}_{M^n}} \left[ \hat{A}_b^t(s, a) \mathbf{1}\{s \in \mathcal{K}^n\} \right] \leq \frac{\log(A)}{\eta} + \eta T W^2 \leq 2W \sqrt{\log(A) T}.$$ 

Hence, for regret on $M_n$, we have:

$$\sum_{t=1}^{T} (V_{M^n}^t - V_{M^n}^t)$$

$$\leq \sum_{t=1}^{T} \mathbb{E}_{(s,a) \sim \tilde{d}_{M^n}} \left[ \hat{A}_b^t(s, a) \mathbf{1}\{s \in \mathcal{K}^n\} \right] + \sum_{t=1}^{T} \left( \mathbb{E}_{(s,a) \sim \tilde{d}_{M^n}} \left( A_b^t(s, a) - \hat{A}_b^t(s, a) \right) \mathbf{1}\{s \in \mathcal{K}^n\} \right)$$

$$\leq 2W \sqrt{\log(A) T} + \sum_{t=1}^{T} \left( \mathbb{E}_{(s,a) \sim \tilde{d}_{M^n}} \left( A_b^t(s, a) - \hat{A}_b^t(s, a) \right) \mathbf{1}\{s \in \mathcal{K}^n\} \right).$$

Now using the fact that $\pi^t$ never picks $a^\dagger$, we have $V_{M^n}^t = V_{b^n}^t$. This concludes the proof. 

Note that the second term of the RHS of the inequality in the above lemma measures the average estimation error of $\hat{A}_b^t$. Below, for PC-PG’s analysis, we bound the critic prediction error under $d^n$.

### B Relationship between $M^n$ and $\mathcal{M}$

We need the following lemma to relate the probability of a known state being visited by $\tilde{\pi}_n$ under $M^n$ and the probability of the same state being visited by $\tilde{\pi}$ under $M_{b^n}$. Note that intuitively as $\tilde{\pi}_n$ always picks $a^\dagger$ outside $\mathcal{K}^n$, it should have smaller probability of visiting the states inside $\mathcal{K}^n$ (once $\tilde{\pi}_n$ escapes, it will be absorbed and will never return back to $\mathcal{K}^n$). Also recall that $M_{b^n}$ and $\mathcal{M}$ share the same underlying transition dynamics. So for any policy, we simply have $d_{M_{b^n}} = d^n$.

The following lemma formally states this.

**Lemma B.1.** Consider any state $s \in \mathcal{K}^n$, we have:

$$\tilde{d}_{M^n}(s, a) \leq d^n(s, a), \forall a \in \mathcal{A},$$

where recall $\tilde{d}_{M^n}$ is the state-action distribution of $\tilde{\pi}_n$ under $M^n$.

**Proof.** We prove by induction. Recall $\tilde{d}_{M^n}$ is the state-action distribution of $\tilde{\pi}_n$ under $M^n$, and $d^n$ is the state-action distribution of $\tilde{\pi}$ under both $M_{b^n}$ and $\mathcal{M}$ as they share the same dynamics.
Starting at $h = 0$, we have:
\[ \tilde{d}_{\mathcal{M}^n,0}(s_0, a) = d^n_0(s_0, a), \]
as $s_0$ is fixed and $s_0 \in \mathcal{K}^n$, and $\tilde{\pi}^n(\cdot | s_0) = \tilde{\pi}(\cdot | s_0)$.

Now assume that at time step $h$, we have that for all $s \in \mathcal{K}^n$, we have:
\[ \tilde{d}_{\mathcal{M}^n,h}(s, a) \leq d^n_h(s, a), \forall a \in \mathcal{A}. \]

Now we proceed to prove that this holds for $h + 1$. By definition, we have that for $s \in \mathcal{K}^n$,
\begin{align*}
\tilde{d}_{\mathcal{M}^n,h+1}(s) &= \sum_{s', a'} \tilde{d}_{\mathcal{M}^n,h}(s', a') P_{\mathcal{M}^n}(s | s', a') \\
&= \sum_{s', a'} \mathbf{1}\{s' \in \mathcal{K}^n\} \tilde{d}_{\mathcal{M}^n,h}(s', a') P_{\mathcal{M}^n}(s | s', a') = \sum_{s', a'} \mathbf{1}\{s' \in \mathcal{K}^n\} \tilde{d}_{\mathcal{M}^n,h}(s', a') P(s | s', a')
\end{align*}
as if $s' \notin \mathcal{K}^n$, $\tilde{\pi}^n$ will deterministically pick $a^\dagger$ (i.e., $a' = a^\dagger$) and $P_{\mathcal{M}^n}(s | s', a^\dagger) = 0$.

On the other hand, for $d^n_{h+1}(s, a)$, we have that for $s \in \mathcal{K}^n$,
\begin{align*}
d^n_{h+1}(s, a) &= \sum_{s', a'} d^n_h(s', a') P(s | s', a') \\
&= \sum_{s', a'} \mathbf{1}\{s' \in \mathcal{K}^n\} d^n_h(s', a') P(s | s', a') + \sum_{s', a'} \mathbf{1}\{s' \notin \mathcal{K}^n\} d^n_h(s', a') P(s | s', a') \\
&\geq \sum_{s', a'} \mathbf{1}\{s' \in \mathcal{K}^n\} d^n_h(s', a') P(s | s', a') \\
&\geq \sum_{s', a'} \mathbf{1}\{s' \in \mathcal{K}^n\} \tilde{d}_{\mathcal{M}^n,h}(s', a') P(s | s', a') = \tilde{d}_{\mathcal{M}^n,h+1}(s).
\end{align*}

Using the fact that $\tilde{\pi}^n(\cdot | s) = \tilde{\pi}(\cdot | s)$ for $s \in \mathcal{K}^n$, we conclude that the inductive hypothesis holds at $h + 1$ as well. Thus it holds for all $h$. Using the definition of average state-action distribution, we conclude the proof.

We now establish a standard simulation lemma-style result to link the performance of policies on $\mathcal{M}^n$ to the performance on the real MDP $\mathcal{M}$, before bounding the error in the lemma using a linear bandits potential function argument as sketched above. These arguments allow us to translate the error bounds from Appendix [A] from the augmented MDP $\mathcal{M}^n$ to the actual MDP $\mathcal{M}$.

**Lemma B.2 (Policy Performances on $\mathcal{M}^n$, $\mathcal{M}_0$, $\mathcal{M}$).** At each episode $n$, denote $\{\pi^t\}_{t=1}^T$ as the sequence of policies generated from NPG in that episode. we have that for $\tilde{\pi}^n$ and $\pi^t$ for any $t \in [T]$:
\begin{align*}
V_{\mathcal{M}^n} &\geq V^n_{\mathcal{M}}, \\
V_{\mathcal{M}} &\geq V^n_{\mathcal{M}} - \frac{1}{1 - \gamma} \left( \sum_{(s, a)\notin\mathcal{K}^n} d^n(s, a) \right).
\end{align*}
Proof. Note that when running $\tilde{\pi}^n$ under $M^n$, once $\tilde{\pi}^n$ visits $s \not\in K^n$, it will be absorbed into $s$ and keeps looping there and receiving the maximum reward $1$. Note that $\tilde{\pi}$ receives reward no more than $1$ and in $M$ we do not have reward bonus.

Recall that $\pi^t$ never takes $a^\dagger$. Hence $d^t(s, a) = d^t_{M^n}(s, a)$ for all $(s, a)$. Recall that the reward bonus is defined as $\frac{1}{1-\gamma}1\{(s, a) \not\in K^n\}$.

The lemma below relates the escaping probability to an elliptical potential function and quantifies the progress made by the algorithm by the maximum information gain quantity.

**Lemma B.3** (Potential Function Argument). Consider the sequence of policies $\{\pi^n\}_{n=1}^N$ generated from Algorithm 2. We have:

$$\sum_{n=0}^{N-1} V^{\pi_{n+1}} - \sum_{n=0}^{N-1} V^{\pi_n+1}_{b^n} - \frac{2I_N(\lambda)}{\beta(1-\gamma)}.$$

Proof. Denote the eigen-decomposition of $\Sigma_n^{\text{cov}}$ as $U \Lambda U^\top$ and $\Sigma_n = \mathbb{E}_{(s,a) \sim d^n} \phi(s,a) \phi(s,a)^\top$. We have:

$$\text{tr} \left( \Sigma_{n+1}^{\text{cov}} (\Sigma_n^{\text{cov}})^{-1} \right) = \mathbb{E}_{(s,a) \sim d^{n+1}} \text{tr} \left( \phi(s,a) \phi(s,a)^\top (\Sigma_n^{\text{cov}})^{-1} \right)$$

$$= \mathbb{E}_{(s,a) \sim d^{n+1}} \phi(s,a)^\top (\Sigma_n^{\text{cov}})^{-1} \phi(s,a)$$

$$\geq \mathbb{E}_{(s,a) \sim d^{n+1}} \left[ 1\{(s, a) \not\in K^n\} \phi(s,a)^\top (\Sigma_n^{\text{cov}})^{-1} \phi(s,a) \right] \geq \beta \mathbb{E}_{(s,a) \sim d^{n+1}} 1\{(s, a) \not\in K^n\}$$

together with Lemma B.2, which implies that

$$V_{b^n}^{\pi_{n+1}} - V^{\pi_{n+1}} \leq \frac{\text{tr} \left( \Sigma_{n+1}^{\text{cov}} (\Sigma_n^{\text{cov}})^{-1} \right)}{\beta(1-\gamma)}.$$

Now call Lemma G.2, we have:

$$\sum_{n=0}^{N} \left( V_{b^n}^{\pi_{n+1}} - V^{\pi_{n+1}} \right) \leq \frac{2\log(\det(\Sigma_{\text{cov}}^N) / \det(\lambda I))}{\beta(1-\gamma)} \leq \frac{2I_N(\lambda)}{\beta(1-\gamma)}$$

where we use the definition of information gain $I_N(\lambda).$ \qed

## C Analysis of PC-PG for the Agnostic Setting (Theorem 4.3)

In this section, we analyze the performance of PC-PG using the NPG results we derived from the previous section. We begin with an assumption and a theorem statement which is the most general sample complexity result for PC-PG and from which all the statements of Section 4 follow.

We first formally state the assumption of transfer bias $\varepsilon_{bias}$ which we have used as the condition in NPG analysis in Lemma C.1.

The following theorem states the detailed sample complexity of PC-PG (a detailed version of Theorem 4.3).
Theorem C.1 (Main Result: Sample Complexity of PC-PG). Fix $\delta \in (0, 1/2)$ and $\epsilon \in (0, \frac{1}{1-\gamma})$.

Setting hyperparameters as follows:

$$T = \frac{4W^2 \log(A)}{(1-\gamma)^2 \epsilon^2}, \quad \lambda = 1, \quad \beta = \frac{\epsilon^2 (1-\gamma)^2}{4W^2}, \quad N \geq \frac{4W^2 I_N(1)}{(1-\gamma)^3 \epsilon^3},$$

$$M = \frac{144W^4 I_N(1)^2 \ln(NT/\delta)}{\epsilon^6 (1-\gamma)^{10}}, \quad K = 32N^2 \log \left( \frac{N d}{\delta} \right).$$

Under Assumption 4.1, with probability at least $1 - 2\delta$, we have:

$$\max_{n \in [N]} V_{\pi^n} \geq V_{\tilde{\pi}} - \frac{2\sqrt{A\epsilon_{bias}}}{1-\gamma} - 4\epsilon,$$

for any comparator $\tilde{\pi} \in \Pi_{\text{linear}}$, with at most total number of samples:

$$\frac{c\nu W^2 I_N(1)^3 \ln(A)}{\epsilon^{11}(1-\gamma)^{15}},$$

where $c$ is a universal constant, and $\nu$ contains only log terms:

$$\nu = \ln \left( \frac{4\hat{d}W^2 I_N(1)}{(1-\gamma)^3 \epsilon^3 \delta} \right) + \ln \left( \frac{16W^4 \ln(A) I_N(1)}{\epsilon^5(1-\gamma)^5 \delta} \right).$$

Remark C.1. Note that in the above theorem, we require that the number of iterations $N$ to satisfy the constraint $N \geq 4W^2 I_N(1)/((1-\gamma)^3 \epsilon^3)$. The specific $N$ thus depends on the form of the maximum information gain $I_N(1)$. For instance, when $\phi(s,a) \in \mathbb{R}^d$ with $\|\phi\|_2 \leq 1$, we have $I_N(1) \leq d \log(N+1)$. Hence setting $N \geq \frac{8W^2 d}{(1-\gamma)^3 \epsilon^3} \ln \left( \frac{4W^2 d}{(1-\gamma)^3 \epsilon^3} \right)$ suffices. Another example is when $\phi$ lives in an RKHS with RBF kernel. In this case, we have $I_N(1) = O(\log(N)^{d_{s,a}})$ (Srinivas et al. [2010]), where $d_{s,a}$ stands for the dimension of the concatenated vector of state and action. In this case, we can set $N = O \left( \frac{W^2}{(1-\gamma)^3 \epsilon^3} \ln \left( \frac{W^2}{(1-\gamma)^3 \epsilon^3} \right)^{d_{s,a}} \right)$.

In the rest of this section, we prove the theorem. Given the analysis of Appendix A, proving the theorem requires the following steps at a high-level:

1. Bounding the number of outer iterations $N$ in order to obtain a desired accuracy $\epsilon$. Intuitively, this requires showing that the probability with which we can reach an unknown state with a positive reward bonus is appropriately small. We carry out this bounding by using arguments from the analysis of linear bandits [Dani et al., 2008]. At a high-level, if there is a good probability of reaching unknown states, then NPG finds them based on our previous analysis as these states carry a high reward. But every time we find such states, the covariance matrix of the resulting policy contains directions not visited by the previous cover with a large probability (or else the quadratic form defining the unknown states would be small). In a $d$-dimensional linear space, the number of times we can keep finding significantly new directions is roughly $O(d)$ (or more precisely based on the intrinsic dimension), which allows us to bound the number of required outer episodes.
2. Bounding the prediction error of the critic in Lemma [A.1] This can be done by a standard regression analysis and we use a specific result for stochastic gradient descent to fit the critic.

3. Errors from empirical covariance matrices instead of their population counterparts have to be accounted for as well, and this is done by using standard inequalities on matrix concentration [Tropp et al. 2015].

C.1 **Proof of Theorem C.1**

We recall that we perform linear regression from \( \phi(s, a) \) to \( Q_{b_n}^\pi(s, a) - b^n(s, a) \), and set \( \hat{A}_{b_n}^t(s, a) \) as

\[
\hat{A}_{b_n}^t(s, a) = (b^n(s, a) + \theta^t \cdot \phi(s, a)) - \mathbb{E}_{a' \sim \pi^*_a}[b^n(s, a') + \theta^t \cdot \phi(s, a')]
\]

where for notation simplicitly, we denote centered bonus \( \bar{b}^{n, t}(s, a) = b^n(s, a) - \mathbb{E}_{a' \sim \pi^*_a}b^n(s, a') \), and centered feature \( \bar{\phi}^t(s, a) = \phi(s, a) - \mathbb{E}_{a' \sim \pi^*_a}\phi(s, a') \).

**Lemma C.1** (Variance and Bias Tradeoff). Assume that at episode \( n \) we have \( \phi(s, a) \top (\Sigma_{\text{cov}}^n)^{-1} \phi(s, a) \leq \beta \) for \((s, a) \in K^n \). At iteration \( t \) inside episode \( n \), let us denote a best on-policy fit as \( \hat{\theta}^* \in \arg\min_{\|\theta\| \leq W} \mathbb{E}_{(s, a) \sim \rho_{\text{cov}}^n} ((Q_{b_n}^\pi(s, a) - b^n(s, a)) - \theta \cdot \phi(s, a))^2 \). Assume the following condition is true for all \( t \in [T] \):

\[
L (\theta^t; \rho_{\text{cov}}^n, Q_{b_n}^t - b^n) \leq \min_{\|\theta\| \leq W} L (\theta; \rho_{\text{cov}}^n, Q_{b_n}^t - b^n) + \varepsilon_{\text{stat}},
\]

where \( \varepsilon_{\text{stat}} \in \mathbb{R}^+ \). Then under [Assumption 4.1] (with \( \bar{\pi} \) as the comparator policy here), we have that for all \( t \in [T] \):

\[
\mathbb{E}_{(s, a) \sim \bar{a}; \text{Mn}} \left( A_{b_n}^t(s, a) - \hat{A}_{b_n}^t(s, a) \right) I\{s \in K^n\} \leq 2\sqrt{A\varepsilon_{\text{bias}}} + 2\sqrt{\beta W^2} + 2\sqrt{\beta n \varepsilon_{\text{stat}}}.
\]

**Proof.** We first show that under condition 1 above, \( \mathbb{E}_{(s, a) \sim \rho_{\text{cov}}^n} (\theta^*_t \phi(s, a) - \theta^t \phi(s, a))^2 \) is bounded by \( \varepsilon_{\text{stat}} \).

\[
\mathbb{E}_{(s, a) \sim \rho_{\text{cov}}^n} (Q_{b_n}^t(s, a) - b^n(s, a) - \theta^t \cdot \phi(s, a))^2 = \mathbb{E}_{(s, a) \sim \rho_{\text{cov}}^n} (Q_{b_n}^t(s, a) - b^n(s, a) - \theta^*_t \cdot \phi(s, a))^2
\]

\[
= \mathbb{E}_{(s, a) \sim \rho_{\text{cov}}^n} (\theta^*_t \cdot \phi(s, a) - \theta^t \cdot \phi(s, a))^2 + 2\mathbb{E}_{(s, a) \sim \rho_{\text{cov}}^n} (Q_{b_n}^t(s, a) - b^n(s, a) - \theta^*_t \cdot \phi(s, a)) (\theta^*_t - \theta^t) \phi(s, a)^\top \phi(s, a) + \theta^t - \theta^*_t)^2.
\]

Note that \( \theta^* \) is one of the minimizers of the constrained square loss \( \mathbb{E}_{(s, a) \sim \rho_{\text{cov}}^n} (Q_{b_n}^t(s, a) - b^n(s, a) - \theta^t \cdot \phi(s, a))^2 \), via first-order optimality, we have:

\[
\mathbb{E}_{(s, a) \sim \rho_{\text{cov}}^n} (Q_{b_n}^t(s, a) - b^n(s, a) - \theta^*_t \cdot \phi(s, a)) (\phi(s, a)^\top (\theta - \theta^*_t) \geq 0,
\]

for any \( \|\theta\| \leq W \), which implies that:

\[
\mathbb{E}_{(s, a) \sim \rho_{\text{cov}}^n} (\theta^t \cdot \phi(s, a) - \theta^t \cdot \phi(s, a))^2 \leq \mathbb{E}_{(s, a) \sim \rho_{\text{cov}}^n} (Q_{b_n}^t(s, a) - b^n(s, a) - \theta^t \cdot \phi(s, a))^2 - \mathbb{E}_{(s, a) \sim \rho_{\text{cov}}^n} (Q_{b_n}^t(s, a) - b^n(s, a) - \theta^*_t \cdot \phi(s, a))^2 \leq \varepsilon_{\text{stat}}.
\]
We first bound term A above. 

\[ \mathbf{E}_{(s,a) \sim d^n} \phi(s,a)\phi(s,a) + \lambda I = n \left( \mathbf{E}_{(s,a) \sim d^n} \phi(s,a)\phi(s,a) + \lambda/n I \right). \]

Denote \( \Sigma_n = \sum_{i=1}^n \mathbf{E}_{(s,a)} \phi(s,a)\phi(s,a)^T + \lambda/n I \). We have:

\[ \left( \theta_s^* - \theta_t^* \right) \mathbf{E}_{(s,a)} \phi(s,a)\phi(s,a)^T + \lambda/n I \left( \theta_s^* - \theta_t^* \right) \leq \varepsilon_{stat} + \frac{\lambda}{n} W^2. \]

Hence for any \((s,a) \in \mathcal{K}^n\), we must have the following point-wise estimation error:

\[ \left| \phi(s,a)^T \left( \theta_s^* - \theta_t^* \right) \right| \leq \|\phi(s,a)\|_{\Sigma_n^{-1}} \|\theta_s^* - \theta_t^*\|_{\Sigma_n} \leq \sqrt{3n\varepsilon_{stat} + \beta\lambda W^2}. \]  

Now we bound term B above. We have:

\[ \mathbf{E}_{(s,a) \sim d^n} \left( A^a(n, s, a) - \bar{A}^a_t(n, s, a) \right) \mathbf{1}\{s \in \mathcal{K}^n\} \]

We first bound term A above.

\[ \mathbf{E}_{(s,a) \sim d^n} \left( A^a(n, s, a) - \bar{A}^a_t(n, s, a) \right) \mathbf{1}\{s \in \mathcal{K}^n\} \]

where the first inequality uses CS inequality, the second inequality uses [Lemma B.1] for \( s \in \mathcal{K}^n \), and the last inequality uses the change of variable over action distributions and [Assumption 4.1].

Now we bound term B above. We have:

\[ \mathbf{E}_{(s,a) \sim d^n} \left( \theta_s^* \phi(s,a) - \theta_t^* \phi(s,a) \right) \mathbf{1}\{s \in \mathcal{K}^n\} \]

Combine term A and term B together, we conclude the proof.
Combine the above lemma and Lemma A.1, we can see that as long as the on-policy critic achieves small statistical error (i.e., $\epsilon_{\text{stat}}$ is small), and our features $\phi(s, a)$ are sufficient to represent Q functions in a linear form (i.e., $\epsilon_{\text{bias}}$ is small), then we can guarantee inside episode $n$, NPG succeeds by finding a policy that has low regret with respect to the comparator $\tilde{\pi}$:

$$\max_{t \in [T]} V_{b_n}^t \geq V_{\mathcal{M}^n} - \frac{1}{1 - \gamma} \left( 2W \sqrt{\frac{\log(A)}{T}} + 2\sqrt{A\epsilon_{\text{bias}}} + 2\sqrt{\beta \lambda W^2} + 2\sqrt{\beta n \epsilon_{\text{stat}}} \right). \quad (9)$$

The term that contains $\epsilon_{\text{stat}}$ comes from the statistical error induced from constrained linear regression. Note that in general, $\epsilon_{\text{stat}}$ decays in the rate of $O(1/\sqrt{M})$ with $M$ being the total number of data samples used for linear regression (line 6 in Algorithm 3), and $\epsilon_{\text{stat}}$ usually does not polynomially depend on dimension of $\phi(s, a)$ explicitly. See Lemma G.1 for an example where linear regression is solved via stochastic gradient descent.

Using Lemma B.3, now we can transfer the regret we computed under the sequence of models $\{\mathcal{M}_{b_n}\}$ to regret under $\mathcal{M}$. Recall that $V^\pi$ denotes $V^\pi(s_0)$ and $V^n$ is in short of $V^{\pi^n}$.

**Lemma C.2.** Assume the condition in Lemma C.1 and Assumption 4.1 hold. For the sequence of policies $\{\pi^n\}_{n=1}^N$, we have:

$$\max_{n \in [N]} V^n \geq V^{\pi} - \frac{1}{1 - \gamma} \left( 2W \sqrt{\frac{\log(A)}{T}} + 2\sqrt{A\epsilon_{\text{bias}}} + 2\sqrt{\beta \lambda W^2} + 2\sqrt{\beta N \epsilon_{\text{stat}}} + \frac{2\mathcal{I}_N(\lambda)}{N\beta} \right).$$

**Proof.** First combine Lemma A.1 and Lemma C.1, we have:

$$\frac{1}{N} \sum_{n=0}^{N-1} V_{b_n}^{n+1} \geq \frac{1}{N} \sum_{n=0}^{N-1} V_{\mathcal{M}^n}^{\pi^n} - \frac{1}{1 - \gamma} \left( 2W \sqrt{\frac{\log(A)}{T}} + 2\sqrt{A\epsilon_{\text{bias}}} + 2\sqrt{\beta \lambda W^2} + 2\sqrt{\beta N \epsilon_{\text{stat}}} \right).$$

Use Lemma B.2 and Lemma B.3 we have:

$$\frac{1}{N} \sum_{n=1}^{N} V^n \geq V^{\pi} - \frac{1}{1 - \gamma} \left( 2W \sqrt{\frac{\log(A)}{T}} + 2\sqrt{A\epsilon_{\text{bias}}} + 2\sqrt{\beta \lambda W^2} + 2\sqrt{\beta N \epsilon_{\text{stat}}} + \frac{\mathcal{I}_N(\lambda)}{N\beta} \right),$$

which concludes the proof. \qed

The following theorem shows that setting hyperparameters properly, we can guarantee to learn a near optimal policy.

**Theorem C.2.** Assume the conditions in Lemma C.1 and Assumption 4.1 hold. Fix $\epsilon \in (0, 1/(4(1 - \gamma)))$. Setting hyperparameters as follows:

$$T = \frac{4W^2 \log(A)}{(1 - \gamma)^2 \epsilon^2}, \quad \lambda = 1, \quad \beta = \frac{e^2(1 - \gamma)^2}{4W^2},$$

$$N \geq \frac{4W^2 \mathcal{I}_N(1)}{(1 - \gamma)^3 \epsilon^3}, \quad \epsilon_{\text{stat}} = \frac{e^3(1 - \gamma)^3}{4\mathcal{I}_N(1)},$$

41
we have:

$$\max_{n \in [N]} V^n \geq V^\hat{\pi} - \frac{2\sqrt{A_{\text{bias}}}}{1 - \gamma} - 4\epsilon.$$ 

Proof. The theorem can be easily verified by substituting the values of hyperparameters into Lemma C.2.

The above theorem indicates that we need to control the $\epsilon_{\text{stat}}$ statistical error from linear regression to be small in the order of $\tilde{O}(\epsilon^3(1 - \gamma)^3)$. Recall that $M$ is the total number of samples we used for each linear regression. If $\epsilon_{\text{stat}} = \tilde{O}
left(\frac{1}{\sqrt{M}}\right)$, then we roughly will need $M$ to be in the order of $\tilde{\Omega}(1/\epsilon^6(1 - \gamma)^6)$. Note that we do on-policy fit in each iteration $t$ inside each episode $n$, thus we will pay total number of samples in the order of $M \times (TN)$.

Another source of samples is the samples used to estimate covariance matrices $\Sigma^n$. As $\phi$ could be infinite dimensional, we need matrix concentration without explicit dependency on dimension of $\phi$. Leveraging matrix Bernstein inequality with matrix intrinsic dimension, the following lemma shows concentration results of $\hat{\Sigma}^n$ on $\Sigma^n$, and of $\hat{\Sigma}^n_{\text{cov}}$ on $\Sigma^n_{\text{cov}}$.

Lemma C.3 (Estimating Covariance Matrices). Set $\lambda = 1$. Define $\hat{d}$ as:

$$\hat{d} = \max_{\pi} \text{tr} (\Sigma^n) / \|\Sigma^n\|,$$

i.e., the maximum intrinsic dimension of the covariance matrix from a mixture policy. For $K \geq 32N^2 \ln \left(\frac{\hat{d}N/\delta}{\epsilon^3}\right)$ (a parameter in Algorithm 2), with probability at least $1 - \delta$, for any $n \in [N]$, we have for all $x$ with $\|x\| \leq 1$,

$$(1/2)x^\top (\Sigma^n_{\text{cov}})^{-1} x \leq x^\top (\hat{\Sigma}^n_{\text{cov}})^{-1} x \leq 2x^\top (\Sigma^n_{\text{cov}})^{-1} x.$$ 

Proof. The proof of the above lemma is simply Lemma G.4.

We are now ready to prove Theorem C.1.

Proof of Theorem C.1. Assume the event in Lemma C.3 holds. In this case, we have for all $n \in [N]$,

$$(1/2)x^\top (\Sigma^n_{\text{cov}})^{-1} x \leq x^\top (\hat{\Sigma}^n_{\text{cov}})^{-1} x \leq 2x^\top (\Sigma^n_{\text{cov}})^{-1} x,$$

for all $\|x\| \leq 1$ and the total number of samples used for estimating covariance matrices is:

$$N \times K = N \times \left(32N^2 \ln \left(\frac{\hat{d}N/\delta}{\epsilon^3}\right)\right) = 32N^3 \ln \left(\hat{d}N/\delta\right) \quad (10)$$

$$= (32 \times 64) \mathcal{I}_N(1)^3W^6 \epsilon^9(1 - \gamma)^9 \ln \left(\frac{4\hat{d}W^2\mathcal{I}_N(1)}{(1 - \gamma)^3\epsilon^3\delta}\right) = c_1\nu_1\mathcal{I}_N(1)^3W^6 \epsilon^9(1 - \gamma)^9, \quad (11)$$

42
where $c_1$ is a constant and $\nu_2$ contains log-terms $\nu := \ln \left( \frac{4d\hat{W}^2\mathcal{I}_N(1)}{(1-\gamma)^3e^2d} \right)$.

Since we set known state-action pair as $\phi(s, a) \top \left( \hat{\Sigma}_n^{\text{cov}} \right)^{-1} \phi(s, a) \leq \beta$, then we must have that for any $(s, a) \in \mathcal{K}_n$, we have:

$$\phi(s, a) \top \left( \Sigma_n^{\text{cov}} \right)^{-1} \phi(s, a) \leq 2\beta,$$

and any $(s, a) \notin \mathcal{K}_n$, we have:

$$\phi(s, a) \top \left( \Sigma_n^{\text{cov}} \right)^{-1} \phi(s, a) \geq \frac{1}{2} \beta.$$

This allows us to call Theorem C.2. From Theorem C.2, we know that we need to set $M$ (number of samples for linear regression) large enough such that

$$\varepsilon_{\text{stat}} = \frac{\varepsilon^3(1-\gamma)^3}{4\mathcal{I}_N(1)},$$

Using Lemma G.1 for linear regression, we know that with probability at least $1 - \delta$, for any $n, t$, $\varepsilon_{\text{stat}}$ scales in the order of:

$$\varepsilon_{\text{stat}} = \sqrt{\frac{9W^4\log(NT/\delta)}{(1-\gamma)^4M}},$$

where we have taken union bound over all episodes $n \in [N]$ and all iterations $t \in [T]$. Now solve for $M$, we have:

$$M = \frac{144W^4\mathcal{I}_N(1)^2\ln(NT/\delta)}{\varepsilon^6(1-\gamma)^{10}}$$

Considering every episode $n \in [N]$ and every iteration $t \in [T]$, we have the total number of samples needed for NPG is:

$$NT \cdot M = \frac{4W^2\mathcal{I}_N(1)}{\varepsilon^3(1-\gamma)^3} \times \frac{4W^2\log(A)}{(1-\gamma)^2e^2} \times \frac{144W^4\mathcal{I}_N(1)^2\ln(NT/\delta)}{\varepsilon^6(1-\gamma)^{10}} = \frac{c_2W^8\mathcal{I}_N(1)^3\ln(A)}{\varepsilon^{11}(1-\gamma)^{15}} \cdot \ln \left( \frac{16W^4\ln(A)\mathcal{I}_N(1)}{e^5(1-\gamma)^5\delta} \right) = \frac{c_2\nu_2W^8\mathcal{I}_N(1)^3\ln(A)}{\varepsilon^{11}(1-\gamma)^{15}},$$

where $c_2$ is a positive universal constant, and $\nu_2$ only contains log terms:

$$\nu_2 = \ln \left( \frac{16W^4\ln(A)\mathcal{I}_N(1)}{e^5(1-\gamma)^5\delta} \right).$$

Combine two sources of samples, we have that the total number of samples is bounded as:

$$\frac{c_2\nu_2W^8\mathcal{I}_N(1)^3\ln(A)}{\varepsilon^{11}(1-\gamma)^{15}} + \frac{c_1\nu_2W^6\mathcal{I}_N(1)^3}{\varepsilon^9(1-\gamma)^9},$$

This concludes the proof. \qed
D  Analysis of PC-PG for Linear MDPs (Theorem 4.1)

For linear MDP $\mathcal{M}$, recall that we assume the following parameters’ norms are bounded:

$$
\|u^T \mu\| \leq \xi \in \mathbb{R}^+, \quad \|\theta\| \leq \omega \in \mathbb{R}^+, \quad \forall v, \text{ s.t. } \|v\|_\infty \leq 1.
$$

With these bounds on linear MDP’s parameters, we can show that for any policy $\pi$, we have $Q^\pi(s, a) = w^\pi \cdot \phi(s, a)$, with $\|w^\pi\| \leq \omega + V_{\text{max}} \xi$, where $V_{\text{max}} = \max_{s, \pi} V^\pi(s)$ is the maximum possible expected total value ($V_{\text{max}}$ is at most $r_{\text{max}}/(1 - \gamma)$ with $r_{\text{max}}$ being the maximum possible immediate reward).

At every episode $n$, recall that NPG is optimizing the MDP $\mathcal{M}_{b^n} = \{P, r(s, a) + b^n(s, a)\}$ with $P, r$ being the true transition and reward of $\mathcal{M}$ which is linear under $\phi(s, a)$.

Due to the reward bonus $b^n(s, a)$ in $\mathcal{M}_{b^n}$, $\mathcal{M}_{b^n}$ is not necessarily a linear MDP under $\phi(s, a)$ ($P$ is still linear under $\phi$ but $r(s, a) + b^n(s, a)$ it not linear anymore). Here we leverage an observation that we know $b^n(s, a)$ (as we designed it), and $Q^\pi(s, a; r + b^n) - b^n(s, a)$ is linear with respect to $\phi$ for any $(s, a) \in S \times A$. The following claim state this observation formally.

**Claim D.1** (Linear Property of $(Q^\pi(s, a; r + b^n) - b^n(s, a))$ under $\phi$). Consider any policy $\pi$ and any reward bonus $b^n(s, a) \in [0, 1/(1 - \gamma)]$. We have that:

$$
Q^\pi(s, a; r + b^n) - b^n(s, a) = w \cdot \phi(s, a), \forall s, a.
$$

Further we have $\|w\| \leq \omega + \xi/(1 - \gamma)^2$.

**Proof.** By definition of $Q$-function, we have:

$$
Q^\pi(s, a; r + b^n) = r(s, a) + b^n(s, a) + \gamma \phi(s, a)^T \sum_{s'} \mu(s') V^\pi(s'; r + b^n) \\
= b^n(s, a) + \phi(s, a) \cdot (\theta + \gamma \mu^T V^\pi(\cdot; r + b^n)) := b^n(s, a) + \phi(s, a) \cdot w,
$$

where note that $w$ is independent of $(s, a)$. Rearrange terms, we prove that $Q^\pi(s, a; r + b^n) - b^n(s, a) = w \cdot \phi(s, a)$.

Further, using the norm bounds we have for $\theta$ and $\mu$, and the fact that $\|V^\pi(\cdot; r + b^n)\|_\infty \leq 1/(1 - \gamma)^2$, we conclude the proof. 

The above claim supports our specific choice of critic $\hat{A}^t_{b^n}$ in the algorithm, where we recall that we perform linear regression from $\phi(s, a)$ to $Q^\pi_{b^n}(s, a) - b^n(s, a)$, and set $\hat{A}^t_{b^n}(s, a)$ as

$$
\hat{A}^t_{b^n}(s, a) = (b^n(s, a) + \theta^t \cdot \phi(s, a)) - \mathbb{E}_{a' \sim \pi^t}[b^n(s, a') + \theta^t \cdot \phi(s, a')]
= b^{n,t}(s, a) + \theta^t \cdot \tilde{\phi}^t(s, a),
$$

where $b^{n,t}(s, a) = b^n(s, a) - \mathbb{E}_{a' \sim \pi^t} b^n(s, a'),$ and $\tilde{\phi}^t(s, a) = \phi(s, a) - \mathbb{E}_{a' \sim \pi^t} \phi(s, a')$.

We now prove [Theorem 4.1] by showing that $\epsilon_{\text{bias}}$ is zero.

**Lemma D.1.** Consider Assumption 4.1. For any episode $n$, iteration $t$, we have $\epsilon_{\text{bias}} = 0$. 

44
Proof. At iteration $t$, denote $\theta^*_t$ as the linear parameterization of $Q^t_{\theta^n}(s, a) - b^n(s, a)$, i.e., $\theta^*_t \cdot \phi(s, a) = Q^t_{\theta^n}(s, a) - b^n(s, a)$ (see Claim D.1 for the existence of $\theta^*_t$). We know that $\theta^*_t \in \argmin_{\theta \in \mathbb{R}^d} L(\theta; \rho^n, Q^t_{\theta^n} - b^n)$, as $L(\theta^*_t; \rho^n, Q^t_{\theta^n} - b^n) = 0$. This indicates that $\theta^*_t$ is one of the best on-policy fit. Now when transfer $\theta^*_t$ to a different distribution $d^n \pi^* \mathcal{Unif}_A$, we simply have:

$$\mathbb{E}_{(s,a) \sim d^n \pi^* \mathcal{Unif}_A} \left( \theta^*_t \cdot \phi(s, a) - (Q^t_{\theta^n}(s, a) - b^n(s, a)) \right)^2 = 0.$$ 

This concludes the proof.

We can now conclude the proof of Theorem 4.1 by invoking Theorem 4.3 with $\epsilon_{bias} = 0$. \qed

## E Analysis of PC-PG for State-Aggregation (Theorem 4.2)

In this section, we analyze Theorem 4.2 for state-aggregation. Similar to the analysis for linear MDP, we provide a variance bias tradeoff lemma that is analogous to Lemma C.1. However, unlike linear MDP, here due to model-misspecification from state-aggregation, the transfer error $\epsilon_{bias}$ will not be zero. But we will show that the transfer error is related to a term that is an expected model-misspecification averaged over a fixed comparator’s state distribution.

First recall the definition of state aggregation $\phi : S \times A \rightarrow \mathbb{Z}$. We abuse the notation a bit, and denote $\phi(s, a) = 1\{\phi(s, a) = z\} \in \mathbb{R}^{\mathbb{Z}}$, i.e., the feature vector $\phi$ indicates which $z$ the state action pair $(s, a)$ is mapped to. The following claim reasons the approximation of $Q$ values under state aggregation.

**Claim E.1.** Consider any MDP with transition $P$ and reward $r$. Denote aggregation error $\epsilon_z$ as:

$$\max \{\|P(\cdot|s, a) - P(\cdot|s', a')\|_1, |r(s, a) - r(s', a')|\} \leq \epsilon_z, \forall (s, a), (s', a'), \text{ s.t., } \phi(s, a) = \phi(s', a') = z.$$

Then, for any policy $\pi, (s, a), (s', a'), z$, such that $\phi(s, a) = \phi(s', a') = z$, we have:

$$|Q^\pi(s, a) - Q^\pi(s', a')| \leq \frac{r_{max} \epsilon_z}{1 - \gamma},$$

where $r(s, a) \in [0, r_{max}]$ for $r_{max} \in \mathbb{R}^+$.

**Proof.** Starting from the definition of $Q^\pi$, we have:

$$|Q^\pi(s, a) - Q^\pi(s', a')| = |r(s, a) - r(s', a')| + \gamma |\mathbb{E}_{x' \sim P_{s,a}} V^\pi(s') - \mathbb{E}_{x' \sim P_{s',a'}} V^\pi(s')|$$

$$\leq \epsilon_z + \frac{r_{max} \gamma}{1 - \gamma} \|P_{s,a} - P_{s',a'}\|_1 \leq \frac{r_{max} \epsilon_z}{1 - \gamma},$$

where we use the assumption that $\phi(s, a) = \phi(s', a') = z$, and the fact that value function $\|V\|_\infty \leq r_{max}/(1 - \gamma)$ as $r(s, a) \in [0, r_{max}]$. \qed

Now we state the bias and variance tradeoff lemma for state aggregation.

\}
Lemma E.1 (Bias and Variance Tradeoff for State Aggregation). Set $W := \sqrt{|\mathcal{Z}|}/(1 - \gamma)^2$. Consider any episode $n$. Assume that we have $\phi(s, a) \perp (\Sigma^{n}_{cov})^{-1} \phi(s, a) \leq \beta \in \mathbb{R}^+$ for $(s, a) \in \mathcal{K}^n$, and the following condition is true for all $t \in \{0, \ldots, T - 1\}$:

$$L^t(\theta^t; \rho^t_{cov}, Q^t_{b^n} - b^n) \leq \min_{\theta: ||\theta|| \leq W} L^t(\theta; \rho^t_{cov}, Q^t_{b^n} - b^n) + \epsilon_{stat} \in \mathbb{R}^+.$$ 

We have that for all $t \in \{0, \ldots, T - 1\}$ at episode $n$:

$$\mathbb{E}_{(s,a) \sim \tilde{d}_{stat}} \left( A^t_{b^n}(s, a) - \hat{A}^t_{b^n}(s, a) \right) 1\{s \in \mathcal{K}^n\} \leq 2\sqrt{\beta}(W^2 + 2\sqrt{\beta \epsilon_{stat}} + \frac{2\mathbb{E}_{(s,a) \sim \tilde{d}^2} \max_a [\epsilon_{\phi(s,a)}]}{(1 - \gamma)^2}.$$ 

Note that comparing to Lemma C.1, the above lemma replaces $\sqrt{\Lambda_{bias}}$ by the average model-misspecification $\mathbb{E}_{(s,a) \sim \tilde{d}^2} \max_a [\epsilon_{\phi(s,a)}]$. 

Proof. We first compute one of the minimizers of $L^t(\theta; \rho^t_{cov}, Q^t_{b^n} - b^n)$. Recall the definition of $L^t(\theta; \rho^t_{cov}, Q^t_{b^n} - b^n)$, we have:

$$\mathbb{E}_{(s,a) \sim \rho^{n}_{cov}} \left( \theta \cdot \phi(s, a) - Q^{n}_{b^n}(s, a) + b^n(s, a) \right)^2 = \mathbb{E}_{(s,a) \sim \rho^{n}_{cov}} \sum_z 1\{\phi(s, a) = z\} \left( \theta_z - Q^{n}_{b^n}(s, a) + b^n(s, a) \right)^2,$$

which means that for $\theta^*_{z}$, we have:

$$\sum_{s,a} \rho^{n}_{cov}(s, a) 1\{\phi(s, a) = z\} \left( \theta_z - Q^{n}_{b^n}(s, a) + b^n(s, a) \right) = 0,$$

which implies that $\theta^*_{z} := \frac{\sum_{s,a} \rho^{n}_{cov}(s, a) 1\{\phi(s, a) = z\} \left( Q^{n}_{b^n}(s, a) - b^n(s, a) \right)}{\sum_{s,a} \rho^{n}_{cov}(s, a) 1\{\phi(s, a) = z\}}$. Note that $|\theta^*_{z}| \leq \frac{1}{(1 - \gamma)^2}$, hence $||\theta^*||_2 \leq \sqrt{|\mathcal{Z}|}/(1 - \gamma)^2 := W$.

Hence, for any $s''', a'''$ such that $\phi(s''', a''') = z$, we must have:

$$\left| \theta^*_{z} - (Q^{n}_{b^n}(s''', a''') - b^n(s''', a''')) \right| = \left| \sum_{s,a} \rho^{n}_{cov}(s, a) 1\{\phi(s, a) = z\} \left( Q^{n}_{b^n}(s, a) - b^n(s, a) \right) - Q^{n}_{b^n}(s''', a''') + b^n(s''', a''') \right| \leq \frac{\epsilon_z}{(1 - \gamma)^2},$$

where we use Claim E.1 and the fact that $r(s, a) + b^n(s, a) \in [0, 1/(1 - \gamma)]$, and the fact that $b^n(s, a) = b^n(s''', a''')$ if $\phi(s, a) = \phi(s''', a''')$ as the bonus is defined under feature $\phi$. 

46
With \( \theta^* \) and its optimality condition for loss \( L^t(\theta; \rho^n_{\text{cov}}) \), we can prove the same point-wise estimation guarantee, i.e., for any \((s, a) \in \mathcal{K}^n\), we have:

\[
\left| \phi(s, a) \cdot (\theta^t - \theta^*_a) \right| \leq \sqrt{\beta n \epsilon_{\text{stat}}} + \lambda W^2.
\]

Now we bound \( \mathbb{E}_{(s,a)\sim \tilde{d}_{\mathcal{M}^n}} \left( A^n_{b^n}(s, a) - \tilde{A}^t_{b^n}(s, a) \right) 1\{s \in \mathcal{K}^n\} \) as follows.

\[
= \mathbb{E}_{(s,a)\sim \tilde{d}_{\mathcal{M}^n}} \left( A^n_{b^n}(s, a) - \tilde{b}^n(s, a) - \theta^t_a \cdot \tilde{\phi}(s, a) \right) 1\{s \in \mathcal{K}^n\} + \mathbb{E}_{(s,a)\sim \tilde{d}_{\mathcal{M}^n}} (\theta^*_a \cdot \tilde{\phi}(s, a) - \theta^t_a \cdot \tilde{\phi}(s, a)) 1\{s \in \mathcal{K}^n\}.
\]

Again, for term B, we can use the point-wise estimation error to bound it as:

\[
\text{term B} \leq 2\sqrt{\beta \lambda W^2} + 2\sqrt{\beta n \epsilon_{\text{stat}}}.
\]

For term A, we have:

\[
\mathbb{E}_{(s,a)\sim \tilde{d}_{\mathcal{M}^n}} \left( A^n_{b^n}(s, a) - \tilde{b}^n(s, a) - \theta^t_a \cdot \tilde{\phi}(s, a) \right) 1\{s \in \mathcal{K}^n\} \\
\leq \mathbb{E}_{(s,a)\sim \tilde{d}_{\mathcal{M}^n}} |Q^n_{b^n}(s, a) - b^n(s, a) - \theta^*_a \cdot \phi(s, a)| 1\{s \in \mathcal{K}^n\} \\
+ \mathbb{E}_{s\sim \tilde{d}_{\mathcal{M}^n}, a\sim \pi^*_t} \left| Q^n_{b^n}(s, a) - b^n(s, a) + \theta^*_a \cdot \phi(s, a) \right| 1\{s \in \mathcal{K}^n\} \\
\leq \mathbb{E}_{(s,a)\sim \bar{d}} \left| Q^n_{b^n}(s, a) - b^n(s, a) - \theta^*_a \cdot \phi(s, a) \right| + \mathbb{E}_{s\sim \bar{d}, a\sim \pi^*_t} \left| Q^n_{b^n}(s, a) - b^n(s, a) + \theta^*_a \cdot \phi(s, a) \right|,
\]

where last inequality uses Lemma B.1 for \( s \in \mathcal{K}^n \) to switch from \( \tilde{d}_{\mathcal{M}^n} \) to \( \bar{d} \) — the state-action distribution of the comparator \( \tilde{\pi} \) in the real MDP \( \mathcal{M} \).

Note that for any \( d \in S \times A \), we have:

\[
\mathbb{E}_{(s,a)\sim \bar{d}} \left| Q^n_{b^n}(s, a) - b^n(s, a) - \theta^*_a \cdot \phi(s, a) \right| \\
\leq \sum_z \mathbb{E}_{(s,a)\sim \bar{d}} 1\{\phi(s, a) = z\} \left| Q^n_{b^n}(s, a) - b^n(s, a) - \theta^*_a \cdot \phi(s, a) \right| \leq \mathbb{E}_{(z)\sim \bar{d}} \frac{\epsilon_z}{(1 - \gamma)^2} = \frac{\mathbb{E}_{(s,a)\sim \bar{d}} \epsilon_{\phi(s,a)}}{(1 - \gamma)^2}.
\]

With this, we have:

\[
\text{term A} \leq \mathbb{E}_{(s,a)\sim \bar{d}} \left| Q^n_{b^n}(s, a) - b^n(s, a) - \theta^*_a \cdot \phi(s, a) \right| + \mathbb{E}_{s\sim \bar{d}, a\sim \pi^*_t} \left| -Q^n_{b^n}(s, a) + b^n(s, a) + \theta^*_a \cdot \phi(s, a) \right| \\
\leq \mathbb{E}_{s\sim \bar{d}} \max_a \left| Q^n_{\pi^*_t}(s, a) - b^n(s, a) - \theta^*_a \cdot \phi(s, a) \right| + \mathbb{E}_{s\sim \bar{d}} \max_a \left| -Q^n_{\pi^*_t}(s, a) + b^n(s, a) + \theta^*_a \cdot \phi(s, a) \right| \\
\leq 2 \left( \mathbb{E}_{s\sim \bar{d}} \max_a \left| Q^n_{b^n}(s, a) - b^n(s, a) - \theta^*_a \cdot \phi(s, a) \right| \right) \leq \frac{2 \mathbb{E}_{s\sim \bar{d}} \max_a \epsilon_{\phi(s,a)}}{(1 - \gamma)^2}.
\]

Combine term A and term B, we conclude the proof.

The rest of the proof of Theorem 4.2 is almost identical to the proof of Theorem C.1 with \( \sqrt{A \epsilon_{\text{bias}}} \) in Theorem C.1 being replaced by \( \frac{2 \mathbb{E}_{s\sim \bar{d}} \max_a \epsilon_{\phi(s,a)}}{(1 - \gamma)^2} \).
F Analysis of PC-PG for the Partially Well-specified Models (Corollary 4.1)

Proof of Corollary 4.1 The proof involves showing that the transfer error is 0. Specifically, we will show the following: consider any state-action distribution $\rho$, and any policy $\pi$, and any bonus function $b$ with bounded value on all $b(s,a)$, there exists $\theta_*$ as one of the best on-policy fit, i.e., $\theta_* \in \arg \min_{\theta,||\theta||\leq W} \mathbb{E}_{(s,a) \sim \rho} (\theta \cdot \phi(s,a) - (Q^\pi(s,a) - b(s,a)))^2$, such that:

$$
\mathbb{E}_{(s,a) \sim d^\pi} (Q^\pi(s,a) - b(s,a) - \theta_* \cdot \phi(s,a))^2 = 0,
$$
i.e., the transfer error is zero.

Let us denote a minimizer of $\mathbb{E}_{(s,a) \sim \rho} (\theta \cdot \phi(s,a) - b(s,a) - Q^\pi(s,a))^2$ as $\tilde{\theta}$. We can modify the first three bits of $\tilde{\theta}$. We set $\tilde{\theta}_1 = Q^\pi(s_0, L) - b(s_0, L) = 1/2 - b(s_0, L)$, $\tilde{\theta}_2 = Q^\pi(s_0, R) - b(s_0, R)$, and $\tilde{\theta}_3 = Q^\pi(s_1, a) - b(s_1, a) = -b(s_1, a)$ for any $a \in \{L, R\}$. Denote this new vector as $\theta_*$. Note that due to the construction of $\phi$ (the feature vectors associated with states inside the binary tree is orthogonal to the span of $\phi$), we can verify that $\theta_*$ is also the minimizer of $\mathbb{E}_{(s,a) \sim \rho} (\theta \cdot \phi(s,a) - (Q^\pi(s,a) - b(s,a)))^2$.

For $\theta_*$, we have $\theta_* \cdot \phi(s_0, a) = Q^\pi(s_0, a) - b(s_0, a)$ for $a \in \{L, R\}$, and $\theta_* \cdot \phi(s_1, a) = Q^\pi(s_1, a) - b(s_1, a)$ for $a \in \{L, R\}$, thus, we can verify that $Q^\pi(s_0, a) - b(s_0, a) = \theta_* \cdot \phi(s_0, a)$ and $Q^\pi(s_1, a) - b(s_1, a) = \theta_* \cdot \phi(s_1, a)$ for $a \in \{L, R\}$. Since $\pi^*$ only visits $s_0$ and $s_1$, we can conclude that $\mathbb{E}_{(s,a) \sim d^\pi} (Q^\pi(s,a) - b(s,a) - \theta_* \cdot \phi(s,a))^2 = 0$.

With $\varepsilon_{bias} = 0$, we can conclude the proof by recalling Theorem C.1.

G Auxiliary Lemmas

Lemma G.1 (Dimension-free Least Square Guarantees). Consider the following learning process. Initialize $\theta_0 = 0$. For $i = 1, \ldots, N$, draw $x_i, y_i \sim \nu$, $y_i \in [0, H]$, $\|x_i\| \leq 1$; Set $\theta_{i+1} = \prod_{\eta_i = \{\theta, ||\theta|| \leq W\}} (\theta_i - \eta_i(\theta_i \cdot x - y_i)x_i)$ with $\eta_i = (W^2)/((W + H)\sqrt{N})$. Set $\theta = \frac{1}{N} \sum_{i=1}^{N} \theta_i$, we have that with probability at least $1 - \delta$:

$$
\mathbb{E}_{x \sim \nu} \left[ (\theta \cdot x - \mathbb{E} [y|x])^2 \right] \leq \mathbb{E}_{x \sim \nu} \left[ (\theta^* \cdot x - \mathbb{E} [y|x])^2 \right] + \frac{R \sqrt{\ln(1/\delta)}}{\sqrt{N}},
$$

with any $\theta^*$ such that $\|\theta^*\| \leq W$ and $R = 3(W^2 + WH)$ which is dimension free and only depends on the norms of the feature and $\theta^*$ and the bound on $y$.

Proof. Note that we compute $\theta_i$ using Projected Online Gradient Descent [Zinkevich, 2003] on the sequence of loss functions $(\theta \cdot x_i - y_i)^2$. Using the projected online gradient descent regret guarantee, we have that:

$$
\sum_{i=1}^{N} (\theta_i \cdot x_i - y_i)^2 \leq \sum_{i=1}^{N} (\theta^* \cdot x_i - y_i)^2 + R(W + H) \sqrt{N}.
$$
Denote random variable \( z_i = (\theta_i \cdot x_i - y_i)^2 - (\theta^* \cdot x_i - y_i)^2 \). Denote \( \mathbb{E}_i \) as the expectation taken over the randomness at step \( i \) conditioned on all history \( t = 1 \) to \( i - 1 \). Note that for \( \mathbb{E}_i[z_i] \), we have:

\[
\mathbb{E}_i \left[ (\theta_i \cdot x - y)^2 - (\theta^* \cdot x - y)^2 \right] = \mathbb{E}_i \left[ (\theta_i \cdot x - \mathbb{E}[y|x])^2 \right] - \mathbb{E}_i \left[ 2(\theta_i \cdot x - \mathbb{E}[y|x])(\mathbb{E}[y|x] - y) - (\theta^* \cdot x - \mathbb{E}[y|x])^2 + 2(\theta^* \cdot x - \mathbb{E}[y|x])(\mathbb{E}[y|x] - y) \right] = \mathbb{E}_i \left[ (\theta_i \cdot x - \mathbb{E}[y|x])^2 - (\theta^* \cdot x - \mathbb{E}[y|x])^2 \right],
\]

where we use \( \mathbb{E}[\mathbb{E}[y|x] - y] = 0 \). Also for \( |z_i| \), we can show that for \( |z_i| \) we have:

\[
|z_i| = |(\theta_i \cdot x_i - \theta^* \cdot x_i)(\theta_i \cdot x_i + \theta^* \cdot x_i - 2y_i)| \leq W(2W + 2H) = 2W(W + H).
\]

Note that \( z_i \) forms a Martingale difference sequence. Using Azuma-Hoeffding’s inequality, we have that with probability at least \( 1 - \delta \):

\[
\left| \sum_{i=1}^{N} z_i - \sum_{i=1}^{N} \mathbb{E}_i \left[ (\theta_i \cdot x - \mathbb{E}[y|x])^2 - (\theta^* \cdot x - \mathbb{E}[y|x])^2 \right] \right| \leq 2W(W + H)\sqrt{\ln(1/\delta)N},
\]

which implies that:

\[
\sum_{i=1}^{N} \mathbb{E}_i \left[ (\theta_i \cdot x - \mathbb{E}[y|x])^2 - (\theta^* \cdot x - \mathbb{E}[y|x])^2 \right] \leq \sum_{i=1}^{N} z_i + 2W(W + H)\sqrt{\ln(1/\delta)N}
\]

\[
\leq 2W(W + H)\sqrt{\ln(1/\delta)N} + Q\sqrt{N}.
\]

Apply Jensen’s inequality on the LHS of the above inequality, we have that:

\[
\mathbb{E} \left( \theta \cdot x - \mathbb{E}[y|x] \right)^2 \leq \mathbb{E} \left( \theta^* \cdot x - \mathbb{E}[y|x] \right)^2 + (Q + 2W(W + H))\sqrt{\frac{\ln(1/\delta)}{N}}.
\]

\[\square\]

**Lemma G.2.** Consider the following process. For \( n = 1, \ldots, N, M_n = M_{n-1} + \Sigma_n \) with \( M_0 = \lambda I \) and \( \Sigma_n \) being PSD matrix with eigenvalues upper bounded by 1. We have that:

\[
2 \log \det(M_N) - 2 \log \det(\lambda I) \geq \sum_{n=1}^{N} \text{Tr} \left( \Sigma_i M_{i-1}^{-1} \right).
\]

**Proof.** Note that \( M_0 \) is PD, and since \( \Sigma_n \) is PSD for all \( n \), we must have \( M_n \) being PD as well. Using matrix inverse lemma, we have:

\[
\det(M_{n+1}) = \det(M_n) \det(I + M_n^{-1/2}\Sigma_{n+1}M_n^{-1/2}).
\]

Add log on both sides of the above equality, we have:

\[
\log \det(M_{n+1}) = \log \det(M_n) + \log \det(I + M_n^{-1/2}\Sigma_{n+1}M_n^{-1/2}).
\]
Denote the eigenvalues of $M_{n+1}^{-1/2} \Sigma_{n+1} M_{n+1}^{-1/2}$ as $\sigma_1, \ldots, \sigma_d$, we have:

$$\log \det(M_{n+1}) = \log \det(M_n) + \sum_{i=1}^d \log(1 + \sigma_i)$$

Note that $\sigma_i \leq 1$, and we have $\log(1 + x) \geq x/2$ for $x \in [0, 1]$. Hence, we have:

$$\log \det(M_{n+1}) \geq \log \det(M_n) + \sum_{i=1}^d \sigma_i/2 = \log \det(M_n) + \frac{1}{2} \text{Tr} \left( M_n^{-1/2} \Sigma_{n+1} M_n^{-1/2} \right)$$

$$= \log \det(M_n) + \frac{1}{2} \text{Tr} \left( \Sigma_{n+1} M_n^{-1} \right),$$

where we use the fact that $\text{Tr}(AB) = \text{Tr}(BA)$ and the trace of PSD matrix is the sum of its eigenvalues. Sum over from $n = 0$ to $N$ and cancel common terms, we conclude the proof. □

**Lemma G.3** (Covariance Matrix Concentration). Given $\nu \in \Delta(\mathcal{S} \times \mathcal{A})$ and $N$ i.i.d samples \{s_i, a_i\} ∼ ν. Denote $\Sigma = \mathbb{E}_{(s, a) \sim \nu} \phi(s, a) \phi(s, a)\top$ and $X_i = \phi(s_i, a_i) \phi(s_i, a_i)\top$ and $X = \sum_{i=1}^N X_i$. Note that $N\Sigma = \mathbb{E}[X] = \sum_{i=1}^N \mathbb{E}[X_i]$. Then, with probability at least $1 - \delta$, we have that:

$$\left| x\top \left( \sum_{i=1}^N \phi(s_i, a_i) \phi(s_i, a_i)\top / N - \Sigma \right) x \right| \leq \frac{2 \ln(4\tilde{d}/\delta)}{3N} + \sqrt{\frac{2 \ln(4\tilde{d}/\delta)}{N}},$$

with $\tilde{d} = \text{Tr}(\Sigma)/\|\Sigma\|$ being the intrinsic dimension of $\Sigma$.

**Proof.** Denote random matrix $X_i = \phi(s_i, a_i) \phi(s_i, a_i)\top - \Sigma$. Note that the maximum eigenvalue of $X_i$ is upper bounded by 1. Also note that $\mathbb{E}[X_i] = 0$ for all $i$. Denote $V = \sum_{i=1}^N \mathbb{E}[X_i^2]$. For any $i$, consider $X_i^2$. Denote the eigendecomposition of $X_i$ as $U_i \Lambda_i U_i\top$. We have $X_i^2 = U_i \Lambda_i^2 U_i\top$. Note that the maximum absolute value of the eigenvalues of $X_i$ is bounded by 1. Hence the maximum eigenvalue of $X_i^2$ is bounded by 1 as well. Hence $\mathbb{E}[X_i^2]$’s maximum eigenvalue is also upper bounded by 1. This implies that $\|V\| \leq N$.

Now apply Matrix Bernstein inequality [Tropp et al., 2015], we have that for any $t \geq \sqrt{N} + 1/3$,

$$\Pr \left( \sigma_{\text{max}} \left( \sum_{i=1}^N X_i \right) \geq t \right) \leq 4\tilde{d} \exp \left( \frac{-t^2/2}{N + t/3} \right).$$

Since $\sigma_{\text{max}} \left( \sum_{i=1}^N X_i \right) = N \sigma_{\text{max}} \left( \sum_{i=1}^N X_i/N \right)$, we get that:

$$\Pr \left( \sigma_{\text{max}} \left( \sum_{i=1}^N X_i/N \right) \geq \epsilon \right) \leq 4\tilde{d} \exp \left( \frac{-\epsilon^2 N/2}{1 + \epsilon/3} \right),$$

for any $\epsilon \geq 1/\sqrt{N} + 1/3N$. Set $4d \exp(-\epsilon^2 N/(2(1 + \epsilon/3))) = \delta$, we get:

$$\epsilon = \frac{2 \ln(4\tilde{d}/\delta)}{3N} + \sqrt{\frac{2 \ln(4\tilde{d}/\delta)}{N}},$$

50
which is trivially bigger than $1/\sqrt{N} + 1/(3N)$ as long as $d \geq 1$ and $\delta \leq 1$. This concludes that with probability at least $1 - \delta$, we have:

$$
\sigma_{\max} \left( \sum_{i=1}^{N} \phi(s_i, a_i)\phi(s_i, a_i)^{T} / N - \Sigma \right) \leq \frac{2 \ln(4d/\delta)}{3N} + \sqrt{\frac{2 \ln(4d/\delta)}{N}}.
$$

We can repeat the same analysis for random matrices $\{X_i := \Sigma - \phi(s_i, a_i)\phi(s_i, a_i)^{T}\}$ and we can show that with probability at least $1 - \delta$, we have:

$$
\sigma_{\max} \left( \Sigma - \sum_{i=1}^{N} \phi(s_i, a_i)\phi(s_i, a_i)^{T} / N \right) \leq \frac{2 \ln(4d/\delta)}{3N} + \sqrt{\frac{2 \ln(4d/\delta)}{N}}.
$$

Hence, with probability $1 - \delta$, for any $x$, we have:

$$
x^T \left( \Sigma - \sum_{i=1}^{N} \phi(s_i, a_i)\phi(s_i, a_i)^{T} / N \right) x \leq \frac{2 \ln(32d/\delta)}{3N} + \sqrt{\frac{2 \ln(32d/\delta)}{N}},
$$

$$
x^T \left( \sum_{i=1}^{N} \phi(s_i, a_i)\phi(s_i, a_i)^{T} / N - \Sigma \right) x \leq \frac{2 \ln(32d/\delta)}{3N} + \sqrt{\frac{2 \ln(32d/\delta)}{N}}.
$$

This concludes the proof.

**Lemma G.4** (Concentration with the Inverse of Covariance Matrix). Consider a fixed $N$. Given $N$ distributions $\nu_1, \ldots, \nu_N$ with $\nu_i \in \Delta(S \times A)$, assume we draw $K$ i.i.d samples from $\nu_i$ and form $\hat{\Sigma}^i = \sum_{j=1}^{K} \phi_j \phi_j^T / K$ for all $i$. Denote $\Sigma = \sum_{i=1}^{N} \mathbb{E}_{(s,a) \sim \nu_i} \phi(s,a)\phi(s,a)^{T} + \lambda I$ and $\hat{\Sigma} = \sum_{i=1}^{N} \hat{\Sigma}^i + \lambda I$ with $\lambda \in (0,1]$. Setting $K = 32N^2 \log \left( \frac{8Nd}{\delta} \right) / \lambda^2$, with probability at least $1 - \delta$, we have:

$$
\frac{1}{2} x^T (\Sigma + \lambda I)^{-1} x \leq x^T (\hat{\Sigma} + \lambda I)^{-1} x \leq 2x^T (\Sigma + \lambda I)^{-1} x,
$$

for all $x$ with $\|x\|_2 \leq 1$.

**Proof.** Denote $\Sigma^i = \mathbb{E}_{(s,a) \sim \nu_i} \phi(x_i, a_i)\phi(x_i, a_i)^{T}$. Denote $\eta(K) = \frac{2 \ln(8Nd/\delta)}{3K} + \sqrt{\frac{2 \ln(8Nd/\delta)}{K}}$. From Lemma G.3 we know that with probability $1 - \delta$, for all $i$, we have:

$$
\Sigma^i + \eta(K)I + (\lambda/N)I \succeq \hat{\Sigma}^i + (\lambda/N)I \succeq \Sigma^i - \eta(K)I + (\lambda/N)I,
$$

which implies that:

$$
\Sigma + N\eta(K)I + \lambda I \succeq \hat{\Sigma} + \lambda I \succeq \Sigma - N\eta(K)I + \lambda I,
$$

which further implies that:

$$
(\Sigma - N\eta(K)I + \lambda I)^{-1} \succeq (\hat{\Sigma} + \lambda I)^{-1} \succeq (\Sigma + N\eta(K)I + \lambda I)^{-1},
$$
under the condition that \( N\eta(K) \leq \lambda \) which holds under the condition of \( K \). Let \( U\Lambda U^\top \) be the eigendecomposition of \( \Sigma \).

\[
\begin{align*}
    x^\top \left( \hat{\Sigma} + \lambda I \right)^{-1} x - x^\top (\Sigma + \lambda I)^{-1} x \\
    = \sum_i \left( (\sigma_i + \lambda - N\eta(K))^{-1} - (\sigma_i + \lambda)^{-1} \right) (x \cdot u_i)^2
\end{align*}
\]

Since \( \sigma_i + \lambda \geq 2N\eta(K) \) as \( \sigma_i \geq 0 \) and \( N\eta(K) \leq \lambda / 2 \), we have that \( 2(\sigma_i + \lambda - N\eta(K)) \geq \sigma_i + \lambda \), which implies that \( (1/2)(\sigma_i + \lambda - K\eta(N))^{-1} \leq (\sigma_i + \lambda)^{-1} \). Hence, we have:

\[
x^\top \left( \hat{\Sigma} + \lambda I \right)^{-1} x - x^\top (\Sigma + \lambda I)^{-1} x \leq \sum_{i=1}^n (u_i \cdot x)^2 (\sigma_i + \lambda)^{-1} = x^\top (\Sigma + \lambda I)^{-1} x.
\]

The analysis for the other direction is similar. This concludes the proof. \( \square \)

## H Experimental Details

### H.1 Algorithm Implementation

We implemented two versions of the algorithm: one with a reward bonus which is added to the environment reward (shown in Algorithm 4), and one which performs reward-free exploration, optionally followed by reward-based exploitation using the policy cover as a start distribution (shown in Algorithm 5).

Both of these use NPG as a subroutine, which performs policy optimization using the restart distribution induced by a policy mixture \( \Pi_{\text{mix}} \). The implementation of NPG is described in Algorithm 6. We sample states from the restart distribution by randomly sampling a roll-in policy from the cover and a horizon length \( h' \), and following the sampled policy for \( h' \) steps. Rewards gathered during these roll-in steps are not used for optimization. With probability \( \epsilon \), a random action is taken at the beginning of the rollout. We then roll out using the current policy being optimized, and use the rewards gathered for optimization. The policy parameters can be updated using any policy gradient method, we used PPO [Schulman et al., 2017] in our experiments.

For all experiments, we optimized the policy mixture weights \( \alpha_1, \ldots, \alpha_n \) at each episode using 2000 steps of gradient descent, using an Adam optimizer and a learning rate of 0.001. All implementations are done in PyTorch [Paszke et al., 2019], and build on the codebase of [Shangtong, 2018]. Experiments were run on a GPU cluster which consisted of a mix of 1080Ti, TitanV, K40, P100 and V100 GPUs.

### H.2 Environments

#### H.2.1 Bidirectional Diabolical Combination Lock

The environment consists of a start state \( s_0 \) where the agent is placed (deterministically) at the beginning of every episode. The action space consists of 10 discrete actions, \( \mathcal{A} = \{1, 2, \ldots, 10\} \). In
Algorithm 4 PC-PG (reward bonus version)

1: Require: kernel function $\phi : S \times A \to \mathbb{R}^d$
2: Initialize policy $\pi_1$ randomly
3: Initialize policy mixture $\Pi_{\text{mix}} \leftarrow \{\pi_1\}$
4: Initialize episode buffer: $\mathcal{R} \leftarrow \emptyset$
5: for episode $n = 1, \ldots K$ do
6:   for trajectory $k = 1, \ldots K$ do
7:     Gather trajectory $\tau_k = \{s_h^{(k)}, a_h^{(k)}\}_{h=1}^H$ following $\pi_n$
8:     $\mathcal{R} \leftarrow \mathcal{R} \cup \{(s_h^{(k)}, a_h^{(k)})\}_{h=1}^H$
9:   end for
10: Compute empirical covariance matrix: $\hat{\Sigma}_n = \sum_{(s,a) \in \mathcal{R}} \phi(s,a)\phi(s,a)^\top$
11: Define exploration bonus: $b_n(s,a) = \phi(s,a)^\top \hat{\Sigma}_n^{-1} \phi(s,a)$
12: Optimize policy mixture weights: $\alpha^{(n)} = \arg\min_{\alpha=(\alpha_1,\ldots,\alpha_n),\alpha_i \geq 0,\sum_i \alpha_i = 1} \log \det \left[ \sum_{i=1}^n \alpha_i \hat{\Sigma}_i \right]$  
13: $\pi_{n+1} \leftarrow \text{NPG}(\pi_n, \Pi_{\text{mix}}, \alpha^{(n)}, N_{\text{update}}, r + b_n)$
14: $\Pi_{\text{mix}} \leftarrow \Pi_{\text{mix}} \cup \{\pi_{n+1}\}$
15: end for

Algorithm 5 PC-PG (reward-free exploration version)

1: Require: kernel function $\phi : S \times A \to \mathbb{R}^d$
2: Initialize policy $\pi_1$ randomly
3: Initialize policy mixture $\Pi_{\text{mix}} \leftarrow \{\pi_1\}$
4: Initialize episode buffer: $\mathcal{R} \leftarrow \emptyset$
5: for episode $n = 1, \ldots K$ do
6:   for trajectory $k = 1, \ldots K$ do
7:     Gather trajectory $\tau_k = \{s_h^{(k)}, a_h^{(k)}\}_{h=1}^H$ following $\pi_n$
8:     $\mathcal{R} \leftarrow \mathcal{R} \cup \{(s_h^{(k)}, a_h^{(k)})\}_{h=1}^H$
9:   end for
10: Compute empirical covariance matrix: $\hat{\Sigma}_n = \sum_{(s,a) \in \mathcal{R}} \phi(s,a)\phi(s,a)^\top$ 
11: Define exploration bonus: $b_n(s,a) = \phi(s,a)^\top \hat{\Sigma}_n^{-1} \phi(s,a)$
12: Optimize policy mixture weights: $\alpha^{(n)} = \arg\min_{\alpha=(\alpha_1,\ldots,\alpha_n),\alpha_i \geq 0,\sum_i \alpha_i = 1} \log \det \left[ \sum_{i=1}^n \alpha_i \hat{\Sigma}_i \right]$  
13: $\pi_{n+1} \leftarrow \text{NPG}(\pi_n, \Pi_{\text{mix}}, \alpha^{(n)}, N_{\text{update}})$
14: $\Pi_{\text{mix}} \leftarrow \Pi_{\text{mix}} \cup \{\pi_{n+1}\}$
15: end for
16: Initialize policy $\pi_{\text{exploit}}$ randomly
17: $\pi_{\text{exploit}} \leftarrow \text{NPG}(\pi_{\text{exploit}}, \Pi_{\text{mix}}, \alpha^{(K)}, N_{\text{update}}, r)$

$s_0$, actions $1-5$ lead the agent to the initial state of the first lock and actions $6-10$ lead the agent to the initial state of the second lock. Each lock $l$ consists of $3H$ states, indexed by $s_{1,l}^h, s_{2,l}^h, s_{3,l}^h$ for $h \in \{1,\ldots,H\}$. A high reward of $R_l$ is obtained at the last states $s_{1,l}^H, s_{2,l}^H$. The states $\{s_{3,l}^h\}_{h=1}^H$
Algorithm 6 NPG(\(\pi, \Pi_{\text{mix}}, \alpha, N_{\text{update}}, r\))

1: **Input** policy \(\pi\), policy mixture \(\Pi_{\text{mix}} = \{\pi_1, \ldots, \pi_n\}\), mixture weights \((\alpha_1, \ldots, \alpha_n)\), optional reward bonus \(b : S \times A \rightarrow [0, 1]\)

2: **for** policy update \(j = 1, \ldots, N_{\text{update}}\) **do**

3: Sample roll in policy index \(j \sim \text{Multinomial}\{\alpha_1, \ldots, \alpha_n\}\)

4: Sample roll in horizon index \(h' \sim \text{Uniform}\{0, \ldots, H - 1\}\)

5: Sample start state \(s_0 \sim P(s_0)\)

6: **for** \(h = 1, \ldots, h'\) **do**

7: \(a_h \sim \pi_j(s_h)\), \(s_{h+1} \sim P(\cdot|s_h, a_h)\)

8: **end for**

9: **for** \(h = h' + 1, \ldots, H\) **do**

10: \(a_h \sim \pi(\cdot|s_h)\) (\(\epsilon\)-greedy if \(h = h' + 1\))

11: \(s_{h+1}, r_{h+1} \sim P(\cdot|s_h, a_h)\)

12: **end for**

13: Perform policy gradient update on return \(R = \sum_{h=h'}^{H} r(s_h, a_h)\)

14: **end for**

15: Return \(\pi\)

are all “dead states” which yield 0 reward. Once the agent is in a dead state \(s_{3,h}^l\), it transitions deterministically to \(s_{3,h+1}^l\); thus entering a dead state at any time makes it impossible to obtain the final reward \(R^l\). At each “good” state \(s_{1,h}^l\) or \(s_{2,h}^l\), a single action leads the agent (stochastic with equal probability) to one of the next good states \(s_{1,h+1}^l, s_{2,h+1}^l\). All other 9 actions lead the agent to the dead state \(s_{3,h+1}^l\). The correct action changes at every horizon length \(h\) and the stochastic nature of the transitions precludes algorithms which plan deterministically. In addition, the agent receives a negative reward of \(-1/H\) for transitioning to a good state, and a reward of 0 for transitioning to a dead state. Therefore, a locally optimal solution is to learn a policy which transitions to a dead state as quickly as possible, since this avoids the \(-1/H\) penalty.

States are encoded using a binary vector. The start state \(s_0\) is simply the zero vector. In each lock, the state \(s_{i,h}^l\) is encoded as a binary vector which is the concatenation of one-hot encodings of \(i, h, l\).

One of the locks (randomly chosen) gives a final reward of 5, while the other lock gives a final reward of 2. Therefore, in addition to the locally optimal policy of quickly transitioning to the dead state (with return 0), another locally optimal solution is to explore the lock with reward 2 and gather the reward there. This leads to a return of \(V = 2 - \sum_{h=1}^{H} \frac{1}{H} = 1\), whereas the optimal return for going to the end of lock with reward 5 is \(V^* = 5 - \sum_{h=1}^{H} \frac{1}{H} = 4\). In order to ensure that the optimal reward is discovered for every lock, the agent must therefore explore both locks to the end. We used Algorithm 5 for this environment.

### H.2.2 Mountain Car

We used the MountainCarContinuous-v0 OpenAI Gym environment at [https://gym.openai.com/envs/MountainCarContinuous-v0/](https://gym.openai.com/envs/MountainCarContinuous-v0/) This environment has a 2-dimensional
continuous state space and a 1-dimensional continuous action space. We used Algorithm 4 for this environment.

H.2.3 Mazes

We used the source code from https://github.com/junhyukoh/value-prediction-network/blob/master/maze.py to implement the maze environment, with the following modifications: i) the blue channel (originally representing the goal) is set to zero ii) the same maze is used across all episodes iii) the reward is set to be a constant 0. We set the maze size to be $20 \times 20$. There are 5 actions: \{up, down, left, right, no-op\}. We used Algorithm 5 for this environment, omitting the exploitation step.

H.3 Hyperparameters

All methods were based on the PPO implementation of [Shangtong, 2018]. For the Diabolical Combination Lock and the MountainCar environments, we used the same policy network architecture: a 2-layer fully connected network with 64 hidden units at each layer and ReLU non-linearities. For the Diabolical Combination Lock environment, the last layer outputs a softmax over 10 actions and for Mountain Car the last layer outputs the parameters of a 1D Gaussian. For the Maze environments, we used a convolutional network with 2 convolutional layers (32 kernels of size $3 \times 3$ for the first, 64 kernels of size $3 \times 3$ for the second, both with stride 2), followed by a single fully-connected layer with 512 hidden units, and a final linear layer mapping to a softmax over the 5 actions. In all cases the RND network has the same architecture as the policy network, except that the last linear layer mapping hidden units to actions is removed. We found that tuning the intrinsic reward coefficient was important for getting good performance for RND. Hyperparameters are shown in Tables 2 and 3.

Table 2: PPO+RND Hyperparameters for Combolock and Mountain Car

| Hyperparameter               | Values Considered       | Final Value (Combolock) | Final Value (Mountain Car) |
|------------------------------|-------------------------|-------------------------|---------------------------|
| Learning Rate                | $10^{-3}, 5 \cdot 10^{-4}, 10^{-4}$ | $10^{-3}$             | $10^{-3}$                 |
| Hidden Layer Size            | 64                      | 64                      | 64                        |
| $\tau_{GAE}$                 | 0.95                    | 0.95                    | 0.95                      |
| Gradient Clipping            | 5.0                     | 5.0                     | 5.0                       |
| Entropy Bonus                | 0.01                    | 0.01                    | 0.01                      |
| PPO Ratio Clip               | 0.2                     | 0.2                     | 0.2                       |
| PPO Minibatch Size           | 160                     | 160                     | 160                       |
| PPO Optimization Epochs      | 5                       | 5                       | 5                         |
| Intrinsic Reward Normalization | true, false         | false                   | false                     |
| Intrinsic Reward coefficient | $0.5, 1, 10, 10^2, 10^3, 10^4$ | $10^3$               | $10^3$                    |
| Extrinsic Reward coefficient | 1.0                     | 1.0                     | 1.0                       |
### Table 3: PPO+RND Hyperparameters for Mazes

| Hyperparameter                  | Values Considered            | Final Value |
|--------------------------------|------------------------------|-------------|
| Learning Rate                  | $10^{-3}, 5\times10^{-4}, 10^{-4}$ | $10^{-3}$  |
| Hidden Layer Size              | 512                          | 512         |
| $\tau_{\text{GAE}}$           | 0.95                         | 0.95        |
| Gradient Clipping              | 0.5                          | 0.5         |
| Entropy Bonus                  | 0.01                         | 0.01        |
| PPO Ratio Clip                 | 0.1                          | 0.1         |
| PPO Minibatch Size             | 128                          | 128         |
| PPO Optimization Epochs        | 10                           | 10          |
| Intrinsic Reward Normalization | true, false                  | true        |
| Intrinsic Reward coefficient   | $1, 10, 10^2, 10^3, 10^4$    | $10^3$      |

The hyperparameters used for PC-PG are given in Tables 4 and 5. For the Diabolical Combination Lock experiments, we used a kernel $\phi(s, a) = s$, where $s$ is the binary vector encoding the state described in Section H.2.1. For Mountain Car, we used a Random Kitchen Sinks kernel [Rahimi and Recht, 2009] with 10 features using the following implementation: [https://scikit-learn.org/stable/modules/generated/sklearn.kernel_approximation.RBFSampler.html](https://scikit-learn.org/stable/modules/generated/sklearn.kernel_approximation.RBFSampler.html). For the Maze environments, we used a randomly initialized convolutional network with the same architecture as the RND network as a kernel.

### Table 4: PC-PG Hyperparameters for Combolock and Mountain Car

| Hyperparameter                  | Values Considered            | Final Value (Combolock) | Final Value (MountainCar) |
|--------------------------------|------------------------------|-------------------------|---------------------------|
| Learning Rate                  | $10^{-3}, 5\times10^{-4}, 10^{-4}$ | $10^{-3}$               | $5\times10^{-4}$          |
| Hidden Layer Size              | 64                           | 64                      | 64                        |
| $\tau_{\text{GAE}}$           | 0.95                         | 0.95                    | 0.95                      |
| Gradient Clipping              | 5.0                          | 5.0                     | 5.0                       |
| Entropy Bonus                  | 0.01                         | 0.01                    | 0.01                      |
| PPO Ratio Clip                 | 0.2                          | 0.2                     | 0.2                       |
| PPO Minibatch Size             | 160                          | 160                     | 160                       |
| PPO Optimization Epochs        | 5                            | 5                       | 5                         |
| $\epsilon$-greedy sampling    | 0, 0.01, 0.05                | 0.05                    | 0.05                      |
| Hyperparameter            | Values Considered          | Final Value   |
|--------------------------|---------------------------|---------------|
| Learning Rate            | $10^{-3}, 5 \cdot 10^{-4}, 10^{-4}$ | $5 \cdot 10^{-4}$ |
| Hidden Layer Size        | 512                       | 512           |
| $\tau_{\text{GAE}}$     | 0.95                      | 0.95          |
| Gradient Clipping        | 0.5                       | 0.5           |
| Entropy Bonus            | 0.01                      | 0.01          |
| PPO Ratio Clip           | 0.1                       | 0.1           |
| PPO Minibatch Size       | 128                       | 128           |
| PPO Optimization Epochs  | 10                        | 10            |
| $\epsilon$-greedy sampling | 0.05                    | 0.05          |