Optimality and Approximation with Policy Gradient Methods in Markov Decision Processes

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Abstract

Policy gradient methods are among the most effective methods in challenging reinforcement learning problems with large state and/or action spaces. However, little is known about even their most basic theoretical convergence properties, including: if and how fast they converge to a globally optimal solution (say with a sufficiently rich policy class); how they cope with approximation error due to using a restricted class of parametric policies; or their finite sample behavior. Such characterizations are important not only to compare these methods to their approximate value function counterparts (where such issues are relatively well understood, at least in the worst case), but also to help with more principled approaches to algorithm design.

This work provides provable characterizations of computational, approximation, and sample size issues with regards to policy gradient methods in the context of discounted Markov Decision Processes (MDPs). We focus on both: 1) "tabular" policy parameterizations, where the optimal policy is contained in the class and where we show global convergence to the optimal policy, and 2) restricted policy classes, which may not contain the optimal policy and where we provide agnostic learning results. One insight of this work is in formalizing the importance how a favorable initial state distribution provides a means to circumvent worst-case exploration issues. Overall, these results place policy gradient methods under a solid theoretical footing, analogous to the global convergence guarantees of iterative value function based algorithms.

1 Introduction

Policy gradient methods have a long history in the reinforcement learning (RL) literature [Williams, 1992, Sutton et al., 1999, Konda and Tsitsiklis, 2000, Kakade, 2001] and are an attractive class of algorithms as they are applicable to any differentiable policy parameterization; admit easy extensions to function approximation; easily incorporate structured state and action spaces; are easy to

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implement in a simulation based, model-free manner. Owing to their flexibility and generality, there has also been a flurry of improvements and refinements to make these ideas work robustly with deep neural network based approaches (see e.g. Schulman et al. [2015, 2017]).

Despite the large body of empirical work around these methods, their convergence properties are only established at a relatively coarse level; in particular, the folklore guarantee is that these methods converge to a stationary point of the objective, assuming adequate smoothness properties hold and assuming either exact or unbiased estimates of a gradient can be obtained (with appropriate regularity conditions on the variance). However, this local convergence viewpoint does not address some of the most basic theoretical convergence questions, including: 1) if and how fast they converge to a globally optimal solution (say with a sufficiently rich policy class); 2) how they cope with approximation error due to using a restricted class of parametric policies; or 3) their finite sample behavior. These questions are the focus of this work.

Overall, these results place policy gradient methods under a solid theoretical footing, analogous to the global convergence guarantees of iterative value function based algorithms. They may also provide a starting point to both further study the first-order (and second-order) convergence properties of these methods and provide more principled approaches to address their shortcomings.

1.1 Our Contributions

This work focuses on first-order and quasi second-order policy gradient methods which directly work in the space of some parameterized policy class (rather than through value estimation). We characterize computational, approximation, and sample size issues with regards to these methods in the context of a discounted Markov Decision Process (MDP). We focus on: 1) tabular policy parameterizations, where there is one parameter per state-action pair so the policy class is *complete* in that it contains the optimal policy, and 2) restricted policy classes, which may not contain the optimal policy, and, as such, policy gradient methods applied to these classes can be viewed as a function approximation technique. Note that policy gradient methods for discrete action MDPs work in the space of stochastic policies, which permits the policy class to be differentiable.

One central issue which repeatedly arises in our analysis can be crudely thought of as the issue of exploration. More precisely, the functional form of the policy gradient weighs the states in the MDP in proportion to the frequency with which the current policy visits that state, while in order to obtain an optimal policy, the policy must be improved at states which may not be visited often under the current policy (see Kakade [2003] for discussion). One of the contributions in the analysis herein is in quantifying this issue through the use of a certain *distribution mismatch coefficient* (see Table 1, caption).

We now discuss our contributions in the context of both tabular parameterizations (which always contain the optimal policy) and restricted parameterizations.

Tabular case: We consider three algorithms: two of which are first order methods, projected gradient ascent (on the simplex) and gradient ascent (with a softmax policy parameterization), and the third algorithm, natural policy gradient ascent, can be viewed as a quasi second-order method (or preconditioned first-order method). Table 1 summarizes our main results in this case: upper

Algorithm	Iteration complexity	
Projected Gradient Ascent on Simplex (Thm 4.2)	$O\left(\frac{ \mathcal{S} \mathcal{A} }{(1-\gamma)^6\epsilon^2} \left\ \frac{d_{\rho}^{\pi^*}}{\mu} \right\ _{\infty}^2\right)$	
Policy Gradient, softmax parameterization (Thm 5.1)	asymptotic	
Policy Gradient + relative entropy regularization, softmax parameterization (Cor 5.4)	$O\left(\frac{ \mathcal{S} ^2 \mathcal{A} ^2}{(1-\gamma)^6 \epsilon^2} \left\ \frac{d_{\rho}^{\pi^*}}{\mu} \right\ _{\infty}^2\right)$	
MDP Experts Algorithm [Even-Dar et al., 2009]	$O\left(\frac{\log A }{(1-\gamma)^4\epsilon^2}\right)$	
MD-MPI Geist et al. [2019]	$\frac{2 + (1 - \gamma) \log \mathcal{A} }{(1 - \gamma)^3 \epsilon}$	
Natural Policy Gradient (NPG) softmax parameterization (Thm 5.7)	$\frac{2}{(1-\gamma)^2\epsilon}$	

Table 1: Iteration Complexities for the Tabular Case: A summary of the number of iterations required by different algorithms to return a policy π satisfying $\mathbb{E}_{s\sim\rho}[V^\star(s)-V^\pi(s)]\leq\epsilon$, assuming access to exact policy gradients. First three algorithms optimize the objective $\mathbb{E}_{s\sim\mu}[V^\pi(s)]$, where μ is the initial starting state distribution; as we show, this implies a guarantee with respect to all starting state distributions ρ . The MDP has $|\mathcal{S}|$ states, $|\mathcal{A}|$ actions, and discount factor $0\leq\gamma<1$; the worst case ratio $\left\|\frac{d_\rho^{\pi^\star}}{\mu}\right\|_\infty=\max_s\left(\frac{d_\rho^{\pi^\star}(s)}{\mu(s)}\right)$ is termed the distribution mismatch coefficient, where, roughly speaking, $d_\rho^{\pi^\star}(s)$ is the fraction of time spent in state s when executing the optimal policy (see (4)), when started in the state $s_0\sim\rho$. Both the MDP Experts Algorithm [Even-Dar et al., 2009] and MD-MPI algorithm [Geist et al., 2019] (see Corollary 3) imply guarantees for the same update rule as the NPG for the softmax parameterization. NPG directly optimizes $\mathbb{E}_{s\sim\rho}[V^\pi(s)]$ and incurs no distribution mismatch coefficient dependence. See Section 2 for further discussion.

bounds on the number of iterations taken by these algorithms to find an ϵ -optimal policy, when we have access to exact policy gradients.

Arguably, the most natural starting point for an analysis of policy gradient methods is to consider directly doing gradient ascent on the policy simplex itself and then to project back onto the simplex if the constraint is violated after a gradient update; we refer to this algorithm as projected gradient ascent on the simplex. Using a notion of gradient domination, our results provably show that any first-order stationary point of the value function results in an approximately optimal policy, under certain regularity assumptions, which allows for a global convergence analysis by directly appealing to results in the non-convex optimization literature.

A more practical and commonly used parameterization is the softmax parameterization, where the simplex constraint is explicitly enforced by the exponential parameterization, thus avoiding projections. To our knowledge, we provide the first global convergence guarantees using only first-order gradient information for the widely-used softmax parameterization. Our first result for this parameterization establishes the asymptotic convergence of the policy gradient algorithm; the analysis challenge here is that the optimal policy (which is deterministic) is attained by sending the softmax parameters to infinity. In order to establish a convergence rate to optimality for the softmax parameterization, we then consider a relative entropy regularizer and provide an iteration complexity bound that is polynomial in all relevant quantities. The use of our relative entropy regularizer is critical to avoiding collapsing gradients, an issue discussed in practice; in particular, the more general approach of entropy based regularizers is fairly common in practice (e.g. see [Williams and Peng, 1991, Mnih et al., 2016, Peters et al., 2010, Abdolmaleki et al., 2018, Ahmed et al., 2019]). One notable distinction, which we discuss later, is that we consider the *relative* entropy as a regularizer rather than the entropy.

For these aforementioned algorithms, the convergence rates depend on a certain distribution mismatch coefficient $\left\|\frac{d_{\rho}^{\pi^{\star}}}{\mu}\right\|_{\infty}$ (see Table 1 caption). Here ρ is the state distribution under which we measure the sub-optimality of our policy and μ is the initial distribution over the states in our optimization objective. Somewhat informally, $d_{\rho}^{\pi^{\star}}$ is a distribution over states which represents the fraction of time that an optimal policy spends in any given state, when started from a state drawn according to ρ . This dependence suggests we desire μ to have sufficient coverage over all the states in the MDP. Furthermore, we provide a lower bound that shows such a term is unavoidable for first-order methods, even when exact gradients are available.

We then consider the Natural Policy Gradient (NPG) algorithm [Kakade, 2001] (also see Bagnell and Schneider [2003], Peters and Schaal [2008]), which can be considered a quasi second-order method due to the use of its particular preconditioner, and provide an iteration complexity to achieve an ϵ -optimal policy that is at most $\frac{2}{(1-\gamma)^{2\epsilon}}$ iterations, improving upon previous related results of [Even-Dar et al., 2009, Geist et al., 2019] (see Table 1 caption and Section 2). Note the convergence rate has *no* dependence on the number of states, the number of actions, or the distribution mismatch coefficient. Note that this dimension-free rate does not contradict the lower bounds on sample complexity of RL [Azar et al., 2013], since we assume exact gradient evaluations. We provide a simple and concise proof for the convergence rate analysis by extending the approach developed in [Even-Dar et al., 2009], which uses a mirror descent style of analysis [Nemirovsky and Yudin, 1983, Cesa-Bianchi and Lugosi, 2006, Shalev-Shwartz et al., 2012] and also handles the non-concavity of the policy optimization problem.

Note this result shows how the variable preconditioner in the natural gradient method improves over the standard gradient ascent algorithm. The dimension free aspect of this convergence rate is worth reflecting on, especially given the widespread use of the natural policy gradient algorithm along with variants such as the Trust Region Policy Optimization (TRPO) algorithm [Schulman et al., 2015]; our results may help to provide analysis of a more general family of variable metric algorithms (see for example Neu et al. [2017]).

Algorithm	Measure of approximation error	Iteration complexity	Accuracy
Approx. Value/Policy Iteration [Bertsekas and Tsitsiklis, 1996]	ϵ_{∞} : the ℓ_{∞} worst-case error of values	$\frac{1}{1-\gamma}\log\frac{1}{\epsilon_{\text{opt}}}$	$\epsilon_{ m opt} + \frac{2\epsilon_{\infty}}{(1-\gamma)^2}$
Approx. Policy Iteration, with concentrability [Munos, 2005, Antos et al., 2008]	ϵ_1 : an ℓ_1 average-case approx. notion	$\frac{1}{1-\gamma}\log\frac{1}{\epsilon_{\text{opt}}}$	$\epsilon_{ m opt} + rac{2C_{ ho,\mu}\epsilon_1}{(1-\gamma)^2}$
Conservative Policy Iteration [Kakade and Langford, 2002]	ϵ_1 : an ℓ_1 average-case approx. notion	$O\left(\frac{1}{\epsilon_1^2}\right)$	$\left\ \frac{d_{\rho}^{\pi^{\star}}}{\mu} \right\ _{\infty} \frac{\epsilon_1}{(1-\gamma)^2}$
Natural Policy Gradient (Cor 6.5)	ϵ_2 : an ℓ_2 average-case approx. notion	$O\left(\frac{1}{(1-\gamma)^2\epsilon_{\rm opt}^2}\right)$	$\epsilon_{\mathrm{opt}} + \sqrt{\left\ \frac{d_{\rho}^{\pi^{\star}}}{\mu}\right\ _{\infty}} \frac{\epsilon_{2}}{(1-\gamma)^{3}}$
Projected Gradient Ascent (Cor 6.14)	ϵ_1 : an ℓ_1 average-case approx. notion	$O\left(\frac{1}{(1-\gamma)^6\epsilon_{\rm opt}^2}\right)$	$\epsilon_{ m opt} + \left\ \frac{d_{ ho}^{\pi^{\star}}}{\mu} \right\ _{\infty} \frac{\epsilon_{1}}{(1-\gamma)^{3}}$

Overview of Approximate Methods: Summary of the iteration complexities and notion of approximation error for different algorithms to return a policy π satisfying $\mathbb{E}_{s\sim\rho}[V^{\star}(s)-V^{\pi}(s)]\leq\epsilon$; see Section 2 for a more in-depth discussion. Different methods use different notions of approximation as indicated in the rows of the table (sample complexities are not directly considered but instead may be thought of as part of the approximation error). For approximate dynamic programming methods, the relevant error is the worst case, ℓ_{∞} -error in approximating a value function, e.g. $\epsilon_{\infty} = \max_{s,a} |Q^{\pi}(s,a) - \widehat{Q}^{\pi}(s,a)|$, where \widehat{Q}^{π} is what an estimation oracle returns during the course of the algorithm. The second row is a refinement of this approach, under the assumption that the concentrability coefficient [Munos, 2005], $C_{\rho,\mu}$, is bounded (see Lemma 12 in Antos et al. [2008]); Appendix F and Scherrer [2014] shows how the concentrability coefficient is essentially an upper bound on the distribution mismatch coefficient. For Conservative Policy Iteration, $\epsilon_1 = \mathbb{E}_{s \sim \mu}[\max_{a \in \mathcal{A}} A^{\pi}(s, a) - \sum_{a \in \mathcal{A}} \pi'(a|s) A^{\pi}(s, a)]$, where π' is the policy returned by the approximate policy improvement oracle (called the ϵ -greedy policy chooser), for an input policy π (see Kakade and Langford [2002] for details). Scherrer [2014] provide a more detailed comparison of CPI and approximate dynamic programming methods, along with a guarantee for a related algorithm, Policy Search by Dynamic Programming (PSDP) [Bagnell et al., 2004], which enjoys an improved iteration complexity over CPI. For our methods, $\epsilon_{\rm opt}$ is the error of the computational procedure trying to find a stationary point of the underlying optimization problem; we drop problem dependent factors in the iteration complexities stated in the table for our methods.

Function Approximation: We now summarize our results with regards to policy gradient methods in the setting where we work with a restricted policy class, which may not contain the optimal

policy. In this sense, these methods can be viewed as approximate methods. Table 2 provides a summary along with the comparisons to some relevant approximate dynamic programming methods.

The focus in the function approximation setting is to avoid the worst-case " ℓ_{∞} " guarantees that are inherent to approximate dynamic programming methods [Bertsekas and Tsitsiklis, 1996] (see the first row in Table 2). Here there are largely two lines of provable guarantees: those methods which utilize a problem dependent parameter (the concentrability coefficient [Munos, 2005]) to provide more refined dynamic programming guarantees (e.g. see Munos [2005], Szepesvári and Munos [2005], Antos et al. [2008], Farahmand et al. [2010]) and those which work with a restricted policy class, making incremental updates, such as Conservative Policy Iteration (CPI) [Kakade and Langford, 2002] and Policy Search by Dynamic Programming (PSDP) [Bagnell et al., 2004] (also see [Scherrer and Geist, 2014, Scherrer, 2014]). We discuss the former class of guarantees in more detail in Section 2 (also see Appendix F and Scherrer [2014] for how the concentrability coefficient is essentially an upper bound on the distribution mismatch coefficient).

The reason to focus on average case guarantees is that it supports the applicability of *supervised machine learning* methods to solve the underlying approximation problem. This is because supervised learning methods, like classification and regression, typically only have bounds on the expected error under a distribution, as opposed to worst-case guarantees over all possible inputs.

One key contribution of this work is in precisely quantifying the notion of (average case) approximation error that is relevant for policy gradient methods; for the natural gradient method, we quantify this in terms of the *compatible function approximation error* [Sutton et al., 1999], while for projected gradient descent, we quantify this in terms of the *Bellman policy error* (the latter being a novel notion we introduce). Furthermore, due to the direct nature of policy gradient methods and due to our precise quantification of approximation error, we are able to provide finite sample and computational complexity results for the natural gradient algorithm. In particular, we provide a model-free, linear time algorithm for the natural policy gradient, requiring only simulation based rollouts (or restarts) in Section 6.1.2.

Note that for both CPI and for policy gradient methods, there is a distribution mismatch coefficient, in place of either the ℓ_{∞} error bound in classical dynamic programming or the concentrability coefficient in the approximate versions. The significance of this is that it formalizes how having a favorable initial state distribution provides a means to circumvent worst-case amplification of approximation error, and we provide a more detailed comparison of these assumptions in Section 2.

We finally observe the importance of iterative algorithms which make incremental updates: NPG, CPI, and PSDP all make small changes to the policy from one iteration to the next, and these algorithms all have improved guarantees over approximate dynamic programming methods. One significant advantage of NPG is that the explicit parametric policy representation in NPG (and other policy gradient methods) leads to a succinct policy representation in comparison to CPI, PSDP, or related boosting-style methods [Scherrer and Geist, 2014], where the representation complexity of the policy of the latter class of methods grows linearly in the number of iterations (since these methods add one policy to the ensemble per iteration). This increased representation complexity is likely why the latter class of algorithms are less widely used in practice.

2 Related Work

We now discuss related work, roughly in the order which reflects our presentation of results in the previous section.

For the direct policy parameterization in the tabular case, we make use of a gradient domination-like property, namely any first-order stationary point of the policy value is approximately optimal up to a distribution mismatch coefficient. A variant of this result also appears in Theorem 2 of Scherrer and Geist [2014], which itself can be viewed as a generalization of the approach in Kakade and Langford [2002]. In contrast to CPI [Kakade and Langford, 2002] and the more general boosting-based approach in Scherrer and Geist [2014], we phrase this approach as a Polyak-like gradient domination property [Polyak, 1963] in order to directly allow for the transfer of any advances in non-convex optimization to policy optimization in RL. More broadly, it is worth noting the global convergence of policy gradients for Linear Quadratic Regulators [Fazel et al., 2018] also goes through a similar proof approach of gradient domination.

Empirically, the recent work of Ahmed et al. [2019] investigates related issues to those studied here, and also uncovers the value of regularization in policy optimization, even with exact gradients. This is very related to our use of relative entropy for the case of entropic regularization.

For our convergence results of the natural policy gradient algorithm in the tabular setting, there are close connections between our results and the works of Even-Dar et al. [2009], Geist et al. [2019]. Even-Dar et al. [2009] provides provable online regret guarantees in changing MDPs utilizing experts algorithms (also see Neu et al. [2010], Abbasi-Yadkori et al. [2019]); as a special case, their MDP Experts Algorithm is equivalent to the natural policy gradient algorithm with the softmax policy parameterization. While the convergence results due to Even-Dar et al. [2009] were not specifically designed for this setting, it is instructive to see what it implies due to the close connections between optimization and regret [Cesa-Bianchi and Lugosi, 2006, Shalev-Shwartz et al., 2012]. The Mirror Descent-Modified Policy Iteration (MD-MPI) algorithm [Geist et al., 2019] with negative entropy as the Bregman divergence results in an identical algorithm as NPG for softmax parameterization in the tabular case; Corollary 3 [Geist et al., 2019] applies to our updates, leading to a bound worse by a $1/(1-\gamma)$ factor and also has dependence on $|\mathcal{A}|$, albeit logarithmic (see Table 1). Our proof for this case is simple and concise, which may be of independent interest. Also worth noting is the Dynamic Policy Programming of Azar et al. [2012], which is an actorcritic algorithm with a softmax parameterization; this algorithm, even though not identical, comes with similar guarantees in terms of its rate (it is weaker in terms of an additional $1/(1-\gamma)$ factor) than the NPG algorithm.

We now turn to function approximation, starting with a discussion of iterative algorithms which make incremental updates in which the next policy is effectively constrained to be close to the previous policy, such as in CPI and PSDP [Bagnell et al., 2004]. Here, the work in Scherrer and Geist [2014] show how CPI is part of broader family of boosting-style methods. Also, with regards to PSDP, the work in Scherrer [2014] shows how PSDP actually enjoys an improved iteration complexity over CPI, namely $O(\log 1/\epsilon_{\rm opt})$ vs. $O(1/\epsilon_{\rm opt}^2)$. It is worthwhile to note that both NPG and projected gradient descent are also both incremental algorithms.

We now discuss the approximate dynamic programming results characterized in terms of the concentrability coefficient. While the approximate dynamic programming results typically require

 ℓ_{∞} bounded errors, which is quite stringent, the notion of concentrability (originally due to [Munos, 2005]) permits sharper bounds in terms of average case function approximation error, provided that the concentrability coefficient is bounded (e.g. see Munos [2005], Szepesvári and Munos [2005], Antos et al. [2008]). Chen and Jiang [2019] provide a more detailed discussion on this quantity. Based on this problem dependent constant being bounded, Munos [2005], Szepesvári and Munos [2005] and Antos et al. [2008] provide meaningful sample size and error bounds for approximate dynamic programming methods, where there is a data collection policy (under which valuefunction fitting occurs) that induces a concentrability coefficient. We discuss the definition of concentrability coefficient in detail in Appendix F, where we also show that the distribution mismatch coefficient in our results can be upper bounded in terms of (essentially) the concentrability coefficient and could be much smaller in general. This is because these concentrability coefficients require a bound for state distributions induced by all policies π , while our distribution mismatch coefficient is only a regularity assumption on a single policy, π^* . Notably, the distribution mismatch coefficient is finite for a well-chosen distribution μ (namely $d_{\rho}^{\pi^*}$) in any MDP, while a finite concentrability coefficient is a restriction on the MDP dynamics itself (see Chen and Jiang [2019]). The more refined quantities defined by Farahmand et al. [2010] partially alleviate some of these concerns, but their assumptions still implicitly constrain the MDP dynamics, like the finiteness of the concentrability coefficient.

In terms of the concentrability coefficient, there are a notable set of provable average case guarantees for the MD-MPI algorithm [Geist et al., 2019] (see also [Azar et al., 2012, Scherrer et al., 2015]), which are stated in terms of various norms of function approximation error. MD-MPI is a class of algorithms for approximate planning under regularized notions of optimality in MDPs. Specifically, Geist et al. [2019] analyze a family of actor-critic style algorithms, where there are both approximate value functions updates and approximate policy updates. As a consequence of utilizing approximate value function updates for the critic, the guarantees of Geist et al. [2019] are stated with dependencies on concentrability coefficients, which makes the results hard to compare to ours directly (though the discussion in Appendix F is relevant here). Furthermore, it is not evident what the computational or statistical complexities of this approach are.

When dealing with function approximation, computational and statistical complexities are relevant because they determine the effectiveness of approximate updates with finite samples. With regards to sample complexity, the work in Szepesvári and Munos [2005], Antos et al. [2008] provide finite sample rates (as discussed above), further generalized to actor-critic methods in Azar et al. [2012], Scherrer et al. [2015]. In our direct policy optimization approach, the analysis of both computational and statistical complexities are straightforward due to that we can leverage known statistical and computational results from the stochastic approximation literature. In particular, we use the stochastic approximation results in Bach and Moulines [2013] (also see Jain et al. [2016, 2017]), to design a simple, linear time, inexact Newton method for the natural policy gradient algorithm.

In terms of the algorithmic updates for the function approximation setting, our development of NPG bears similarity to the natural actor-critic algorithm Peters and Schaal [2008], for which some asymptotic guarantees under finite concentrability coefficients are obtained in Bhatnagar et al. [2009]. While both updates seek to minimize the compatible function approximation error, we perform

streaming updates based on stochastic optimization using Monte Carlo estimates for values. In contrast Peters and Schaal [2008] utilize Least Squares Temporal Difference methods [Boyan, 1999] to minimize the loss. As a consequence, their updates additionally make linear approximations to the value functions in order to estimate the advantages; our approach is flexible in allowing for wide family of smoothly differentiable policy classes.

Finally, we remark on two related concurrent works. The work of Bhandari and Russo [2019] provides gradient domination-like conditions under which there is (asymptotic) global convergence to the optimal policy. Their results are applicable to the projected gradient descent algorithm; however, they are not applicable to gradient descent with the softmax parameterization (see the discussion in Section 5 herein for the challenges with regards to the softmax case). Bhandari and Russo [2019] also provide global convergence results beyond MDPs. Also, Liu et al. [2019] provide an analysis of the TRPO algorithm [Schulman et al., 2015] with neural network parameterizations, which bears resemblance to our natural policy gradient analysis. In particular, Liu et al. [2019] utilize ideas from both Even-Dar et al. [2009] (with a mirror descent style of analysis) along with Cai et al. [2019] (to handle approximation with neural networks) to provide conditions under which TRPO returns a near optimal policy. Liu et al. [2019] do not explicitly consider the case where the policy class is not complete (i.e when there is approximation).

3 Setting

A (finite) Markov Decision Process (MDP) $M = (\mathcal{S}, \mathcal{A}, P, r, \gamma, \rho)$ is specified by: a finite state space \mathcal{S} ; a finite action space \mathcal{A} ; a transition model P where P(s'|s,a) is the probability of transitioning into state s' upon taking action a in state s; a reward function $r: \mathcal{S} \times \mathcal{A} \rightarrow [0,1]$ where r(s,a) is the immediate reward associated with taking action a in state s; a discount factor $\gamma \in [0,1)$; a starting state distribution ρ over \mathcal{S} .

A deterministic, stationary policy $\pi: \mathcal{S} \to \mathcal{A}$ specifies a decision-making strategy in which the agent chooses actions adaptively based on the current state, i.e., $a_t = \pi(s_t)$. The agent may also choose actions according to a stochastic policy $\pi: \mathcal{S} \to \Delta(\mathcal{A})$ (where $\Delta(\mathcal{A})$ is the probability simplex over \mathcal{A}), and, overloading notation, we write $a_t \sim \pi(\cdot|s_t)$.

A policy induces a distribution over trajectories $\tau = (s_t, a_t, r_t)_{t=0}^{\infty}$, where s_0 is drawn from the starting state distribution ρ , and, for all subsequent timesteps $t, a_t \sim \pi(\cdot|s_t)$ and $s_{t+1} \sim P(\cdot|s_t, a_t)$. The value function $V^{\pi}: \mathcal{S} \to \mathbb{R}$ is defined as the discounted sum of future rewards starting at state s and executing π , i.e.

$$V^{\pi}(s) := \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^{t} r(s_{t}, a_{t}) | \pi, s_{0} = s\right],$$

where the expectation is with respect to the randomness of the trajectory τ induced by π in M. Since we assume that $r(s,a) \in [0,1]$, we have $0 \le V^{\pi}(s) \le \frac{1}{1-\gamma}$. We further define $V^{\pi}(\rho)$ as the expected value under the initial state distribution ρ , i.e.

$$V^{\pi}(\rho) := \mathbb{E}_{s_0 \sim \rho}[V^{\pi}(s_0)].$$

The action-value (or Q-value) function $Q^{\pi}: \mathcal{S} \times \mathcal{A} \to \mathbb{R}$ and the *advantage* function $A^{\pi}: \mathcal{S} \times \mathcal{A} \to \mathbb{R}$ are defined as:

$$Q^{\pi}(s,a) = \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^{t} r(s_{t}, a_{t}) | \pi, s_{0} = s, a_{0} = a\right], \quad A^{\pi}(s,a) := Q^{\pi}(s,a) - V^{\pi}(s).$$

The goal of the agent is to find a policy π that maximizes the expected value from the initial state, i.e. the optimization problem the agent seeks to solve is:

$$\max_{\pi} V^{\pi}(\rho) \tag{1}$$

where the max is over all policies. The famous theorem of Bellman and Dreyfus [1959] shows there exists a policy π^* which simultaneously maximizes $V^{\pi}(s_0)$, for all states $s_0 \in \mathcal{S}$.

Policy Parameterizations. This work studies ascent methods for the optimization problem:

$$\max_{\theta \in \Theta} V^{\pi_{\theta}}(\rho),$$

where $\{\pi_{\theta} | \theta \in \Theta\}$ is some class of parametric (stochastic) policies. We consider a number of different policy classes. The first two are *complete* in the sense that any stochastic policy can be represented in the class. The final class may be restrictive. These classes are as follows:

• Direct parameterization: The policies are parameterized by

$$\pi_{\theta}(a|s) = \theta_{s,a},\tag{2}$$

where $\theta \in \Delta(\mathcal{A})^{|\mathcal{S}|}$, i.e. θ is subject to $\theta_{s,a} \geq 0$ and $\sum_{a \in \mathcal{A}} \theta_{s,a} = 1$ for all $s \in \mathcal{S}$ and $a \in \mathcal{A}$.

• *Softmax parameterization:* For unconstrained $\theta \in \mathbb{R}^{|\mathcal{S}||\mathcal{A}|}$,

$$\pi_{\theta}(a|s) = \frac{\exp(\theta_{s,a})}{\sum_{a' \in A} \exp(\theta_{s,a'})}.$$
(3)

The softmax parameterization is also complete.

• Restricted parameterizations: We also study parametric classes $\{\pi_{\theta} | \theta \in \Theta\}$ that may not contain all stochastic policies. Here, the best we may hope for is an agnostic result where we do as well as the best policy in this class.

While the softmax parameterization is the more natural parametrization among the two complete policy classes, it is also insightful to consider the direct parameterization.

It is worth explicitly noting that $V^{\pi_{\theta}}(s)$ is non-concave in θ for both the direct and the softmax parameterizations, so the standard tools of convex optimization are not applicable. For completeness, we formalize this as follows (with a proof in Appendix A, along with an example in Figure 1):

Lemma 3.1. There is an MDP M (described in Figure 1) such that the optimization problem $V^{\pi_{\theta}}(s)$ is not concave for both the direct and softmax parameterizations.

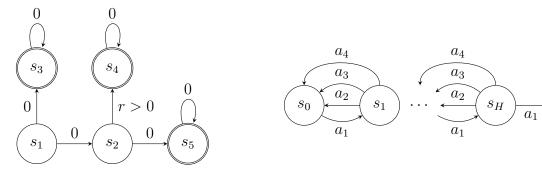


Figure 1: A simple deterministic MDP corresponding to Lemma 3.1 where $V^{\pi_{\theta}}(s)$ is non-concave. The numbers on arrows represent the rewards for each action.

Figure 2: A deterministic, chain MDP of length H+2. We consider a policy where $\pi(a|s)=\theta_{s,a}$ for $i=1,2,\ldots,H$. Rewards are 0 everywhere other than $r(s_{H+1},a_1)=1$.

 a_1

 s_{H+1}

Policy gradients. In order to introduce these methods, it is useful to define the discounted state visitation distribution $d_{s_0}^{\pi}$ of a policy π as:

$$d_{s_0}^{\pi}(s) := (1 - \gamma) \sum_{t=0}^{\infty} \gamma^t \Pr^{\pi}(s_t = s | s_0)$$
(4)

where $\Pr^{\pi}(s_t = s | s_0)$ is the state visitation probability that $s_t = s$, after we execute π starting at state s_0 . Again, we overload notation and write:

$$d_{\rho}^{\pi}(s) = \mathbb{E}_{s_0 \sim \rho} \left[d_{s_0}^{\pi}(s) \right].$$

where d_{ρ}^{π} is the discounted state visitation distribution under initial distribution ρ . The policy gradient functional form (see e.g. Williams [1992], Sutton et al. [1999]) is then:

$$\nabla_{\theta} V^{\pi_{\theta}}(s_0) = \frac{1}{1 - \gamma} \mathbb{E}_{s \sim d_{s_0}^{\pi_{\theta}}} \mathbb{E}_{a \sim \pi_{\theta}(\cdot|s)} \left[\nabla_{\theta} \log \pi_{\theta}(a|s) Q^{\pi_{\theta}}(s, a) \right]. \tag{5}$$

Furthermore, if we are working with a differentiable parameterization of $\pi_{\theta}(\cdot|s)$ that explicitly constrains $\pi_{\theta}(\cdot|s)$ to be in the simplex, i.e. $\pi_{\theta} \in \Delta(\mathcal{A})^{|\mathcal{S}|}$ for all θ , then we also have:

$$\nabla_{\theta} V^{\pi_{\theta}}(s_0) = \frac{1}{1 - \gamma} \mathbb{E}_{s \sim d_{s_0}^{\pi_{\theta}}} \mathbb{E}_{a \sim \pi_{\theta}(\cdot|s)} \left[\nabla_{\theta} \log \pi_{\theta}(a|s) A^{\pi_{\theta}}(s, a) \right]. \tag{6}$$

Note the above gradient expression does not hold for the direct parameterization. ¹

The performance difference lemma. The following lemma is helpful throughout:

¹This is since $\sum_a \nabla_\theta \pi_\theta(a|s) = 1$ is not explicitly maintained by the direct parameterization, without resorting to projections.

Lemma 3.2. (The performance difference lemma [Kakade and Langford, 2002]) For all policies π , π' and states s_0 ,

$$V^{\pi}(s_0) - V^{\pi'}(s_0) = \frac{1}{1 - \gamma} \mathbb{E}_{s \sim d_{s_0}^{\pi}} \mathbb{E}_{a \sim \pi(\cdot|s)} \left[A^{\pi'}(s, a) \right].$$

For completeness, we provide a proof in Appendix A.

The distribution mismatch coefficient. We often characterize the difficulty of the exploration problem faced by our policy optimization algorithms when maximizing the objective $V^{\pi}(\mu)$ through the following notion of distribution mismatch coefficient.

Definition 3.3 (Distribution mismatch coefficient). Given a policy π and measures $\rho, \mu \in \Delta(\mathcal{S})$, we refer to $\left\|\frac{d_{\rho}^{\pi}}{\mu}\right\|_{\infty}$ as the *distribution mismatch coefficient* of π relative to μ . Here, $\frac{d_{\rho}^{\pi}}{\mu}$ denotes componentwise division.

We often instantiate this coefficient with μ as the initial state distribution used in a policy optimization algorithm, ρ as the distribution to measure the sub-optimality of our policies, and some policy $\pi^* \in \operatorname{argmax}_{\pi \in \Pi} V^{\pi}(\rho)$, given a policy class Π .

Notation. Following convention, we use V^{\star} and Q^{\star} to denote $V^{\pi^{\star}}$ and $Q^{\pi^{\star}}$ respectively. For iterative algorithms which obtain policy parameters $\theta^{(t)}$ at iteration t, we let $\pi^{(t)}$, $V^{(t)}$ and $A^{(t)}$ denote the corresponding quantities parameterized by $\theta^{(t)}$, i.e. $\pi_{\theta^{(t)}}$, $V^{\theta^{(t)}}$ and $V^{\theta^{(t)}}$, respectively. For vectors u and v, we use $\frac{u}{v}$ to denote the componentwise ratio; $u \geq v$ denotes a componentwise inequality; we use the standard convention where $\|v\|_2 = \sqrt{\sum_i v_i^2}$, $\|v\|_1 = \sum_i |v_i|$, and $\|v\|_{\infty} = \max_i |v_i|$.

4 Warmup: Directly Parameterized Policy Classes

Our starting point is, arguably, the simplest first-order method: we directly take gradient ascent updates on the policy simplex itself and then project back onto the simplex if the constraints are violated after a gradient update. This algorithm is projected gradient ascent on the direct policy parametrization of the MDP, where the parameters are the state-action probabilities, i.e. $\theta_{s,a} = \pi_{\theta}(a|s)$ (see (2)). As noted in Lemma 3.1, $V^{\pi_{\theta}}(s)$ is non-concave in the parameters π_{θ} . Here, we first prove that $V^{\pi_{\theta}}(\mu)$ satisfies a Polyak-like gradient domination condition [Polyak, 1963], and this tool helps in providing convergence rates. The basic approach was also used in the analysis of CPI [Kakade and Langford, 2002]; related gradient domination-like lemmas also appeared in Scherrer and Geist [2014].

It is instructive to consider this special case due the connections it makes to the non-convex optimization literature. We also provide a lower bound that essentially shows this coefficient is not avoidable among first-order methods, which has implications to algorithms whose runtime appeals to the curvature of saddle points (e.g. [Nesterov and Polyak, 2006, Ge et al., 2015, Jin et al., 2017]).

For the direct policy parametrization where $\theta_{s,a} = \pi_{\theta}(a|s)$, the gradient is:

$$\frac{\partial V^{\pi}(\mu)}{\partial \pi(a|s)} = \frac{1}{1-\gamma} d^{\pi}_{\mu}(s) Q^{\pi}(s,a),\tag{7}$$

using (5). In particular, for this parameterization, we may write $\nabla_{\pi}V^{\pi}(\mu)$ instead of $\nabla_{\theta}V^{\pi_{\theta}}(\mu)$.

4.1 Gradient Domination

Informally, we say a function $f(\theta)$ satisfies a gradient domination property if for all $\theta \in \Theta$,

$$f(\theta^*) - f(\theta) = O(G(\theta)),$$

where $\theta^* \in \operatorname{argmax}_{\theta' \in \Theta} f(\theta')$ and where $G(\theta)$ is some suitable scalar notion of first-order stationarity, which can be considered a measure of how large the gradient is (see [Karimi et al., 2016, Bolte et al., 2007, Attouch et al., 2010]). Thus if one can find a θ that is (approximately) a first-order stationary point, then the parameter θ will be near optimal (in terms of function value). Such conditions are a standard device to establishing global convergence in non-convex optimization, as they effectively rule out the presence of bad critical points. In other words, given such a condition, quantifying the convergence rate for a specific algorithm, like say projected gradient ascent, will require quantifying the rate of its convergence to a first-order stationary point, for which one can invoke standard results from the optimization literature.

The following lemma shows that the direct policy parameterization satisfies a notion of gradient domination. This is the basic approach used in the analysis of CPI [Kakade and Langford, 2002]; a variant of this lemma also appears in Scherrer and Geist [2014]. We give a proof for completeness.

While we are interested in the value $V^{\pi}(\rho)$, it is helpful to consider the gradient with respect to another state distribution $\mu \in \Delta(\mathcal{S})$.

Lemma 4.1 (Gradient domination). For the direct policy parameterization (as in (2)), for all state distributions $\mu, \rho \in \Delta(S)$, we have

$$V^{\star}(\rho) - V^{\pi}(\rho) \leq \left\| \frac{d_{\rho}^{\pi^{\star}}}{d_{\mu}^{\pi}} \right\|_{\infty} \max_{\bar{\pi}} (\bar{\pi} - \pi)^{\top} \nabla_{\pi} V^{\pi}(\mu)$$
$$\leq \frac{1}{1 - \gamma} \left\| \frac{d_{\rho}^{\pi^{\star}}}{\mu} \right\|_{\infty} \max_{\bar{\pi}} (\bar{\pi} - \pi)^{\top} \nabla_{\pi} V^{\pi}(\mu),$$

where the max is over the set of all policies, i.e. $\bar{\pi} \in \Delta(\mathcal{A})^{|\mathcal{S}|}$.

Before we provide the proof, a few comments are in order with regards to the performance measure ρ and the optimization measure μ . Subtly, note that although the gradient is with respect to $V^{\pi}(\mu)$, the final guarantee applies to *all* distributions ρ . The significance is that even though we may be interested in our performance under ρ , it may be helpful to optimize under the distribution μ . To see this, note the lemma shows that a sufficiently small gradient magnitude in the feasible

directions implies the policy is nearly optimal in terms of its value, but only if the state distribution of π , i.e. d^{π}_{μ} , adequately covers the state distribution of some optimal policy π^* . Here, it is also worth recalling the theorem of Bellman and Dreyfus [1959] which shows there exists a single policy π^* that is simultaneously optimal for all starting states s_0 . Note that the hardness of the exploration problem is captured through the distribution mismatch coefficient (Definition 3.3).

Proof:[of Lemma 4.1] By the performance difference lemma (Lemma 3.2),

$$V^{*}(\rho) - V^{\pi}(\rho) = \frac{1}{1 - \gamma} \sum_{s,a} d_{\rho}^{\pi^{*}}(s) \pi^{*}(a|s) A^{\pi}(s,a)$$

$$\leq \frac{1}{1 - \gamma} \sum_{s,a} d_{\rho}^{\pi^{*}}(s) \max_{\bar{a}} A^{\pi}(s,\bar{a})$$

$$= \frac{1}{1 - \gamma} \sum_{s} \frac{d_{\rho}^{\pi^{*}}(s)}{d_{\mu}^{\pi}(s)} \cdot d_{\mu}^{\pi}(s) \max_{\bar{a}} A^{\pi}(s,\bar{a})$$

$$\leq \frac{1}{1 - \gamma} \left(\max_{s} \frac{d_{\rho}^{\pi^{*}}(s)}{d_{\mu}^{\pi}(s)} \right) \sum_{s} d_{\mu}^{\pi}(s) \max_{\bar{a}} A^{\pi}(s,\bar{a}), \tag{8}$$

where the last inequality follows since $\max_{\bar{a}} A^{\pi}(s, \bar{a}) \ge 0$ for all states s and policies π . We wish to upper bound (8). We then have:

$$\begin{split} \sum_{s} \frac{d^{\pi}_{\mu}(s)}{1 - \gamma} \max_{\bar{a}} A^{\pi}(s, \bar{a}) &= \max_{\bar{\pi} \in \Delta(\mathcal{A})^{|S|}} \sum_{s, a} \frac{d^{\pi}_{\mu}(s)}{1 - \gamma} \bar{\pi}(a|s) A^{\pi}(s, a) \\ &= \max_{\bar{\pi} \in \Delta(\mathcal{A})^{|S|}} \sum_{s, a} \frac{d^{\pi}_{\mu}(s)}{1 - \gamma} (\bar{\pi}(a|s) - \pi(a|s)) A^{\pi}(s, a) \\ &= \max_{\bar{\pi} \in \Delta(\mathcal{A})^{|S|}} \sum_{s, a} \frac{d^{\pi}_{\mu}(s)}{1 - \gamma} (\bar{\pi}(a|s) - \pi(a|s)) Q^{\pi}(s, a) \\ &= \max_{\bar{\pi} \in \Delta(\mathcal{A})^{|S|}} (\bar{\pi} - \pi)^{\top} \nabla_{\pi} V^{\pi}(\mu) \end{split}$$

where the first step follows since \max_{π} is attained at an action which maximizes $A^{\pi}(s,\cdot)$ (per state); the second step follows as $\sum_{a} \pi(a|s) A^{\pi}(s,a) = 0$; the third step uses $\sum_{a} (\bar{\pi}(a|s) - \pi(a|s)) V^{\pi}(s) = 0$ for all s; and the final step follows from the gradient expression (see (7)). Using this in (8),

$$V^{\star}(\rho) - V^{\pi}(\rho) \leq \left\| \frac{d_{\rho}^{\pi^{\star}}}{d_{\mu}^{\pi}} \right\|_{\infty} \max_{\bar{\pi} \in \Delta(\mathcal{A})^{|\mathcal{S}|}} (\bar{\pi} - \pi)^{\top} \nabla_{\pi} V^{\pi}(\mu)$$
$$\leq \frac{1}{1 - \gamma} \left\| \frac{d_{\rho}^{\pi^{\star}}}{\mu} \right\|_{\infty} \max_{\bar{\pi} \in \Delta(\mathcal{A})^{|\mathcal{S}|}} (\bar{\pi} - \pi)^{\top} \nabla_{\pi} V^{\pi}(\mu).$$

where the last step follows due to $\max_{\bar{\pi} \in \Delta(\mathcal{A})^{|\mathcal{S}|}} (\bar{\pi} - \pi)^{\top} \nabla_{\pi} V^{\pi}(\mu) \geq 0$ for any policy π and $d^{\pi}_{\mu}(s) \geq (1 - \gamma)\mu(s)$ (see (4)).

In a sense, the use of an appropriate μ circumvents the issues of strategic exploration. It is natural to ask whether this additional term is necessary, a question which we return to. First, we provide a convergence rate for the projected gradient descent algorithm.

4.2 Convergence Rates for Projected Gradient Descent

Using this notion of gradient domination, we now give an iteration complexity bound for projected gradient ascent over the probability simplex $\Delta(\mathcal{A})^{|\mathcal{S}|}$. The projected gradient ascent algorithm updates

$$\pi^{(t+1)} = P_{\Delta(A)^{|S|}}(\pi^{(t)} + \eta \nabla_{\pi} V^{(t)}(\mu)), \tag{9}$$

where $P_{\Delta(A)^{|S|}}$ is the projection on the probability simplex $\Delta(A)^{|S|}$.

Theorem 4.2. The projected gradient ascent algorithm (9) on $V^{\pi}(\mu)$ with stepsize $\eta = \frac{(1-\gamma)^3}{2\gamma|\mathcal{A}|}$ satisfies for all distributions $\rho \in \Delta(\mathcal{S})$,

$$\min_{t < T} \left\{ V^{\star}(\rho) - V^{(t)}(\rho) \right\} \le \epsilon \quad \text{whenever} \quad T > \frac{64\gamma |\mathcal{S}||\mathcal{A}|}{(1-\gamma)^{6} \epsilon^{2}} \left\| \frac{d_{\rho}^{\pi^{\star}}}{\mu} \right\|_{\infty}^{2}.$$

A proof is provided in Appendix B.1. The proof first invokes a standard iteration complexity result of projected gradient ascent to show that the gradient magnitude with respect to all feasible directions is small. More concretely, we show the policy is ϵ -stationary², that is, for all $\pi_{\theta} + \delta \in \Delta(\mathcal{A})^{|\mathcal{S}|}$ and $\|\delta\|_2 \leq 1$, $\delta^{\top} \nabla_{\pi} V^{\pi_{\theta}}(\mu) \leq \epsilon$. We then use Lemma 4.1 to complete the proof.

4.3 A Lower Bound: Vanishing Gradients, Saddle Points, and The Necessity of the Distribution Mismatch Coefficient

To understand the necessity of the distribution mismatch coefficient in Lemma 4.1 and Theorem 4.2, let us first give an informal argument that some condition on the state distribution of π , or equivalently μ , is necessary for stationarity to imply optimality. For example, in a sparsereward MDP (where the agent is only rewarded upon visiting some small set of states), a policy that does visit *any* rewarding states will have zero gradient, even though it is arbitrarily suboptimal in terms of values. Below, we give a more quantitative version of this intuition, which demonstrates that even if π chooses all actions with reasonable probabilities (and hence the agent will visit all states if the MDP is connected), then there is an MDP where a large fraction of the policies π have vanishingly small gradients, and yet these policies are highly suboptimal in terms of their value.

Concretely, consider the chain MDP of length H+2 shown in Figure 2. The starting state of interest is state s_0 and the discount factor $\gamma = H/(H+1)$. Suppose we work with the direct parameterization, where $\pi_{\theta}(a|s) = \theta_{s,a}$ for $a = a_1, a_2, a_3$ and $\pi_{\theta}(a_4|s) = 1 - \theta_{s,a_1} - \theta_{s,a_2} - \theta_{s,a_3}$. Note we do not over-parameterize the policy. For this MDP and policy structure, if we were to initialize the probabilities over actions, say deterministically, then there is an MDP (obtained by permuting the actions) where all the probabilities for a_1 will be less than 1/4.

²See Appendix B.1 for discussion on this definition.

The following result not only shows that the gradient is exponentially small (in H), it also shows that many higher order derivatives, up to $O(H/\log H)$, are also exponentially small (in H).

Lemma 4.3 (Vanishing gradients at suboptimal parameters). Consider the chain MDP of Figure 2, with $\gamma = H/(H+1)$, and with the direct policy parameterization (with $3|\mathcal{S}|$ parameters, as described in the text above). Suppose θ is such that $0 < \theta < 1$ (componentwise) and $\theta_{s,a_1} < 1/4$ (for all states s). For all $k \leq \frac{H}{40 \log(2H)} - 1$, we have $\|\nabla_{\theta}^k V^{\pi_{\theta}}(s_0)\| \leq (1/3)^{H/4}$, where $\nabla_{\theta}^k V^{\pi_{\theta}}(s_0)$ is a tensor of the k_{th} order derivatives of $V^{\pi_{\theta}}(s_0)$ and the norm is the operator norm of the tensor. Furthermore, $V^*(s_0) - V^{\pi_{\theta}}(s_0) \geq (H+1)/8 - (H+1)^2/3^H$.

This lemma also suggests that results in the non-convex optimization literature, on escaping from saddle points, e.g. [Nesterov and Polyak, 2006, Ge et al., 2015, Jin et al., 2017], do not directly imply global convergence due to that the higher order derivatives are small.

Remark 4.4. (Exact vs. Approximate Gradients) The chain MDP of Figure 2, is a common example where sample based estimates of gradients will be 0 under random exploration strategies; there is an exponentially small (in H) chance of hitting the goal state under a random exploration strategy. Note that this lemma is with regards to exact gradients. This suggests that even with exact computations (along with using exact higher order derivatives) we might expect numerical instabilities.

The proof is provided in Appendix B.2. The lemma illustrates that lack of good exploration can indeed be detrimental in policy gradient algorithms, since the gradient can be small either due to π being near-optimal, or, simply because π does not visit advantageous states often enough. In this sense, it also demonstrates the necessity of the distribution mismatch coefficient in Lemma 4.1.

5 The Softmax Parameterization

We now consider the softmax policy parameterization (3). Here, we still have a non-concave optimization problem in general, as shown in Lemma 3.1, though we do show that global optimality can be reached under certain regularity conditions. From a practical perspective, the softmax parameterization of policies is preferable to the direct parameterization, since the parameters θ are unconstrained and standard unconstrained optimization algorithms can be employed. However, optimization over this policy class creates other challenges as we study in this section, as the optimal policy (which is deterministic) is attained by sending the parameters to infinity.

We study three algorithms for this problem. The first performs direct policy gradient descent on the objective without modification, while the second adds entropic regularization to keep the parameters from becoming too large, as a means to ensure adequate exploration. Finally, we study the natural policy gradient algorithm and establish a global optimality result with no dependence on the distribution mismatch coefficient or dimension-dependent factors.

³The operator norm of a k_{th} -order tensor $J \in \mathbb{R}^{d^{\otimes k}}$ is defined as $\sup_{u_1,\dots,u_k \in \mathbb{R}^d : ||u_i||_2 = 1} \langle J, u_1 \otimes \dots \otimes u_d \rangle$.

For the softmax parameterization, the gradient takes the form:

$$\frac{\partial V^{\pi_{\theta}}(\mu)}{\partial \theta_{s,a}} = \frac{1}{1 - \gamma} d_{\mu}^{\pi_{\theta}}(s) \pi_{\theta}(a|s) A^{\pi_{\theta}}(s,a) \tag{10}$$

(see Lemma C.1 for a proof).

5.1 Asymptotic Convergence, without Regularization

Due to the exponential scaling with the parameters θ in the softmax parameterization, *any* policy that is nearly deterministic will have gradients close to 0. In spite of this difficulty, we provide a positive result that GD asymptotically converges to the global optimum for the softmax parameterization.

The update rule for gradient descent is:

$$\theta^{(t+1)} = \theta^{(t)} + \eta \nabla_{\theta} V^{(t)}(\mu).$$
 (11)

Theorem 5.1 (Global convergence for softmax parameterization). Assume we follow the gradient descent update rule as specified in Equation 11 and that the distribution μ is strictly positive i.e. $\mu(s) > 0$ for all states s. Suppose $\eta \leq \frac{(1-\gamma)^2}{5}$, then we have that for all states s, $V^{(t)}(s) \to V^{\star}(s)$ as $t \to \infty$.

Remark 5.2. (Strict positivity of μ and exploration) Theorem 5.1 assumed that optimization distribution μ was *strictly* positive, i.e. $\mu(s) > 0$ for all states s. We leave it is an open question of whether or not gradient descent will globally converge if this condition is not met.

The complete proof is provided in the Appendix C.1. We now discuss the subtleties in the proof and show why the softmax parameterization precludes a direct application of the gradient domination lemma. In order to utilize the gradient domination property, we would desire to show that: $\nabla_{\pi}V^{\pi}(\mu) \to 0$. However, using the functional form of the softmax parameterization (see Lemma C.1) and (7), we have that:

$$\frac{\partial V^{\pi_{\theta}}(\mu)}{\partial \theta_{s,a}} = \frac{1}{1 - \gamma} d_{\mu}^{\pi_{\theta}}(s) \pi_{\theta}(a|s) A^{\pi_{\theta}}(s,a) = \pi_{\theta}(a|s) \frac{\partial V^{\pi_{\theta}}(\mu)}{\partial \pi_{\theta}(a|s)}.$$

Hence, we see that even if $\nabla_{\theta}V^{\pi_{\theta}}(\mu) \to 0$, we are not guaranteed that $\nabla_{\pi}V^{\pi_{\theta}}(\mu) \to 0$.

We now briefly discuss the main technical challenge in the proof. The proof first shows that the sequence $V^{(t)}(s)$ is monotone increasing pointwise, i.e. for *every* state s, $V^{(t+1)}(s) \geq V^{(t)}(s)$ (Lemma C.2). This implies the existence of a limit $V^{(\infty)}(s)$ by the monotone convergence theorem (Lemma C.3). Based on these limiting quantities $V^{(\infty)}(s)$ and $Q^{(\infty)}(s,a)$, define the following limiting sets for each state s:

$$I_0^s := \{a|Q^{(\infty)}(s,a) = V^{(\infty)}(s)\}$$

$$I_+^s := \{a|Q^{(\infty)}(s,a) > V^{(\infty)}(s)\}$$

$$I_-^s := \{a|Q^{(\infty)}(s,a) < V^{(\infty)}(s)\}.$$

The challenge is to then show that, for all states s, the set I_+^s is the empty set, which would immediately imply $V^{(\infty)}(s) = V^\star(s)$. The proof proceeds by contradiction, assuming that I_+^s is non-empty. Using that I_+^s is non-empty and that the gradient tends to zero in the limit, i.e. $\nabla_\theta V^{\pi_\theta}(\mu) \to 0$, we have that for all $a \in I_+^s$, $\pi^{(t)}(a|s) \to 0$ (see (10)). This, along with the functional form of the softmax parameterization, implies that there is divergence (in magnitude) among the set of parameters associated with *some* action a at state s, i.e. that $\max_{a \in \mathcal{A}} |\theta_{s,a}^{(t)}| \to \infty$. The primary technical challenge in the proof is to then use this divergence along with the dynamics of gradient descent to show that I_+^s is empty via a contradiction.

We leave it as a question for future work as to characterizing the convergence rate, which we conjecture is exponentially slow in some of the relevant quantities. Here, we turn to a regularization based approach to ensure convergence at a polynomial rate.

5.2 Polynomial Convergence with Relative Entropy Regularization

Due to the exponential scaling with the parameters θ , policies can rapidly become near deterministic, when optimizing under the softmax parameterization, which can result in slow convergence. Indeed a key challenge in the asymptotic analysis in the previous section was to handle the growth of the absolute values of parameters to infinity. A common practical remedy for this is to use entropy-based regularization to keep the probabilities from getting too small [Williams and Peng, 1991, Mnih et al., 2016], and we study gradient ascent on a similarly regularized objective in this section. Recall that the relative-entropy for distributions p and q is defined as: $\mathrm{KL}(p,q) := \mathbb{E}_{x \sim p}[-\log q(x)/p(x)]$. Denote the uniform distribution over a set \mathcal{X} by $\mathrm{Unif}_{\mathcal{X}}$, and define the following relative-entropy regularized objective as:

$$L_{\lambda}(\theta) := V^{\pi_{\theta}}(\mu) - \lambda \mathbb{E}_{s \sim \text{Unif}_{\mathcal{S}}} \left[\text{KL}(\text{Unif}_{\mathcal{A}}, \pi_{\theta}(\cdot|s)) \right]$$
$$= V^{\pi_{\theta}}(\mu) + \frac{\lambda}{|\mathcal{S}| |\mathcal{A}|} \sum_{s,a} \log \pi_{\theta}(a|s) + \lambda \log |\mathcal{A}|, \qquad (12)$$

where λ is a regularization parameter. The constant (i.e. the last term) is not relevant with regards to optimization. This regularizer is different from the more commonly utilized entropy regularizer as in Mnih et al. [2016], a point which we return to in Remark 5.5.

The policy gradient ascent updates for $L_{\lambda}(\theta)$ are given by:

$$\theta^{(t+1)} = \theta^{(t)} + \eta \nabla_{\theta} L_{\lambda}(\theta^{(t)}). \tag{13}$$

Our next theorem shows that approximate first-order stationary points of the entropy-regularized objective are approximately globally optimal, provided the regularization is sufficiently small.

Theorem 5.3. (*Relative entropy regularization*) Suppose θ is such that:

$$\|\nabla_{\theta} L_{\lambda}(\theta)\|_{2} \le \epsilon_{opt}$$

and $\epsilon_{opt} \leq \lambda/(2|\mathcal{S}||\mathcal{A}|)$. Then we have that for all starting state distributions ρ :

$$V^{\pi_{\theta}}(\rho) \geq V^{\star}(\rho) - \frac{2\lambda}{1-\gamma} \left\| \frac{d_{\rho}^{\pi^{\star}}}{\mu} \right\|_{\infty}.$$

Proof: The proof consists of showing that $\max_a A^{\pi_{\theta}}(s, a) \leq 2\lambda/(\mu(s)|\mathcal{S}|)$ for all states. To see that this is sufficient, observe that by the performance difference lemma (Lemma 3.2),

$$V^{\star}(\rho) - V^{\pi_{\theta}}(\rho) = \frac{1}{1 - \gamma} \sum_{s,a} d_{\rho}^{\pi^{\star}}(s) \pi^{\star}(a|s) A^{\pi_{\theta}}(s,a)$$

$$\leq \frac{1}{1 - \gamma} \sum_{s} d_{\rho}^{\pi^{\star}}(s) \max_{a \in \mathcal{A}} A^{\pi_{\theta}}(s,a)$$

$$\leq \frac{1}{1 - \gamma} \sum_{s} 2d_{\rho}^{\pi^{\star}}(s) \lambda / (\mu(s)|\mathcal{S}|)$$

$$\leq \frac{2\lambda}{1 - \gamma} \max_{s} \left(\frac{d_{\rho}^{\pi^{\star}}(s)}{\mu(s)}\right).$$

which would then complete the proof.

We now proceed to show that $\max_a A^{\pi_{\theta}}(s,a) \leq 2\lambda/(\mu(s)|\mathcal{S}|)$. For this, it suffices to bound $A^{\pi_{\theta}}(s,a)$ for any state-action pair s,a where $A^{\pi_{\theta}}(s,a) \geq 0$ else the claim is trivially true. Consider an (s,a) pair such that $A^{\pi_{\theta}}(s,a) > 0$. Using the policy gradient expression for the softmax parameterization (see Lemma C.1),

$$\frac{\partial L_{\lambda}(\theta)}{\partial \theta_{s,a}} = \frac{1}{1 - \gamma} d_{\mu}^{\pi_{\theta}}(s) \pi_{\theta}(a|s) A^{\pi_{\theta}}(s,a) + \frac{\lambda}{|\mathcal{S}|} \left(\frac{1}{|\mathcal{A}|} - \pi_{\theta}(a|s) \right) . \tag{14}$$

The gradient norm assumption $\|\nabla_{\theta}L_{\lambda}(\theta)\|_{2} \leq \epsilon_{\mathrm{opt}}$ implies that:

$$\epsilon_{\text{opt}} \ge \frac{\partial L_{\lambda}(\theta)}{\partial \theta_{s,a}} = \frac{1}{1 - \gamma} d_{\mu}^{\pi_{\theta}}(s) \pi_{\theta}(a|s) A^{\pi_{\theta}}(s,a) + \frac{\lambda}{|\mathcal{S}|} \left(\frac{1}{|\mathcal{A}|} - \pi_{\theta}(a|s) \right)$$
$$\ge \frac{\lambda}{|\mathcal{S}|} \left(\frac{1}{|\mathcal{A}|} - \pi_{\theta}(a|s) \right),$$

where we have used where $A^{\pi_{\theta}}(s, a) \geq 0$. Rearranging and using our assumption $\epsilon_{\text{opt}} \leq \lambda/(2|\mathcal{S}|\,|\mathcal{A}|)$,

$$\pi_{\theta}(a|s) \ge \frac{1}{|\mathcal{A}|} - \frac{\epsilon_{\text{opt}}|\mathcal{S}|}{\lambda} \ge \frac{1}{2|\mathcal{A}|}.$$

Solving for $A^{\pi_{\theta}}(s, a)$ in (14), we have:

$$A^{\pi_{\theta}}(s, a) = \frac{1 - \gamma}{d_{\mu}^{\pi_{\theta}}(s)} \left(\frac{1}{\pi_{\theta}(a|s)} \frac{\partial L_{\lambda}(\theta)}{\partial \theta_{s,a}} + \frac{\lambda}{|\mathcal{S}|} \left(1 - \frac{1}{\pi_{\theta}(a|s)|\mathcal{A}|} \right) \right)$$

$$\leq \frac{1 - \gamma}{d_{\mu}^{\pi_{\theta}}(s)} \left(2|\mathcal{A}|\epsilon_{\text{opt}} + \frac{\lambda}{|\mathcal{S}|} \right)$$

$$\leq 2\frac{1 - \gamma}{d_{\mu}^{\pi_{\theta}}(s)} \frac{\lambda}{|\mathcal{S}|}$$

$$\leq 2\lambda/(\mu(s)|\mathcal{S}|),$$

where the penultimate step uses $\epsilon_{\rm opt} \leq \lambda/(2|\mathcal{S}||\mathcal{A}|)$ and the final step uses $d_{\mu}^{\pi_{\theta}}(s) \geq (1-\gamma)\mu(s)$. This completes the proof.

By combining the above theorem with standard results on the convergence of gradient ascent, we obtain the following corollary.

Corollary 5.4. (Iteration complexity with relative entropy regularization) Let $\beta_{\lambda} := \frac{8\gamma}{(1-\gamma)^3} + \frac{2\lambda}{|\mathcal{S}|}$. Starting from any initial $\theta^{(0)}$, consider the updates (13) with $\lambda = \frac{\epsilon(1-\gamma)}{2\left\|\frac{d_{\rho}^{\pi}}{\mu}\right\|_{\infty}}$ and $\eta = 1/\beta_{\lambda}$. Then for all starting state distributions ρ , we have

$$\min_{t < T} \left\{ V^{\star}(\rho) - V^{(t)}(\rho) \right\} \le \epsilon \quad \text{whenever} \quad T \ge \frac{320|\mathcal{S}|^2|\mathcal{A}|^2}{(1 - \gamma)^6 \, \epsilon^2} \left\| \frac{d_{\rho}^{\pi^{\star}}}{\mu} \right\|_{\infty}^2.$$

See Appendix C.2 for the proof. The corollary shows the importance of balancing how the regularization parameter λ is set relative to the desired accuracy ϵ , as well as the importance of the initial distribution μ to obtain global optimality.

Remark 5.5. (Entropy vs. relative entropy regularization) The more commonly considered regularizer is the entropy [Mnih et al., 2016] (also see Ahmed et al. [2019] for a more detailed empirical investigation), where the regularizer would be:

$$\frac{1}{|\mathcal{S}|} \sum_{s} H(\pi_{\theta}(\cdot|s)) = \frac{1}{|\mathcal{S}|} \sum_{s} \sum_{a} -\pi_{\theta}(a|s) \log \pi_{\theta}(a|s).$$

Note that the entropy is far less aggressive in penalizing small probabilities, in comparison to the relative entropy. In particular, the entropy regularizer is always bounded between 0 and $\log |\mathcal{A}|$, while the relative entropy (against the uniform distribution over actions), is bounded between 0 and infinity, where it tends to infinity as probabilities tend to 0. We leave it is an open question if a polynomial convergence rate is achievable with the more common entropy regularizer; our polynomial convergence rate using the KL regularizer crucially relies on the aggressive nature in which the relative entropy prevents small probabilities.

5.3 Dimension-free Convergence of Natural Policy Gradient Ascent

We now show the Natural Policy Gradient algorithm, with the softmax parameterization (3), obtains an improved iteration complexity. The NPG algorithm defines a Fisher information matrix (induced by π), and performs gradient updates in the geometry induced by this matrix as follows:

$$F_{\rho}(\theta) = \mathbb{E}_{s \sim d_{\rho}^{\pi_{\theta}}} \mathbb{E}_{a \sim \pi_{\theta}(\cdot|s)} \Big[\nabla_{\theta} \log \pi_{\theta}(a|s) \Big(\nabla_{\theta} \log \pi_{\theta}(a|s) \Big)^{\top} \Big]$$

$$\theta^{(t+1)} = \theta^{(t)} + \eta F_{\rho}(\theta^{(t)})^{\dagger} \nabla_{\theta} V^{(t)}(\rho), \tag{15}$$

where M^{\dagger} denotes the Moore-Penrose pseudoinverse of the matrix M. Throughout this section, we restrict to using the initial state distribution $\rho \in \Delta(\mathcal{S})$ in our update rule in (15) (so our optimization

measure μ and the performance measure ρ are identical). Also, we restrict attention to states $s \in \mathcal{S}$ reachable from ρ , since, without loss of generality, we can exclude states that are not reachable under this start state distribution⁴.

We leverage a particularly convenient form the update takes for the softmax parameterization (see Kakade [2001]). For completeness, we provide a proof in Appendix C.3.

Lemma 5.6. For the softmax parameterization (3), the NPG updates (15) take the form:

$$\theta^{(t+1)} = \theta^{(t)} + \frac{\eta}{1-\gamma} A^{(t)}$$
 and $\pi^{(t+1)}(a|s) = \pi^{(t)}(a|s) \frac{\exp(\eta A^{(t)}(s,a)/(1-\gamma))}{Z_t(s)},$

where
$$Z_t(s) = \sum_{a \in A} \pi^{(t)}(a|s) \exp(\eta A^{(t)}(s,a)/(1-\gamma)).$$

The updates take a strikingly simple form in this special case; they are identical to the classical multiplicative weights updates [Freund and Schapire, 1997, Cesa-Bianchi and Lugosi, 2006] for online linear optimization over the probability simplex, where the linear functions are specified by the advantage function of the current policy at each iteration. Notably, there is no dependence on the state distribution $d_{\rho}^{(t)}$, since the pseudoinverse of the Fisher information cancels out the effect of the state distribution in NPG. We now provide a dimension free convergence rate of this algorithm.

Theorem 5.7 (Global convergence for Natural Policy Gradient Ascent). Suppose we run the NPG updates (15) using $\rho \in \Delta(S)$ and with $\theta^{(0)} = 0$. Fix $\eta > 0$. For all T > 0, we have:

$$V^{(T)}(\rho) \ge V^*(\rho) - \frac{\log |\mathcal{A}|}{\eta T} - \frac{1}{(1-\gamma)^2 T}.$$

In particular, setting $\eta \geq (1 - \gamma)^2 \log |\mathcal{A}|$, we see that NPG finds an ϵ -optimal policy in a number of iterations that is at most:

$$T \le \frac{2}{(1-\gamma)^2 \epsilon},$$

which has no dependence on the number of states or actions, despite the non-concavity of the underlying optimization problem.

The proof strategy we take borrows ideas from the online regret framework in changing MDPs (in [Even-Dar et al., 2009]); here, we provide a faster rate of convergence than the analysis implied by Even-Dar et al. [2009] or by Geist et al. [2019]. We also note that while this proof is obtained for the NPG updates, it is known in the literature that in the limit of small stepsizes, NPG and TRPO updates are closely related (e.g. see Schulman et al. [2015], Neu et al. [2017], Rajeswaran et al. [2017]).

First, the following improvement lemma is helpful:

Lemma 5.8 (Improvement lower bound for NPG). For the iterates $\pi^{(t)}$ generated by the NPG updates (15), we have for all starting state distributions μ

$$V^{(t+1)}(\mu) - V^{(t)}(\mu) \ge \frac{(1-\gamma)}{n} \mathbb{E}_{s \sim \mu} \log Z_t(s) \ge 0.$$

⁴Specifically, we restrict the MDP to the set of states $\{s \in \mathcal{S} : \exists \pi \text{ such that } d^{\pi}_{\rho}(s) > 0\}.$

Proof: First, let us show that $\log Z_t(s) \ge 0$. To see this, observe:

$$\log Z_t(s) = \log \sum_a \pi^{(t)}(a|s) \exp(\eta A^{(t)}(s,a)/(1-\gamma))$$

$$\geq \sum_a \pi^{(t)}(a|s) \log \exp(\eta A^{(t)}(s,a)/(1-\gamma)) = \frac{\eta}{1-\gamma} \sum_a \pi^{(t)}(a|s) A^{(t)}(s,a) = 0.$$

where the inequality follows by Jensen's inequality on the concave function $\log x$ and the final equality uses $\sum_a \pi^{(t)}(a|s) A^{(t)}(s,a) = 0$. Using $d^{(t+1)}$ as shorthand for $d^{(t+1)}_{\mu}$, the performance difference lemma implies:

$$V^{(t+1)}(\mu) - V^{(t)}(\mu) = \frac{1}{1 - \gamma} \mathbb{E}_{s \sim d^{(t+1)}} \sum_{a} \pi^{(t+1)}(a|s) A^{(t)}(s, a)$$

$$= \frac{1}{\eta} \mathbb{E}_{s \sim d^{(t+1)}} \sum_{a} \pi^{(t+1)}(a|s) \log \frac{\pi^{(t+1)}(a|s) Z_{t}(s)}{\pi^{(t)}(a|s)}$$

$$= \frac{1}{\eta} \mathbb{E}_{s \sim d^{(t+1)}} \text{KL}(\pi_{s}^{(t+1)} || \pi_{s}^{(t)}) + \frac{1}{\eta} \mathbb{E}_{s \sim d^{(t+1)}} \log Z_{t}(s)$$

$$\geq \frac{1}{\eta} \mathbb{E}_{s \sim d^{(t+1)}} \log Z_{t}(s) \geq \frac{1 - \gamma}{\eta} \mathbb{E}_{s \sim \mu} \log Z_{t}(s).$$

where the last step uses that $d^{(t+1)} = d_{\mu}^{(t+1)} \ge (1-\gamma)\mu$, componentwise (by (4)), and that $\log Z_t(s) \ge 0$.

With this lemma, we now prove Theorem 5.7.

Proof:[of Theorem 5.7] Since ρ is fixed, we use d^* as shorthand for $d_{\rho}^{\pi^*}$; we also use π_s as shorthand for the vector of $\pi(\cdot|s)$. By the performance difference lemma (Lemma 3.2),

$$V^{\pi^{\star}}(\rho) - V^{(t)}(\rho) = \frac{1}{1 - \gamma} \mathbb{E}_{s \sim d^{\star}} \sum_{a} \pi^{\star}(a|s) A^{(t)}(s, a)$$

$$= \frac{1}{\eta} \mathbb{E}_{s \sim d^{\star}} \sum_{a} \pi^{\star}(a|s) \log \frac{\pi^{(t+1)}(a|s) Z_{t}(s)}{\pi^{(t)}(a|s)}$$

$$= \frac{1}{\eta} \mathbb{E}_{s \sim d^{\star}} \left(\text{KL}(\pi_{s}^{\star}||\pi_{s}^{(t)}) - \text{KL}(\pi_{s}^{\star}||\pi_{s}^{(t+1)}) + \sum_{a} \pi^{\star}(a|s) \log Z_{t}(s) \right)$$

$$= \frac{1}{\eta} \mathbb{E}_{s \sim d^{\star}} \left(\text{KL}(\pi_{s}^{\star}||\pi_{s}^{(t)}) - \text{KL}(\pi_{s}^{\star}||\pi_{s}^{(t+1)}) + \log Z_{t}(s) \right),$$

where we have used the closed form of our updates from Lemma 5.6 in the second step. By applying Lemma 5.8 with d^* as the starting state distribution, we have:

$$\frac{1}{n} \mathbb{E}_{s \sim d^{\star}} \log Z_{t}(s) \leq \frac{1}{1 - \gamma} \left(V^{(t+1)}(d^{\star}) - V^{(t)}(d^{\star}) \right)$$

which gives us a bound on $\mathbb{E}_{s \sim d^*} \log Z_t(s)$.

Using the above equation and that $V^{(t+1)}(\rho) \ge V^{(t)}(\rho)$ (as $V^{(t+1)}(s) \ge V^{(t)}(s)$ for all states s by Lemma 5.8), we have:

$$V^{\pi^{\star}}(\rho) - V^{(T-1)}(\rho) \leq \frac{1}{T} \sum_{t=0}^{T-1} (V^{\pi^{\star}}(\rho) - V^{(t)}(\rho))$$

$$\leq \frac{1}{\eta T} \sum_{t=0}^{T-1} \mathbb{E}_{s \sim d^{\star}} (KL(\pi_{s}^{\star} || \pi_{s}^{(t)}) - KL(\pi_{s}^{\star} || \pi_{s}^{(t+1)})) + \frac{1}{\eta T} \sum_{t=0}^{T-1} \mathbb{E}_{s \sim d^{\star}} \log Z_{t}(s)$$

$$\leq \frac{\mathbb{E}_{s \sim d^{\star}} KL(\pi_{s}^{\star} || \pi^{(0)})}{\eta T} + \frac{1}{(1 - \gamma)T} \sum_{t=0}^{T-1} \left(V^{(t+1)}(d^{\star}) - V^{(t)}(d^{\star}) \right)$$

$$= \frac{\mathbb{E}_{s \sim d^{\star}} KL(\pi_{s}^{\star} || \pi^{(0)})}{\eta T} + \frac{V^{(T)}(d^{\star}) - V^{(0)}(d^{\star})}{(1 - \gamma)T}$$

$$\leq \frac{\log |\mathcal{A}|}{\eta T} + \frac{1}{(1 - \gamma)^{2}T}.$$

The proof is completed using that $V^{(T)}(\rho) \ge V^{(T-1)}(\rho)$.

6 Restricted Policy Classes and Function Approximation

We now analyze the case of using restricted parametric classes

$$\Pi = \{ \pi_{\theta} | \theta \in \Theta \subseteq \mathbb{R}^d \}$$
 (16)

that may not contain all stochastic policies. We focus on obtaining agnostic results, where we seek to do as well as the best policy in this class. We consider smooth policy classes, with and without additional constraints on the parameter θ .

Recall a function $f: \mathbb{R}^d \to \mathbb{R}$ is said to be β -smooth if for all $x, x' \in \mathbb{R}^d$:

$$\|\nabla f(x) - \nabla f(x')\|_2 \le \beta \|x - x'\|_2$$

and, due to Taylor's theorem, recall that this implies:

$$\left| f(x') - f(x) - \nabla f(x) \cdot (x' - x) \right| \le \frac{\beta}{2} \|x' - x\|_2^2.$$
 (17)

6.1 Natural Policy Gradient for Unconstrained Policy Classes

This section studies policy classes parameterized by some parameter $\theta \in \mathbb{R}^d$. In contrast with the tabular results in the previous sections, the policies classes that we are often interested in are not fully expressive, e.g. $d \ll |\mathcal{S}||\mathcal{A}|$ (indeed $|\mathcal{S}|$ or $|\mathcal{A}|$ need not even be finite for the results in this section); in this sense, we are in the regime of function approximation.

We now consider the (unconstrained) policy optimization problem:

$$\max_{\theta \in \mathbb{R}^d} V^{\pi_{\theta}}(\rho)$$

for some state distribution ρ . As before, while we are interested in $V^{\pi_{\theta}}(\rho)$, we shall see that optimization with respect to a different distribution μ is also important in the approximate case.

Let us more abstractly consider an update rule of the form

$$\theta^{(t+1)} = \theta^{(t)} + \eta w^{(t)} \,. \tag{18}$$

where $w^{(t)}$ is either the exact NPG update rule or a (sample based) approximation to it.

To analyze NPG for restricted policy classes, we leverage a close connection of the NPG update rule (15) to the notion of *compatible function approximation* [Sutton et al., 1999], as formalized in Kakade [2001]. It is helpful to consider a distribution ν over state-action pairs, i.e. $\nu \in \Delta(\mathcal{S}) \times \Delta(\mathcal{A})$. For a weight vector $w \in \mathbb{R}^d$ and with respect to ν and θ , define the compatible function approximation error L_{ν} and the minimal compatible function approximation error L_{ν}^{\star} as:

$$L_{\nu}(w;\theta) := \mathbb{E}_{s,a\sim\nu} \left[\left(A^{\pi_{\theta}}(s,a) - w \cdot \nabla_{\theta} \log \pi_{\theta}(a|s) \right)^{2} \right], \quad L_{\nu}^{\star}(\theta) := \min_{w} L_{\nu}(w;\theta). \tag{19}$$

As shown in Kakade [2001], the NPG update rule (15) can be viewed as the minimizer of a certain function approximation problem: precisely, if we take $\nu(s,a) = d_{\rho}^{\pi_{\theta}}(s)\pi_{\theta}(a|s)$, then

$$F_{\rho}(\theta)^{\dagger} \nabla_{\theta} V^{\theta}(\rho) \in \operatorname{argmin}_{w} L_{\nu}(w; \theta).$$
 (20)

This is a straightforward consequence of the first order optimality conditions. Consequently, when the minimizer is unique, then the NPG update direction is precisely identified by minimizing the regression problem implied by the compatible function approximation error. When the solution is not unique, we allow the use of any minimizer of $L_{\nu}(w;\theta)$ and prove that this does not affect the convergence properties of the algorithm, beyond the norm of the solution we find.

This observation also opens a direct pathway to approximate updates where we can solve the regression problems with samples. Furthermore, if the minimal compatible function approximation error is 0, then Thm 5.7 already establishes that global convergence occurs for the NPG update rule. The more often encountered scenario is when the minimal compatible function error is nonzero, as is likely to happen when the parameterization using θ does not represent all possible policies.

Let us gain further intuition to this concept by recalling the result of Sutton et al. [1999].

Remark 6.1. (Compatible function approximation) Consider the state-action visitation distribution under π starting from μ , i.e.

$$\nu(s,a) = d^{\pi_{\theta}}_{\mu}(s)\pi_{\theta}(a|s)$$

and the minimizer

$$w^*(\theta) \in \operatorname{argmin}_w L_{\nu}(w; \theta).$$

Let us denote the best linear predictor of $A^{\pi_{\theta}}(s,a)$ using $\nabla_{\theta} \log \pi_{\theta}(a|s)$ by $\widehat{A}^{\pi_{\theta}}(s,a)$, i.e.

$$\widehat{A}^{\pi_{\theta}}(s, a) := w^{\star}(\theta) \cdot \nabla_{\theta} \log \pi_{\theta}(a|s).$$

As shown in Sutton et al. [1999], the first order optimality conditions for $\widehat{A}^{\pi_{\theta}}(s,a)$ being the best linear predictor directly imply that:

$$\nabla_{\theta} V^{\pi_{\theta}}(\mu) = \frac{1}{1 - \gamma} \mathbb{E}_{s \sim d_{\mu}^{\pi_{\theta}}} \mathbb{E}_{a \sim \pi_{\theta}(\cdot|s)} \left[\nabla_{\theta} \log \pi_{\theta}(a|s) A^{\pi_{\theta}}(s, a) \right]$$
$$= \frac{1}{1 - \gamma} \mathbb{E}_{s \sim d_{\mu}^{\pi_{\theta}}} \mathbb{E}_{a \sim \pi_{\theta}(\cdot|s)} \left[\nabla_{\theta} \log \pi_{\theta}(a|s) \widehat{A}^{\pi_{\theta}}(s, a) \right].$$

In other words, computing the gradient with the best linear approximation, $\widehat{A}^{\pi_{\theta}}(s, a)$, instead of $A^{\pi_{\theta}}(s, a)$ results in identical outcomes.

Our convergence rates assume that the policy class is smooth in the sense that $\log \pi_{\theta}$ is a smooth function of θ .

Assumption 6.2. (Policy Smoothness) Assume for all $s \in \mathcal{S}$, $a \in \mathcal{A}$ that $\log \pi_{\theta}(a|s)$ is a β -smooth function of θ (recall (17)).

Note that this assumption is a strict generalization of our previous analysis for the softmax parameterization in the tabular setting. In fact, we present a more general example of a policy class satisfying Assumption 6.2 below.

Example 6.3 (Linear softmax policies). For any state, action pair s, a, suppose we have a feature mapping $\phi_{s,a} \in \mathbb{R}^d$ with $\|\phi_{s,a}\|_2^2 \leq \beta$. Let us consider the policy class

$$\pi_{\theta}(a|s) = \frac{\exp(\theta \cdot \phi_{s,a})}{\sum_{a' \in \mathcal{A}} \exp(\theta \cdot \phi_{s,a'})}$$

with $\theta \in \mathbb{R}^d$. Then $\log \pi_{\theta}(a|s)$ is a β -smooth function.

To gain further intuition about the compatible function approximation error, we can specialize it to the linear setting of Example 6.3. Here, $\nabla_{\theta} \log \pi_{\theta}(a|s) = \widetilde{\phi}_{s,a}$, where $\widetilde{\phi}_{s,a} = \phi_{s,a} - \mathbb{E}_{a' \sim \pi_{\theta}(\cdot|s)}[\phi_{s,a'}]$ is the centered version of $\phi_{s,a}$. Thus, we get

$$L_{\nu}(w;\theta) = \mathbb{E}_{s,a\sim\nu} \left[\left(A^{\pi_{\theta}}(s,a) - w \cdot \widetilde{\phi}_{s,a} \right)^{2} \right].$$

That is, the compatible function approximation error measures the expressivity of our parameterization in how well linear functions of the parameterization can capture the policy's advantage function. More generally, the error provides a particularly useful characterization of the policy class expressivity for NPG updates as characterized in the main result of this section (Theorem 6.4).

Our main technical result of this section quantifies the effect of error in the compatible function approximation. The theorem is stated in an abstract manner, so that it can be subsequently utilized in concrete settings to deal with optimization and statistical error. The theorem relates the compatible function approximation errors on an arbitrary sequence $\{w^{(t)}, \theta^{(t)}\}$ to the sub-optimality of the resulting policy.

Theorem 6.4. (NPG approximation) Fix a comparison policy π and a state distribution ρ . Define ν as the induced state-action measure under π , i.e.

$$\nu(s,a) = d_{\rho}^{\pi}(s)\pi(a|s).$$

Suppose that the update rule (18) starts with $\theta^{(0)} = 0$ and uses the (arbitrary) sequence of weights $w^{(0)}, \ldots, w^{(T)}$; that Assumption 6.2 holds; and that for all t < T,

$$\frac{1}{T} \sum_{t=0}^{T-1} L_{\nu}(w^{(t)}; \theta^{(t)}) \le \widetilde{\epsilon}_{approx}, \quad \|w^{(t)}\|_{2} \le W.$$

We have that:

$$\min_{t < T} \left\{ V^{\pi}(\rho) - V^{(t)}(\rho) \right\} \le \frac{1}{1 - \gamma} \left(\sqrt{\widetilde{\epsilon}_{approx}} + \frac{\log |\mathcal{A}|}{\eta T} + \frac{\eta \beta W^2}{2} \right).$$

Proof: First, by smoothness (see Equation (17)),

$$\log \frac{\pi^{(t+1)}(a|s)}{\pi^{(t)}(a|s)} \geq \nabla_{\theta} \log \pi^{(t)}(a|s) \cdot (\theta^{(t+1)} - \theta^{(t)}) - \frac{\beta}{2} \|\theta^{(t+1)} - \theta^{(t)}\|_{2}^{2}$$
$$= \eta \nabla_{\theta} \log \pi^{(t)}(a|s) \cdot w^{(t)} - \eta^{2} \frac{\beta}{2} \|w^{(t)}\|_{2}^{2}.$$

We use d as shorthand for d_{ρ}^{π} (note ρ and π are fixed); we also use π_s as shorthand for the vector $\pi(\cdot|s)$. By the performance difference lemma (Lemma 3.2),

$$\begin{split} &\mathbb{E}_{s\sim d}\left(\mathrm{KL}(\pi_{s}||\pi_{s}^{(t)}) - \mathrm{KL}(\pi_{s}||\pi_{s}^{(t+1)})\right) \\ &= \mathbb{E}_{s\sim d}\,\mathbb{E}_{a\sim\pi(\cdot|s)}\left[\log\frac{\pi^{(t+1)}(a|s)}{\pi^{(t)}(a|s)}\right] \\ &\geq \eta\mathbb{E}_{s\sim d}\,\mathbb{E}_{a\sim\pi(\cdot|s)}\left[\nabla_{\theta}\log\pi^{(t)}(a|s)\cdot w^{(t)}\right] - \eta^{2}\frac{\beta}{2}\|w^{(t)}\|_{2}^{2} \qquad \text{(using previous display)} \\ &= \eta\mathbb{E}_{s\sim d}\,\mathbb{E}_{a\sim\pi(\cdot|s)}\left[A^{(t)}(s,a)\right] - \eta^{2}\frac{\beta}{2}\|w^{(t)}\|_{2}^{2} \\ &+ \eta\mathbb{E}_{s\sim d}\,\mathbb{E}_{a\sim\pi(\cdot|s)}\left[\nabla_{\theta}\log\pi^{(t)}(a|s)\cdot w^{(t)} - A^{(t)}(s,a)\right] \\ &\geq (1-\gamma)\eta\bigg(V^{\pi}(\rho) - V^{(t)}(\rho)\bigg) - \eta^{2}\frac{\beta}{2}\|w^{(t)}\|_{2}^{2} \\ &- \eta\sqrt{\mathbb{E}_{s\sim d}\,\mathbb{E}_{a\sim\pi(\cdot|s)}\left[\left(\nabla_{\theta}\log\pi^{(t)}(a|s)\cdot w^{(t)} - A^{(t)}(s,a)\right)^{2}\right]} \qquad \text{(Lemma 3.2 and Jensen)} \\ &\geq (1-\gamma)\eta\bigg(V^{\pi}(\rho) - V^{(t)}(\rho)\bigg) - \eta^{2}\frac{\beta}{2}W^{2} - \eta\sqrt{L_{\nu}(w^{(t)};\theta^{(t)})}. \end{split}$$

Rearranging, we have:

$$V^{\pi}(\rho) - V^{(t)}(\rho) \\ \leq \frac{1}{1 - \gamma} \left(\frac{1}{\eta} \mathbb{E}_{s \sim d} \left(\text{KL}(\pi_s || \pi_s^{(t)}) - \text{KL}(\pi_s || \pi_s^{(t+1)}) \right) + \frac{\eta \beta}{2} W^2 + \sqrt{L_{\nu}(w^{(t)}; \theta^{(t)})} \right)$$

Proceeding,

$$\frac{1}{T} \sum_{t=0}^{T-1} (V^{\pi}(\rho) - V^{(t)}(\rho)) \leq \frac{1}{\eta T (1-\gamma)} \sum_{t=0}^{T-1} \mathbb{E}_{s \sim d} \left(\text{KL}(\pi_{s} || \pi_{s}^{(t)}) - \text{KL}(\pi_{s} || \pi_{s}^{(t+1)}) \right) \\
+ \frac{1}{T (1-\gamma)} \sum_{t=0}^{T-1} \left(\frac{\eta \beta W^{2}}{2} + \sqrt{L_{\nu}(w^{(t)}; \theta^{(t)})} \right) \\
\leq \frac{\mathbb{E}_{s \sim d} \text{KL}(\pi_{s} || \pi^{(0)})}{\eta T (1-\gamma)} + \frac{\eta \beta W^{2}}{2 (1-\gamma)} + \frac{\sqrt{\tilde{\epsilon}_{approx}}}{1-\gamma} \\
\leq \frac{\log |\mathcal{A}|}{\eta T (1-\gamma)} + \frac{\eta \beta W^{2}}{2 (1-\gamma)} + \frac{\sqrt{\tilde{\epsilon}_{approx}}}{1-\gamma}$$

where we have used the definition of $\tilde{\epsilon}_{approx}$ and convexity in the second to last step.

6.1.1 Convergence Rate using Exact Natural Policy Gradients

In order to leverage Theorem 6.4 for obtaining concrete convergence rates, we start with the simplest setting where we have access to exact natural policy gradients, or equivalently (due to Equation 20), we use the exact minimizer of $L_{\nu^{(t)}}(w;\theta^{(t)})$ at each iteration t. In the next subsection, we consider a sample-based approximation scheme.

The difficulty with applying Theorem 6.4 is that, ideally, we seek to ensure that $L_{\nu}(w; \theta^{(t)})$ is small, where ν is the unknown state-action measure of a comparator policy π . Like previous results, we use an exploratory initial distribution over states and actions to partially address this issue as described below.

Formally, we consider a (slightly) more general version of the natural policy gradient algorithm, and we provide an agnostic learning result for this algorithm (where we compare to the best policy in the policy class). Instead of using a starting state distribution μ over states, the generalized version uses a starting distribution ν_0 over state-action pairs. Analogous to d_{μ}^{π} , this starting state-action distribution induces a state-action visitation distribution ν_0 , defined as:

$$\nu_{\nu_0}^{\pi}(s,a) := (1-\gamma)\mathbb{E}_{s_0,a_0 \sim \nu_0} \sum_{t=0}^{\infty} \gamma^t \Pr^{\pi}(s_t = s, a_t = a | s_0, a_0)$$
(21)

where $\Pr^{\pi}(s_t = s, a_t = a | s_0, a_0)$ is the state-action visitation probability that $s_t = s$ and $a_t = a$, after starting at state s_0 , taking action a_0 , and following π thereafter. As per our convention, $\nu^{(t)}$ is shorthand for $\nu_{\nu_0}^{\pi^{(t)}}$.

We now consider the update rule:

$$w^{(t)} \in \operatorname{argmin}_{w} L_{\nu^{(t)}}(w; \theta^{(t)}). \tag{22}$$

which exactly computes a minimizer (of a least squares objective function); the following subsection provides a finite sample version. This form is a more general version than that of (20); the generality is helpful in the following corollary, which provides a (worst-case) upper bound in terms of ν_0 .

Corollary 6.5. (Agnostic Learning with NPG) Suppose that we follow the update rule in (22) starting with $\theta^{(0)} = 0$. Fix a state distribution ρ and a state-action distribution ν_0 ; let $\pi^* = \pi_{\theta^*}$ the best policy in Π for ρ , i.e. $\theta^* \in \operatorname{argmax}_{\theta \in \Theta} V^{\pi_{\theta}}(\rho)$. Define ν^* as the induced state-action measure under π^* , i.e.

$$\nu^{\star}(s,a) = d_{\rho}^{\pi^{\star}}(s)\pi^{\star}(a|s).$$

Suppose $\eta = \sqrt{2 \log |\mathcal{A}|/(\beta W^2 T)}$; Assumption 6.2 holds; and that for all t < T,

$$L_{\nu^{(t)}}^{\star}(\theta^{(t)}) \le \epsilon_{approx}, \quad \|w^{(t)}\|_2 \le W.$$

We have that:

$$\min_{t < T} \left\{ V^{\pi^{\star}}(\rho) - V^{(t)}(\rho) \right\} \le \left(\frac{W\sqrt{2\beta \log |\mathcal{A}|}}{(1 - \gamma)} \right) \cdot \frac{1}{\sqrt{T}} + \sqrt{\frac{1}{(1 - \gamma)^3} \left\| \frac{\nu^{\star}}{\nu_0} \right\|_{\infty}} \epsilon_{approx}.$$

Proof: Since $\nu^{(t)}(s, a) \ge (1 - \gamma)\nu_0(s, a)$,

$$L_{\nu^{\star}}(w^{(t)}; \theta^{(t)}) \leq \left\| \frac{\nu^{\star}}{\nu^{(t)}} \right\|_{\infty} \cdot L_{\nu^{(t)}}(w^{(t)}; \theta^{(t)}) \leq \left\| \frac{\nu^{\star}}{\nu^{(t)}} \right\|_{\infty} \cdot \epsilon_{\text{approx}} \leq \frac{1}{(1 - \gamma)} \left\| \frac{\nu^{\star}}{\nu_{0}} \right\|_{\infty} \cdot \epsilon_{\text{approx}}.$$

Using this in Theorem 6.4 with the choice of η completes the proof.

When $\epsilon_{\rm approx}=0$, as in the tabular setting, the term depending on distribution mismatch coefficient disappears, consistent with Theorem 5.7. However, the convergence rate is only $O(\sqrt{1/T})$ instead of the O(1/T) bound there. This is because obtaining the fast rate in the function approximation regime appears to require even stronger conditions on the distributions (including $\nu^{(t+1)}$) under which the approximation errors are controlled at each round t.

Remark 6.6. (Dual Norm Error Bounds) Note that the $\ell_1 - \ell_\infty$ Hölder's inequality used in the first inequality of the proof is just one upper bound we can obtain to capture the measure mismatch between $\nu^{(t)}$ and ν^* , which may be overly conservative in some situations. For instance, an alternative Cauchy-Schwarz inequality would yield a bound depending on the second moment of the ratio, with a worse exponent on $\epsilon_{\rm approx}$. These alternatives are all valid upper bounds on the performance of the algorithm and are just part of the analysis. This observation is notable due to that it is perhaps helpful to state performance bounds (say for actor-critic methods) in terms of dual norms (e.g. Geist et al. [2019]).

6.1.2 Sample and Computational Complexity of the Natural Policy Gradient

So far we have assumed access to population quantities such as exact policy gradients, or the ability to minimize the compatible function approximation error (19) exactly. However, practical policy gradient algorithms typically use empirical estimates of these quantities. We now focus on the finite sample complexity of the NPG algorithm and show that the additional burden of using empirical quantities instead of their population counterparts is relatively small. Using the stochastic approximation results in Bach and Moulines [2013] (also see Jain et al. [2016, 2017]), we can design what is essentially an inexact Newton method for the NPG algorithm.

Algorithm 1 Sample-based Natural Policy Gradient with Function Approximation

Require: Learning rate η , SGD learning rate α , number of SGD iterations N, and simulation access to the MDP M under starting state-action distribution ν_0 .

- 1: Initialize $\theta^{(0)} = 0$.
- 2: **for** $t = 0, 1, \dots, T 1$ **do**
- Initialize $w_0 = 0$ 3:
- for i = 0, 1, ..., N 1 do 4:
- Sample $s, a \sim \nu^{(t)}$. Sample $a' \sim \nu^{(t)}(a|s)$. 5:
- Continue the episode by executing π starting from s, a, using a termination probability 6: of $1 - \gamma$. Let $\widehat{Q}(s, a)$ be the cumulative (undiscounted) reward from this episode.
- 7: Estimate

$$g_i = \left(w_i \cdot \nabla_{\theta} \log \pi^{(t)}(a|s) - \widehat{Q}(s,a)\right) \nabla_{\theta} \log \pi^{(t)}(a|s) + \widehat{Q}(s,a) \nabla_{\theta} \log \pi^{(t)}(a'|s).$$

Update w: 8:

$$w_{i+1} = w_i - \alpha g_i.$$

- end for 9:
- 10:
- Set $\widehat{w}^{(t)} = \frac{1}{N} \sum_{i=1}^{N} w_i$. Update $\theta^{(t+1)} = \theta^{(t)} + \eta \widehat{w}^{(t)}$. 11:
- **12: end for**

The algorithm proceeds in epochs, where in each epoch t the algorithm estimates $\widehat{w}^{(t)}$ using a sample based procedure and then updates $\theta^{(t)}$ according to:

$$\theta^{(t+1)} = \theta^{(t)} + \eta \widehat{w}^{(t)}. \tag{23}$$

Within each epoch, we use the average SGD update rule (specified in Algorithm 1) to learn $\widehat{w}^{(t)}$. In particular, within the episode, the update rule for w is:

$$w \leftarrow w - \alpha \widehat{\nabla_w L_{\nu^{(t)}}}(w; \theta^{(t)}),$$

where $\widehat{\nabla_w L_{\nu^{(t)}}}(w;\theta^{(t)})$ is an unbiased estimate of the gradient and α is a constant learning rate. After N updates, the average SGD algorithm returns the running average of the weight vectors encountered during the N updates; this average is used for $\widehat{w}^{(t)}$.

The algorithm is presented in Algorithm 1. Here, we assume access to an episodic environment, where in each episode the agent is started in some $(s_0, a_0) \sim \nu_0$; the agent then chooses actions after observing the state; the agent is able to terminate the episode at will. Note that to obtain an unbiased estimate of an infinite discounted reward (e.g. to estimate $Q^{\pi}(s,a)$), we can simulate the process by using a termination probability of $1-\gamma$, and then the *undiscounted* sum is an unbiased estimate of the expected discounted sum $Q^{\pi}(s,a)$. To understand the gradient estimator used in

the algorithm, observe that:

$$\nabla_{w} L_{\nu^{(t)}}(w;\theta) = 2\mathbb{E}_{s,a\sim\nu^{(t)}} \left[\left(w \cdot \nabla_{\theta} \log \pi_{\theta}(a|s) - A^{\pi_{\theta}}(s,a) \right) \nabla_{\theta} \log \pi_{\theta}(a|s) \right]$$

$$= 2\mathbb{E}_{s,a\sim\nu^{(t)}} \left[\left(w \cdot \nabla_{\theta} \log \pi_{\theta}(a|s) - Q^{\pi_{\theta}}(s,a) \right) \nabla_{\theta} \log \pi_{\theta}(a|s) \right]$$

$$+2\mathbb{E}_{s,a\sim\nu^{(t)}} \left[V^{\pi_{\theta}}(s) \nabla_{\theta} \log \pi_{\theta}(a|s) \right]. \tag{24}$$

The algorithm estimates the last term by obtaining conditionally independent estimates (independent conditioned on state s) of $V^{\pi_{\theta}}(s)$ and $\nabla_{\theta} \log \pi_{\theta}(a|s)$.

In order to state our main result for the algorithm, we make the following two assumptions on the policies and the MDP as described below.

Assumption 6.7. (Lipschitz Policy) Assume $\|\nabla_{\theta} \log \pi^{(t)}(a|s)\|_2 \leq B$.

Assumption 6.8. (Bounded Error and Weights) Suppose we follow the sample based NPG update rule specified in Algorithm 1. Define $w^{(t)} := \operatorname{argmin}_w L_{\nu^{(t)}}(w; \theta^{(t)})$. Suppose that for all t < T,

$$\mathbb{E}\bigg[L_{\nu^{(t)}}^{\star}(\boldsymbol{\theta}^{(t)})\bigg] \leq \epsilon_{\mathrm{approx}}, \quad \mathbb{E}\bigg[\|\widehat{w}^{(t)}\|_2^2\bigg] \leq \widehat{W}^2, \quad \mathbb{E}\bigg[\|\boldsymbol{w}^{(t)}\|_2^2\bigg] \leq W^2,$$

where the expectation is with respect to the randomness in $\theta^{(t)}$ in Algorithm 1 (under the parameter choices of the algorithm).

Remark 6.9. (A bias-variance tradeoff) Both W and \widehat{W} may be large when $\nabla^2_w L_\nu(w;\theta)$ is poorly conditioned. As in supervised learning, we can explicitly enforce bounds on these norms via projections; our results can be modified appropriately to account for this constraint. In particular, constraining to w such that $\|w\|_2 \leq W$ increases the approximation error, as the relevant error is then $\min_{w: \|w\|_2 \leq W} L_\nu(w;\theta)$ instead of $\min_w L_\nu(w;\theta)$ (see Theorem 6.4), while it decreases the variance in the algorithm (we can appeal to margin based bounds that have no explicit d dependence).

Corollary 6.10. (Sample and Computational Complexity of NPG) Suppose that we follow the sample based NPG update rule specified in Algorithm 1, starting with $\theta^{(0)} = 0$ and using N episodes per update of $\theta^{(t)}$. Fix a state distribution ρ and a state-action distribution ν_0 ; let $\pi^* = \pi_{\theta^*}$ where $\theta^* \in \operatorname{argmax}_{\theta \in \Theta} V^{\pi_{\theta}}(\rho)$; and define $\nu^*(s, a) = d_{\rho}^{\pi^*}(s)\pi^*(a|s)$.

Suppose $\eta = \sqrt{2 \log |\mathcal{A}|/(\beta \widehat{W}^2 T)}$, $\alpha = 1/B$, and assumptions 6.2, 6.7, and 6.8 hold. We have:

$$\mathbb{E}\left[\min_{t < T} \left\{ V^{\pi^{\star}}(\rho) - V^{(t)}(\rho) \right\} \right] \leq \left(\frac{\widehat{W}\sqrt{2\beta \log |\mathcal{A}|}}{(1 - \gamma)}\right) \cdot \frac{1}{\sqrt{T}} + \sqrt{\frac{1}{(1 - \gamma)^3}} \left\| \frac{\nu^{\star}}{\nu_0} \right\|_{\infty} \left(\sqrt{\epsilon_{approx}} + \frac{4\sqrt{d} \left(BW + 1/(1 - \gamma)\right)}{\sqrt{N}}\right).$$

Furthermore, each episode has expected length $2/(1-\gamma)$ so the expected number of total samples is $2NT/(1-\gamma)$; the total number of gradient computations $\nabla_{\theta} \log \pi^{(t)}(a|s)$ is 2NT; the total number of scalar multiplies, divides, and additions is $O(dNT + NT/(1-\gamma))$.

When $N \to \infty$, we recover the result of Corollary 6.5 for exact NPG updates. Using samples, we obtain the usual additional penalty scaling as $1/\sqrt{N}$, with the dimension dependence arising out of the analysis of averaged SGD (see e.g. Bach and Moulines [2013]). The dimension factor can be removed at the expense of a worse dependence on N, if we maintain bounded iterates w_i during each inner update in Algorithm 1, possibly by projecting on a scaled ℓ_2 ball.

Proof: First, by convexity, we have:

$$\mathbb{E}\left[\sqrt{\frac{1}{T}\sum_{t=0}^{T-1}L_{\nu^{\star}}(w^{(t)};\theta^{(t)})}\right] \leq \sqrt{\frac{1}{T}\sum_{t=0}^{T-1}\mathbb{E}\left[L_{\nu^{\star}}(w^{(t)};\theta^{(t)})\right]}.$$

The proof bounds $L_{\nu^*}(w^{(t)}; \theta^{(t)})$.

Using that $\nu_t(s, a) \ge (1 - \gamma)\nu_0(s, a)$, we have

$$\begin{split} & \mathbb{E} \bigg[L_{\nu^{\star}}(\widehat{w}^{(t)}; \boldsymbol{\theta}^{(t)}) \bigg] \leq \mathbb{E} \bigg[\bigg\| \frac{\nu^{\star}}{\nu^{(t)}} \bigg\|_{\infty} L_{\nu^{(t)}}(\widehat{w}^{(t)}; \boldsymbol{\theta}^{(t)}) \bigg] \\ & \leq \frac{1}{(1 - \gamma)} \bigg\| \frac{\nu^{\star}}{\nu_{0}} \bigg\|_{\infty} \mathbb{E} \bigg[L_{\nu^{(t)}}(\widehat{w}^{(t)}; \boldsymbol{\theta}^{(t)}) \bigg] \\ & = \frac{1}{(1 - \gamma)} \bigg\| \frac{\nu^{\star}}{\nu_{0}} \bigg\|_{\infty} \left(\mathbb{E} \bigg[L_{\nu^{(t)}}^{\star}(\boldsymbol{\theta}^{(t)}) \bigg] + \mathbb{E} \bigg[L_{\nu^{(t)}}(\widehat{w}^{(t)}; \boldsymbol{\theta}^{(t)}) \bigg] - \mathbb{E} \bigg[L_{\nu^{(t)}}^{\star}(\boldsymbol{\theta}^{(t)}) \bigg] \right) \\ & \leq \frac{1}{(1 - \gamma)} \bigg\| \frac{\nu^{\star}}{\nu_{0}} \bigg\|_{\infty} \left(\epsilon_{\text{approx}} + \mathbb{E} \bigg[L_{\nu^{(t)}}(\widehat{w}^{(t)}; \boldsymbol{\theta}^{(t)}) \bigg] - \mathbb{E} \bigg[L_{\nu^{(t)}}^{\star}(\boldsymbol{\theta}^{(t)}) \bigg] \right) \end{split}$$

In order to control the difference of the last two terms in the above bound, we would like to say that $\widehat{w}^{(t)}$ approximately minimizes $L_{\nu^{(t)}}(w;\theta^{(t)})$. We first note that the algorithm is indeed performing averaged SGD on $L_{\nu^{(t)}}(w;\theta^{(t)})$ in the inner loop since $\mathbb{E}[g_i|w_i] = \nabla_w L_{\nu^{(t)}}(w_i;\theta^{(t)})$. This is seen as Line 6 computes an unbiased estimate of $Q^{(t)}(s,a)$ with $s,a \sim \nu^{(t)}$, and this estimate is independent of w_i . Since $a' \sim \pi^{(t)}(\cdot|s)$ is further independent of everything else, we obtain

$$\begin{split} \mathbb{E}[g_{i}|w_{i}] &= \mathbb{E}[(w_{i} \cdot \nabla_{\theta} \log \pi^{(t)}(a|s) - \widehat{Q}(s,a))\nabla_{\theta} \log \pi^{(t)}(a|s) + \widehat{Q}(s,a)\nabla_{\theta} \log \pi^{(t)}(a'|s) \mid w_{i}] \\ &= \mathbb{E}_{(s,a) \sim \nu^{(t)}}[w_{i} \cdot \nabla_{\theta} \log \pi^{(t)}(a|s)\nabla_{\theta} \log \pi^{(t)}(a|s)] - \mathbb{E}_{(s,a) \sim \nu^{(t)}}[\nabla_{\theta} \log \pi^{(t)}(a|s)\mathbb{E}[\widehat{Q}(s,a)|s,a]] \\ &+ \mathbb{E}_{(s,a) \sim \nu^{(t)}}[\mathbb{E}[\widehat{Q}(s,a)|s,a]\mathbb{E}[\nabla_{\theta} \log \pi(a'|s)|s,a]] \\ &= \mathbb{E}_{(s,a) \sim \nu^{(t)}}[w_{i} \cdot \nabla_{\theta} \log \pi^{(t)}(a|s)\nabla_{\theta} \log \pi^{(t)}(a|s)] - \mathbb{E}_{(s,a) \sim \nu^{(t)}}[\nabla_{\theta} \log \pi^{(t)}(a|s)Q^{(t)}(s,a)] \\ &+ \mathbb{E}_{(s,a) \sim \nu^{(t)}}[Q^{(t)}(s,a)\mathbb{E}[\nabla_{\theta} \log \pi(a'|s)|s]] \\ &= \mathbb{E}_{(s,a) \sim \nu^{(t)}}[w_{i} \cdot \nabla_{\theta} \log \pi^{(t)}(a|s)\nabla_{\theta} \log \pi^{(t)}(a|s)] - \mathbb{E}_{(s,a) \sim \nu^{(t)}}[\nabla_{\theta} \log \pi^{(t)}(a|s)Q^{(t)}(s,a)] \\ &+ \mathbb{E}_{(s,a') \sim \nu^{(t)}}[V^{(t)}(s)\nabla_{\theta} \log \pi(a'|s)], \end{split}$$

where the final equality uses that both a and a' are drawn independently from $\pi^{(t)}(\cdot|s)$ conditional on s. The final expression exactly matches the form of the gradient shown in Equation 24, showing that our gradient estimates are indeed unbiased.

Using Theorem 1 from Bach and Moulines [2013] along with Assumption 6.7, we have:

$$\mathbb{E}\bigg[L_{\nu^{(t)}}(\widehat{w}^{(t)};\theta^{(t)})\bigg] - \mathbb{E}\bigg[L_{\nu^{(t)}}^{\star}(\theta^{(t)})\bigg] \leq \frac{2\left(\sigma\sqrt{d} + BW\right)^2}{N},$$

where σ is a uniform upper bound on the minimum variance of the regression problem underlying $w^{(t)}$. Following Bach and Moulines [2013], we recall the definition of σ . First, define the random vector $g_{\star}^{(t)}$ as the stochastic gradient at the optimal solution $w^{(t)}$, i.e.

$$g_{\star}^{(t)} := \left(w^{(t)} \cdot \nabla_{\theta} \log \pi^{(t)}(a|s) - \widehat{Q}(s,a) \right) \nabla_{\theta} \log \pi^{(t)}(a|s) + \widehat{Q}(s,a) \nabla_{\theta} \log \pi^{(t)}(a'|s).$$

The variance σ^2 is defined such that:

$$\mathbb{E}_{s,a \sim \nu^{(t)}} \left[g_{\star}^{(t)} (g_{\star}^{(t)})^{\top} \right] \preceq \sigma^2 \nabla_w^2 L_{\nu^{(t)}} (w^{(t)}; \theta^{(t)})$$

holds (also see Jain et al. [2016, 2017] for a sharper definition). It is straightforward to verify that $\sigma \leq B \|w^{(t)}\|_2 + 2/(1-\gamma)$, which completes the proof of the error bound.

We now argue each episode has expected length $2/(1-\gamma)$. Sampling $s, a \sim \nu^{(t)}$, in Line 6, can be obtained in expected time $1/(1-\gamma)$: we simulate the process under ν_0 and π_0 and accept the current state action pair with probability $1-\gamma$. We then obtain an unbiased estimate of $Q^{\pi}(s,a)$, in Line 6, by further simulating the process by using a termination probability of $1-\gamma$. Each of these two steps uses an expected number of samples that is $1/(1-\gamma)$.

From the proof, it is also evident that the multiplier of the dimension term can be instead replaced by the smaller term σ which we have upper bounded for ease of exposition within the proof.

6.2 Projected Policy Gradient for Constrained Policy Classes

We now consider a generalization of the structural assumption on the policies beyond the smooth, unconstrained case in the previous section. Let $\Pi = \{\pi_{\theta} : \theta \in \Theta\}$, where $\Theta \subseteq \mathbb{R}^d$ is a convex set, be the feasible set of all policies. Note that while we assume Θ is a convex set (in order to be able to efficiently do projections), we do not assume that the mapping from θ to π_{θ} is convex (as was the case in direct policy parameterization for the tabular setting). In this section, we show a convergence guarantee that applies to such policy parameterizations when using the projected gradient algorithm. We first recall the definition of ϵ -stationarity (see Appendix B.1 for discussion): a policy π_{θ} parameterized by θ is ϵ -stationary for $V^{\pi_{\theta}}(\mu)$ if for all $\theta + \delta \in \Theta$ and $\|\delta\|_2 \leq 1$, we have

$$\delta^{\top} \nabla_{\theta} V^{\pi_{\theta}}(\mu) = \mathbb{E}_{s \sim d_{\mu}^{\pi_{\theta}}} \left[\sum_{a \in \mathcal{A}} \frac{1}{1 - \gamma} \delta^{\top} \nabla_{\theta} \pi_{\theta}(s, a) Q^{\pi_{\theta}}(s, a) \right] \le \epsilon.$$
 (25)

Following our convention, we suppress the dependence on the starting state distribution μ when it is clear from the context. In this section, we show that any such ϵ -stationary point induces a

near-optimal policy from the class Π , modulo a distribution mismatch coefficient analogous to our result in Theorem 4.2. In order to develop such a result for the function approximation setting, we need some additional notation. Given a policy π_{θ} , let us define π_{θ}^+ as the greedy policy with respect to π_{θ} 's advantage function, i.e. π_{θ}^+ is deterministic and

if
$$\pi_{\theta}^+(a|s) = 1$$
, then $a \in \operatorname{argmax}_{a' \in \mathcal{A}} A^{\pi_{\theta}}(s, a')$.

When doing policy improvement with function approximation, it is natural to measure the error in approximating the 1-step improvement relative to any policy in the class. With this intuition, we define the *Bellman policy error* in approximating π_{θ}^+ as

$$L_{\text{BPE}}(\theta; w) = \mathbb{E}_{s \sim d_{\mu}^{\pi_{\theta}}} \left[\sum_{a \in \mathcal{A}} \left| \pi_{\theta}^{+}(a|s) - \pi_{\theta}(a|s) - w^{\top} \nabla_{\theta} \pi_{\theta}(a|s) \right| \right]$$

$$= \mathbb{E}_{s \sim d_{\mu}^{\pi_{\theta}}} \left[\| \pi_{\theta}^{+}(\cdot|s) - \pi_{\theta}(\cdot|s) - w^{\top} \nabla_{\theta} \pi_{\theta}(\cdot|s) \|_{1} \right],$$
(26)

where $||x||_1$ denotes the ℓ_1 norm of a vector x.

Since the stationarity of a parameter θ measures the effect of local perturbations on the function value, it is natural to also quantify the Bellman policy error based on perturbations centered around θ . Precisely, we define the best fit weight vector with respect to the Bellman policy error as

$$w^{\star}(\theta) = \operatorname{argmin}_{w \in \mathbb{R}^d : w + \theta \in \Theta} L_{\text{BPE}}(\theta; w). \tag{27}$$

We also use the shorthand:

$$L_{\text{BPE}}(\theta) = L_{\text{BPE}}(\theta; w^{\star}(\theta)).$$

It is easily seen that in the direct policy parameterization for the tabular setting, $L_{\text{BPE}}(\theta) = 0$, since

$$L_{\text{BPE}}(\theta; w) = \mathbb{E}_{s \sim d_{\mu}^{\pi_{\theta}}} \left[\sum_{a \in \mathcal{A}} \left| \pi_{\theta}^{+}(a|s) - \theta_{s,a} - w_{s,a} \right| \right].$$

which is 0 provided we set $w_{s,a} = \pi_{\theta}^+(a|s) - \theta_{s,a}$. We now argue that the Bellman policy error is the relevant measure for how function approximation enters into the suboptimality of a policy found by projected first-order methods. We note that the property of $L_{\text{BPE}}(\theta) = 0$ for all $\theta \in \Theta$ is related to notions such as *policy completeness* from prior work [Dann et al., 2018], further motivating this error as a relevant measure of the expressivity of a policy class. Related notions also appear in the analysis of CPI [Kakade and Langford, 2002, Scherrer and Geist, 2014], which measure the gap between the advantage of π_{θ}^+ relative to π_{θ} . In contrast, L_{BPE} evaluates the error in approximating π^+ by updating π_{θ} along the gradient direction, which is natural in the context of first-order methods.

We now show an analog of the gradient domination result (Lemma 4.1) in the setting of function approximation.

Theorem 6.11. Given any starting state distribution ρ , suppose we find an ϵ_{opt} -stationary point θ of $V^{\pi_{\theta}}(\mu)$, as in (25), satisfying $L_{BPE}(\theta) \leq \epsilon_{approx}$. Let $\pi^{\star} = \pi_{\theta^{\star}}$ where $\theta^{\star} \in \operatorname{argmax}_{\theta \in \Theta} V^{\pi_{\theta}}(\rho)$. We have the guarantee

$$V^{\pi^*}(\rho) - V^{\pi_{\theta}}(\rho) \le \frac{1}{(1 - \gamma)^3} \left\| \frac{d_{\rho}^{\pi^*}}{\mu} \right\|_{\infty} \left(\epsilon_{approx} + (1 - \gamma)^2 (1 + \|w^*(\theta)\|_2) \epsilon_{opt} \right).$$

See Appendix D for the proof. In order to further turn this result into a convergence rate on the number of iterations of a projected policy gradient method, we make two regularity assumptions, namely Lipschitz continuity and smoothness, on the policy class which we state below.

Assumption 6.12 (Lipschitz continuous and smooth policies). Assume that for all $\theta, \theta' \in \Theta$ and for all $s \in S$ and $a \in A$, we have

$$|\pi_{\theta}(a|s) - \pi_{\theta'}(a|s)| \le \beta_1 \|\theta - \theta'\|_2$$
 (\beta_1-Lipschitz)
$$\|\nabla_{\theta}\pi_{\theta}(a|s) - \nabla_{\theta}\pi_{\theta'}(a|s)\|_2 \le \beta_2 \|\theta - \theta'\|_2$$
 (\beta_2-smooth)

Linear policies satisfy the requisite assumptions on continuity and smoothness.

Example 6.13 (Linear Policy). For any state, action pair (s, a), suppose we have a feature mapping $\phi_{s,a} \in \mathbb{R}^d$ with $\|\phi_{s,a}\|_2 \leq B$. Let us consider the policy class

$$\pi_{\theta}(a|s) = \phi_{s,a}^{\top} \theta \text{ for } \theta \in \Theta, \quad \text{where } \Theta = \{\theta : \pi_{\theta} \in \Delta_{|\mathcal{A}|}\}.$$

Here, Θ is a convex set since the pre-image of Δ_A under a linear function is convex.

We study the projected gradient descent updates, which initialize at some $\theta^{(0)}$ and update

$$\theta^{(t+1)} = \mathcal{P}_{\Theta}(\theta^{(t)} + \eta \nabla_{\theta} V^{(t)}(\mu)), \tag{28}$$

where \mathcal{P}_{Θ} denotes projections onto the convex set Θ . We show the following convergence rate for these updates.

Corollary 6.14. Suppose that Assumption 6.12 holds and for our definitions (26)-(27) of $L_{BPE}(\theta)$ and $w^{\star}(\theta)$, assume for all t < T

$$L_{BPE}(\theta^{(t)}) \le \epsilon_{approx}$$
 and $\|w^*(\theta^{(t)})\|_2 \le W^*$.

Let

$$\beta = \frac{\beta_2 |\mathcal{A}|}{(1-\gamma)^2} + \frac{2\gamma \beta_1^2 |\mathcal{A}|^2}{(1-\gamma)^3}.$$

Then, projected gradient ascent (28) with stepsize $\eta = \frac{1}{\beta}$ satisfies for all starting state distributions ρ and for any other policy $\pi^* \in \Pi$,

$$\min_{t < T} \left\{ V^{\star}(\rho) - V^{(t)}(\rho) \right\} \le \frac{1}{(1 - \gamma)^3} \left\| \frac{d_{\rho}^{\pi^{\star}}}{\mu} \right\|_{\infty} \epsilon_{approx} + (W^{\star} + 1)\epsilon, \text{ for } T \ge \frac{8\beta}{(1 - \gamma)^3 \epsilon^2} \left\| \frac{d_{\rho}^{\pi^{\star}}}{\mu} \right\|_{\infty}^2.$$

We present the proof in Appendix D, which utilizes standard non-convex optimization results (e.g. [Beck, 2017, Theorem 10.15]) for the convergence of projected gradient ascent on smooth functions over a convex set.

7 Discussion

This work provides a systematic study of the convergence properties of policy optimization techniques in MDPs, both in the tabular and the function approximation settings. At the very core, our results imply that the non-convexity of the policy optimization problem is not the fundamental challenge for typical variants of the policy gradient approach. This is evidenced by the global convergence results which we establish and that demonstrate the relative niceness of the underlying optimization problem. At the same time, our results do highlight that insufficient exploration can lead to the convergence to sub-optimal policies, as is also observed in practice. Conversely, we can expect typical policy gradient algorithms to find the best policy from amongst those whose state-visitation distribution is adequately aligned with the policies we discover.

We show that the nature and severity of the exploration term differs in different policy optimization approaches, as well as based on the noise in gradient computation. For instance, we find that doing policy gradient in its standard form for both the direct and softmax parameterizations can be slow to converge, particularly in the face of distribution mismatch, even when policy gradients are computed exactly. Natural policy gradient, on the other hand, enjoys a fast dimension-free convergence when we are in tabular settings with exact gradients. On the other hand, for the function approximation setting, or when using finite samples, all algorithms suffer to some degree from the exploration issue captured through the distribution mismatch coefficient.

Finally, we also identify concrete measures of the expressivity of a policy class as required in different algorithms such as the natural policy gradient or projected policy gradient. While similar quantities have certainly been studied and introduced in prior works, we concretely connect them with the convergence rates of these techniques and also show how questions of exploration interplay with these quantities.

In the interest of scope, we omit certain issues in our study, but which should be important questions for future research. We do not consider the effects of standard variance reduction techniques like use of control variates or actor-critic approaches to policy optimization. We also do not investigate the question of how good initial state distribution μ might be designed to improve the convergence properties, which is effectively the exploration problem in reinforcement learning. We hope that our study, combined with future results along the lines mentioned above, can serve as a means to design more principled approaches to reinforcement learning.

Finally, one direction to make further progress is to provide sharper *problem dependent* rates, in terms of the underlying MDP at hand. While our distribution mismatch coefficient can always be made finite unlike concentrability coefficient-style measures, it does ignore properties of the MDP dynamics, and combining the two sets of ideas might pave the way for a sharper analysis or improved algorithms.

Acknowledgments

Sham Kakade acknowledges funding from the Washington Research Foundation for Innovation in Data-intensive Discovery, the ONR award N00014-18-1-2247, and the DARPA award FA8650-18-2-7836. Jason D. Lee acknowledges support of the ARO under MURI Award W911NF-11-1-0303.

This is part of the collaboration between US DOD, UK MOD and UK Engineering and Physical Research Council (EPSRC) under the Multidisciplinary University Research Initiative.

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A Proofs for Section 3

Proof:[of Lemma 3.1] Recall the MDP in Figure 1. Note that since actions in terminal states s_3 , s_4 and s_5 do not change the expected reward, we only consider actions in states s_1 and s_2 . Let the "up/above" action as a_1 and "right" action as a_2 . Note that

$$V^{\pi}(s_1) = \pi(a_2|s_1)\pi(a_1|s_2) \cdot r$$

Consider

$$\theta^{(1)} = (\log 1, \log 3, \log 3, \log 3), \quad \theta^{(2)} = (-\log 1, -\log 3, -\log 3, -\log 1)$$

where θ is written as a tuple $(\theta_{a_1,s_1}, \theta_{a_2,s_1}, \theta_{a_1,s_2}, \theta_{a_2,s_2})$. Then, for the softmax parameterization, we get

$$\pi^{(1)}(a_2|s_1) = \frac{3}{4}; \quad \pi^{(1)}(a_1|s_2) = \frac{3}{4}; \quad V^{(1)}(s_1) = \frac{9}{16}r$$

and

$$\pi^{(2)}(a_2|s_1) = \frac{1}{4}; \quad \pi^{(2)}(a_1|s_2) = \frac{1}{4}; \quad V^{(2)}(s_1) = \frac{1}{16}r$$

Also, for $\theta^{\text{(mid)}} = \frac{\theta^{(1)} + \theta^{(2)}}{2}$

$$\pi^{\text{(mid)}}(a_2|s_1) = \frac{1}{2}; \quad \pi^{\text{(mid)}}(a_1|s_2) = \frac{1}{2}; \quad V^{\text{(mid)}}(s_1) = \frac{1}{4}r$$

This gives

$$V^{(1)}(s_1) + V^{(2)}(s_1) > 2V^{\text{(mid)}}(s_1)$$

which shows that V^{π} is non-concave.

Proof:[of Lemma 3.2] Let $\Pr^{\pi}(\tau|s_0 = s)$ denote the probability of observing a trajectory τ when starting in state s and following the policy π . Using a telescoping argument, we have:

$$V^{\pi}(s) - V^{\pi'}(s) = \mathbb{E}_{\tau \sim \Pr^{\pi}(\tau|s_{0}=s)} \left[\sum_{t=0}^{\infty} \gamma^{t} r(s_{t}, a_{t}) \right] - V^{\pi'}(s)$$

$$= \mathbb{E}_{\tau \sim \Pr^{\pi}(\tau|s_{0}=s)} \left[\sum_{t=0}^{\infty} \gamma^{t} \left((r(s_{t}, a_{t}) + V^{\pi'}(s_{t}) - V^{\pi'}(s_{t}) \right) \right] - V^{\pi'}(s)$$

$$= \mathbb{E}_{\tau \sim \Pr^{\pi}(\tau|s_{0}=s)} \left[\sum_{t=0}^{\infty} \gamma^{t} \left(r(s_{t}, a_{t}) + \gamma V^{\pi'}(s_{t+1}) - V^{\pi'}(s_{t}) \right) \right]$$

$$\stackrel{(a)}{=} \mathbb{E}_{\tau \sim \Pr^{\pi}(\tau|s_{0}=s)} \left[\sum_{t=0}^{\infty} \gamma^{t} \left(r(s_{t}, a_{t}) + \gamma \mathbb{E}[V^{\pi'}(s_{t+1})|s_{t}, a_{t}] - V^{\pi'}(s_{t}) \right) \right]$$

$$= \mathbb{E}_{\tau \sim \Pr^{\pi}(\tau|s_{0}=s)} \left[\sum_{t=0}^{\infty} \gamma^{t} A^{\pi'}(s_{t}, a_{t}) \right] = \frac{1}{1 - \gamma} \mathbb{E}_{s' \sim d_{s}^{\pi}} \mathbb{E}_{a \sim \pi(\cdot|s)} \gamma^{t} A^{\pi'}(s', a),$$

where (a) uses the tower property of conditional expectations and the final equality follows from the definition of d_s^{π} .

B Proofs for Section 4

B.1 Proofs for Section 4.2

We first define first-order optimality for constrained optimization.

Definition B.1 (First-order Stationarity). A policy $\pi_{\theta} \in \Delta(\mathcal{A})^{|S|}$ is ϵ -stationary with respect to the initial state distribution μ if

$$G(\pi_{\theta}) := \max_{\pi_{\theta} + \delta \in \Delta(\mathcal{A})^{|S|}, \|\delta\|_{2} \le 1} \delta^{\top} \nabla_{\pi} V^{\pi_{\theta}}(\mu) \le \epsilon.$$

where $\Delta(\mathcal{A})^{|S|}$ is the set of all policies.

Due to that we are working with the direct parameterization (see (2)), we drop the θ subscript.

Remark B.2. If $\epsilon = 0$, then the definition simplifies to $\delta^{\top} \nabla_{\pi} V^{\pi}(\mu) \leq 0$. Geometrically, δ is a feasible direction of movement since the probability simplex $\Delta(\mathcal{A})^{|S|}$ is convex. Thus the gradient is negatively correlated with any feasible direction of movement, and so π is first-order stationary.

Proposition B.3. Let $V^{\pi}(\mu)$ be β -smooth in π . Define the gradient mapping

$$G^{\eta} = \frac{1}{\eta} \left(P_{\Delta(\mathcal{A})^{|S|}} (\pi + \eta \nabla_{\pi} V^{\pi}(\mu)) - \pi \right),$$

and the update rule for the projected gradient is $\pi^+ = \pi + \eta G^{\eta}$. If $||G^{\eta}||_2 \le \epsilon$, then

$$\max_{\pi+\delta \in \Delta(A)^{|\mathcal{S}|}, \ \|\delta\|_2 \leq 1} \delta^\top \nabla_\pi V^{\pi^+}(\mu) \leq \epsilon \big(\eta\beta + 1\big).$$

Proof: By Lemma 3 of Ghadimi and Lan [2016],

$$\nabla_{\pi} V^{\pi^+}(\mu) \in N_{\Delta(\mathcal{A})^{|\mathcal{S}|}}(\pi^+) + \epsilon(\eta\beta + 1)B_2,$$

where B_2 is the unit ℓ_2 ball, and $N_{\Delta(\mathcal{A})^{|\mathcal{S}|}}$ is the normal cone of the product simplex $\Delta(\mathcal{A})^{|\mathcal{S}|}$. Since $\nabla_{\pi}V^{\pi^+}(\mu)$ is $\epsilon(\eta\beta+1)$ distance from the normal cone and δ is in the tangent cone, then $\delta^{\top}\nabla_{\pi}V^{\pi^+}(\mu) \leq \epsilon(\eta\beta+1)$.

Proof:[of Theorem 4.2] We first define

$$G^{\eta}(\pi) = \frac{1}{\eta} (\pi - P_{\Delta(A)^{|S|}}(\pi + \eta \nabla_{\pi} V^{(t)}(\mu)))$$

From Lemma E.3, we have $V^{\pi}(s)$ is β -smooth for all states s (and also hence $V^{\pi}(\mu)$ is also β -smooth) with $\beta = \frac{2\gamma |\mathcal{A}|}{(1-\gamma)^3}$. Then, from Beck [2017][Theorem 10.15], we have that for $G^{\eta}(\pi)$ with step-size $\eta = \frac{1}{\beta}$,

$$\min_{t=0,1,\dots,T-1} \|G^{\eta}(\pi^{(t)})\|_2 \le \frac{\sqrt{2\beta(V^{\star}(\mu) - V^{(0)}(\mu))}}{\sqrt{T}}$$

Then, from Proposition B.3, we have

$$\min_{t=0,1,\dots,T} \max_{\pi^{(t)}+\delta \in \Delta(A)^{|\mathcal{S}|}, \ \|\delta\|_2 \leq 1} \delta^\top \nabla_\pi V^{\pi^{(t+1)}}(\mu) \leq (\eta\beta+1) \frac{\sqrt{2\beta(V^\star(\mu)-V^{(0)}(\mu))}}{\sqrt{T}}$$

Observe that

$$\max_{\bar{\pi} \in \Delta(A)^{|\mathcal{S}|}} (\bar{\pi} - \pi)^{\top} \nabla_{\pi} V^{\pi}(\mu) = 2\sqrt{|\mathcal{S}|} \max_{\bar{\pi} \in \Delta(A)^{|\mathcal{S}|}} \frac{1}{2\sqrt{|\mathcal{S}|}} (\bar{\pi} - \pi)^{\top} \nabla_{\pi} V^{\pi}(\mu)$$

$$\leq 2\sqrt{|\mathcal{S}|} \max_{\pi + \delta \in \Delta(A)^{|\mathcal{S}|}, \|\delta\|_{2} \leq 1} \delta^{\top} \nabla_{\pi} V^{\pi}(\mu)$$

where the last step follows as $\|\bar{\pi} - \pi\|_2 \le 2\sqrt{|\mathcal{S}|}$. And then using Lemma 4.1 and $\eta\beta = 1$, we have

$$\min_{t=0,1,\dots,T} V^{\star}(\rho) - V^{(t)}(\rho) \leq \frac{4\sqrt{|\mathcal{S}|}}{1-\gamma} \left\| \frac{d_{\rho}^{\pi^{\star}}}{\mu} \right\|_{\infty} \frac{\sqrt{2\beta(V^{\star}(\mu) - V^{(0)}(\mu))}}{\sqrt{T}}$$

We can get our required bound of ϵ , if we set T such that

$$\frac{4\sqrt{|\mathcal{S}|}}{1-\gamma} \left\| \frac{d_{\rho}^{\pi^{\star}}}{\mu} \right\| \frac{\sqrt{2\beta(V^{\star}(\mu) - V^{(0)}(\mu))}}{\sqrt{T}} \le \epsilon$$

or, equivalently,

$$T \ge \frac{32|\mathcal{S}|\beta(V^{\star}(\mu) - V^{(0)}(\mu))}{(1 - \gamma)^2 \epsilon^2} \left\| \frac{d_{\rho}^{\pi^{\star}}}{\mu} \right\|_{\infty}^2.$$

Using $V^{\star}(\mu) - V^{(0)}(\mu) \leq \frac{1}{1-\gamma}$ and $\beta = \frac{2\gamma|\mathcal{A}|}{(1-\gamma)^3}$ from Lemma E.3 leads to the desired result.

B.2 Proofs for Section 4.3

Recall the MDP in Figure 2. Each trajectory starts from the initial state s_0 , and we use the discount factor $\gamma = H/(H+1)$. Recall that we work with the direct parameterization, where $\pi_{\theta}(a|s) = \theta_{s,a}$ for $a = a_1, a_2, a_3$ and $\pi_{\theta}(a_4|s) = 1 - \theta_{s,a_1} - \theta_{s,a_2} - \theta_{s,a_3}$. Note that since states s_0 and s_{H+1} only have once action, therefore, we only consider the parameters for states s_1 to s_H . For this policy class and MDP, let P^{θ} be the state transition matrix under π_{θ} , i.e. $[P^{\theta}]_{s,s'}$ is the probability of going from state s_1 to s_2 under policy s_3 :

$$[P^{\theta}]_{s,s'} = \sum_{a \in A} \pi_{\theta}(a|s) P(s'|s,a).$$

For the MDP illustrated in Figure 2, the entries of this matrix are given as:

$$[P^{\theta}]_{s,s'} = \begin{cases} \theta_{s,a_1} & \text{if } s' = s_{i+1} \text{ and } s = s_i \text{ with } 1 \le i \le H \\ 1 - \theta_{s,a_1} & \text{if } s' = s_{i-1} \text{ and } s = s_i \text{ with } 1 \le i \le H \\ 1 & \text{if } s' = s_1 \text{ and } s = s_0 \\ 1 & \text{if } s' = s = s_{H+1} \\ 0 & \text{otherwise} \end{cases}$$
 (29)

With this definition, we recall that the value function in the initial state s_0 is given by

$$V^{\pi_{\theta}}(s_0) = \mathbb{E}_{\tau \sim \pi_{\theta}}[\sum_{t=0}^{\infty} \gamma^t r_t] = e_0^T (I - \gamma P^{\theta})^{-1} r,$$

where e_0 is an indicator vector for the starting state s_0 . From the form of the transition probabilities (29), it is clear that the value function only depends on the parameters θ_{s,a_1} in any state s. While care is needed for derivatives as the parameters across actions are related by the simplex feasibility constraints, we have assumed each parameter is strictly positive, so that an infinitesimal change to any parameter other than θ_{s,a_1} does not affect the policy value and hence the policy gradients. With this understanding, we succinctly refer to θ_{s,a_1} as θ_s in any state s. We also refer to the state s_i simply as i to reduce subscripts.

For convenience, we also define \bar{p} (resp. \underline{p}) to be the largest (resp. smallest) of the probabilities θ_s across the states $s \in [1, H]$ in the MDP.

In this section, we prove Lemma 4.3, that is: for $0 < \theta < 1$ (componentwise across states and actions), $\bar{p} \leq 1/4$, and for all $k \leq \frac{H}{40 \log(2H)} - 1$, we have $\|\nabla_{\theta}^k V^{\pi_{\theta}}(s_0)\| \leq (1/3)^{H/4}$, where $\nabla_{\theta}^k V^{\pi_{\theta}}(s_0)$ is a tensor of the k_{th} order. Furthermore, we seek to show $V^{\star}(s_0) - V^{\pi_{\theta}}(s_0) \geq (H + 1)/8 - (H + 1)^2/3^H$ (where θ^{\star} are the optimal policy's parameters).

It is easily checked that $V^{\pi_{\theta}}(s_0) = M_{0,H+1}^{\theta}$, where

$$M^{\theta} := (I - \gamma P^{\theta})^{-1}$$

since the only rewards are obtained in the state s_{H+1} . In order to bound the derivatives of the expected reward, we first establish some properties of the matrix M^{θ} .

Lemma B.4. Suppose
$$\bar{p} \leq 1/4$$
. Fix any $\alpha \in \left[\frac{1-\sqrt{1-4\gamma^2\bar{p}(1-\underline{p})}}{2\gamma(1-\underline{p})}, \max\left\{\frac{1+\sqrt{1-4\gamma^2\bar{p}(1-\underline{p})}}{2\gamma(1-\underline{p})}, 1\right\}\right]$. Then

1.
$$M_{a,b} \leq \frac{\alpha^{b-a-1}}{1-\gamma}$$
 for $0 \leq a \leq b \leq H$.

2.
$$M_{a,H+1}^{\theta} \leq \frac{\gamma \bar{p}}{1-\gamma} M_{a,H}^{\theta} \leq \frac{\gamma \bar{p}}{(1-\gamma)^2} \alpha^{H-a}$$
 for $0 \leq a \leq H$.

Proof: Let $\rho_{a,b}^k$ be the normalized discounted probability of reaching b, when the initial state is a, in k steps, that is

$$\rho_{a,b}^{k} := (1 - \gamma) \sum_{i=0}^{k} [(\gamma P^{\theta})^{i}]_{a,b}, \tag{30}$$

where we recall the convention that U^0 is the identity matrix for any square matrix U. Observe that $0 \le \rho_{a,b}^k \le 1$, and, based on the form (29) of P^{θ} , we have the recursive relation for all k > 0:

$$\rho_{a,b}^{k} = \begin{cases} \gamma(1 - \theta_{b+1})\rho_{a,b+1}^{k-1} + \gamma\theta_{b-1}\rho_{a,b-1}^{k-1} & \text{if } 1 < b < H \\ \gamma\theta_{H-1}\rho_{a,H-1}^{k-1} & \text{if } b = H \\ \gamma\theta_{H}\rho_{a,H}^{k-1} + \gamma\rho_{a,H+1}^{k-1} & \text{if } b = H+1 \text{ and } a < H+1 \\ 1 - \gamma & \text{if } b = H+1 \text{ and } a = H+1 \\ \gamma(1 - \theta_{2})\rho_{a,2}^{k-1} + \gamma\rho_{a,0}^{k-1} & \text{if } b = 0 \end{cases}$$

$$(31)$$

Note that $\rho_{a,b}^0=0$ for $a\neq b$ and $\rho_{a,b}^0=1-\gamma$ for a=b. Now let us inductively prove that for all $k\geq 0$

$$\rho_{a,b}^k \le \alpha^{b-a} \quad \text{for} \quad 1 \le a \le b \le H. \tag{32}$$

Clearly this holds for k=0 since $\rho_{a,b}^0=0$ for $a\neq b$ and $\rho_{a,b}^0=1-\gamma$ for a=b. Now, assuming the bound for all steps till k-1, we now prove it for k case by case.

For a = b the result follows since

$$\rho_{a,b}^k \leq 1 = \alpha^{b-a}$$
.

For 1 < b < H and a < b, observe that the recursion (31) and the inductive hypothesis imply that

$$\begin{split} \rho_{a,b}^k &\leq \gamma (1 - \theta_{b+1}) \alpha^{b+1-a} + \gamma \theta_{b-1} \alpha^{b-1-a} \\ &= \alpha^{b-a-1} \left(\gamma (1 - \theta_{b+1}) \alpha^2 + \gamma \theta_{b-1} \right) \\ &\leq \alpha^{b-a-1} \left(\gamma (1 - \underline{p}) \alpha^2 + \gamma \overline{p} \right) \\ &= \alpha^{b-a-1} \left(\alpha + \gamma (1 - p) \alpha^2 - \alpha + \gamma \overline{p} \right) \leq \alpha^{b-a}, \end{split}$$

where the last inequality follows since $\alpha^2\gamma(1-\underline{p})-\alpha+\gamma\bar{p}\leq 0$ due to that α is within the roots of this quadratic equation. Note the discriminant term in the square root is non-negative provided $\bar{p}<1/4$, since the condition along with the knowledge that $\underline{p}\leq\bar{p}$ ensures that $4\gamma^2\bar{p}(1-\underline{p})\leq 1$.

For b = H and a < H, we observe that

$$\begin{split} \rho_{a,b}^k &\leq \gamma \theta_{H-1} \, \alpha^{H-1-a} \\ &= \alpha^{H-a} \frac{\gamma \theta_{H-1}}{\alpha} \\ &\leq \alpha^{H-a} \big(\frac{\gamma \bar{p}}{\alpha} \big) \leq \alpha^{H-a} \big(\gamma (1 - \underline{p}) \alpha + \frac{\gamma \bar{p}}{\alpha} \big) \leq \alpha^{H-a}. \end{split}$$

This proves the inductive claim (note that the cases of b=a=1 and b=a=H are already handled in the first part above). Next, we prove that for all $k \ge 0$

$$\rho_{0,b}^k \le \alpha^{b-1}.$$

Clearly this holds for k=0 and $b\neq 0$ since $\rho_{0,b}^0=0$. Furthermore, for all $k\geq 0$ and b=0,

$$\rho_{0,b}^k \le 1 \le \alpha^{b-1},$$

since $\alpha \le 1$ by construction and b = 0. Now, we consider the only remaining case when k > 0 and $b \in [1, H + 1]$. By (29), observe that for k > 0 and $b \in [1, H + 1]$,

$$[(P^{\theta})^{i}]_{0,b} = [(P^{\theta})^{i-1}]_{1,b}, \tag{33}$$

for all $i \ge 1$. Using the definition of $\rho_{a,b}^k$ (30) for k > 0 and $b \in [1, H+1]$,

$$\begin{split} \rho_{0,b}^k &= (1-\gamma) \sum_{i=0}^k [(\gamma P^\theta)^i]_{0,b} = (1-\gamma)[(\gamma P^\theta)^0]_{0,b} + (1-\gamma) \sum_{i=1}^k [(\gamma P^\theta)^i]_{0,b} \\ &= 0 + (1-\gamma) \sum_{i=1}^k \gamma^i [(P^\theta)^i]_{0,b} \qquad \qquad \text{(since } b \geq 1) \\ &= (1-\gamma) \sum_{i=1}^k \gamma^i \left[(P^\theta)^{i-1} \right]_{1,b} \qquad \qquad \text{(using Equation (33))} \\ &= (1-\gamma) \gamma \sum_{j=0}^{k-1} \gamma^j [(P^\theta)^j]_{1,b} \qquad \qquad \text{(By substituting } j = i-1) \\ &= \gamma \rho_{1,b}^{k-1} \qquad \qquad \text{(using Equation (30))} \\ &\leq \alpha^{b-1} \qquad \qquad \text{(using Equation (32) and } \gamma, \alpha \leq 1) \end{split}$$

Hence, for all $k \ge 0$

$$\rho_{0,b}^k \leq \alpha^{b-1}$$

In conjunction with Equation (32), the above display gives for all $k \ge 0$,

$$\rho_{a,b}^k \le \alpha^{b-a} \quad \text{for} \quad 1 \le a \le b \le H$$

$$\rho_{a,b}^k \le \alpha^{b-a-1} \quad \text{for} \quad 0 = a \le b \le H$$

Also observe that

$$M_{a,b}^{\theta} = \lim_{k \to \infty} \frac{\rho_{a,b}^k}{1 - \gamma}.$$

Since the above bound holds for all $k \geq 0$, it also applies to the limiting value $M_{a,b}^{\theta}$, which shows that

$$M_{a,b} \le \frac{\alpha^{b-a}}{1-\gamma} \le \frac{\alpha^{b-a-1}}{1-\gamma}$$
 for $1 \le a \le b \le H$

$$M_{a,b} \le \frac{\alpha^{b-a-1}}{1-\gamma}$$
 for $0 = a \le b \le H$

which completes the proof of the first part of the lemma.

For the second claim, from recursion (31) and b = H + 1 and a < H + 1

$$\rho_{a,H+1}^k = \gamma \theta_H \rho_{a,H}^{k-1} + \gamma \rho_{a,H+1}^{k-1} \le \gamma \bar{p} \rho_{a,H}^{k-1} + \gamma \rho_{a,H+1}^{k-1},$$

Taking the limit of $k \to \infty$, we see that

$$M_{a,H+1}^{\theta} \le \gamma \bar{p} M_{a,H} + \gamma M_{a,H+1}^{\theta}.$$

Rearranging the terms in the above bound yields the second claim in the lemma. Using the lemma above, we now bound the derivatives of M^{θ} .

Lemma B.5. The k_{th} order partial derivatives of M satisfy:

$$\left| \frac{\partial^k M_{0,H+1}}{\partial \theta_{\beta_1} \dots \partial \theta_{\beta_k}} \right| \le \frac{\bar{p} \, 2^k \, \gamma^{k+1} \, k! \, \alpha^{H-2k}}{(1-\gamma)^{k+2}}.$$

where β denotes a k dimensional vector with entries in $\{1, 2, ..., H\}$.

Proof: Since we know that $\nabla_{\theta} M = M \nabla_{\theta} (I - \gamma P^{\theta}) M$, using the form of P^{θ} in (29), we get for any $h \in [1, H]$

$$\frac{\partial M_{a,b}}{\partial \theta_h} = -\gamma \sum_{i,j=0}^{H+1} M_{a,i} \frac{\partial P_{i,j}}{\partial \theta_h} M_{j,b} = \gamma M_{a,h} (M_{h-1,b} - M_{h+1,b})$$
(34)

where the second equality follows since $P_{h,h+1} = \theta_h$ and $P_{h,h-1} = 1 - \theta_h$ are the only two entries in the transition matrix which depend on θ_h for $h \in [1, H]$.

Next, let us consider a k_{th} order partial derivative of $M_{0,H+1}$, denoted as $\frac{\partial^k M_{0,H+1}}{\partial \theta_\beta}$. Note that β can have repeated entries to capture higher order derivative with respect to some parameter. We prove by induction for all $k \geq 1$, $\frac{\partial^k M_{0,H+1}}{\partial \theta_\beta}$ can be written as $\sum_{n=1}^N c_n \zeta_n$ where

- 1. $|c_n| = \gamma^k$ and $N \le 2^k k!$,
- 2. Each monomial ζ_n is of the form $M_{i_1,j_1} \dots M_{i_{k+1},j_{k+1}}$, $i_1 = 0$, $j_{k+1} = H+1$, $j_l \leq H$ and $i_{l+1} = j_l \pm 1$ for all $l \in [1,k]$.

The base case k = 1 follows from Equation (34), as we can write for any $h \in [H]$

$$\frac{\partial M_{0,H+1}}{\partial \theta_h} = \gamma M_{0,h} M_{h-1,H+1} - \gamma M_{0,h} M_{h+1,H+1}$$

Clearly, the induction hypothesis is true with $|c_n| = \gamma$, N = 2, $i_1 = 0$, $j_2 = H + 1$, $j_1 \le H$ and $i_2 = j_1 \pm 1$. Now, suppose the claim holds till k - 1. Then by the chain rule:

$$\frac{\partial^k M_{0,H+1}}{\partial \theta_{\beta_1} \dots \partial \theta_{\beta_k}} = \frac{\partial^{\frac{\partial^{k-1} M_{0,H+1}}{\partial \theta_{\beta}/1}}}{\partial \theta_{\beta_1}},$$

where $oldsymbol{eta}^{/i}$ is the vector $oldsymbol{eta}$ with the i_{th} entry removed. By inductive hypothesis,

$$\frac{\partial^{k-1} M_{0,H+1}}{\partial \theta_{\beta^{/1}}} = \sum_{n=1}^{N} c_n \zeta_n$$

where

- 1. $|c_n| = \gamma^{k-1}$ and $N \le 2^{k-1}(k-1)!$,
- 2. Each monomial ζ_n is of the form $M_{i_1,j_1} \dots M_{i_k,j_k}$, $i_1 = 0$, $j_k = H+1$, $j_l \leq H$ and $i_{l+1} = j_l \pm 1$ for all $l \in [1, k-1]$.

In order to compute the $(k)_{th}$ derivative of $M_{0,H+1}$, we have to compute derivative of each monomial ζ_n with respect to θ_{β_1} . Consider one of the monomials in the $(k-1)_{th}$ derivative, say, $\zeta = M_{i_1,j_1} \dots M_{i_k,j_k}$. We invoke the chain rule as before and replace one of the terms in ζ , say M_{i_m,j_m} , with $\gamma M_{i_m,\beta_1} M_{\beta_1-1,j_m} - \gamma M_{i_m,\beta_1} M_{\beta_1+1,j_m}$ using Equation 34. That is, the derivative of each entry gives rise to two monomials and therefore derivative of ζ leads to 2k monomials which can be written in the form $\zeta' = M_{i'_1,j'_1} \dots M_{i'_{k+1},j'_{k+1}}$ where we have the following properties (by appropriately reordering terms)

- 1. $i'_{l}, j'_{l} = i_{l}, j_{l}$ for l < m
- 2. $i'_{l}, j'_{l} = i_{l-1}, j_{l-1}$ for l > m+1
- 3. $i'_m, j'_m = i_m, \beta_1$ and $i'_{m+1}, j'_{m+1} = j_m \pm 1, j_m$

Using the induction hypothesis, we can write

$$\frac{\partial^k M_{0,H+1}}{\partial \theta_{\beta_1} \dots \partial \theta_{\beta_k}} = \sum_{n=0}^{N'} c'_n \zeta'_n$$

where

- 1. $|c'_n| = \gamma |c_n| = \gamma^k$, since as shown above each coefficient gets multiplied by $\pm \gamma$.
- 2. $N' \le 2k2^{k-1}(k-1)! = 2^kk!$, since as shown above each monomial ζ leads to 2k monomials ζ' .
- 3. Each monomial ζ'_n is of the form $M_{i_1,j_1} \dots M_{i_{k+1},j_{k+1}}$, $i_1 = 0$, $j_{k+1} = H+1$, $j_l \leq H$ and $i_{l+1} = j_l \pm 1$ for all $l \in [1,k]$.

This completes the induction.

Next we prove a bound on the magnitude of each of the monomials which arise in the derivatives of $M_{0,H+1}$. Specifically, we show that for each monomial $\zeta = M_{i_1,j_1} \dots M_{i_{k+1},j_{k+1}}$, we have

$$|M_{i_1,j_1} \dots M_{i_{k+1},j_{k+1}}| \le \frac{\gamma \bar{p} \alpha^{H-2k}}{(1-\gamma)^{k+2}}$$
 (35)

We observe that it suffices to only consider pairs of indices i_l, j_l where $i_l < j_l$. Since $|M_{i,j}| \le \frac{1}{1-\gamma}$ for all i, j,

$$\left| \prod_{l=1}^{k+1} M_{i'_{l}, j'_{l}} \right| \leq \left| \prod_{1 \leq l \leq k : i'_{l} < j'_{l}} M_{i'_{l}, j'_{l}} \right| \prod_{1 \leq l \leq k : i'_{l} \geq j'_{l}} \frac{1}{1 - \gamma} \left| M_{i'_{k+1}, j'_{k+1}} \right|$$

$$= \left| \prod_{1 \leq l \leq k : i'_{l} < j'_{l}} M_{i'_{l}, j'_{l}} \right| \prod_{1 \leq l \leq k : i'_{l} \geq j'_{l}} \frac{1}{1 - \gamma} \left| M_{i'_{k+1}, H+1} \right|$$
(by the inductive claim shown above)
$$\leq \frac{\alpha^{\sum_{\{1 \leq l \leq k : i'_{l} < j'_{l}\}} j'_{l} - i'_{l} - 1}}{(1 - \gamma)^{k}} \frac{\gamma \bar{p} \alpha^{H - i'_{k+1}}}{(1 - \gamma)^{2}}$$
(using Lemma B.4, parts 1 and 2 on the first and last terms resp.)
$$= \frac{\gamma \bar{p} \alpha^{\sum_{\{1 \leq l \leq k+1 : i'_{l} < j'_{l}\}} j'_{l} - i'_{l} - 1}}{(1 - \gamma)^{k+2}}$$
(36)

(36)

The last step follows from $H+1=j'_{k+1}\geq i'_{k+1}$. Note that

$$\sum_{\{1 \le l \le k+1 : i_l' < j_l'\}} j_l' - i_l' \ge \sum_{l=1}^{k+1} j_l' - i_l' = j_{k+1}' - i_1' + \sum_{l=1}^{k} (j_{l+1}' - i_l') \ge H + 1 - k \ge 0$$

where the first inequality follows from adding only non-positive terms to the sum, the second equality follows from rearranging terms and the third inequality follows from $i_1'=0, j_{k+1}'=H+1$ and $i'_{l+1} = j'_l \pm 1$ for all $l \in [1, k]$. Therefore,

$$\sum_{\{1 \le l \le k+1 : i'_l < j'_l\}} j'_l - i'_l - 1 \ge H - 2k$$

Using Equation (36) and $\alpha \leq 1$ with above display gives

$$\left| \prod_{l=1}^{k+1} M_{i'_l, j'_l} \right| \le \frac{\gamma \bar{p} \alpha^{H-2k}}{(1-\gamma)^{k+2}}$$

This proves the bound. Now using the claim that

$$\frac{\partial^k M_{0,H+1}}{\partial \theta_{\beta}} = \sum_{n=1}^N c_n \zeta_n$$

where $|c_n| = \gamma^k$ and $N \leq 2^k k!$, we have shown that

$$\left| \frac{\partial^k M_{0,H+1}}{\partial \theta_{\beta}} \right| \leq \frac{\bar{p} \, 2^k \, \gamma^{k+1} \, k! \, \alpha^{H-2k}}{(1-\gamma)^{k+2}},$$

which completes the proof.

We are now ready to prove Lemma 4.3.

Proof:[Proof of Lemma 4.3] The k_{th} order partial derivative of $V^{\pi_{\theta}}(s_0)$ is equal to

$$\frac{\partial^k V^{\pi_{\theta}}(s_0)}{\partial \theta_{\beta_1} \dots \partial \theta_{\beta_h}} = \frac{\partial^k M_{0,H+1}^{\theta}}{\partial \theta_{\beta_1} \dots \partial \theta_{\beta_k}}.$$

Given vectors u^1, \ldots, u^k which are unit vectors in \mathbb{R}^{H^k} (we denote the unit sphere by \mathbb{S}^{H^k}), the norm of this gradient tensor is given by:

$$\|\nabla_{\theta}^{k}V^{\pi_{\theta}}(s_{0})\| = \max_{u^{1},\dots,u^{k}\in\mathbb{S}^{H^{k}}} \left| \sum_{\boldsymbol{\beta}\in[H]^{k}} \frac{\partial^{k}V^{\pi_{\theta}}(s_{0})}{\partial\theta_{\beta_{1}}\dots\partial\theta_{\beta_{k}}} u_{\beta_{1}}^{1}\dots u_{\beta_{k}}^{k} \right|$$

$$\leq \max_{u^{1},\dots,u^{k}\in\mathbb{S}^{H^{k}}} \sqrt{\sum_{\boldsymbol{\beta}\in[H]^{k}} \left(\frac{\partial^{k}V^{\pi_{\theta}}(s_{0})}{\partial\theta_{\beta_{1}}\dots\partial\theta_{\beta_{k}}} \right)^{2}} \sqrt{\sum_{\boldsymbol{\beta}\in[H]^{k}} \left(u_{\beta_{1}}^{1}\dots u_{\beta_{k}}^{k} \right)^{2}}$$

$$= \max_{u^{1},\dots,u^{k}\in\mathbb{S}^{H^{k}}} \sqrt{\sum_{\boldsymbol{\beta}\in[H]^{k}} \left(\frac{\partial^{k}V^{\pi_{\theta}}(s_{0})}{\partial\theta_{\beta_{1}}\dots\partial\theta_{\beta_{k}}} \right)^{2}} \sqrt{\prod_{i=1}^{k} \|u^{i}\|_{2}^{2}}$$

$$= \sqrt{\sum_{\boldsymbol{\beta}\in[H]^{k}} \left(\frac{\partial^{k}V^{\pi_{\theta}}(s_{0})}{\partial\theta_{\beta_{1}}\dots\partial\theta_{\beta_{k}}} \right)^{2}} = \sqrt{\sum_{\boldsymbol{\beta}\in[H]^{k}} \left(\frac{\partial^{k}M_{0,H+1}^{\theta}}{\partial\theta_{\beta_{1}}\dots\partial\theta_{\beta_{k}}} \right)^{2}}$$

$$\leq \sqrt{\frac{H^{k}\bar{p}^{2} 2^{2k} \gamma^{2k+2} (k!)^{2} \alpha^{2H-4k}}{(1-\gamma)^{2k+4}}},$$

where the last inequality follows from Lemma B.5. In order to proceed further, we need an upper bound on the smallest admissible value of α . To do so, let us consider all possible parameters θ such that $\bar{p} \leq 1/4$ in accordance with the theorem statement. In order to bound α , it suffices to place an upper bound on the lower end of the range for α in Lemma B.4 (note Lemma B.4 holds for any choice of α in the range). Doing so, we see that

$$\frac{1 - \sqrt{1 - 4\gamma^2 \bar{p}(1 - \underline{p})}}{2\gamma(1 - \underline{p})} \le \frac{1 - 1 + 2\gamma\sqrt{\bar{p}(1 - \underline{p})}}{2\gamma(1 - \underline{p})}$$
$$= \sqrt{\frac{\bar{p}}{1 - \underline{p}}} \le \sqrt{\frac{4\bar{p}}{3}},$$

where the first inequality uses $\sqrt{x-y} \ge \sqrt{x} - \sqrt{y}$, by triangle inequality while the last inequality uses $p \le \bar{p} \le 1/4$.

Hence, we have the bound

$$\max_{u^{1},\dots,u^{k}\in\mathbb{S}^{H^{k}}} \left| \sum_{\beta\in[H]^{h}} \frac{\partial^{k}V^{\pi_{\theta}}(s_{0})}{\partial\theta_{\beta_{1}}\dots\partial\theta_{\beta_{k}}} u_{\beta_{1}}^{1}\dots u_{\beta_{k}}^{k} \right| \leq \sqrt{\frac{H^{k}\bar{p}^{2} 2^{2k} \gamma^{2k+2} (k!)^{2} (\frac{4\bar{p}}{3})^{H-2k}}{(1-\gamma)^{2k+4}}} \\
\stackrel{(a)}{\leq} \sqrt{(H+1)^{2k+4} H^{k}\bar{p}^{2} 2^{2k} \gamma^{2k+2} (k!)^{2} (\frac{4\bar{p}}{3})^{H-2k}} \\
\stackrel{(b)}{\leq} \sqrt{(2H)^{2k+4} H^{k} 2^{2k} (H)^{2k} (\frac{4\bar{p}}{3})^{H-2k}} \\
= \sqrt{(2)^{4k+4} (H)^{5k+4} (\frac{4\bar{p}}{3})^{H-2k}}$$

where (a) uses $\gamma = H/(H+1)$, (b) follows since $\bar{p} \leq 1$, $H, k \geq 1$, $\gamma \leq 1$ and $k \leq H$. Requiring that the gradient norm be no larger than $(\frac{4\bar{p}}{3})^{H/4}$, we would like to satisfy

$$(2)^{4k+4}(H)^{5k+4}\left(\frac{4\bar{p}}{3}\right)^{H-2k} \le \left(\frac{4\bar{p}}{3}\right)^{H/2},$$

for which it suffices to have

$$k \le k_0 := \frac{\frac{H}{2}\log(3/4\bar{p}) - \log(2^4H^4)}{\log(2^4H^5) + 2\log(3/4\bar{p})}.$$

Since,

$$\begin{split} &\frac{\frac{H}{2}\log(3/4\bar{p}) - \log(2^4H^4)}{\log(2^4H^5) + 2\log(3/4\bar{p})} \\ &\stackrel{(a)}{\geq} \frac{\frac{H}{2}\log(3/4\bar{p}) - \log(2^4H^4)}{2\log(2^4H^5)2\log(3/4\bar{p})} \\ &\stackrel{\geq}{\geq} \frac{H}{8\log(2^4H^5)} - \frac{\log(2^4H^4)}{4\log(2^4H^5)\log(3/4\bar{p})} \\ &\stackrel{(b)}{\geq} \frac{H}{8\log(2^4H^5)} - \frac{\log(2^4H^4)}{4\log(2^4H^4)\log(3)} \\ &\stackrel{\geq}{\geq} \frac{H}{40\log(2H)} - 1 \end{split}$$

where (a) follows from $a+b \le 2ab$ when $a, b \ge 1$, (b) follows from $H \ge 1$ and $\bar{p} \le 1/4$. Therefore, in order to obtain the smallest value of k_0 for all choices of $0 \le \bar{p} < 1/4$, we further lower bound k_0 as

$$k_0 \ge \frac{H}{40\log(2H)} - 1,$$

Thus, the norm of the gradient is bounded by $(\frac{4\bar{p}}{3})^{H/4} \le (1/3)^{H/4}$ for all $k \le \frac{H}{40\log(2H)} - 1$ as long as $\bar{p} \le 1/4$, which gives the first part of the lemma.

For the second part, note that the optimal policy always chooses the action a_1 , and gets a discounted reward of

$$\gamma^{H+2}/(1-\gamma) = (H+1)\left(1-\frac{1}{H+1}\right)^{H+2} \ge \frac{H+1}{8},$$

where the final inequality uses $(1-1/x)^x \ge 1/8$ for $x \ge 1$. On the other hand, the value of π_{θ} is upper bounded by

$$M_{0,H+1} \le \frac{\gamma \bar{p}\alpha^H}{(1-\gamma)^2} \le \frac{\gamma \bar{p}}{(1-\gamma)^2} \left(\frac{4\bar{p}}{3}\right)^H$$
$$\le \frac{(H+1)^2}{3^H}.$$

This gives the second part of the lemma.

C Proofs for Section 5

We first give a useful lemma about the structure of policy gradients for the softmax parameterization. We use the notation $\Pr^{\pi}(\tau|s_0=s)$ to denote the probability of observing a trajectory τ when starting in state s and following the policy π and $\Pr^{\pi}_{\mu}(\tau)$ be $\mathbb{E}_{s\sim\mu}[\Pr^{\pi}(\tau|s_0=s)]$ for a distribution μ over states.

Lemma C.1. For the softmax policy class, we have:

$$\frac{\partial V^{\pi_{\theta}}(\mu)}{\partial \theta_{s,a}} = \frac{1}{1 - \gamma} d_{\mu}^{\pi_{\theta}}(s) \pi_{\theta}(a|s) A^{\pi_{\theta}}(s,a)$$

Proof: First note that

$$\frac{\partial \log \pi_{\theta}(a|s)}{\partial \theta_{s',a'}} = \mathbb{1}\left[s = s'\right] \left(\mathbb{1}\left[a = a'\right] - \pi_{\theta}(a'|s)\right) \tag{37}$$

where $\mathbb{1}|\mathcal{E}|$ is the indicator of \mathcal{E} being true.

Using this, we have:

$$\frac{\partial V^{\pi_{\theta}}(\mu)}{\partial \theta_{s,a}} = \mathbb{E}_{\tau \sim \Pr_{\mu}^{\pi_{\theta}}} \left[\sum_{t=0}^{\infty} \gamma^{t} \mathbb{1}[s_{t} = s] \Big(\mathbb{1}[a_{t} = a] A^{\pi_{\theta}}(s, a) - \pi_{\theta}(a|s) A^{\pi_{\theta}}(s_{t}, a_{t}) \Big) \right] \\
= \mathbb{E}_{\tau \sim \Pr_{\mu}^{\pi_{\theta}}} \left[\sum_{t=0}^{\infty} \gamma^{t} \mathbb{1}[(s_{t}, a_{t}) = (s, a)] A^{\pi_{\theta}}(s, a) \right] \\
+ \pi_{\theta}(a|s) \sum_{t=0}^{\infty} \gamma^{t} \mathbb{E}_{\tau \sim \Pr_{\mu}^{\pi_{\theta}}} \left[\mathbb{1}[s_{t} = s] A^{\pi_{\theta}}(s_{t}, a_{t}) \right] \\
= \frac{1}{1 - \gamma} \mathbb{E}_{(s', a') \sim d_{\mu}^{\pi_{\theta}}} \left[\mathbb{1}[(s', a') = (s, a)] A^{\pi_{\theta}}(s, a) \right] + 0 \\
= \frac{1}{1 - \gamma} d_{\mu}^{\pi_{\theta}}(s, a) A^{\pi_{\theta}}(s, a),$$

where the second to last step uses that for any policy $\sum_a \pi(a|s) A^{\pi}(s,a) = 0$.

C.1 Proofs for Section 5.1

We now prove Theorem 5.1, i.e. we show that for the updates given by

$$\theta^{(t+1)} = \theta^{(t)} + \eta \nabla V^{(t)}(\mu), \tag{38}$$

policy gradient converges to optimal policy for the softmax parameterization.

We prove this theorem by first proving a series of supporting lemmas. First, we show in Lemma C.2, that $V^{(t)}(s)$ is monotonically increasing for all states s using the fact that for appropriately chosen stepsizes GD makes monotonic improvement for smooth objectives.

Lemma C.2 (Monotonic Improvement in $V^{(t)}(s)$). For all states s and actions a, for updates (38) with learning rate $\eta \leq \frac{(1-\gamma)^2}{5}$, we have

$$V^{(t+1)}(s) \ge V^{(t)}(s); \quad Q^{(t+1)}(s,a) \ge Q^{(t)}(s,a)$$

Proof: The proof will consist of showing that:

$$\sum_{a \in \mathcal{A}} \pi^{(t+1)}(a|s) A^{(t)}(s,a) \ge \sum_{a \in \mathcal{A}} \pi^{(t)}(a|s) A^{(t)}(s,a) = 0.$$
(39)

holds for all states s. To see this, observe that since the above holds for all states s', the performance difference lemma (Lemma 3.2) implies

$$V^{(t+1)}(s) - V^{(t)}(s) = \frac{1}{1 - \gamma} \mathbb{E}_{s' \sim d_s^{\pi(t+1)}} \mathbb{E}_{a \sim \pi^{(t+1)}(\cdot|s')} \left[A^{(t)}(s', a) \right] \ge 0,$$

which would complete the proof.

Let us use the notation $\theta_s \in \mathbb{R}^{|\mathcal{A}|}$ to refer to the vector of $\theta_{s,\cdot}$ for some fixed state s. Define the function

$$F_s(\theta_s) := \sum_{a \in \mathcal{A}} \pi_{\theta_s}(a|s)c(s,a)$$

where c(s,a) is constant, which we later set to be $A^{(t)}(s,a)$; note we do not treat c(s,a) as a function of θ . Thus,

$$\begin{split} & \frac{\partial F_{s}(\theta_{s})}{\partial \theta_{s,a}} \Big|_{\theta_{s}^{(t)}} = \sum_{a' \in \mathcal{A}} \frac{\partial \pi_{\theta_{s}}(a'|s)}{\partial \theta_{s,a}} \Big|_{\theta_{s}^{(t)}} c(s,a') \\ & = \pi^{(t)}(a|s)(1 - \pi^{(t)}(a|s))c(s,a) - \sum_{a' \neq a} \pi^{(t)}(a|s)\pi^{(t)}(a'|s)c(s,a') \\ & = \pi^{(t)}(a|s) \left(c(s,a) - \sum_{a' \in \mathcal{A}} \pi^{(t)}(a'|s)c(s,a') \right) \end{split}$$

Taking c(s, a) to be $A^{(t)}(s, a)$ implies $\sum_{a' \in \mathcal{A}} \pi^{(t)}(a'|s) c(s, a') = \sum_{a' \in \mathcal{A}} \pi^{(t)}(a'|s) A^{(t)}(s, a') = 0$,

$$\frac{\partial F_s(\theta_s)}{\partial \theta_{s,a}}\Big|_{\theta_s^{(t)}} = \pi^{(t)}(a|s)A^{(t)}(s,a) \tag{40}$$

Observe that for the softmax parameterization,

$$\theta_s^{(t+1)} = \theta_s^{(t)} + \eta \nabla_s V^{(t)}(\mu)$$

where ∇_s is gradient w.r.t. θ_s and from Lemma C.1 that:

$$\frac{\partial V^{(t)}(\mu)}{\partial \theta_{s,a}} = \frac{1}{1 - \gamma} d_{\mu}^{\pi^{(t)}}(s) \pi^{(t)}(a|s) A^{(t)}(s,a)$$

This gives using Equation (40)

$$\theta_s^{(t+1)} = \theta_s^{(t)} + \eta \frac{1}{1-\gamma} d_{\mu}^{\pi^{(t)}}(s) \nabla_s F_s(\theta_s) \Big|_{\theta_s^{(t)}}$$

Recall that for a β smooth function, gradient descent will decrease the function value provided that $\eta \leq 1/\beta$ (e.g. see Beck [2017]). Because $F_s(\theta_s)$ is β -smooth for $\beta = \frac{5}{1-\gamma}$ (Lemma E.1 and $\left|A^{(t)}(s,a)\right| \leq \frac{1}{1-\gamma}$), then our assumption that

$$\eta \le \frac{(1-\gamma)^2}{5} = (1-\gamma)\beta^{-1}$$

implies that $\eta \frac{1}{1-\gamma} d_{\mu}^{\pi^{(t)}}(s) \leq 1/\beta$, and so we have

$$F_s(\theta_s^{(t+1)}) \ge F_s(\theta_s^{(t)})$$

which implies (39).

Next, we show the limit for iterates $V^{(t)}(s)$ and $Q^{(t)}(s,a)$ exists for all states s and actions a.

Lemma C.3. For all states s and actions a, there exists values $V^{(\infty)}(s)$ and $Q^{(\infty)}(s,a)$ such that as $t \to \infty$, $V^{(t)}(s) \to V^{(\infty)}(s)$ and $Q^{(t)}(s,a) \to Q^{(\infty)}(s,a)$. Define

$$\Delta = \min_{\{s, a | A^{(\infty)}(s, a) \neq 0\}} |A^{(\infty)}(s, a)|$$

where $A^{(\infty)}(s,a) = Q^{(\infty)}(s,a) - V^{(\infty)}(s)$. Furthermore, there exists a T_0 such that for all $t > T_0$, $s \in \mathcal{S}$, and $a \in \mathcal{A}$, we have

$$Q^{(t)}(s,a) \ge Q^{(\infty)}(s,a) - \Delta/4$$
 (41)

Proof: Observe that $Q^{(t+1)}(s,a) \geq Q^{(t)}(s,a)$ (by Lemma C.2) and $Q^{(t)}(s,a) \leq \frac{1}{1-\gamma}$, therefore by monotone convergence theorem, $Q^{(t)}(s,a) \to Q^{(\infty)}(s,a)$ for some constant $Q^{(\infty)}(s,a)$. Similarly it follows that $V^{(t)}(s) \to V^{(\infty)}(s)$ for some constant $V^{(\infty)}(s)$. Due to the limits existing, this implies we can choose T_0 , such that the result (41) follows.

Based on the limits $V^{(\infty)}(s)$ and $Q^{(\infty)}(s,a)$, define following sets:

$$I_0^s := \{a|Q^{(\infty)}(s,a) = V^{(\infty)}(s)\}$$

$$I_+^s := \{a|Q^{(\infty)}(s,a) > V^{(\infty)}(s)\}$$

$$I_-^s := \{a|Q^{(\infty)}(s,a) < V^{(\infty)}(s)\}.$$

In the following lemmas C.5- C.11, we first show that probabilities $\pi^{(t)}(a|s) \to 0$ for actions $a \in I_+^s \cup I_-^s$ as $t \to \infty$. We then show that for actions $a \in I_-^s$, $\lim_{t \to \infty} \theta_{s,a}^{(t)} = -\infty$ and for all actions $a \in I_+^s$, $\theta^{(t)}(a|s)$ is bounded from below as $t \to \infty$.

Lemma C.4. We have that there exists a T_1 such that for all $t > T_1$, $s \in \mathcal{S}$, and $a \in \mathcal{A}$, we have

$$A^{(t)}(s,a) < -\frac{\Delta}{4} \text{ for } a \in I_{-}^{s}; \quad A^{(t)}(s,a) > \frac{\Delta}{4} \text{ for } a \in I_{+}^{s}$$
 (42)

Proof: Since, $V^{(t)}(s) \to V^{(\infty)}(s)$, we have that there exists $T_1 > T_0$ such that for all $t > T_1$,

$$V^{(t)}(s) > V^{(\infty)}(s) - \frac{\Delta}{4}.$$
 (43)

Using Equation (41), it follows that for $t > T_1 > T_0$, for $a \in I^s_-$

$$\begin{split} A^{(t)}(s,a) &= Q^{(t)}(s,a) - V^{(t)}(s) \\ &\leq Q^{(\infty)}(s,a) - V^{(t)}(s) \\ &\leq Q^{(\infty)}(s,a) - V^{(\infty)}(s) + \Delta/4 \\ &\leq -\Delta + \Delta/4 \\ &< -\Delta/4 \end{split} \qquad \text{(definition of I^s_- and Lemma C.3)}$$

Similarly $A^{(t)}(s,a) = Q^{(t)}(s,a) - V^{(t)}(s) > \Delta/4$ for $a \in I^s_+$ as

$$\begin{split} A^{(t)}(s,a) &= Q^{(t)}(s,a) - V^{(t)}(s) \\ &\geq Q^{(\infty)}(s,a) - \Delta/4 - V^{(t)}(s) \\ &\geq Q^{(\infty)}(s,a) - V^{(\infty)}(s) - \Delta/4 \\ &\geq \Delta - \Delta/4 \\ &> \Delta/4 \end{split} \tag{Lemma C.3}$$
 (Lemma C.2)

which completes the proof.

Lemma C.5. $\frac{\partial V^{(t)}(\mu)}{\partial \theta_{s,a}} \to 0 \text{ as } t \to \infty \text{ for all states } s \text{ and actions } a. \text{ This implies that for } a \in I^s_+ \cup I^s_-, \pi^{(t)}(a|s) \to 0 \text{ and that } \sum_{a \in I^s_0} \pi^{(t)}(a|s) \to 1.$

Proof: Because $V^{\pi_{\theta}}(\mu)$ is smooth and that the learning rate is set below the smooth constant, it follows from standard optimization results (e.g see Beck [2017]) that $\frac{\partial V^{(t)}(\mu)}{\partial \theta_{s,a}} \to 0$ for all states s and actions a. We have from Lemma C.1

$$\frac{\partial V^{(t)}(\mu)}{\partial \theta_{s,a}} = \frac{1}{1 - \gamma} d_{\mu}^{\pi^{(t)}}(s) \pi^{(t)}(a|s) A^{(t)}(s,a).$$

Since, $|A^{(t)}(s,a)| > \frac{\Delta}{4}$ for all $t > T_1$ (from Lemma C.4) for all $a \in I^s_- \cup I^s_+$ and $d^{\pi^{(t)}}_\mu(s) \ge \frac{\mu(s)}{1-\gamma} > 0$ (using the strict positivity of μ in our assumption in Theorem 5.1), we have $\pi^{(t)}(a|s) \to 0$.

Lemma C.6. (Monotonicity in $\theta_{s,a}^{(t)}$). For all $a \in I_+^s$, $\theta_{s,a}^{(t)}$ is strictly in increasing for $t \geq T_1$. For all $a \in I_-^s$, $\theta_{s,a}^{(t)}$ is strictly in decreasing for $t \geq T_1$.

Proof: We have from Lemma C.1

$$\frac{\partial V^{(t)}(\mu)}{\partial \theta_{s,a}} = \frac{1}{1 - \gamma} d_{\mu}^{\pi^{(t)}}(s) \pi^{(t)}(a|s) A^{(t)}(s,a)$$

From Lemma C.4, we have for all $t > T_1$

$$A^{(t)}(s,a) > 0 \text{ for } a \in I^s_+; \quad A^{(t)}(s,a) < 0 \text{ for } a \in I^s_-$$

Since $d_{\mu}^{\pi^{(t)}}(s) > 0$ and $\pi^{(t)}(a|s) > 0$ for the softmax parameterization, we have for all $t > T_1$

$$\frac{\partial V^{(t)}(\mu)}{\partial \theta_{s,a}} > 0 \text{ for } a \in I_+^s; \quad \frac{\partial V^{(t)}(\mu)}{\partial \theta_{s,a}} < 0 \text{ for } a \in I_-^s$$

This implies for all $a \in I_+^s$, $\theta_{s,a}^{(t+1)} - \theta_{s,a}^{(t)} = \frac{\partial V^{(t)}(\mu)}{\partial \theta_{s,a}} > 0$ i.e. $\theta_{s,a}^{(t)}$ is strictly increasing for $t \geq T_1$. The second claim follows similarly.

Lemma C.7. For all s where $I_+^s \neq \emptyset$, we have that:

$$\max_{a \in I_0^s} \theta_{s,a}^{(t)} \to \infty, \quad \min_{a \in \mathcal{A}} \theta_{s,a}^{(t)} \to -\infty$$

Proof: Since $I_+^s \neq \emptyset$, there exists some action $a_+ \in I_+^s$. From Lemma C.5,

$$\pi^{(t)}(a_+|s) \to 0$$
, as $t \to \infty$

or equivalently by softmax parameterization,

$$\frac{\exp(\theta_{s,a_+}^{(t)})}{\sum_a \exp(\theta_{s,a}^{(t)})} \to 0, \text{ as } t \to \infty$$

From Lemma C.6, for any action $a \in I_+^s$ and in particular for a_+ , $\theta_{s,a_+}^{(t)}$ is monotonically increasing for $t > T_1$. That is the numerator in previous display is monotonically increasing. Therefore, the denominator should go to infinity i.e.

$$\sum_{a} \exp(\theta_{s,a}^{(t)}) \to \infty, \text{ as } t \to \infty.$$

From Lemma C.5,

$$\sum_{a \in I_0^s} \pi^{(t)}(a|s) \to 1, \text{ as } t \to \infty$$

or equivalently

$$\frac{\sum_{a \in I_0^s} \exp(\theta_{s,a}^{(t)})}{\sum_{a} \exp(\theta_{s,a}^{(t)})} \to 1, \text{ as } t \to \infty$$

Since, denominator goes to ∞ ,

$$\sum_{a \in I_0^s} \exp(\theta_{s,a}^{(t)}) \to \infty, \text{ as } t \to \infty$$

which implies

$$\max_{a \in I_0^s} \theta_{s,a}^{(t)} \to \infty$$
, as $t \to \infty$

Note this also implies $\max_{a\in\mathcal{A}}\theta_{s,a}^{(t)}\to\infty$. The last part of the proof is completed using that the gradients sum to 0, i.e. $\sum_a \frac{\partial V^{(t)}(\mu)}{\partial \theta_{s,a}}=0$. From gradient sum to 0, we get that $\sum_{a\in\mathcal{A}}\theta_{s,a}^{(t)}=\sum_{a\in\mathcal{A}}\theta_{s,a}^{(0)}:=c$ for all t>0 where c is defined as the sum (over \mathcal{A}) of initial parameters. That is $\min_{a\in\mathcal{A}}\theta_{s,a}^{(t)}<-\frac{1}{|\mathcal{A}|}\max_{a\in\mathcal{A}}\theta_{s,a}^{(t)}+c$. Since, $\max_{a\in\mathcal{A}}\theta_{s,a}^{(t)}\to\infty$, the result follows.

Lemma C.8. Suppose $a_+ \in I_+^s$. For any $a \in I_0$, if there exists $a \ t \ge T_0$ such that $\pi^{(t)}(a|s) \le \pi^{(t)}(a_+|s)$, then for all $\tau \ge t$, $\pi^{(\tau)}(a|s) \le \pi^{(\tau)}(a_+|s)$.

Proof: The proof is inductive. Suppose $\pi^{(t)}(a|s) \leq \pi^{(t)}(a_+|s)$, this implies from Lemma C.1

$$\frac{\partial V^{(t)}(\mu)}{\partial \theta_{s,a}} = \frac{1}{1 - \gamma} d_{\mu}^{(t)}(s) \pi^{(t)}(a|s) \left(Q^{(t)}(s, a) - V^{(t)}(s) \right) \\
\leq \frac{1}{1 - \gamma} d_{\mu}^{(t)}(s) \pi^{(t)}(a_{+}|s) \left(Q^{(t)}(s, a_{+}) - V^{(t)}(s) \right) = \frac{\partial V^{(t)}(\mu)}{\partial \theta_{s,a_{+}}}.$$

where the second to last step follows from $Q^{(t)}(s,a_+) \geq Q^{(\infty)}(s,a_+) - \Delta/4 \geq Q^{(\infty)}(s,a) + \Delta - \Delta/4 > Q^{(t)}(s,a)$ for $t > T_0$. This implies that $\pi^{(t+1)}(a|s) \leq \pi^{(t+1)}(a_+|s)$ which completes the proof.

Consider an arbitrary $a_+ \in I_+^s$. Let us partition the set I_0^s into $B_0^s(a_+)$ and $\bar{B}_0^s(a_+)$ as follows: $B_0^s(a_+)$ is the set of all $a \in I_0^s$ such that for all $t \ge T_0$, $\pi^{(t)}(a_+|s) < \pi^{(t)}(a|s)$, and $\bar{B}_0^s(a_+)$ contains the remainder of the actions from I_0^s . We drop the argument (a_+) when clear from the context.

Lemma C.9. Suppose $I_+^s \neq \emptyset$. For all $a_+ \in I_+^s$, we have that $B_0^s(a_+) \neq \emptyset$ and that

$$\sum_{a \in B_0^s(a_+)} \pi^{(t)}(a|s) \to 1, \text{ as } t \to \infty.$$

This implies that:

$$\max_{a \in B_0^s(a_+)} \theta_{s,a}^{(t)} \to \infty.$$

Proof: Let $a_+ \in I_+^s$. Consider any $a \in \bar{B}_0^s$. Then, by definition of \bar{B}_0^s , there exists $t' > T_0$ such that $\pi^{(t)}(a_+|s) \ge \pi^{(t)}(a|s)$. From Lemma C.8, for all $\tau > t \ \pi^{(\tau)}(a_+|s) \ge \pi^{(\tau)}(a|s)$. Also, since $\pi^{(t)}(a_+|s) \to 0$, this implies

$$\pi^{(t)}(a|s) \to 0 \text{ for all } a \in \bar{B}_0^s$$

Since, $B_0^s \cup \bar{B}_0^s = I_0^s$ and $\sum_{a \in I_0^s} \pi^{(t)}(a|s) \to 1$ (from Lemma C.5), this implies that $B_0^s \neq \emptyset$ and that means

$$\sum_{a \in B_0^s} \pi^{(t)}(a|s) \to 1, \text{ as } t \to \infty,$$

which completes the proof of the first claim. The proof of the second claim is identical to the proof in Lemma C.7 where instead of $\sum_{a \in I_0^s} \pi^{(t)}(a|s) \to 1$, we use $\sum_{a \in B_0^s} \pi^{(t)}(a|s) \to 1$.

Lemma C.10. Consider any s where $I_+^s \neq \emptyset$. Then, for any $a_+ \in I_+^s$, there exists an iteration T_{a_+} such that for all $t > T_{a_+}$,

$$\pi^{(t)}(a_+|s) > \pi^{(t)}(a|s)$$

for all $a \in \bar{B}_0^s(a_+)$.

Proof: The proof follows from definition of $\bar{B}_0^s(a_+)$. That is if $a \in \bar{B}_0^s(a_+)$, then there exists a iteration $t_a > T_0$ such that $\pi^{(t_a)}(a_+|s) > \pi^{(t_a)}(a|s)$. Then using Lemma C.8, for all $\tau > t_a$, $\pi^{(\tau)}(a_+|s) > \pi^{(\tau)}(a|s)$. Choosing

$$T_{a_+} = \max_{a \in B_0^s(a_+)} t_a$$

completes the proof.

Lemma C.11. For all actions $a \in I_+^s$, we have that $\theta_{s,a}^{(t)}$ is bounded from below as $t \to \infty$. For all actions $a \in I^s$, we have that $\theta_{s,a}^{(t)} \to -\infty$ as $t \to \infty$.

Proof: For the first claim, from Lemma C.6, we know that after T_1 , $\theta_{s,a}^{(t)}$ is strictly increasing for $a \in I_+^s$, i.e. for all $t > T_1$

$$\theta_{s,a}^{(t)} \ge \theta_{s,a}^{(T_1)}$$
.

For the second claim, we know that after T_1 , $\theta_{s,a}^{(t)}$ is strictly decreasing for $a \in I_-^s$ (Lemma C.6). Therefore, by monotone convergence theorem, $\lim_{t\to\infty}\theta_{s,a}^{(t)}$ exists and is either $-\infty$ or some constant θ_0 . We now prove the second claim by contradiction. Suppose $a \in I_-^s$ and that there exists a θ_0 , such that $\theta_{s,a}^{(t)} > \theta_0$, for $t \geq T_1$. By Lemma C.7, there must exist an action where $a' \in \mathcal{A}$ such that

$$\lim \inf_{t \to \infty} \theta_{s,a'}^{(t)} = -\infty. \tag{44}$$

Let us consider some $\delta > 0$ such that $\theta_{s,a'}^{(T_1)} \geq \theta_0 - \delta$. Now for $t \geq T_1$ define $\tau(t)$ as follows: $\tau(t) = k$ if k is the largest iteration in the interval $[T_1,t]$ such that $\theta_{s,a'}^{(k)} \geq \theta_0 - \delta$ (i.e. $\tau(t)$ is the latest iteration before $\theta_{s,a'}$ crosses below $\theta_0 - \delta$). Define $\mathcal{T}^{(t)}$ as the subsequence of iterations $\tau(t) < t' < t$ such that $\theta_{s,a'}^{(t')}$ decreases, i.e.

$$\frac{\partial V^{(t')}(\mu)}{\partial \theta_{s,a'}} \le 0, \text{ for } \tau(t) < t' < t.$$

Define Z_t as the sum (if $\mathcal{T}^{(t)} = \emptyset$, we define $Z_t = 0$):

$$Z_t = \sum_{t' \in \mathcal{T}^{(t)}} \frac{\partial V^{(t')}(\mu)}{\partial \theta_{s,a'}}.$$

For non-empty $\mathcal{T}^{(t)}$, this gives:

$$Z_{t} = \sum_{t' \in \mathcal{T}^{(t)}} \frac{\partial V^{(t')}(\mu)}{\partial \theta_{s,a'}} \leq \sum_{t' = \tau(t) - 1}^{t - 1} \frac{\partial V^{(t')}(\mu)}{\partial \theta_{s,a'}} \leq \sum_{t' = \tau(t)}^{t - 1} \frac{\partial V^{(t')}(\mu)}{\partial \theta_{s,a'}} + \frac{1}{1 - \gamma^{2}}$$
$$= \frac{1}{\eta} (\theta_{s,a'}^{(t)} - \theta_{s,a'}^{(\tau(t))}) + \frac{1}{1 - \gamma^{2}} \leq \frac{1}{\eta} \left(\theta_{s,a'}^{(t)} - (\theta_{0} - \delta)\right) + \frac{1}{1 - \gamma^{2}},$$

where we have used that $|\frac{\partial V^{(t')}(\mu)}{\partial \theta_{s,a'}}| \leq 1/(1-\gamma)$. By (44), this implies that:

$$\lim\inf_{t\to\infty}Z_t=-\infty.$$

For any $\mathcal{T}^{(t)} \neq \emptyset$, this implies that for all $t' \in \mathcal{T}^{(t)}$, from Lemma C.1

$$\left| \frac{\partial V^{(t')}(\mu)/\partial \theta_{s,a}}{\partial V^{(t')}(\mu)/\partial \theta_{s,a'}} \right| = \left| \frac{\pi^{(t')}(a|s)A^{(t')}(s,a)}{\pi^{(t')}(a'|s)A^{(t')}(s,a')} \right| \ge \exp\left(\theta_0 - \theta_{s,a'}^{(t')}\right) \frac{(1-\gamma)\Delta}{4}$$
$$\ge \exp\left(\delta\right) \frac{(1-\gamma)\Delta}{4}$$

where we have used that $|A^{(t')}(s,a')| \leq 1/(1-\gamma)$ and $|A^{(t')}(s,a)| \geq \frac{\Delta}{4}$ for all $t' > T_1$ (from Lemma C.4). Note that since $\frac{\partial V^{(t')}(\mu)}{\partial \theta_{s,a}} < 0$ and $\frac{\partial V^{(t')}(\mu)}{\partial \theta_{s,a'}} < 0$ over the subsequence $\mathcal{T}^{(t)}$, the sign of the inequality reverses. In particular, for any $\mathcal{T}^{(t)} \neq \emptyset$

$$\frac{1}{\eta} (\theta_{s,a}^{(T_1)} - \theta_{s,a}^{(t)}) = \sum_{t'=T_1}^{t-1} \frac{\partial V^{(t')}(\mu)}{\partial \theta_{s,a}} \le \sum_{t' \in \mathcal{T}^{(t)}} \frac{\partial V^{(t')}(\mu)}{\partial \theta_{s,a}}$$

$$\le \exp\left(\delta\right) \frac{(1 - \gamma)\Delta}{4} \sum_{t' \in \mathcal{T}^{(t)}} \frac{\partial V^{(t')}(\mu)}{\partial \theta_{s,a'}}$$

$$= \exp\left(\delta\right) \frac{(1 - \gamma)\Delta}{4} Z_t$$

where the first step follows from that $\theta_{s,a}^{(t)}$ is monotonically decreasing, i.e. $\frac{\partial V^{(t)}(\mu)}{\partial \theta_{s,a}} < 0$ for $t \notin \mathcal{T}$ (Lemma C.6). Since,

$$\lim \inf_{t \to \infty} Z_t = -\infty,$$

this contradicts that $\theta_{s,a}^{(t)}$ is lower bounded from below, which completes the proof.

Lemma C.12. Consider any s where $I_+^s \neq \emptyset$. Then, for any $a_+ \in I_+^s$

$$\sum_{a \in B_0^s(a_+)} \theta_{s,a}^{(t)} \to \infty, \ as \ t \to \infty$$

Proof: Consider any $a \in B_0^s$. We have by definition of B_0^s that $\pi^{(t)}(a_+|s) < \pi^{(t)}(a|s)$ for all $t > T_0$. This implies by the softmax parameterization that $\theta_{s,a_+}^{(t)} < \theta_{s,a}^{(t)}$. Since, $\theta_{s,a_+}^{(t)}$ is lower bounded as $t \to \infty$ (using Lemma C.11), this implies $\theta_{s,a}^{(t)}$ is lower bounded as $t \to \infty$ for all $a \in B_0^s$. This in conjunction with $\max_{a \in B_0^s(a_+)} \theta_{s,a}^{(t)} \to \infty$ implies

$$\sum_{a \in B_0^s} \theta_{s,a}^{(t)} \to \infty,\tag{45}$$

which proves this claim.

We are now ready to complete the proof for Theorem 5.1. We prove it by showing that I_+^s is empty for all states s or equivalently $V^{(t)}(s_0) \to V^{\star}(s_0)$ as $t \to \infty$.

Proof:[Proof for Theorem 5.1] Suppose the set I_+^s is non-empty for some s, else the proof is complete. Let $a_+ \in I_+^s$. Then, from Lemma C.12,

$$\sum_{a \in B_0^s} \theta_{s,a}^{(t)} \to \infty,\tag{46}$$

Now we proceed by showing a contradiction. For $a \in I_-^s$, we have that since $\frac{\pi^{(t)}(a|s)}{\pi^{(t)}(a_+|s)} = \exp(\theta_{s,a}^{(t)} - \theta_{s,a_+}^{(t)}) \to 0$ (as $\theta_{s,a_+}^{(t)}$ is lower bounded and $\theta_{s,a}^{(t)} \to -\infty$ by Lemma C.11), there exists $T_2 > T_0$ such that

$$\frac{\pi^{(t)}(a|s)}{\pi^{(t)}(a_+|s)} < \frac{(1-\gamma)\Delta}{16|\mathcal{A}|}$$

or, equivalently,

$$-\sum_{a \in I^s} \frac{\pi^{(t)}(a|s)}{1-\gamma} > -\pi^{(t)}(a_+|s)\frac{\Delta}{16}.$$
(47)

For $a \in \bar{B}_0^s$, we have $A^{(t)}(s,a) \to 0$ (by definition of set I_0^s and $\bar{B}_0^s \subset I_0^s$) and $1 < \frac{\pi^{(t)}(a_+|s)}{\pi^{(t)}(a|s)}$ for all $t > T_{a_+}$ from Lemma C.10. Thus, there exists $T_3 > T_2, T_{a_+}$ such that

$$|A^{(t)}(s,a)| < \frac{\pi^{(t)}(a_+|s)}{\pi^{(t)}(a|s)} \frac{\Delta}{16|\mathcal{A}|}$$

which implies

$$\sum_{a \in \bar{B}_0^s} \pi^{(t)}(a|s)|A^{(t)}(s,a)| < \pi^{(t)}(a_+|s)\frac{\Delta}{16}$$

$$-\pi^{(t)}(a_+|s)\frac{\Delta}{16} < \sum_{a \in \bar{B}_0^s} \pi^{(t)}(a|s)A^{(t)}(s,a) < \pi^{(t)}(a_+|s)\frac{\Delta}{16}$$
(48)

We have for $t > T_3$, from $\sum_{a \in \mathcal{A}} \pi^{(t)}(a|s) A^{(t)}(s,a) = 0$,

$$\begin{split} 0 &= \sum_{a \in I_0^s} \pi^{(t)}(a|s) A^{(t)}(s,a) + \sum_{a \in I_+^s} \pi^{(t)}(a|s) A^{(t)}(s,a) + \sum_{a \in I_-^s} \pi^{(t)}(a|s) A^{(t)}(s,a) \\ &\geq \sum_{a \in B_0^s} \pi^{(t)}(a|s) A^{(t)}(s,a) + \sum_{a \in \bar{B}_0^s} \pi^{(t)}(a|s) A^{(t)}(s,a) + \pi^{(t)}(a_+|s) A^{(t)}(s,a_+) \\ &\quad + \sum_{a \in I_-^s} \pi^{(t)}(a|s) A^{(t)}(s,a) \\ &\geq \sum_{a \in B_0^s} \pi^{(t)}(a|s) A^{(t)}(s,a) + \sum_{a \in \bar{B}_0^s} \pi^{(t)}(a|s) A^{(t)}(s,a) + \pi^{(t)}(a_+|s) \frac{\Delta}{4} - \sum_{a \in I_-^s} \frac{\pi^{(t)}(a|s)}{1 - \gamma} \\ &\stackrel{(c)}{>} \sum_{a \in B_0^s} \pi^{(t)}(a|s) A^{(t)}(s,a) - \pi^{(t)}(a_+|s) \frac{\Delta}{16} + \pi^{(t)}(a_+|s) \frac{\Delta}{4} - \pi^{(t)}(a_+|s) \frac{\Delta}{16} \\ &> \sum_{a \in B_0^s} \pi^{(t)}(a|s) A^{(t)}(s,a) \end{split}$$

where in the step (a), we used $A^{(t)}(s,a)>0$ for all actions $a\in I^s_+$ for $t>T_3>T_1$ from Lemma C.4. In the step (b), we used $A^{(t)}(s,a_+)\geq \frac{\Delta}{4}$ for $t>T_3>T_1$ from Lemma C.4 and $A^{(t)}(s,a)\geq -\frac{1}{1-\gamma}$. In the step (c), we used Equation (47) and left inequality in (48). This implies that for all $t>T_3$

$$\sum_{a \in B_0^s} \frac{\partial V^{(t)}(\mu)}{\partial \theta_{s,a}} < 0$$

This contradicts Equation (46) which requires

$$\lim_{t \to \infty} \sum_{a \in B_0^s} \left(\theta_{s,a}^{(t)} - \theta_{s,a}^{(T_3)} \right) = \eta \sum_{t=T_3}^{\infty} \sum_{a \in B_0^s} \frac{\partial V^{(t)}(\mu)}{\partial \theta_{s,a}} \to \infty.$$

Therefore, the set I_+^s must be empty, which completes the proof.

C.2 Proofs for Section 5.2

Proof: [of Corollary 5.4] Using Theorem 5.3, the desired optimality gap ϵ will follow if we set

$$\lambda = \frac{\epsilon (1 - \gamma)}{2 \left\| \frac{d_{\rho}^{\pi^{*}}}{\mu} \right\|_{\infty}} \tag{49}$$

and if $\|\nabla_{\theta}L_{\lambda}(\theta)\|_{2} \leq \lambda/(2|\mathcal{S}||\mathcal{A}|)$. In order to complete the proof, we need to bound the iteration complexity of making the gradient sufficiently small.

Since the optimization is deterministic and unconstrained, we can appeal to standard results such as from Ghadimi and Lan [2013] which give that after T iterations of gradient ascent with stepsize of $1/\beta_{\lambda}$, we have

$$\min_{t \le T} \|\nabla_{\theta} V^{(t)}(\mu)\|_{2}^{2} \le \frac{2\beta_{\lambda}(V^{\star}(\mu) - V^{(0)}(\mu))}{T} \le \frac{2\beta_{\lambda}}{(1 - \gamma)T},$$

where β_{λ} is an upper bound on the smoothness of $L_{\lambda}(\theta)$. We seek to ensure

$$\epsilon_{\text{opt}} \le \sqrt{\frac{2\beta_{\lambda}}{(1-\gamma)T}} \le \frac{\lambda}{2|\mathcal{S}||\mathcal{A}|}$$

Choosing $T \geq \frac{8\beta_{\lambda} |\mathcal{S}|^2 |\mathcal{A}|^2}{(1-\gamma)^{\lambda^2}}$ satisfies the above inequality. By Lemma E.4), we can take $\beta_{\lambda} = \frac{8\gamma}{(1-\gamma)^3} + \frac{2\lambda}{|\mathcal{S}|}$, and so

$$\frac{8\beta_{\lambda} |\mathcal{S}|^{2} |\mathcal{A}|^{2}}{(1-\gamma)^{\lambda^{2}}} \leq \frac{64 |\mathcal{S}|^{2} |\mathcal{A}|^{2}}{(1-\gamma)^{4} \lambda^{2}} + \frac{16 |\mathcal{S}| |\mathcal{A}|^{2}}{(1-\gamma)^{\lambda}}$$

$$\leq \frac{80 |\mathcal{S}|^{2} |\mathcal{A}|^{2}}{(1-\gamma)^{4} \lambda^{2}}$$

$$= \frac{320 |\mathcal{S}|^{2} |\mathcal{A}|^{2}}{(1-\gamma)^{6} \epsilon^{2}} \left\| \frac{d_{\rho}^{\pi^{\star}}}{\mu} \right\|_{\infty}^{2}$$

where we have used that $\lambda < 1$. This completes the proof.

C.3 Proofs for Section 5.3

Proof:[of Lemma 5.6] Following the definition of compatible function approximation in Sutton et al. [1999], which was also invoked in Kakade [2001], for a vector $w \in \mathbb{R}^{|\mathcal{S}||\mathcal{A}|}$, we define the error function

$$L^{\theta}(w) = \mathbb{E}_{s \sim d_{\theta}^{\pi_{\theta}}, a \sim \pi_{\theta}(a|s)} (w^{\top} \nabla_{\theta} \log \pi_{\theta}(a|s) - A^{\pi_{\theta}}(s, a))^{2}.$$

Let w_{θ}^{\star} be the minimizer of $L^{\theta}(w)$ with the smallest ℓ_2 norm. Then by definition of Moore-Penrose pseudoinverse, it is easily seen that

$$w_{\theta}^{\star} = F_{\rho}(\theta)^{\dagger} \mathbb{E}_{s \sim d_{\rho}^{\pi_{\theta}}, a \sim \pi_{\theta}(a|s)} [\nabla_{\theta} \log \pi_{\theta}(a|s) A^{\pi_{\theta}}(s, a)] = (1 - \gamma) F_{\rho}(\theta)^{\dagger} \nabla_{\theta} V^{\pi_{\theta}}(\rho).$$

In other words, w_{θ}^{\star} is precisely proportional to the NPG update direction. Note further that for the Softmax policy parameterization, we have by (37),

$$w^{\top} \nabla_{\theta} \log \pi_{\theta}(a|s) = w_{s,a} - \sum_{a' \in \mathcal{A}} w_{s,a'} \pi_{\theta}(a'|s).$$

Since $\sum_{a\in\mathcal{A}}\pi(a|s)A^{\pi}(s,a)=0$, this immediately yields that $L^{\theta}(A^{\pi_{\theta}})=0$. However, this might not be the unique minimizer of L^{θ} , which is problematic since $w^{\star}(\theta)$ as defined in terms of the Moore-Penrose pseudoinverse is formally the smallest norm solution to the least-squares problem, which $A^{\pi_{\theta}}$ may not be. However, given any vector $v\in\mathbb{R}^{|\mathcal{S}||\mathcal{A}|}$, let us consider solutions of the form $A^{\pi_{\theta}}+v$. Due to the form of the derivatives of the policy for the softmax parameterization (recall Equation 37), we have for any state s, a such that s is reachable under ρ ,

$$v^{\top} \nabla_{\theta} \log \pi_{\theta}(a|s) = \sum_{a' \in A} (v_{s,a'} \mathbb{1}[a = a'] - v_{s,a'} \pi_{\theta}(a'|s)) = v_{s,a} - \sum_{a' \in A} v_{s,a'} \pi(a'|s).$$

Note that here we have used that π_{θ} is a stochastic policy with $\pi_{\theta}(a|s) > 0$ for all actions a in each state s, so that if a state is reachable under ρ , it will also be reachable using π_{θ} , and hence the zero derivative conditions apply at each reachable state. For $A^{\pi_{\theta}} + v$ to minimize L^{θ} , we would like $v^{\top}\nabla_{\theta}\log\pi_{\theta}(a|s) = 0$ for all s, a so that $v_{s,a}$ is independent of the action and can be written as a constant c_s for each s by the above equality. Hence, the minimizer of $L^{\theta}(w)$ is determined up to a state-dependent offset, and

$$F_{\rho}(\theta)^{\dagger} \nabla_{\theta} V^{\pi_{\theta}}(\rho) = \frac{A^{\pi_{\theta}}}{1 - \gamma} + v,$$

where $v_{s,a} = c_s$ for some $c_s \in \mathbb{R}$ for each state s and action a. Finally, we observe that this yields the updates

$$\theta^{(t+1)} = \theta^{(t)} + \frac{\eta}{1-\gamma} A^{(t)} + \eta v \quad \text{and} \quad \pi^{(t+1)}(a|s) = \pi^{(t)}(a|s) \frac{\exp(\eta A^{(t)}(s,a)/(1-\gamma) + \eta c_s)}{Z_t(s)}.$$

Owing to the normalization factor $Z_t(s)$, the state dependent offset c_s cancels in the updates for π , so that resulting policy is invariant to the specific choice of c_s . Hence, we pick $c_s \equiv 0$, which yields the statement of the lemma.

D Proofs of Section 6.2

First, the following result, closely related to Proposition B.3 but restated here for the parametric policy case, is helpful.

Proposition D.1. Let $V^{\pi_{\theta}}(\mu)$ be β -smooth in θ . Define the gradient mapping as

$$G^{\eta} = \frac{1}{\eta} \left(P_{\Theta}(\theta + \eta \nabla_{\theta} V^{\pi_{\theta}}(\mu)) - \theta \right),$$

and the update rule of projected gradient is $\theta^+ = \theta + \eta G^{\eta}$. If $\|G^{\eta}\|_2 \le \epsilon$ for some η , then,

$$\max_{\theta + \delta \in \Theta, \ \|\delta\|_2 \le 1} \delta^\top \nabla_{\theta} V^{\pi_{\theta^+}}(\mu) \le \epsilon (\eta \beta + 1). \tag{50}$$

Proof: By Lemma 3 of Ghadimi and Lan [2016],

$$\nabla V^{\pi_{\theta^+}}(\mu) \in N_{\Theta}(\theta^+) + \epsilon(\eta\beta + 1)B_2, \tag{51}$$

where B_2 is the unit ℓ_2 ball, and N_{Θ} is the normal cone of the convex set Θ . Since $\nabla_{\theta}V^{\pi_{\theta^+}}(\mu)$ is $\epsilon(\eta\beta+1)$ distance from the normal cone and δ is in the tangent cone, then $\delta^{\top}\nabla_{\theta}V^{\pi_{\theta^+}}(\mu) \leq \epsilon(\eta\beta+1)$, which completes the proof.

Proof:[of Theorem 6.11] Let us use $d^{\pi_{\theta}}(s)$ as shorthand for $d^{\pi_{\theta}}_{\mu}(s)$. Let π^{\star} be the optimal policy in the class Π . By the performance difference lemma,

$$V^{\pi^{\star}}(\rho) - V^{\pi_{\theta}}(\rho) = \frac{1}{1 - \gamma} \mathbb{E}_{s \sim d_{\rho}^{\pi^{\star}}} \left[\sum_{a \in \mathcal{A}} \pi^{\star}(a|s) A^{\pi_{\theta}}(s, a) \right]$$

$$\leq \frac{1}{1 - \gamma} \mathbb{E}_{s \sim d_{\rho}^{\pi^{\star}}} \left[\max_{a \in \mathcal{A}} A^{\pi_{\theta}}(s, a) \right]$$

$$\leq \frac{1}{1 - \gamma} \left\| \frac{d_{\rho}^{\pi^{\star}}}{d^{\pi_{\theta}}} \right\|_{\infty} \mathbb{E}_{s \sim d^{\pi_{\theta}}} \left[\max_{a \in \mathcal{A}} A^{\pi_{\theta}}(s, a) \right].$$

where the final step uses that $\max_{a \in \mathcal{A}} A^{\pi_{\theta}}(s, a) \geq 0$. Continuing,

$$V^{\pi^*}(\rho) - V^{\pi_{\theta}}(\rho) \leq \frac{1}{1 - \gamma} \left\| \frac{d_{\rho}^{\pi^*}}{d^{\pi_{\theta}}} \right\|_{\infty} \mathbb{E}_{s \sim d^{\pi_{\theta}}} \left[\sum_{a \in \mathcal{A}} (\pi_{\theta}^{+}(a|s) - \pi_{\theta}(a|s)) A^{\pi_{\theta}}(s, a) \right]$$
$$= \frac{1}{1 - \gamma} \left\| \frac{d_{\rho}^{\pi^*}}{d^{\pi_{\theta}}} \right\|_{\infty} \mathbb{E}_{s \sim d^{\pi_{\theta}}} \left[\sum_{a \in \mathcal{A}} (\pi_{\theta}^{+}(a|s) - \pi_{\theta}(a|s)) Q^{\pi_{\theta}}(s, a) \right],$$

where the first inequality uses $\sum_a \pi_{\theta}(a|s) A^{\pi_{\theta}}(s,a) = 0$ for all policies π and states s, while the equality follows since $\sum_a (\pi_{\theta}^+(a|s) - \pi_{\theta}(a|s)) V^{\pi_{\theta}}(s) = 0$ for all states s.

By adding and subtracting $w^*(\theta)$ in the above, we have

$$V^{\pi^{\star}}(\rho) - V^{\pi_{\theta}}(\rho)$$

$$\leq \frac{1}{1-\gamma} \left\| \frac{d_{\rho}^{\pi^{\star}}}{d^{\pi_{\theta}}} \right\|_{\infty} \mathbb{E}_{s \sim d^{\pi_{\theta}}} \left[\sum_{a \in \mathcal{A}} \left(\pi_{\theta}^{+}(a|s) - \pi_{\theta}(a|s) - w^{\star}(\theta)^{T} \nabla_{\theta} \pi_{\theta}(a|s) \right) Q^{\pi_{\theta}}(s, a) \right]$$

$$+ \frac{1}{1-\gamma} \left\| \frac{d_{\rho}^{\pi^{\star}}}{d^{\pi_{\theta}}} \right\|_{\infty} \mathbb{E}_{s \sim d^{\pi_{\theta}}} \left[\sum_{a \in \mathcal{A}} w^{\star}(\theta)^{T} \nabla_{\theta} \pi_{\theta}(a|s) Q^{\pi_{\theta}}(s, a) \right]$$

$$\leq \frac{1}{(1-\gamma)^{2}} \left\| \frac{d_{\rho}^{\pi^{\star}}}{d^{\pi_{\theta}}} \right\|_{\infty} \mathbb{E}_{s \sim d^{\pi_{\theta}}} \left[\sum_{a \in \mathcal{A}} |\pi_{\theta}^{+}(a|s) - \pi_{\theta}(a|s) - w^{\star}(\theta)^{T} \nabla_{\theta} \pi_{\theta}(a|s) | \right]$$

$$+ \frac{1}{1-\gamma} \left\| \frac{d_{\rho}^{\pi^{\star}}}{d^{\pi_{\theta}}} \right\|_{\infty} \mathbb{E}_{s \sim d^{\pi_{\theta}}} \left[\sum_{a \in \mathcal{A}} w^{\star}(\theta)^{T} \nabla_{\theta} \pi_{\theta}(a|s) Q^{\pi_{\theta}}(s, a) \right]$$

$$\leq \frac{\epsilon_{\text{approx}}}{(1-\gamma)^{2}} \left\| \frac{d_{\rho}^{\pi^{\star}}}{d^{\pi_{\theta}}} \right\|_{\infty} + \left\| \frac{d_{\rho}^{\pi^{\star}}}{d^{\pi_{\theta}}} \right\|_{\infty} w^{\star}(\theta)^{T} \nabla_{\theta} V^{\pi_{\theta}}(\mu)$$

$$(52)$$

where have used our definition 27 of $w^*(\theta)$ and ϵ_{approx} in the last step.

Now define $\delta:=\frac{1}{\max\{1,\|w^\star(\theta)\|_2\}}w^\star(\theta)$. Then , it is easily verified that $\|\delta\|_2\leq 1$. Also, note that $\theta+\delta$ lies on the line connecting θ and $\theta+w^\star(\theta)$. To see this, observe that since $\theta,\theta+w^\star(\theta)\in\Theta$, then by convexity of Θ , we have $\theta+\delta\in\Theta$. Using our assumption that θ is an $\epsilon_{\rm opt}$ -stationary point,

$$\delta^{\top} \nabla_{\theta} V^{\pi_{\theta}}(\mu) \le \epsilon_{\text{opt}}.$$

Substituting this in Equation (52), we obtain

$$V^{\pi^{\star}}(\rho) - V^{\pi_{\theta}}(\rho) \leq \frac{\epsilon_{\text{approx}}}{(1 - \gamma)^{2}} \left\| \frac{d_{\rho}^{\pi^{\star}}}{d^{\pi_{\theta}}} \right\|_{\infty} + \max\{1, \|w^{\star}(\theta)\|_{2}\} \left\| \frac{d_{\rho}^{\pi^{\star}}}{d^{\pi_{\theta}}} \right\|_{\infty} \delta^{T} \nabla_{\theta} V^{\pi_{\theta}}(\mu)$$

$$\leq \frac{1}{(1 - \gamma)^{2}} \left\| \frac{d_{\rho}^{\pi^{\star}}}{d^{\pi_{\theta}}} \right\|_{\infty} \left(\epsilon_{\text{approx}} + (1 - \gamma)^{2} \max\{1, \|w^{\star}(\theta)\|_{2}\} \epsilon_{\text{opt}} \right)$$

$$\leq \frac{1}{(1 - \gamma)^{3}} \left\| \frac{d_{\rho}^{\pi^{\star}}}{\mu} \right\|_{\infty} \left(\epsilon_{\text{approx}} + (1 - \gamma)^{2} (1 + \|w^{\star}(\theta)\|_{2}) \epsilon_{\text{opt}} \right),$$

where the last inequality uses $d^{\pi_{\theta}}(s) = d^{\pi_{\theta}}_{\mu}(s) \ge (1 - \gamma)\mu(s)$.

Proof:[of Corollary 6.14] From Lemma E.5, $V^{\pi_{\theta}}(s)$ is β -smooth for all states s (and hence $V^{\pi_{\theta}}(\mu)$ is also β -smooth) in $\theta \in \Theta$. From Beck [2017][Theorem 10.15], for projected gradient ascent on β -smooth functions over convex set with step-size $\eta = \frac{1}{\beta}$, we can bound the projected gradient $G^{\eta}(\theta)$ with,

$$\min_{t=0,1,\dots,T-1} \|G^{\eta}(\theta^{(t)})\|_2 \le \frac{\sqrt{2\beta(V^{\star}(\mu) - V^{(0)}(\mu))}}{\sqrt{T}}$$

Then, using this bound on the projected gradient, from Proposition D.1, we have

$$\min_{t=0,1,...,T} \delta^{\top} \nabla_{\theta} V^{\pi^{(t)}}(\mu) \leq (\eta \beta + 1) \frac{\sqrt{2\beta (V^{\star}(\mu) - V^{(0)}(\mu))}}{\sqrt{T}}$$

And then using Theorem 6.11 and $\eta\beta = 1$, we have

$$\min_{t=0,1,\dots,T} V^{\star}(\rho) - V^{(t)}(\rho) \\
\leq \frac{1}{(1-\gamma)^3} \left\| \frac{d_{\rho}^{\pi^{\star}}}{\mu} \right\|_{\infty} \left(\epsilon_{\text{approx}} + 2(1-\gamma)^2 \max_{t=0,1,\dots,T} (\|w^{\star}(\theta^{(t)})\|_2 + 1) \frac{\sqrt{2\beta(V^{\star}(\mu) - V^{(0)}(\mu))}}{\sqrt{T}} \right)$$

Substituting

$$V^{\star}(\mu) - V^{(0)}(\mu) \le \frac{1}{1 - \gamma},$$
$$T > \frac{8\beta}{(1 - \gamma)^3 \epsilon^2} \left\| \frac{d_{\rho}^{\pi^{\star}}}{\mu} \right\|_{\infty}^2$$

gives the required bound.

E Smoothness Proofs

Various convergence guarantees we show leverage results from smooth, non-convex optimization. In this section, we collect the various results on smoothness of policies and value functions in the different parameterizations which are needed in our analysis.

Define the Hadamard product of two vectors:

$$[x \odot y]_i = x_i y_i$$

Define diag(x) for a column vector x as the diagonal matrix with diagonal as x.

Lemma E.1 (Smoothness for softmax parameterization). Fix a state s. Let $\theta_s \in \mathbb{R}^{|\mathcal{A}|}$ be the column vector of parameters for state s. Let $\pi_{\theta}(\cdot|s)$ be the corresponding vector of action probabilities given by the softmax parameterization. For some fixed vector $c \in \mathbb{R}^{|\mathcal{A}|}$, define:

$$F(\theta) := \pi_{\theta}(\cdot|s) \cdot c = \sum_{a} \pi_{\theta}(a|s)c_{a}.$$

Then

$$\|\nabla_{\theta_s} F(\theta_s) - \nabla_{\theta_s} F(\theta_s')\|_2 \le \beta \|\theta_s - \theta_s'\|_2$$

where

$$\beta = 5||c||_{\infty}.$$

Proof: For notational convenience, we do not explicitly state the s dependence. For the softmax parameterization, we have that

$$\nabla_{\theta} \pi_{\theta} = \operatorname{diag}(\pi_{\theta}) - \pi_{\theta} \pi_{\theta}^{\top}.$$

We can then write (as $\nabla_{\theta} \pi_{\theta}$ is symmetric),

$$\nabla_{\theta}(\pi_{\theta} \cdot c) = (\operatorname{diag}(\pi_{\theta}) - \pi_{\theta} \pi_{\theta}^{\top}) c = \pi_{\theta} \odot c - (\pi_{\theta} \cdot c) \pi_{\theta}$$
(53)

and therefore

$$\nabla_{\theta}^{2}(\pi_{\theta} \cdot c) = \nabla_{\theta}(\pi_{\theta} \odot c - (\pi_{\theta} \cdot c)\pi_{\theta}).$$

For the first term, we get

$$\nabla_{\theta}(\pi_{\theta} \odot c) = \operatorname{diag}(\pi_{\theta} \odot c) - \pi_{\theta}(\pi_{\theta} \odot c)^{\top},$$

and the second term, we can decompose by chain rule

$$\nabla_{\theta}((\pi_{\theta} \cdot c)\pi_{\theta}) = (\pi_{\theta} \cdot c)\nabla_{\theta}\pi_{\theta} + (\nabla_{\theta}(\pi_{\theta} \cdot c))\pi_{\theta}^{\top}$$

Substituting these back, we get

$$\nabla_{\theta}^{2}(\pi_{\theta} \cdot c) = \operatorname{diag}(\pi_{\theta} \odot c) - \pi_{\theta}(\pi_{\theta} \odot c)^{\top} - (\pi_{\theta} \cdot c)\nabla_{\theta}\pi_{\theta} - (\nabla_{\theta}(\pi_{\theta} \cdot c))\pi_{\theta}^{\top}. \tag{54}$$

Note that

$$\begin{split} & \max(\left\|\operatorname{diag}(\pi_{\theta} \odot c)\right\|_{2}, \left\|\pi_{\theta} \odot c\right\|_{2}, \left|\pi_{\theta} \cdot c\right|) \leq \left\|c\right\|_{\infty} \\ & \left\|\nabla_{\theta} \pi_{\theta}\right\|_{2} = \left\|\operatorname{diag}(\pi_{\theta}) - \pi_{\theta} \pi_{\theta}^{\top}\right\|_{2} \leq 1 \\ & \left\|\nabla_{\theta} (\pi_{\theta} \cdot c)\right\|_{2} \leq \left\|\pi_{\theta} \odot c\right\|_{2} + \left\|(\pi_{\theta} \cdot c) \pi_{\theta}\right\|_{2} \leq 2 \|c\|_{\infty}, \end{split}$$

which gives

$$\left\| \nabla_{\theta}^{2}(\pi_{\theta} \cdot c) \right\|_{2} \le 5\|c\|_{\infty}.$$

Before we prove the smoothness results for $\nabla_{\pi}V^{\pi}(s_0)$ and $\nabla_{\theta}V^{\pi_{\theta}}(s_0)$, we prove the following helpful lemma. This lemma is general and not specific to the direct or softmax policy parameterizations.

Lemma E.2. Let $\pi_{\alpha} := \pi_{\theta + \alpha u}$ and let $\widetilde{V}(\alpha)$ be the corresponding value at a fixed state s_0 , i.e.

$$\widetilde{V}(\alpha) := V^{\pi_{\alpha}}(s_0).$$

Assume that

$$\sum_{a \in \mathcal{A}} \left| \frac{d\pi_{\alpha}(a|s_0)}{d\alpha} \right|_{\alpha=0} \le C_1, \quad \sum_{a \in \mathcal{A}} \left| \frac{d^2\pi_{\alpha}(a|s_0)}{(d\alpha)^2} \right|_{\alpha=0} \le C_2$$

Then

$$\max_{\|u\|_{2}=1} \left| \frac{d^{2} \widetilde{V}(\alpha)}{(d\alpha)^{2}} \right|_{\alpha=0} \le \frac{C_{2}}{(1-\gamma)^{2}} + \frac{2\gamma C_{1}^{2}}{(1-\gamma)^{3}}.$$

Proof: Consider a unit vector u and let $\widetilde{P}(\alpha)$ be the state-action transition matrix under π , i.e.

$$[\widetilde{P}(\alpha)]_{(s,a)\to(s',a')} = \pi_{\alpha}(a'|s')P(s'|s,a).$$

We can differentiate $\widetilde{P}(\alpha)$ w.r.t α to get

$$\left[\frac{d\widetilde{P}(\alpha)}{d\alpha}\bigg|_{\alpha=0}\right]_{(s,a)\to(s',a')} = \frac{d\pi_{\alpha}(a'|s')}{d\alpha}\bigg|_{\alpha=0} P(s'|s,a).$$

For an arbitrary vector x,

$$\left[\frac{d\widetilde{P}(\alpha)}{d\alpha} \bigg|_{\alpha=0} x \right]_{s,a} = \sum_{a',s'} \frac{d\pi_{\alpha}(a'|s')}{d\alpha} \bigg|_{\alpha=0} P(s'|s,a) x_{a',s'}$$

and therefore

$$\max_{\|u\|_{2}=1} \left| \left[\frac{d\tilde{P}(\alpha)}{d\alpha} \Big|_{\alpha=0} x \right]_{s,a} \right| = \max_{\|u\|_{2}=1} \left| \sum_{a',s'} \frac{d\pi_{\alpha}(a'|s')}{d\alpha} \Big|_{\alpha=0} P(s'|s,a) x_{a',s'} \right| \\
\leq \sum_{a',s'} \left| \frac{d\pi_{\alpha}(a'|s')}{d\alpha} \Big|_{\alpha=0} P(s'|s,a) |x_{a',s'}| \\
\leq \sum_{a',s'} P(s'|s,a) ||x||_{\infty} \sum_{a'} \left| \frac{d\pi_{\alpha}(a'|s')}{d\alpha} \Big|_{\alpha=0} \right| \\
\leq \sum_{s'} P(s'|s,a) ||x||_{\infty} C_{1} \\
\leq C_{1} ||x||_{\infty}.$$

By definition of ℓ_{∞} norm,

$$\max_{\|u\|_{2}=1} \left\| \frac{d\widetilde{P}(\alpha)}{d\alpha} x \right\|_{\infty} \le C_{1} \|x\|_{\infty}$$

Similarly, differentiating $\widetilde{P}(\alpha)$ twice w.r.t. α , we get

$$\left[\frac{d^2\widetilde{P}(\alpha)}{(d\alpha)^2}\bigg|_{\alpha=0}\right]_{(s,a)\to(s',a')} = \frac{d^2\pi_\alpha(a'|s')}{(d\alpha)^2}\bigg|_{\alpha=0}P(s'|s,a).$$

An identical argument leads to that, for arbitrary x,

$$\max_{\|u\|_2=1} \left\| \frac{d^2 \widetilde{P}(\alpha)}{(d\alpha)^2} \right|_{\alpha=0} x \right\|_{\infty} \le C_2 \|x\|_{\infty}$$

Let $Q^{\alpha}(s_0, a_0)$ be the corresponding Q-function for policy π_{α} at state s_0 and action a_0 . Observe that $Q^{\alpha}(s_0, a_0)$ can be written as:

$$Q^{\alpha}(s_0, a_0) = e_{(s_0, a_0)}^{\mathsf{T}} (\mathbf{I} - \gamma \widetilde{P}(\alpha))^{-1} r = e_{(s_0, a_0)}^{\mathsf{T}} M(\alpha) r$$

where $M(\alpha):=(\mathbf{I}-\gamma\widetilde{P}(\alpha))^{-1}$ and differentiating twice w.r.t α gives:

$$\frac{dQ^{\alpha}(s_0, a)}{d\alpha} = \gamma e_{(s_0, a)}^{\top} M(\alpha) \frac{d\widetilde{P}(\alpha)}{d\alpha} M(\alpha) r,$$

$$\frac{d^2 Q^{\alpha}(s_0, a_0)}{(d\alpha)^2} = 2\gamma^2 e_{(s_0, a_0)}^{\top} M(\alpha) \frac{d\widetilde{P}(\alpha)}{d\alpha} M(\alpha) \frac{d\widetilde{P}(\alpha)}{d\alpha} M(\alpha) r$$

$$+ \gamma e_{(s_0, a_0)}^{\top} M(\alpha) \frac{d^2 \widetilde{P}(\alpha)}{(d\alpha)^2} M(\alpha) r.$$

By using power series expansion of matrix inverse, we can write $M(\alpha)$ as:

$$M(\alpha) = (\mathbf{I} - \gamma \widetilde{P}(\alpha))^{-1} = \sum_{n=0}^{\infty} \gamma^n \widetilde{P}(\alpha)^n$$

which implies that $M(\alpha) \ge 0$ (componentwise) and $M(\alpha)\mathbf{1} = \frac{1}{1-\gamma}\mathbf{1}$, i.e. each row of $M(\alpha)$ is positive and sums to $1/(1-\gamma)$. This implies:

$$\max_{\|u\|_{2}=1} \|M(\alpha)x\|_{\infty} \le \frac{1}{1-\gamma} \|x\|_{\infty}$$

This gives using expression for $\frac{d^2Q^{\alpha}(s_0,a_0)}{(d\alpha)^2}$ and $\frac{dQ^{\alpha}(s_0,a)}{d\alpha}$

$$\begin{aligned} \max_{\|u\|_2 = 1} \left| \frac{d^2 Q^{\alpha}(s_0, a_0)}{(d\alpha)^2} \right|_{\alpha = 0} \right| &\leq 2\gamma^2 \left\| M(\alpha) \frac{d\widetilde{P}(\alpha)}{d\alpha} M(\alpha) \frac{d\widetilde{P}(\alpha)}{d\alpha} M(\alpha) r \right\|_{\infty} \\ &+ \gamma \left\| M(\alpha) \frac{d^2 \widetilde{P}(\alpha)}{(d\alpha)^2} M(\alpha) r \right\|_{\infty} \\ &\leq \frac{2\gamma^2 C_1^2}{(1 - \gamma)^3} + \frac{\gamma C_2}{(1 - \gamma)^2} \\ \max_{\|u\|_2 = 1} \left| \frac{dQ^{\alpha}(s_0, a)}{d\alpha} \right|_{\alpha = 0} \left| \leq \left\| \gamma M(\alpha) \frac{d\widetilde{P}(\alpha)}{d\alpha} M(\alpha) r \right\|_{\infty} \\ &\leq \frac{\gamma C_1}{(1 - \gamma)^2} \end{aligned}$$

Consider the identity:

$$\widetilde{V}(\alpha) = \sum_{a} \pi_{\alpha}(a|s_0) Q^{\alpha}(s_0, a),$$

By differentiating $\widetilde{V}(\alpha)$ twice w.r.t α , we get

$$\frac{d^2\widetilde{V}(\alpha)}{(d\alpha)^2} = \sum_a \frac{d^2\pi_\alpha(a|s_0)}{(d\alpha)^2} Q^\alpha(s_0, a) + 2\sum_a \frac{d\pi_\alpha(a|s_0)}{d\alpha} \frac{dQ^\alpha(s_0, a)}{d\alpha} + \sum_a \pi_\alpha(a|s_0) \frac{d^2Q^\alpha(s_0, a)}{(d\alpha)^2}.$$

Hence,

$$\max_{\|u\|_{2}=1} \left| \frac{d^{2} \widetilde{V}(\alpha)}{(d\alpha)^{2}} \right| \leq \frac{C_{2}}{1-\gamma} + \frac{2\gamma C_{1}^{2}}{(1-\gamma)^{2}} + \frac{2\gamma^{2} C_{1}^{2}}{(1-\gamma)^{3}} + \frac{\gamma C_{2}}{(1-\gamma)^{2}}$$
$$= \frac{C_{2}}{(1-\gamma)^{2}} + \frac{2\gamma C_{1}^{2}}{(1-\gamma)^{3}},$$

which completes the proof.

Using this lemma, we now establish smoothness for: the value functions under the direct policy parameterization; the value functions under Assumption 6.12 for the approximate setting; the relative-entropy regularized objective 12 for the softmax parameterization.

Lemma E.3 (Smoothness for direct parameterization). For all starting states s_0 ,

$$\left\| \nabla_{\pi} V^{\pi}(s_0) - \nabla_{\pi} V^{\pi'}(s_0) \right\|_2 \le \frac{2\gamma |\mathcal{A}|}{(1-\gamma)^3} \left\| \pi - \pi' \right\|_2$$

Proof: By differentiating π_{α} w.r.t α gives

$$\sum_{a \in \mathcal{A}} \left| \frac{d\pi_{\alpha}(a|s_0)}{d\alpha} \right| \le \sum_{a \in \mathcal{A}} |u_{a,s}| \le \sqrt{|\mathcal{A}|}$$

and differentiating again w.r.t α gives

$$\sum_{a \in \mathcal{A}} \left| \frac{d^2 \pi_{\alpha}(a|s_0)}{(d\alpha)^2} \right| = 0$$

Using this with Lemma E.2 with $C_1 = \sqrt{|\mathcal{A}|}$ and $C_2 = 0$, we get

$$\max_{\|u\|_{2}=1} \left| \frac{d^{2} \widetilde{V}(\alpha)}{(d\alpha)^{2}} \right|_{\alpha=0} \le \frac{C_{2}}{(1-\gamma)^{2}} + \frac{2\gamma C_{1}^{2}}{(1-\gamma)^{3}} \le \frac{2\gamma |\mathcal{A}|}{(1-\gamma)^{3}}$$

which completes the proof.

Next we present a smoothness result for the entropy regularized policy optimization problem which we study for the softmax parameterization.

Lemma E.4 (Smoothness for relative entropy regularized softmax). For the softmax parameterization and

$$L_{\lambda}(\theta) = V^{\pi_{\theta}}(\mu) + \frac{\lambda}{|\mathcal{S}| |\mathcal{A}|} \sum_{s,a} \log \pi_{\theta}(a|s),$$

we have that

$$\left\|\nabla_{\theta} L_{\lambda}(\theta) - \nabla_{\theta} L_{\lambda}(\theta')\right\|_{2} \leq \beta_{\lambda} \left\|\theta - \theta'\right\|_{2}$$

where

$$\beta_{\lambda} = \frac{8}{(1-\gamma)^3} + \frac{2\lambda}{|\mathcal{S}|}$$

Proof: Let us first bound the smoothness of $V^{\pi_{\theta}}(\mu)$. Consider a unit vector u. Let $\theta_s \in \mathbb{R}^{|\mathcal{A}|}$ denote the parameters associated with a given state s. We have:

$$\nabla_{\theta_s} \pi_{\theta}(a|s) = \pi_{\theta}(a|s) \left(e_a - \pi(\cdot|s)\right)$$

and

$$\nabla_{\theta_s}^2 \pi_{\theta}(a|s) = \pi_{\theta}(a|s) \left(e_a e_a^{\top} - e_a \pi(\cdot|s)^{\top} - \pi(\cdot|s) e_a^{\top} + 2\pi(\cdot|s) \pi(\cdot|s)^{\top} - \operatorname{diag}(\pi(\cdot|s)) \right),$$

where e_a is a standard basis vector and $\pi(\cdot|s)$ is a vector of probabilities. We also have by differentiating $\pi_{\alpha}(a|s)$ once w.r.t α ,

$$\sum_{a \in \mathcal{A}} \left| \frac{d\pi_{\alpha}(a|s)}{d\alpha} \right|_{\alpha=0} \le \sum_{a \in \mathcal{A}} \left| u^{\top} \nabla_{\theta + \alpha u} \pi_{\alpha}(a|s) \right|_{\alpha=0} \\
\le \sum_{a \in \mathcal{A}} \pi_{\theta}(a|s) \left| u_{s}^{\top} e_{a} - u_{s}^{\top} \pi(\cdot|s) \right| \\
\le \max_{a \in \mathcal{A}} \left(\left| u_{s}^{\top} e_{a} \right| + \left| u_{s}^{\top} \pi(\cdot|s) \right| \right) \le 2$$

Similarly, differentiating once again w.r.t. α , we get

$$\begin{split} \sum_{a \in \mathcal{A}} \left| \frac{d^2 \pi_{\alpha}(a|s)}{(d\alpha)^2} \right|_{\alpha = 0} &| \leq \sum_{a \in \mathcal{A}} \left| u^\top \nabla^2_{\theta + \alpha u} \pi_{\alpha}(a|s) \right|_{\alpha = 0} u \right| \\ &\leq \max_{a \in \mathcal{A}} \left(\left| u_s^\top e_a e_a^\top u_s \right| + \left| u_s^\top e_a \pi(\cdot|s)^\top u_s \right| + \left| u_s^\top \pi(\cdot|s) e_a^\top u_s \right| \\ &+ 2 \left| u_s^\top \pi(\cdot|s) \pi(\cdot|s)^\top u_s \right| + \left| u_s^\top \operatorname{diag}(\pi(\cdot|s)) u_s \right| \right) \\ &\leq 6 \end{split}$$

Using this with Lemma E.2 for $C_1=2$ and $C_2=6$, we get

$$\max_{\|u\|_2=1} \left| \frac{d^2 \widetilde{V}(\alpha)}{(d\alpha)^2} \right|_{\alpha=0} \le \frac{C_2}{(1-\gamma)^2} + \frac{2\gamma C_1^2}{(1-\gamma)^3} \le \frac{6}{(1-\gamma)^2} + \frac{8\gamma}{(1-\gamma)^3} \le \frac{8}{(1-\gamma)^3}$$

or equivalently for all starting states s and hence for all starting state distributions μ ,

$$\|\nabla_{\theta} V^{\pi_{\theta}}(\mu) - \nabla_{\theta} V^{\pi_{\theta'}}(\mu)\|_{2} \le \beta \|\theta - \theta'\|_{2} \tag{55}$$

where $\beta = \frac{8}{(1-\gamma)^3}$.

Now let us bound the smoothness of the regularizer $\frac{\lambda}{|S|}R(\theta)$, where

$$R(\theta) := \frac{1}{|\mathcal{A}|} \sum_{s,a} \log \pi_{\theta}(a|s)$$

We have

$$\frac{\partial R(\theta)}{\partial \theta_{s,a}} = \frac{1}{|\mathcal{A}|} - \pi_{\theta}(a|s).$$

Equivalently,

$$\nabla_{\theta_s} R(\theta) = \frac{1}{|\mathcal{A}|} \mathbf{1} - \pi_{\theta}(\cdot | s).$$

Hence,

$$\nabla^2_{\theta_s} R(\theta) = -\mathrm{diag}(\pi_{\theta}(\cdot|s)) + \pi_{\theta}(\cdot|s)\pi_{\theta}(\cdot|s)^{\top}.$$

For any vector u_s ,

$$\left|u_s^{\top} \nabla_{\theta_s}^2 R(\theta) u_s\right| = \left|u_s^{\top} \operatorname{diag}(\pi_{\theta}(\cdot|s)) u_s - (u_s \cdot \pi_{\theta}(\cdot|s))^2\right| \le 2\|u_s\|_{\infty}^2.$$

Since $\nabla_{\theta_s} \nabla_{\theta_{s'}} R(\theta) = 0$ for $s \neq s'$,

$$\left| u^{\top} \nabla_{\theta}^2 R(\theta) u \right| = \left| \sum_s u_s^{\top} \nabla_{\theta_s}^2 R(\theta) u_s \right| \le 2 \sum_s \|u_s\|_{\infty}^2 \le 2 \|u\|_2^2.$$

Thus R is 2-smooth and $\frac{\lambda}{|S|}R$ is $\frac{2\lambda}{|S|}$ -smooth, which completes the proof.

Finally, we give a bound on smoothness in the function approximation case under Assumption 6.12.

Lemma E.5 (Smoothness under Assumption 6.12). *Assume that for all* θ , $\theta' \in \Theta$ *and for all* $s \in S$ *and* $a \in A$, *we have*

$$|\pi_{\theta}(a|s) - \pi_{\theta'}(a|s)| \le \beta_1 \|\theta - \theta'\|_2$$
 (\beta_1\text{-Lipschitz})
$$\|\nabla_{\theta}\pi_{\theta}(a|s) - \nabla_{\theta}\pi_{\theta'}(a|s)\|_2 \le \beta_2 \|\theta - \theta'\|_2$$
 (\beta_2\text{-smooth})

Then, for all starting states s_0 ,

$$\|\nabla_{\theta} V^{\pi_{\theta}}(s_0) - \nabla_{\theta} V^{\pi_{\theta'}}(s_0)\|_2 \le \beta \|\theta - \theta'\|_2$$

where,

$$\beta = \frac{\beta_2 |\mathcal{A}|}{(1-\gamma)^2} + \frac{2\gamma \beta_1^2 |\mathcal{A}|^2}{(1-\gamma)^3}$$

Proof: By differentiating $\pi_{\alpha}(a|s_0)$ once w.r.t α , we get

$$\sum_{a \in \mathcal{A}} \left| \frac{d\pi_{\alpha}(a|s_0)}{d\alpha} \right|_{\alpha=0} \le \sum_{a \in \mathcal{A}} \left| u^{\top} \nabla_{\theta} \pi_{\theta}(a|s_0) \right|$$

$$\le \sum_{a \in \mathcal{A}} \left\| u \right\|_2 \left\| \nabla_{\theta} \pi_{\theta}(a|s_0) \right\|_2 \le \beta_1 |\mathcal{A}|$$

And differentiating once again w.r.t. α , we get

$$\sum_{a \in \mathcal{A}} \left| \frac{d^2 \pi_{\alpha}(a|s_0)}{(d\alpha)^2} \right|_{\alpha=0} \le \sum_{a \in \mathcal{A}} \left| u^{\top} \nabla_{\theta}^2 \pi_{\theta}(a|s_0) u \right|$$

$$\le \sum_{a \in \mathcal{A}} \left\| \nabla_{\theta}^2 \pi_{\theta}(a|s_0) \right\|_2 \left\| u \right\|_2^2$$

$$\le \beta_2 |\mathcal{A}|$$

Using this with Lemma E.2 for $C_1 = \beta_1 |\mathcal{A}|$ and $C_2 = \beta_2 |\mathcal{A}|$, we get

$$\max_{\|u\|_{2}=1} \left| \frac{d^{2} \widetilde{V}(\alpha)}{(d\alpha)^{2}} \right|_{\alpha=0} \le \frac{C_{2}}{(1-\gamma)^{2}} + \frac{2\gamma C_{1}^{2}}{(1-\gamma)^{3}}$$

$$\le \frac{\beta_{2} |\mathcal{A}|}{(1-\gamma)^{2}} + \frac{2\gamma \beta_{1}^{2} |\mathcal{A}|^{2}}{(1-\gamma)^{3}}$$

which completes the proof.

F Concentrability vs. Distribution Mismatch Coefficients

The concentrability coefficient was introduced in Munos [2005] as a regularity assumption on an MDP to analyze approximate dynamic programming algorithms. Scherrer [2014] provides a more detailed discussion of how various notions of concentrability coefficients relate to the distribution mismatch coefficient. For completeness, we provide a discussion here, and also refer the reader to Scherrer [2014].

We start by a formal definition of these coefficients. For a stationary policy π , let $P^{\pi}: \mathcal{S} \times \mathcal{S}$ denote the matrix of transition probabilities under π so that $[P^{\pi}]_{s,s'}$ is the probability of a transition from s to s' under π .

Definition F.1 (Concentrability coefficient, [Munos, 2005]). Suppose we are given two distributions ρ and μ over S and an integer $m \ge 0$. Define

$$c_{\rho,\mu}(m) := \sup_{\pi_1,\dots,\pi_m} \left\| \frac{\rho P^{\pi_1} \dots P^{\pi_m}}{\mu} \right\|_{\infty}.$$

where the supremum is over a sequence of randomized stationary policies $\pi_1, \dots \pi_m$, where $\pi_i : \mathcal{S} \to \Delta(\mathcal{A})$. The second-order discounted concentrability of future state distributions is defined as

$$C_{\rho,\mu} := (1 - \gamma)^2 \sum_{m>1} m \gamma^{m-1} c_{\rho,\mu}(m).$$

Given these concentrability coefficients, standard results in the approximate value/policy iteration literature present bounds on the sample complexity of finding a near-optimal policy. We present an example of such a result from the work of Antos et al. [2008]. For the result, let $Q_k: \mathcal{S} \times \mathcal{A} \to [0, 1/(1-\gamma)]$ be an arbitrary sequence of functions for $k \geq 0$ and let π_k be the greedy policy relative to Q_k . Let us define

$$\epsilon_k = Q_k - \mathcal{T}^{\pi_k} Q_k, \quad \text{where} \quad \mathcal{T}^{\pi_k} Q(s, a) = r(s, a) + \gamma \mathbb{E}_{s'}[Q(s', \pi(s'))|s, a].$$
 (56)

That is, the ϵ_k captures the Bellman error of the Q value functions Q_k . If $\epsilon_k = 0$ for all k, then the procedure is identical to policy iteration. Antos et al. [2008] provides the following guarantee:

Lemma F.2 (Lemma 12 in Antos et al. [2008]). For any sequence of functions $Q_k : \mathcal{S} \times \mathcal{A} \rightarrow [0, 1/(1-\gamma)]$ for $k \geq 0$ and with ϵ_k as defined in Equation 56, we have

$$\frac{1}{|\mathcal{A}|} \sum_{a \in \mathcal{A}} \mathbb{E}_{s \sim \rho} |Q^{\star}(s, a) - Q^{\pi_k}(s, a)| \leq \frac{2\gamma}{(1 - \gamma)^2} \left(C_{\rho, \mu} \max_{0 \leq k \leq K} \frac{1}{|\mathcal{A}|} \sum_{a \in \mathcal{A}} \mathbb{E}_{s \sim \mu} |\epsilon_k(s, a)| + \gamma^K \right)$$

Based on this lemma, it is possible to further analyze the effect of finite samples by bounding ϵ_k , but we focus on the infinite sample case for the cleanest comparison with our results. In this case, it is easily seen that the first term captures the approximation error, while the second term

in the lemma is the optimization error which decays to 0 as $K \to \infty$. We would like to compare the result with, e.g. Corollary 6.5 from our paper in the function approximation setting. Doing so requires relating the notion of concentrability used here with our assumption of a small distribution mismatch coefficient, which we do next.

We now show the notion of distribution mismatch coefficient used in our analysis is always smaller than an appropriately modified notion of a concentrability coefficient. Let us define

$$C'_{\rho,\mu} = (1 - \gamma)^2 \sum_{m>1} m \gamma^{m-1} c_{\rho,\mu}(m-1).$$
 (57)

where we take $c_{\rho,\mu}(0) = \left\| \frac{\rho}{\mu} \right\|_{\infty}$. The following remark points out that $C'_{\rho,\mu}$ is a more appropriate notion to consider in our setting.

Remark F.3. $(C_{\rho,\mu} \text{ vs } C'_{\rho,\mu})$ Let us consider the special case where $\gamma=0$. Here, if the r(s,a) were known, then an optimal policy should be returned by any algorithm, as is the case in the bound of Lemma F.2. In particular, the results in [Munos, 2005, Antos et al., 2008] (and other results using concentrability) provide optimal policies in the case when $\gamma=0$. In our setting, even if $\gamma=0$, it is unreasonable to expect the algorithm to return an optimal policy, as our algorithm does not have access to r(s,a). $C'_{\rho,\mu}$ is a modified definition to account for this discrepancy, where we change the indexing on time.

We now see that $C'_{\rho,\mu}$ yields an upper bound on the distribution mismatch coefficient due to that concentrability takes a supremum over all non-stationary policies whereas the distribution mismatch coefficient only assumes a bound relative to a fixed π . See Scherrer [2014] for a more detailed discussion.

Lemma F.4. For any distributions ρ , μ over S and for any policy π , we have:

$$\left\| \frac{d_{\rho}^{\pi}}{\mu} \right\|_{\infty} \le \frac{1}{1 - \gamma} C_{\rho, \mu}'.$$

Proof: The proof follows from the observation that Equation (57) takes a supremum over all non-stationary policies, while we are only looking at the distribution induced by π on the LHS. Formally, we have

$$\left\| \frac{d_{\rho}^{\pi}}{\mu} \right\|_{\infty} = (1 - \gamma) \left\| \sum_{m \ge 0} \gamma^m \frac{\rho(P^{\pi})^m}{\mu} \right\|_{\infty}$$

$$\leq (1 - \gamma) \sum_{m \ge 0} \gamma^m \left\| \frac{\rho(P^{\pi})^m}{\mu} \right\|_{\infty}$$

$$\leq (1 - \gamma) \sum_{m \ge 0} (m + 1) \gamma^m \left\| \frac{\rho(P^{\pi})^m}{\mu} \right\|_{\infty}$$

$$\leq (1 - \gamma) \sum_{m \ge 1} m \gamma^{m-1} c_{\rho,\mu}(m - 1) = \frac{1}{1 - \gamma} C'_{\rho,\mu}$$

where we have used that norms satisfy the triangle inequality.

Remark F.5. (Normalization and the additional $\frac{1}{1-\gamma}$ factor) First, let us remark that the concentrability coefficient is a normalized quantity in the sense that $(1-\gamma)^2 \sum_{m\geq 1} m\gamma^{m-1} = 1$. So there is a sense in which the $\frac{1}{1-\gamma}$ factor in our upper bound in the previous lemma is not attributable to the concentrability coefficient not being a normalized quantity. It is unclear if this additional factor is overly pessimistic in natural MDPs.

As an example, we can simplify our Natural Policy Gradient bound from Corollary 6.5 to obtain:

$$\min_{t < T} \left\{ V^{\pi^{\star}}(\rho) - V^{(t)}(\rho) \right\} \le \left(\frac{W\sqrt{2\beta \log |\mathcal{A}|}}{1 - \gamma} \right) \cdot \frac{1}{\sqrt{T}} + \frac{\sqrt{|\mathcal{A}|C'_{\rho,\mu}\epsilon_{\text{approx}}}}{(1 - \gamma)^2} \,.$$

where we have chosen the initial state-action measure $\nu_0(s,a)$ so that $\nu_0(s)=\mu(s)$ and $\nu_0(a|s)$ is the uniform distribution over actions. Thus, we see at a high-level that a bound using the distribution mismatch coefficient directly implies a bound in terms of our adaptation of the concentrability coefficients. However, in general the distribution mismatch coefficient can be much smaller with a suitable choice of μ , even in cases where $C'_{\rho,\mu}$ is infinite since it only demands coverage for one policy rather than all possible non-stationary policies in the MDP.