Essentially Sharp Estimates on the Entropy Regularization Error in Discrete Discounted Markov Decision Processes

Anonymous Authors[1]

Abstract

We study the error introduced by entropy regularization of infinite-horizon discrete discounted Markov decision processes. We show that this error decreases exponentially in the inverse regularization strength both in a weighted KL-divergence and in value with a problem-specific exponent. We provide a lower bound matching our upper bound up to a polynomial factor. Our proof relies on the correspondence of the solutions of entropy-regularized Markov decision processes with gradient flows of the unregularized reward with respect to a Riemannian metric common in natural policy gradient methods. Further, this correspondence allows us to identify the limit of the gradient flow as the generalized maximum entropy optimal policy, thereby characterizing the implicit bias of the Kakade gradient flow which corresponds to a time-continuous version of the natural policy gradient method. We use this to show that for entropy-regularized natural policy gradient methods the overall error decays exponentially in the square root of the number of iterations.

1. Introduction

Entropy regularization plays an important role in reinforcement learning and is usually employed to encourage exploration thereby improving sample complexity and improving convergence of policy optimization techniques (Ahmed et al., 2019). One benefit of entropy regularization is that it corresponds to a strictly convex regularizer in the space of state-action distribution, where the reward optimization problem is equivalent to a linear program. Employing this hidden strong convexity, entropy-regularized vanilla and natural policy gradient methods have been shown to converge exponentially for discrete and continuous problems, for gradient descent and gradient flows, and for tabular methods as well as under function approximation (Mei et al., 2020; Cen et al., 2021; Çaycı et al., 2021; Müller & Montúfar, 2024; Kerimkulov et al., 2023).

Adding entropy regularization changes the optimization problem thereby introducing an error for which a conclusive analysis remains elusive. For general bounded regularizers and regularization strength $\tau \geq 0$ an $O(\tau)$ estimate on the regularization error can be established (Geist et al., 2019), which was subsequently used in the overall error analysis of entropy-regularized natural policy gradients (Dai et al., 2018; Lee et al., 2018). This result covers general regularizers but neither uses the structure of Markov decision processes nor the entropic regularizer. Together with the $O(e^{-\tau k \eta})$ convergence of entropy-regularized natural policy gradients this implies $O(\frac{\log k}{\eta k})$ convergence of the overall error with regularization strength $\tau = \frac{\log k}{\eta k}$, where k denotes the number of iterations, see (Cen et al., 2021).

1.1. Contributions

The main contribution of this article is a sharp analysis of the entropy regularization error in infinite-horizon discrete discounted Markov decision processes. We summarize our contributions as the following:

- *Sharp analysis of entropy regularization.* In Theorem 2.4 and Theorem 2.5 we give essentially matching upper and lower bounds on the entropy regularization error and show exponential convergence $\tilde{O}(e^{-\Delta \tau^{-1}})$ with a problem-dependent exponent $\Delta > 0$, where $\tilde{O}$ hides polynomial factors.

- *Implicit bias.* We show that the gradient flows corresponding to natural policy gradients converge towards the generalized maximum entropy optimal policy characterizing their implicit bias, see Theorem 2.5.

- *Overall error analysis.* We show that for regularized natural policy gradient methods the overall error decreases exponentially in the square-root of the number of iterations $\tilde{O}(e^{-\sqrt{\Delta \eta k/2}})$, see Theorem 2.6.

[1]Anonymous Institution, Anonymous City, Anonymous Region, Anonymous Country. Correspondence to: Anonymous Author <anon.email@domain.com>.

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1.2. Related works

At the core of our argument lies the observation that the optimal regularized policies solve the gradient flow of the unregularized reward with respect to the Kakade metric, which can be seen as the continuous time limit of unregularized natural policy gradient methods for tabular softmax policies. This correspondence uses the isometry between the Kakade metric and the conditional Fisher-Rao metric on the state-action distributions (Müller & Montúfar, 2024), which allows us to use the theory of Hessian gradient flows in convex optimization (Alvarez et al., 2004).

Natural policy gradients are known to converge at a $O(\frac{1}{k})$ rate (Agarwal et al., 2021) which was used in (Khodadadian et al., 2022) to show assymptotic $O(e^{-ck})$ convergence for all $c < \Delta$. Our continuous-time analysis uses similar arguments, but we provide an anytime analysis, an essentially matching lower bound, and show convergence towards the generalized maximum entropy optimal policy.

A continuous-time analysis of gradient flows with respect to the Kakade metric has been conducted for Markov decision processes with discrete and continuous state and action spaces in (Müller & Montúfar, 2024; Kerimkulov et al., 2023). For unregularized reward exponential convergence was established in (Müller & Montúfar, 2024) without control over the exponent or the coefficient. Under the presence of entropy regularization with strength $\tau > 0$ exponential $O(e^{-\tau t})$ convergence was established in (Müller & Montúfar, 2024; Kerimkulov et al., 2023). For gradient flows with respect to the Fisher metric in state-action space exponential convergence $O(e^{-\delta t})$ with a problem specific exponent was established, however, a lower bound is missing there, and the exponent $\delta \leq \Delta$ is dominated by the one for Kakade's gradient flows (Müller et al., 2024).

For unregularized natural actor-critic methods a $O(\log k)$ bound on the distance of the policies to the maximum entropy optimal policy was established by (Hu et al., 2021). Working in continuous time allows us to show exponential convergence towards the generalized maximum entropy optimal policy. A similar algorithmic bias showing convergence to the maximum entropy optimal policy was established for natural policy gradient methods that decrease regularization and increase step sizes during optimization (Li et al., 2023). In contrast to our implicit bias result, this approach considers an asymptotically vanishing but explicit regularization.

1.3. Notation

The *probability simplex* $\Delta_{\mathcal{X}} := \{\mu \in \mathbb{R}^{\mathcal{X}}_{\geq 0} : \sum_{x\in\mathcal{X}} \mu(x) = 1\}$ over a finite set $\mathcal{X}$ denotes all probability vectors. Given a second finite set $\mathcal{Y}$ we can identify the Cartesian product $\Delta^{\mathcal{Y}}_{\mathcal{X}} = \Delta_{\mathcal{X}} \times \cdots \Delta_{\mathcal{X}}$ with the set of stochastic matrices or the set of Markov kernels. We refer to $\Delta^{\mathcal{Y}}_{\mathcal{X}}$ as the *conditional probability polytope* and for $P \in \Delta^{\mathcal{Y}}_{\mathcal{X}}$ we write $P(x|y)$ for the entries of the Markov kernel. Finally, for two vectors $\mu, \nu \in \mathbb{R}^{\mathcal{X}}$ we denote the *Hadamard product* by $\mu \odot \nu \in \mathbb{R}^{\mathcal{X}}$ with entries $(\mu \odot \nu)(x) := \mu(x)\nu(x)$.

2. Main results

We consider a state and action spaces $\mathcal{S}$ and $\mathcal{A}$. The transition dynamics are described by a fixed Markov kernel $P \in \Delta^{\mathcal{S}\times\mathcal{A}}_{\mathcal{S}}$, where $P(s'|s,a)$ describes the probability of transitioning from s to s' under the action a. We consider stochastic memoryless policies $\pi \in \Delta^{\mathcal{S}}_{\mathcal{A}}$ and the discounted infinite-horizon entropy-regularized reward, given by

$$R_\tau(\pi) := (1-\gamma)\mathbb{E}_\pi\Bigg[\sum_{t\in\mathbb{N}} \gamma^t \Big(r(S_t, A_t) - \tau D_{\mathrm{KL}}(\pi(\cdot|S_t), \pi_0(\cdot|S_t)\Big)\Bigg] \tag{1}$$

where $\mu \in \Delta_{\mathcal{S}}$ is an initial distribution over the states, $r \in \mathbb{R}^{\mathcal{S}\times\mathcal{A}}$, and $\gamma \in [0,1)$ is the *discount factor*. Here, the states and actions are produced according to $S_0 \sim \mu$, $A_t \sim \pi(\cdot|S_t)$, $S_{t+1} \sim P(\cdot|S_t, A_t)$ and we refer to $\pi_0 \in \Delta^{\mathcal{S}}_{\mathcal{A}}$ *reference policy* and to $\tau \geq 0$ as the *regularization strength*. It is the goal of this article to understand the error induced by entropy regularization.

Important concepts in Markov decision processes are the *state* and *state-action distributions*

$$d^\pi(s) := (1-\gamma)\sum_{t\in\mathbb{N}} \gamma^t \mathbb{P}^{\pi,\mu}(S_t = s) \quad \text{and} \tag{2}$$

$$\nu^\pi(s,a) := (1-\gamma)\sum_{t\in\mathbb{N}} \gamma^t \mathbb{P}^{\pi,\mu}(S_t = s, A_t = a). \tag{3}$$

Definition 2.1 (Kakade divergence)**.** For two policies $\pi_1, \pi_2 \in \Delta^{\mathcal{S}}_{\mathcal{A}}$ we call

$$D_{\mathrm{K}}(\pi_1, \pi_2) := \sum_{s\in\mathcal{S}} d^{\pi_1}(s) D_{\mathrm{KL}}(\pi_1(\cdot|s), \pi_2(\cdot|s)) \tag{4}$$

the *Kakade divergence* between π_1 and π_2.[1]

A direct computation shows $R_\tau(\pi) = R(\pi) + \tau D_{\mathrm{K}}(\pi, \pi_0)$. Note that the Kakade divergence is not a Bregman divergence, see Remark A.2.

Assumption 2.2 (State exploration). For any $\pi \in \Delta^{\mathcal{S}}_{\mathcal{A}}$ it holds that $d^\pi(s) > 0$ for all $s \in \mathcal{S}$.

Setting 2.3. *Consider a finite discounted Markov decision process* $(\mathcal{S}, \mathcal{A}, P, \gamma, r)$*, an initial distribution* $\mu \in \Delta_{\mathcal{S}}$ *and fix a policy* $\pi_0 \in \mathrm{int}(\Delta^{\mathcal{S}}_{\mathcal{A}})$ *and let Assumption 2.2 hold and denote the optimal reward by* $R^\star := \max\{R(\pi) : \pi \in \Delta^{\mathcal{S}}_{\mathcal{A}}\}$.

[1] Note that D_{K} depends both on the initial distribution $\mu \in \Delta_{\mathcal{S}}$ as well as on the discount factor $\gamma \in [0,1)$.

Further, let $(\pi_t)_{t\geq 0}$ denote the solutions of the entropy-regularized problems

$$\pi_t = \operatorname*{arg\,max}_{\pi\in\Delta_{\mathcal{A}}^{\mathcal{S}}} \left\{ R(\pi) - t^{-1} D_{\mathrm{K}}(\pi,\pi_0) \right\}. \tag{5}$$

We denote the projection onto the optimal policies by

$$\pi^\star = \operatorname*{arg\,min}_{\pi\in\Pi^\star} D_{\mathrm{K}}(\pi,\pi_0), \tag{6}$$

where $\Pi^\star \coloneqq \{\pi \in \Delta_{\mathcal{A}}^{\mathcal{S}} : R(\pi) = R^\star\}$ denotes the set of optimal policies and set $c \coloneqq D_{\mathrm{K}}(\pi^\star,\pi_0)$. Finally, we set

$$\Delta \coloneqq -\max\left\{A^\star(s,a) \neq 0 : s\in\mathcal{S}, a\in\mathcal{A}\right\}, \tag{7}$$

where $A^\star$ is the advantage function under an optimal policy.

Now we give essentially matching upper and lower bounds on the entropy regularization error measured in value.

Theorem 2.4 (Convergence in value)**.** *Consider Setting 2.3. There exist $c_1, c_2 > 0$ such that for $t \geq 1$ it holds that*

$$R^\star - R(\pi_t) \leq c_1 e^{-\Delta(t-1)+\gamma c\log t} \quad \textit{and} \tag{8}$$

$$R^\star - R(\pi_t) \geq c_2 e^{-\Delta(t-1)-c\log t - 2\|r\|_\infty}. \tag{9}$$

We can give the constants in closed form, see Theorem C.2 The distance of the optimal entropy regularized policies decays at the same rate as the suboptimality gap.

Theorem 2.5 (Convergence of policies)**.** *Consider Setting 2.3. It holds that*

$$D_{\mathrm{K}}(\pi^\star,\pi_t) \leq \frac{e^{-\Delta(t-1)+\gamma c\log t}}{1-e^{-\Delta(t-1)+\gamma c\log t}}, \tag{10}$$

if $e^{-\Delta(t-1)+\gamma c\log t} < 1$ which is satisfied for $t > 0$ large enough. Further, for a suitable constant $c_3 > 0$ we have

$$D_{\mathrm{K}}(\pi^\star,\pi_t) \geq c_3 e^{-\Delta(t-1)-c\log t - 2\|r\|_\infty}. \tag{11}$$

As $(\pi_t)_{t\geq 0}$ solve a continuous version of the natural policy gradient method, Theorem 2.5 describes the *implicit bias* of these methods towards a generalized maximum entropy optimal policy, see Remark B.9.

Theorem 2.6 (Overall error analysis)**.** *Consider Setting 2.3 with $t \geq 1$ and assume that $(\pi_k)_{k\in\mathbb{N}}$ are iterates produced by natural policy ascent with a tabular softmax parametrization with stepsize $\eta > 0$. For $t^{-1} = \sqrt{2\Delta/\eta k}$ it holds that*

$$R^\star - R(\pi_k) = O\left(\left(\eta k \Delta^{-1}\right)^{c/2} \cdot e^{-\sqrt{\Delta\eta k/2}}\right). \tag{12}$$

In contrast, unregularized natural policy gradient methods converge at a rate $\tilde{O}(e^{-\Delta\eta k})$ (Khodadadian et al., 2022).

3. Proof structure

Our anlysis relies on the observation that the optimal regularized policies $(\pi_t)_{t\geq 0}$ solve a gradient flow with respect to a Riemannian metric proposed in the context of natural policy gradients. The gradient of the reward with respect to this metric admits an expression via the advantage function which allows for an explicit convergence analysis.

3.1. Geometry of Kakade's metric

The following Riemannian metric was proposed in the context of natural gradients (Kakade, 2001).

Definition 3.1 (Kakade metric)**.** We call the Riemannian metric[2] g^{K} on $\operatorname{int}(\Delta_{\mathcal{A}}^{\mathcal{S}})$ defined by

$$g_\pi^{\mathrm{K}}(v,w) \coloneqq \sum_{s\in\mathcal{S}} d^\pi(s) \sum_{a\in\mathcal{A}} \frac{v(s,a)w(s,a)}{\pi(a|s)} \tag{13}$$

for all $v, w \in T\Delta_{\mathcal{A}}^{\mathcal{S}}$ the *Kakade metric*. For a differentiable function $f\colon \Delta_{\mathcal{A}}^{\mathcal{S}} \to \mathbb{R}$ we denote the corresponding Riemannian gradient by $\nabla^{\mathrm{K}} f(\pi)$.

The following expression of the gradient of the reward with respect to the Kakade metric allows for an explicit convergence analysis of the corresponding gradient flow later.

Theorem 3.2 (Gradient with respect to the Kakade metric)**.** *Let Assumption 2.2 hold. Then for all $\pi \in \operatorname{int}(\Delta_{\mathcal{A}}^{\mathcal{S}})$ and $a \in \mathcal{A}$, $s \in \mathcal{S}$ it holds that*

$$\nabla^{\mathrm{K}} R(\pi)(s,a) = A^\pi(s,a)\pi(a|s), \tag{14}$$

where $\mathcal{A}^\pi \in \mathbb{R}^{\mathcal{S}\times\mathcal{A}}$ denotes the advantage function of π.

Based on the expression of the Kakade gradient, we call

$$\partial_t \pi_t(a|s) = A^{\pi_t}(s,a)\pi_t(a|s) \tag{15}$$

the *Kakade gradient flow*.

The Fisher-Rao metric arises from the negative entropy (Ay et al., 2017), similarly, one can define a conditional version. For $\nu \in \mathbb{R}_{>0}^{\mathcal{S}\times\mathcal{A}}$ we define the *conditional entropy* via

$$H_{A|S}(\nu) \coloneqq \sum_{s\in\mathcal{S},a\in\mathcal{A}} \nu(s,a) \log \frac{\nu(s,a)}{\sum_{a'\in\mathcal{A}} \nu(s,a')}. \tag{16}$$

Definition 3.3 (Conditional Fisher-Rao metric)**.** We call the metric $g^{A|S}$ on $\operatorname{int}(\mathscr{D})$ given by

$$g_\nu^{A|S}(v,w) \coloneqq v^\top \nabla^2 H_{A|S}(\nu) w \quad \text{for } v,w \in T\mathscr{D} \tag{17}$$

the *conditional Fisher-Rao metric* and the denote the corresponding gradient by $\nabla^{A|S}$. We call the corresponding Bregman divergence $D^{A|S}$ the *conditional KL-divergence*.

The maximization of the regularized reward R_τ subject to $\pi \in \Delta_{\mathcal{A}}^{\mathcal{S}}$ is equivalent to the regularized linear program

$$\max r^\top \nu - \tau D_{A|S}(\nu,\nu_0) \quad \text{subject to } \nu \in \mathscr{D}, \tag{18}$$

where $\nu_0 = \nu^{\pi_0}$, see (Neu et al., 2017).

The Kakade metric has been characterized as the pullback of the conditional Fisher-Rao metric.

[2] Under Assumption 2.2 g^{K} is a Riemannian metric.

Theorem 3.4 ((Müller & Montúfar, 2024)). *Consider a finite Markov decision process and let Assumption 2.2 hold. Then the following mapping is an isometry*

$$(\mathrm{int}(\Delta_{\mathcal{A}}^{\mathcal{S}}), g^{\mathrm{K}}) \to (\mathrm{int}(\mathscr{D}), g^{A|S}), \quad \pi \mapsto \nu^{\pi}. \tag{19}$$

As the reward is a linear function of the state-action distributions we can apply results from Hessian gradient flows of linear programs (Alvarez et al., 2004).

Corollary 3.5. *The following statements hold:*

1. Well-posedness: *The Kakade gradient flow* (15) *admits a unique global solution* $(\pi_t)_{t\geq 0}$.
2. Central path property: *For all* $t \geq 0$ *it holds that*
$$\pi_t = \arg\max_{\pi\in\Delta_{\mathcal{A}}^{\mathcal{S}}} \Big\{ R(\pi) - t^{-1} D_{\mathrm{K}}(\pi, \pi_0) \Big\}. \tag{20}$$
3. Sublinear convergence: *For all* $t \geq 0$ *we have*
$$0 \leq R^\star - R(\pi_t) \leq t^{-1} \cdot \min_{\pi^\star\in\Pi^\star} D_{\mathrm{K}}(\pi^\star, \pi_0). \tag{21}$$
4. Implicit bias: *It holds that*
$$\lim_{t\to+\infty} \pi_t = \pi^\star = \arg\min_{\pi\in\Pi^\star} D_{\mathrm{K}}(\pi, \pi_0). \tag{22}$$

Importantly, (20) provides an equivalence between Kakade gradient flows and the solutions of the regularized problems.

3.2. Tight analysis

A central step in our proof is to show that the selection probabilities of suboptimal actions decay exponentially fast in t. This can be seen as a continuous time analogon to (Khodadadian et al., 2022, Lemma 3.4).

Lemma 3.6. *Consider Setting 2.3. Then for all* $t \geq t_0 > 0$, $s \in \mathcal{S}$, *and* $a \in \mathcal{A}$ *it holds that*

$$\pi_t(a|s) \leq \pi_0(a|s) e^{A^\star(s,a)(t-1)+\gamma c \log t + 2\|r\|_\infty} \quad \textit{and}$$
$$\pi_t(a|s) \geq \pi_0(a|s) e^{A^\star(s,a)(t-1)-c \log t - 2\|r\|_\infty}.$$

Proof. We consider the Kakade gradient flow (15). As a consequence of the sublinear convergence (21) it holds that

$$\partial_t \pi_t(a|s) \leq \left(A^\star(s,a) + \frac{\gamma c}{t} \right) \pi_t(a|s) \quad \text{and}$$
$$\partial_t \pi_t(a|s) \geq \left(A^\star(s,a) - \frac{c}{t} \right) \pi_t(a|s)$$

where $c = D(\pi^\star, \pi_0)$. Now, Grönwall's inequality yields

$$\pi_T(a|s) \leq \pi_{t_0}(a|s) e^{A^\star(s,a)(T-t_0)+\gamma c \int_{t_0}^T t^{-1} \mathrm{d}t}$$
$$= \pi_{t_0}(a|s) e^{A^\star(s,a)(T-t_0)+\gamma c \log T - \gamma c \log t_0}$$

and similarly for the lower bound. Further, note that $\|A^\pi\|_\infty \leq 2\|r\|_\infty$ and hence Grönwall yields

$$\pi_0(a|s) e^{-2\|r\|_\infty t_0} \leq \pi_{t_0}(a|s) \leq \pi_0(a|s) e^{2\|r\|_\infty t_0}$$

and choosing $t_0 = 1$ finishes the proof. □

The proofs of the main results presented in Section 2 rely on the following auxiliary results, which proofs we defer to Appendix C. The combination of Lemma 3.6 and the following lemma yields the proof of Theorem 2.4.

Lemma 3.7 (Sub-optimality gap). *For any policy* $\pi \in \Delta_{\mathcal{A}}^{\mathcal{S}}$ *it holds that*

$$R^\star - R(\pi) \leq \frac{2\|r\|_\infty}{1-\gamma} \sum_{s\in\mathcal{S}, a\notin A_s^\star} d^\pi(s)\pi(a|s) \quad \textit{and} \tag{23}$$

$$R^\star - R(\pi) \geq \frac{\Delta}{1-\gamma} \cdot \sum_{s\in\mathcal{S}, a\notin A_s^\star} d^\pi(s)\pi(a|s). \tag{24}$$

The following lemma underlies the proof of Theorem 2.5.

Lemma 3.8. *Let* $\pi^\star \in \Pi^\star$ *be the Kakade projection of* $\pi \in \mathrm{int}(\Delta_{\mathcal{A}}^{\mathcal{S}})$ *onto* $\Pi^\star$. *Then it holds that*

$$D_{\mathrm{K}}(\pi^\star, \pi) \leq \frac{\max_{s\in\mathcal{S}} \sum_{a\notin A_s^\star} \pi(a|s)}{1 - \max_{s\in\mathcal{S}} \sum_{a\notin A_s^\star} \pi(a|s)} \quad \textit{and} \tag{25}$$

$$D_{\mathrm{K}}(\pi^\star, \pi) \geq \sum_{s\in\mathcal{S}} d^\star(s) \sum_{a\notin A_s^\star} \pi(a|s). \tag{26}$$

To estimate the unregularized reward of a policy close to the optimal regularized policy we use the following result.

Lemma 3.9. *With* $c = \frac{\sqrt{2}|\mathcal{S}|\|r\|_\infty}{1-\gamma}$ *for any policy* $\pi \in \Delta_{\mathcal{A}}^{\mathcal{S}}$ *we have*

$$R^\star - R(\pi) \leq R^\star - R(\pi_\tau^\star) + c\|\log \pi_\tau^\star - \log \pi\|_\infty^{\frac{1}{2}}, \tag{27}$$

where $\pi_\tau^\star$ *denotes the optimal regularized policy.*

Entropy-regularized natural policy gradient methods with step size $\eta > 0$ and regularization strength $\tau > 0$ satisfy $\|\log \pi_\tau^\star - \log \pi\|_\infty = O(e^{-\tau\eta k})$ (Cen et al., 2021). This together with Lemma 3.9 yields Theorem 2.6.

4. Conclusion

We provide essentially sharp estimates on the error introduced by entropy regularization in discrete discounted Markov decision processes showing $\tilde{O}(e^{-\Delta\tau^{-1}})$ convergence with a problem-dependent exponent $\Delta > 0$. At the heart lies the observation that the optimal regularized policies solve a gradient flow with respect to a Riemannian metric playing a central role in natural policy gradient methods. The tight estimate on the entropy regularization error leads to an improved $\tilde{O}(e^{-\sqrt{\Delta\eta k/2}})$ overall error analysis of natural policy gradient methods. However, this leaves a gap to the $\tilde{O}(e^{-\Delta\eta k})$ convergence of unregularized natural policy methods that can be addressed in future works.

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A. Preliminaries

In this section we provide background material from the theory of Markov decision processes. We put an emphasis on regularization and see that entropically regularized Markov decision processes are equivalent to a conditional entropic regularization of the linear programming formulation of the Markov decision process. We conclude with a general discussion of regularized linear programs and revisit the central path property, which guarantees that the solutions of regularized linear programs with regularization strength t^{-1} solve the gradient flow of the linear program with respect to the Riemannian metric induced by the convex regularizer.

A.1. Markov decision processes and entropy regularization

We consider a finite set $\mathcal{S}$ of states of some system and a finite set $\mathcal{A}$ of actions that can used to control the state $s \in \mathcal{S}$. The transition dynamics are described by a fixed Markov kernel $P \in \Delta_{\mathcal{S}}^{\mathcal{S}\times\mathcal{A}}$, where $P(s'|s,a)$ describes the probability of transitioning from s to s' under the action a. It is the goal in Markov decision processes and reinforcement learning to design a *policy* $\pi \in \Delta_{\mathcal{A}}^{\mathcal{S}}$. A common optimality criterion is the *discounted infinite horizon reward* given by

$$R(\pi) \coloneqq (1-\gamma)\mathbb{E}_{\mathbb{P}^{\pi,\mu}}\left[\sum_{t\in\mathbb{N}} \gamma^t r(S_t, A_t)\right], \tag{28}$$

where $\mu \in \Delta_{\mathcal{S}}$ is an initial distribution over the states and $\mathbb{P}^{\pi,\mu}$ denotes the law of the Markov process on $\mathcal{S}\times\mathcal{A}$ induced by the iteration

$$S_0 \sim \mu, A_t \sim \pi(\cdot|S_t), S_{t+1} \sim P(\cdot|S_t, A_t), \tag{29}$$

$r \in \mathbb{R}^{\mathcal{S}\times\mathcal{A}}$ is the *instantaneous reward* vector, and $\gamma \in [0,1)$ is the *discount factor*. To encourage exploration it is common to regularize the reward with an entropy term which yields the *entropy regularized* or *KL-regularized* reward

$$R_\tau^\mu(\pi) \coloneqq (1-\gamma)\mathbb{E}_{\mathbb{P}^{\pi,\mu}}\left[\sum_{t\in\mathbb{N}} \gamma^t (r(S_t, A_t) - \tau D_{\mathrm{KL}}(\pi(\cdot|S_t), \pi_0(\cdot|S_t))\right] \tag{30}$$

for some *reference policy* $\pi_0 \in \Delta_{\mathcal{A}}^{\mathcal{S}}$ and *regularization strength* $\tau \geq 0$. The entropy or KL-regularized reward optimization problem is now given by

$$\max R_\tau(\pi) \quad \text{subject to } \pi \in \Delta_{\mathcal{A}}^{\mathcal{S}}. \tag{31}$$

It is our main contribution to provide a sharp analysis of how well a solution of the regularized reward optimization problem approximates the solution of the unregularized problem. In the special case that π_0 is the uniform policy, meaning that $\pi_0(a|s) = |\mathcal{A}|^{-1}$, then the regularization term becomes up to constant equal to the negative entropy $-H(\pi(\cdot|S_t))$.

A central role in theoretical and algorithmic approaches to Markov decision processes and reinforcement learning plays the *value function* $V^\pi \in \mathbb{R}^{\mathcal{S}}$ given by

$$V_\tau^\pi(s) \coloneqq R_\tau^{\delta_s}(\pi) \quad \text{for all } s \in \mathcal{S}, \tag{32}$$

which stores the reward obtained when starting in a deterministic state $s \in \mathcal{S}$. The unregularized and regularized *state-action* or *Q-value functions* are given by

$$Q_\tau(s,a) \coloneqq (1-\gamma)r(s,a) + \gamma \sum_{s'\in\mathcal{S}} V_\tau^\pi(s')P(s'|s,a) \quad \text{for all } s \in \mathcal{S}, a \in \mathcal{A}. \tag{33}$$

In the regularized case, we also define the *soft Q-function* given by

$$q_\tau(s,a) \coloneqq Q_\tau(s,a) - (1-\gamma)\tau \log \pi(a|s) \quad \text{for all } s \in \mathcal{S}, a \in \mathcal{A}. \tag{34}$$

Finally, we define the *advantage function* of a policy π via

$$A_\tau^\pi(s,a) \coloneqq Q_\tau^\pi(s,a) - V_\tau^\pi(s) \tag{35}$$

and the *soft advantage function* via

$$B_\tau^\pi(s,a) := q_\tau^\pi(s,a) - V_\tau^\pi(s). \tag{36}$$

Finally, we define the *optimal reward* and *optimal value functions* via $R^\star := \max_{\pi\in\Delta_{\mathcal{A}}^{\mathcal{S}}} R(\pi)$ and

$$V_\tau^\star(s) := \max_{\pi\in\Delta_{\mathcal{A}}^{\mathcal{S}}} V_\tau^\pi(s) \quad \text{and } Q_\tau^\star(s,a) := \max_{\pi\in\Delta_{\mathcal{A}}^{\mathcal{S}}} Q_\tau^\pi(s,a) \quad \text{for } s\in\mathcal{S}, a\in\mathcal{A} \tag{37}$$

and the *optimal advantage function* via

$$A_\tau^\star(s,a) := Q_\tau^\star(s,a) - V^\star(s) \quad \text{for } s\in\mathcal{S}, a\in\mathcal{A}. \tag{38}$$

It is well known that there are optimal policies $\pi_\tau^\star \in \Delta_{\mathcal{A}}^{\mathcal{S}}$ satisfying $V_\tau^\star = V^{\pi_\tau^\star}$ and $Q_\tau^\star = Q^{\pi_\tau^\star}$, which is known as the Bellman principle, see (Geist et al., 2019). In the unregularized case, the optimal advantage function $A^\star$ satisfies $A^\star(s,a)\le 0$ for all $s\in\mathcal{S}, a\in\mathcal{A}$ and an action $a\in\mathcal{A}$ is optimal in a state $s\in\mathcal{S}$ if and only if $A^\star(s,a)=0$. For $s\in\mathcal{S}$, we denote the set of optimal actions by $A_s^\star := \{a\in\mathcal{A} : A^\star(s,a)=0\}$ and the set of optimal policies is given by

$$\Pi^\star := \left\{\pi\in\Delta_{\mathcal{A}}^{\mathcal{S}} : R(\pi)=R^\star\right\} = \left\{\pi\in\Delta_{\mathcal{A}}^{\mathcal{S}} : \operatorname{supp}(\pi(\cdot|s))\subseteq A_s^\star \text{ for all } s\in\mathcal{S}\right\}. \tag{39}$$

We denote the unregularized value and advantage functions by $V^\pi = V_0^\pi$, $Q^\pi = Q_0^\pi$, $q^\pi = q_0^\pi$, $A^\pi = A_0^\pi$, and $B^\pi = B_0^\pi$. Note that $Q^\pi = q^\pi$ and $A^\pi = B^\pi$.

Of central importance in the theory of Markov decision processes are the *state distributions*, which measure how much time the process spends at the individual states for a given policy $\pi\in\Delta_{\mathcal{A}}^{\mathcal{S}}$. This is formalized by

$$d^\pi(s) = d_\gamma^{\pi,\mu}(s) := (1-\gamma)\sum_{t\in\mathbb{N}} \gamma^t \mathbb{P}^{\pi,\mu}(S_t = s). \tag{40}$$

Note that indeed $d^\pi\in\Delta_{\mathcal{S}}$ by the geometric series. Sometimes, the state distributions are called state frequencies or state occupancy measures.

Definition A.1 (Kakade divergence)**.** For two policies $\pi_1,\pi_2\in\Delta_{\mathcal{A}}^{\mathcal{S}}$ we call

$$D_{\mathrm{K}}(\pi_1,\pi_2) = D_{\mathrm{K}}^\mu(\pi_1,\pi_2) := \sum_{s\in\mathcal{S}} d^{\pi_1}(s) D_{\mathrm{KL}}(\pi_1(\cdot|s),\pi_2(\cdot|s)) \tag{41}$$

the *Kakade divergence* between π_1 and π_2. Note that D_{K} depends both on the initial distribution $\mu\in\Delta_{\mathcal{S}}$ as well as on the discount factor $\gamma\in[0,1)$.

An important property of the Kakade divergence is that

$$R_\tau(\pi) = R(\pi) - \tau D_{\mathrm{K}}(\pi,\pi_0) \quad \text{for all } \pi\in\Delta_{\mathcal{A}}^{\mathcal{S}} \tag{42}$$

and hence the Kakade divergence describes the regularization term in space of policies. Convex optimization problems with a regularizer given by a Bregman divergence are well studied (**?**). We can not directly apply such results as neither R is convex nor D_{K} a Bregman divergence.

Remark A.2 (Kakade's divergence is not Bregman). Bregman divergences are well-studied in convex optimization (Alvarez et al., 2004; Bubeck et al., 2015), however, the Kakade divergence does not fall into this class. Indeed, Bregman divergences are convex in their first argument, which is not generally true for the Kakade divergence. To construct a specific example, where $D_{\mathrm{K}}(\cdot,\pi)$ is not convex, we consider the Markov decision process with two states and actions shown in Figure 1. Further, we choose the reference policy π to be to be the uniform policy and if we consider $\pi_p(a_1|s_i)=p$ for $i=1,2$, then we obtain

$$g(p) := D_{\mathrm{K}}(\pi_p,\pi) = (1-\gamma)\phi(p) + \gamma^2 p^2\phi(p), \tag{43}$$

where $\phi(p) := -p\log p - (1-p)\log(1-p)$. Taking the second derivative yields

$$\partial_p^2 g(p) = -(1-\gamma)\left(\frac{1}{1-p} - \frac{1}{p^2}\right) - \gamma^2\left(\frac{1}{1-p} + \frac{1}{p}\right)p - 2\gamma^2(\log p - \log(1-p)). \tag{44}$$

Taking $p\to 1$ yields $\partial_p^2 g(p)\to -\infty$ showing the non-convexity of g and therefore $D_{\mathrm{K}}(\cdot,\pi)$.

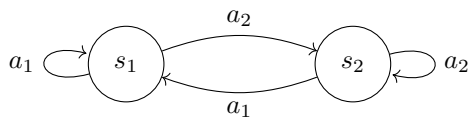

Figure 1. Transition graph of the Markov decision process.

We show later that the Kakade divergence is the pullback of the conditional KL divergence on the space of state-action distributions, which renders the entropy regularized reward optimization problem equivalent to a linear program with a Bregman regularizer.

The following estimate on the regularization error is well known and commonly applied when approximating unregularized Markov decision processes via regularization, see (Geist et al., 2019; Cen et al., 2021).

Proposition A.3 (Sublinear estimate on the entropy regularization error)**.** *Let $\pi_\tau^\star$ denote an optimal policy of the regularized reward $R_\tau(\pi) \coloneqq R(\pi) - \tau D_{\mathrm{K}}(\pi, \pi_0)$ for some $\pi_0 \in \Delta_{\mathcal{A}}^{\mathcal{S}}$ and denote the set of optimal policies by $\Pi^\star$. Then we have*

$$0 \leq R^\star - R(\pi_\tau^\star) \leq \tau \inf_{\pi \in \Pi^\star} D_{\mathrm{K}}(\pi^\star, \pi_0), \tag{45}$$

where $\inf_{\pi \in \Pi^\star} D_{\mathrm{K}}(\pi, \pi_0) < +\infty$ for $\pi_0 \in \operatorname{int}(\Delta_{\mathcal{A}}^{\mathcal{S}})$.

Proof. For any $\pi^\star \in \Pi^\star$ we have

$$R^\star - \tau D_{\mathrm{K}}(\pi^\star, \pi_0) = R_\tau(\pi^\star) \leq R_\tau(\pi_\tau^\star) \leq R(\pi_\tau^\star).$$

Rearranging and taking the infimum over $\Pi^\star$ yields the claim. □

In the remainder we will improve this sublinear estimate $O(\tau)$ on the suboptimality of the entropy optimal regularized policy $\pi_\tau^\star$ to a linear estimate $\tilde{O}(e^{-\Delta\tau^{-1}})$ and provide a lower bound matching up to a polynomial term. Additionally, we provide convergence of the policies.

A.2. State-action geometry of entropy regularization

Similarly to the state-distributions we define the *state-action distribution* of a policy $\pi \in \Delta_{\mathcal{A}}^{\mathcal{S}}$ via

$$\nu^\pi(s, a) = \nu_\gamma^{\pi,\mu}(s, a) \coloneqq (1 - \gamma) \sum_{t \in \mathbb{N}} \gamma^t \mathbb{P}^{\pi,\mu}(S_t = s, A_t = a). \tag{46}$$

Note that by the geometric series, we have $d^\pi \in \Delta_{\mathcal{S}}$ and $\nu^\pi \in \Delta_{\mathcal{S}\times\mathcal{A}}$ for the state and state-action distribution, respectively, and we have $\nu^\pi(s, a) = d^\pi(s)\pi(a|s)$. The state and state-action distributions are also known as *occupancy measures* or *state frequencies* (**?**). An important property of state-action distributions is given by

$$R(\pi) = r^\top \nu^\pi, \tag{47}$$

which can be seen using the dominated convergence theorem.

Proposition A.4 (State-action polytope, (Derman, 1970))**.** *The set $\mathscr{D} = \{\nu^\pi : \pi \in \Delta_{\mathcal{A}}^{\mathcal{S}}\}$ of state-action distributions forms a polytope given by*

$$\mathscr{D} = \Delta_{\mathcal{S}\times\mathcal{A}} \cap \left\{\nu \in \mathbb{R}^{\mathcal{S}\times\mathcal{A}} : \ell_s(\nu) = 0 \textit{ for all } s \in \mathcal{S}\right\}, \tag{48}$$

where

$$\ell_s(\nu) \coloneqq \sum_{a \in \mathcal{A}} \nu(s, a) - \gamma \sum_{a' \in \mathcal{A}, s' \in \mathcal{S}} P(s|s', a')\nu(s', a') - (1 - \gamma)\mu(s). \tag{49}$$

In particular, the characterization of the state-action distributions of a Markov decision process as a polyope shows that the reward optimization problem is equivalent to the linear program

$$\max r^\top \nu \quad \text{subject to } \nu \in \mathscr{D}. \tag{50}$$

Further, it is well known that for a state-action distribution $\nu \in \mathscr{D}$ a policy $\pi \in \Delta_{\mathcal{A}}^{\mathcal{S}}$ with $\nu^\pi = \nu$ can be computed by conditioning (Kallenberg, 1994; Müller & Montufar, 2022)

$$\pi(a|s) = \nu(a|s) := \begin{cases} \frac{\nu(s,a)}{\sum_{a'} \nu(s,a')} & \text{if } \sum_{a'} \nu(s,a') > 0 \text{ and} \\ \frac{1}{|\mathcal{A}|} & \text{otherwise.} \end{cases} \tag{51}$$

The entropy regularized reward optimization problem admits an interpretation as a regularized version of the linear program (50), where the regularizer is given by the conditional entropy.

Definition A.5 (Conditional entropy and KL)**.** For $\nu \in \mathbb{R}_{>0}^{\mathcal{S}\times\mathcal{A}}$ define the *conditional entropy* via

$$H_{A|S}(\nu) := \sum_{s\in\mathcal{S}, a\in\mathcal{A}} \nu(s,a) \log \nu(a|s) = H(\nu) - H(d), \tag{52}$$

where $d(s) := \sum_{a\in\mathcal{A}} \nu(s,a)$. For $\nu_1, \nu_2 \in \mathbb{R}_{>0}^{\mathcal{S}\times\mathcal{A}}$ we call

$$D_{A|S}(\nu_1, \nu_2) := \sum_{s\in\mathcal{S}, a\in\mathcal{A}} \nu_1(s,a) \log \frac{\nu_1(a|s)}{\nu_2(a|s)} = D_{\mathrm{KL}}(\nu_1, \nu_2) - D_{\mathrm{KL}}(d_1, d_2). \tag{53}$$

the *conditional KL-divergence* between ν_1 and ν_2, where $d_i(s) = \sum_{a\in\mathcal{A}} \nu_i(s,a)$.

Direct computation shows that $D_{A|S}$ is the Bregman divergence induced by $H_{A|S}$, see (Neu et al., 2017, A.1).

Proposition A.6 (State-action geometry of entropic regularization)**.** *It holds that*

$$D_{\mathrm{K}}(\pi_1, \pi_2) = D_{A|S}(\nu^{\pi_1}, \nu^{\pi_2}) \quad \textit{for all } \pi_1, \pi_2 \in \Delta_{\mathcal{A}}^{\mathcal{S}} \tag{54}$$

showing the D_{K} is the pull back of the conditional KL-divergence $D_{A|S}$. In particular, the entropy regularized reward optimization problem is equivalent to the regularized linear program

$$\max r^\top \nu - \tau D_{A|S}(\nu, \nu_0) \quad \textit{subject to } \nu \in \mathscr{D}, \tag{55}$$

where $\nu_0 = \nu^{\pi_0}$, meaning that there is a unique solution $\nu_\tau^\star \in \mathrm{int}(\mathscr{D})$ and therefore a unique solution $\pi_\tau^\star \in \mathrm{int}(\Delta_{\mathcal{A}}^{\mathcal{S}})$ of the regularized problem and we have $\nu^{\pi_\tau^\star} = \nu_\tau^\star$.

Proof. This is a direct consequence of $R_\tau(\pi) = r^\top \nu^\pi - \tau D_{A|S}(\nu, \nu_0)$, see also (Neu et al., 2017). □

We recall an expression of the difference of the rewards of two policies in terms of the advantage function and the state-action distribution that is useful tools in many proofs.

Lemma A.7 (Performance difference)**.** *For any two policies $\pi_1, \pi_2 \in \Delta_{\mathcal{S}}^{\mathcal{A}}$ it holds that*

$$R(\pi_1) - R(\pi_2) = \frac{\langle \nu^{\pi_1}, A^{\pi_2} \rangle_{\mathcal{S}\times\mathcal{A}}}{1-\gamma}. \tag{56}$$

The performance difference lemma is well known in the theory of Markov decision and we refer to (Agarwal et al., 2021, Lemma 2). Additionally, we require the following regularity result for the reward function.

A.3. Regularized linear programs and Hessian gradient flows

We have seen that the state-action distributions of the optimal regularized policies $\pi_\tau^\star$ solve the linear program associated to the Markov decision process with a conditional entropic regularization. Here, we see that the solutions of regularized linear programs solve the gradient flow of the unregularized problem with respect to the Riemannian metric induced by the convex regularizer. Whereas these results are known we provide their proof for the sake of completeness and refer to (Alvarez et al., 2004) for a more general discussion of Hessian gradient flows. We work in the following setting.

Setting A.8. *We consider the linear program*

$$\max c^\top x \quad \textit{subject to } x \in P, \tag{57}$$

with cost $c \in \mathbb{R}^d$ and feasible region $P \subseteq \mathbb{R}^d$. Further, we consider a twice continuously differentiable convex function ϕ defined on a neighborhood of $\operatorname{int}(P)$ and assume that $\nabla^2\phi(x)$ is strictly positive definite on TP for all $x \in \operatorname{int}(P)$. We define the Riemannian Hessian metric $g^\phi(v,w) := v^\top \nabla^2\phi(x) w$ on $\operatorname{int}(P)$ and denote the gradient of f with respect to g^ϕ by $\nabla^\phi f$. By $(x_t)_{t\in[0,T)} \subseteq \operatorname{int}(P)$ we denote a solution of the Hessian gradient flows

$$\partial_t x_t = \nabla^\phi f(x_t) \tag{58}$$

with initial condition $\mu_0 \in \operatorname{int}(P)$ and potential $f(\mu) = c^\top \mu$, where $T \in \mathbb{R}_{\geq 0} \cup \{+\infty\}$. Finally, we denote the Bregman divergence induced by ϕ by D_ϕ.

Note that $(x_t)_{t\in[0,T)} \subseteq \operatorname{int}(P)$ solves the Hessian gradient flow (58) if and only if we have

$$\langle \nabla^2\phi(x_t)\partial_t x_t, v\rangle = \langle \nabla f(x_t), v\rangle \quad \text{for all } v \in TP, t \in [0,T). \tag{59}$$

We can now formualte and prove the equivalence property between Hessian gradient flows of linear programs and solutions of regularized linear programs.

Proposition A.9 (Central path property)**.** *Consider Setting A.8. Then the Hessian gradient flow $(x_t)_{t\geq 0}$ of the linear program is characterized by*

$$x_t = \arg\max \left\{ c^\top x - t^{-1} D_\phi(x, x_0) : x \in P \right\} \quad \textit{for all } t \in (0,T). \tag{60}$$

Proof. Let $\hat{x}_t \in P$ denote the unique maximizer of $g(x) := c^\top x - t^{-1} D_\phi(x, x_0)$ over P for $t > 0$, then surely $\hat{x}_t \in \operatorname{int}(P)$. Thus, $\hat{x}_t$ is uniquely determined by $\langle \nabla g(\hat{x}_t), v\rangle = 0$ for all $v \in TP$. Direct computation yields $\nabla g(x) = c - t^{-1}(\nabla\phi(x) - \nabla\phi(x_0))$ and hence $\hat{x}_t$ is uniquely determined by

$$t\langle c, v\rangle = \langle \nabla\phi(\hat{x}_t) - \nabla\phi(x_0), v\rangle \quad \text{for all } v \in TP.$$

On the other hand, for the gradient flow we can use (59) and compute for $v \in TP$

$$\begin{aligned}
\langle \nabla\phi(x_t) - \nabla\phi(x_0), v\rangle &= \int_0^t \partial_s \langle \nabla\phi(x_s), v\rangle \mathrm{d}s \\
&= \int_0^t \langle \nabla^2\phi(x_s)\partial_s x_s, v\rangle \mathrm{d}s \\
&= \int_0^t \langle \nabla f(x_s) x_s, v\rangle \mathrm{d}s \\
&= \int_0^t \langle c, v\rangle \mathrm{d}s = t\langle c, v\rangle.
\end{aligned}$$

This shows $x_t = \hat{x}_t$ as claimed. □

Corollary A.10 (Sublinear convergence)**.** *Consider Setting A.8 and assume that the linear program (57) admits a solution $x^\star \in P$. Then it holds that*

$$c^\top x^\star - c^\top x_t \leq \frac{D_\phi(x^\star, x_0) - D_\phi(x_t, x_0)}{t} \leq \frac{D_\phi(x^\star, x_0)}{t} \quad \textit{for all } t \in [0,T). \tag{61}$$

Proof. By the central path property, we have

$$c^\top x_t - t^{-1} D_\phi(x_t, x_0) \geq c^\top x^\star - t^{-1} D_\phi(x^\star, x_0).$$

Rearranging yields the result. □

Corollary A.11 (Implicit bias of Hessian gradient flows of LPs)**.** *Consider Setting A.8 and denote the face of maximizers of the linear program (57) by $F^\star$. Then it holds that*

$$\lim_{t\to+\infty} x_t = x^\star = \arg\min_{x\in F^\star} D_\phi(x, x_0). \tag{62}$$

In words, the Hessian gradient flow converges to the Bregman projection of x_0 to $F^\star$.

Proof. By compactness of P, the sequence $(x_{t_n})_{n\in\mathbb{N}}$ has at least one accumulation point for any sequence $t_n \to +\infty$. Hence, we can assume without loss of generality that $x_{t_n} \to \hat{x}$ and it remains to identify $\hat{x}$ as the information projection $x^\star \in F^\star$.

Surely, we have $\hat{x} \in F^\star$ as $c^\top \hat{x} = \lim_{n\to\infty} c^\top x_{t_n} = \max_{x\in P} c^\top x$ by Corollary A.10. Further, by the central path property we have for any optimizer $x' \in F^\star$ that

$$c^\top x_t - t^{-1} D_\phi(x_t, x_0) \geq c^\top \hat{x} - t^{-1} D_\phi(x', x_0)$$

and therefore

$$D_\phi(x', x_0) - D_\phi(x_t, x_0) \geq t c^\top (x' - x_t) \geq 0.$$

Hence, we have

$$D_\phi(\hat{x}, x_0) = \lim_{n\to\infty} D_\phi(x_{t_n}, x_0) \leq D_\phi(x', x_0)$$

and can conclude by minimizing over $x' \in F^\star$. □

B. Geometry and Sublinear Convergence of Kakade Gradient Flows

It is our goal to study the solutions $\pi^\star_\tau$ of the entropy regularized reward R_τ. For linear programs we have seen in Appendix A.3 that the solutions of the regularized problems solve the corresponding Hessian gradient flow. Recall, that the entropy regularized reward optimization problem is equivalent to a linear program in state-action space with a conditional KL regularization. Hence, the state-action distributions solve a Hessian gradient flow and hence the policies $\pi^\star_{t^{-1}}$ solve a gradient flow with respect to some metric. In this section we study this Riemannian metric on the space of policies and provide an explicit expression of the gradient dynamics.

B.1. The Kakade metric and policy gradient theorems

We first introduce the Riemannian metric on the policy space that was proposed in the context of natural gradients (Kakade, 2001).

Definition B.1 (Kakade metric)**.** We call the Riemannian metric g^{K} on $\mathrm{int}(\Delta^{\mathcal{S}}_{\mathcal{A}})$ defined by

$$g^{\mathrm{K}}_\pi(v, w) \coloneqq \sum_{s\in\mathcal{S}} d^\pi(s) \sum_{a\in\mathcal{A}} \frac{v(s,a)w(s,a)}{\pi(a|s)} = \mathbb{E}_{\nu^\pi}\left[\frac{v(s,a)}{\pi(a|s)} \cdot \frac{w(s,a)}{\pi(a|s)}\right] \tag{63}$$

for all $v, w \in T\Delta^{\mathcal{S}}_{\mathcal{A}}$ the *Kakade metric*. We denote the induced norm by $\|v\|_{g^{\mathrm{K}}_\pi} \coloneqq g^{\mathrm{K}}_\pi(v,v)^{\frac{1}{2}}$ and for a differentiable function $f\colon \Delta^{\mathcal{S}}_{\mathcal{A}} \to \mathbb{R}$ we denote the corresponding Riemannian gradient by $\nabla^{\mathrm{K}} f(\pi)$.

The Kakade metric has been referred to as the Fisher-Rao metric on $\Delta^{\mathcal{S}}_{\mathcal{A}}$ as this reduces to the Fisher-Rao metric if $|\mathcal{S}| = 1$, see (Kerimkulov et al., 2023). We choose the name Kakade metric here, as there exist multiple extensions of the Fisher-Rao metric to products of simplicies: product metric, i.e., sum of the metrics over the individual factors, or other positive weightings of the metrics of the individual factors, see (Montúfar et al., 2014) for an in-depth discussion of different choices and their invariance properties. Further, the choice of Kakade has been described as the limit of weighted Fisher-Rao metrics on the finite-hoirzon path spaces (Bagnell & Schneider, 2003; Peters et al., 2003). For example in a game-theoretic context, when considering independently chosen strategies of the players, it might be more natural to work with the product metric, i.e., the sum of the Fisher-Rao metrics over the individual factors; this corresponds to the pullback of the Fisher-Rao metric on the simplex of joint distributions under the independence model (Montúfar et al., 2014; Boll et al., 2024). Note that

although the Kakade metric closely connected to the weighted entropy H_{K}, it is not the Hessian metric of H_{K}, in fact, it is not a Hessian metric at all (Müller & Montúfar, 2024, Remark 13).

In general, the Kakade metric is only a pseudo-metric and the following assumption ensures that g^{K} defines a Riemannian metric and we make it for the remainder of our analysis.

Assumption B.2 (State exploration). For any policy $\pi \in \operatorname{int}(\Delta_{\mathcal{A}}^{\mathcal{S}})$ the discounted state distribution is positive, meaning that $d^{\pi}(s) > 0$ for all $s \in \mathcal{S}$.

Kakade gradient flows are well-posed, i.e., admit a unique solution $(\pi_t)_{t\in\mathbb{R}_{\geq 0}}$, both in the unregularized case (Alvarez et al., 2004; Müller & Montúfar, 2024) and the regularized case (Müller, 2023).

The *policy gradient theorem* states that

$$\partial_{\theta_i} R(\pi) = \sum_{s\in\mathcal{S}} d^{\pi_\theta}(s) \sum_{a\in\mathcal{A}} \partial_{\theta_i} \pi_\theta(a|s) A^{\pi_\theta}(s,a) \tag{64}$$

and therefore describes the gradient of the reward via the advantage function (Sutton et al., 1999; Agarwal et al., 2021). Inspired by this, we provide an explicit formula for the gradient of the reward with respect to the Kakade metric.

Theorem B.3 (Gradient with respect to the Kakade metric)**.** *Let Assumption B.2 hold. Then for all $\pi \in \operatorname{int}(\Delta_{\mathcal{A}}^{\mathcal{S}})$ and $a \in \mathcal{A}$, $s \in \mathcal{S}$ it holds that*

$$\nabla^{\mathrm{K}} R(\pi)(s,a) = A^{\pi}(s,a)\pi(a|s). \tag{65}$$

In the proof, we use the following auxiliary result.

Lemma B.4 (Derivatives of state-action distributions, (Müller & Montufar, 2022))**.** *It holds that*

$$\frac{\partial \nu^{\pi}}{\partial \pi(a|s)} = d^{\pi}(s)(I - \gamma P_{\pi}^{T})^{-1} e_{(s,a)}, \tag{66}$$

where $P_{\pi} \in \Delta_{\mathcal{S}\times\mathcal{A}}^{\mathcal{S}\times\mathcal{A}}$ is given by $P_{\pi}(s',a'|s,a) = \pi(a'|s')P(s'|s,a)$.

Proof of Theorem B.3. First, note that $A^{\pi} \odot \pi \in T\Delta_{\mathcal{A}}^{\mathcal{S}}$ where $(A^{\pi} \odot \pi)(s,a) = A^{\pi}(s,a)\pi(a|s)$ and that R and g^{K} can be extended to a neighborhood of $\Delta_{\mathcal{A}}^{\mathcal{S}}$. It suffices to show

$$g_{\pi}^{\mathrm{K}}(A^{\pi} \odot \pi, v) = \partial_v R(\pi) \quad \text{for all } v \in T\Delta_{\mathcal{A}}^{\mathcal{S}}.$$

Since $R(\pi) = r^{\top}\nu^{\pi}$, we have $\frac{\partial R(\pi)}{\partial \pi(a|s)} = r^{\top}\frac{\partial \nu^{\pi}}{\partial \pi(a|s)}$. For any tangent vector $v \in T\Delta_{\mathcal{A}}^{\mathcal{S}}$ we can use Lemma B.4 to compute

$$\begin{aligned}
\partial_v R(\pi) &= \sum_{s\in\mathcal{S},a\in\mathcal{A}} v(s,a)\frac{\partial R(\pi)}{\partial \pi(a|s)} \\
&= \sum_{s\in\mathcal{S},a\in\mathcal{A}} d^{\pi}(s)v(s,a)\left\langle (I-\gamma P_{\pi}^{T})^{-1}e_{(s,a)}, r\right\rangle \\
&= \sum_{s\in\mathcal{S},a\in\mathcal{A}} d^{\pi}(s)v(s,a)\left\langle e_{(s,a)}, (I-\gamma P_{\pi})^{-1}r\right\rangle \\
&= \sum_{s\in\mathcal{S},a\in\mathcal{A}} d^{\pi}(s)v(s,a)\left\langle e_{(s,a)}, Q^{\pi}\right\rangle \\
&= \sum_{s\in\mathcal{S},a\in\mathcal{A}} d^{\pi}(s)v(s,a)Q^{\pi}(s,a) \\
&= \sum_{s\in\mathcal{S},a\in\mathcal{A}} d^{\pi}(s)v(s,a)(Q^{\pi}(s,a) - V^{\pi}(s)) \\
&= g_{\pi}^{\mathrm{K}}(A^{\pi} \odot \pi, v),
\end{aligned}$$

where we have used the Bellman equation $(I-\gamma P_{\pi})^{-1}r = Q^{\pi}$ as well as $\sum_{a\in\mathcal{A}} v(s,a) = 0$. □

Note that the gradient of the reward with respect to the Kakade metric is independent of the initial distribution $\mu \in \Delta_{\mathcal{S}}$ both for the regularized and the unregularized reward.

We have seen that the gradient of the reward function R with respect to the Kakade metric admits an explicit form, see Theorem B.3. This will allow us to provide essentially sharp rates for the corresponding gradient flow.

Definition B.5 (Kakade gradient flow)**.** We call the gradient flow

$$\partial_t \pi_t = \nabla^{\mathrm{K}} R_\tau(\pi_t) \tag{67}$$

the *Kakade gradient flow*. By Theorem B.3, the unregularized Kakade gradient flow satisfies

$$\partial_t \pi_t(a|s) = A^{\pi_t}(s,a)\pi_t(a|s). \tag{68}$$

B.2. State-action geometry of Kakade gradient flows

It is our goal to use tools from Hessian gradient flows, but the Kakade metric is not a Hessian metric. However, it was shown that the policy polytope $\Delta_{\mathcal{A}}^{\mathcal{S}}$ endowed with the Kakade metric is isometric to the state-action polytope with endowed with the Hessian metric induced by the conditional entropy (Müller & Montúfar, 2024). This allow us to borrow from the results on Hessian gradient flows.

Definition B.6 (Conditional Fisher-Rao metric)**.** We call the metric $g^{A|S}$ on $\mathrm{int}(\mathscr{D})$ given by

$$g_d^{A|S}(v,w) \coloneqq v^\top \nabla^2 H_{A|S}(d) w \quad \text{for } v,w \in T\mathscr{D} \tag{69}$$

the *conditional Fisher-Rao metric* and the denote the corresponding gradient by $\nabla^{A|S}$.

It is elementary to check the convexity of $H_{A|S}$ on $\mathbb{R}_{>0}^{\mathcal{A}\times\mathcal{S}}$, but it also easily seen that $\nabla^2 H_{A|S}$ has zero eigenvalues. However, it can be shown that $\nabla^2 H_{A|S}$ is strictly definite on $T\mathscr{D}$ and therefore induces a Riemannian metric on $\mathrm{int}(\mathscr{D})$, see (Müller & Montúfar, 2024).

The following result relates the Kakade metric and Kakade divergence to the Hessian metric and Bregman divergence of the conditional entropy $H_{A|S}$.

Theorem B.7 (State-action geometry of the Kakade metric, (Müller & Montúfar, 2024))**.** *Consider a finite Markov decision process and let Assumption B.2 hold. Then the mapping*

$$\begin{aligned} \Psi\colon (\mathrm{int}(\Delta_{\mathcal{A}}^{\mathcal{S}}), g^{\mathrm{K}}) &\to (\mathrm{int}(\mathscr{D}), g^{A|S}) \\ \pi &\mapsto \nu^\pi \\ \nu(\cdot|\cdot) &\leftarrow\!\shortmid \nu \end{aligned} \tag{70}$$

between policies and state-action distributions is an isometry.

As isometries map gradient flows to gradient flows, Theorem B.7 implies that $(\pi_t)_{t\geq 0}$ solves the Kakade gradient flow $\partial_t R(\pi_t) = \nabla^{\mathrm{K}} R(\pi_t)$ if and only if $(\nu_t)_{t\geq 0} = (\nu^{\pi_t})_{t\geq 0}$ solves the conditional Fisher-Rao gradient flow $\partial_t \nu_t = \nabla^{A|S} f(\nu_t)$ if the following diagram commutes

$$\begin{tikzcd} \Delta_{\mathcal{A}}^{\mathcal{S}} \arrow[r, "\Psi"] \arrow[dr, "R"'] & \mathscr{D} \arrow[d, "f"] \\ & \mathbb{R} \end{tikzcd}, \quad \text{where} \quad \begin{tikzcd} \pi \arrow[r, mapsto] \arrow[dr, mapsto] & \nu^\pi \arrow[d, mapsto] \\ & R(\pi). \end{tikzcd} \tag{71}$$

The isometry property allows us to transfer the theory on Hessian gradient flows of linear programs to Kakade gradient flows despite the Kakade metric not being Hessian.

Corollary B.8 (Implications from Hessian gradient flows)**.** *Let Assumption B.2 hold, denote the set of optimal policies by* $\Pi^\star \coloneqq \{\pi \in \Delta_{\mathcal{A}}^{\mathcal{S}} : R(\pi) = R^\star\}$*, and fix an initial policy* $\pi_0 \in \mathrm{int}(\Delta_{\mathcal{A}}^{\mathcal{S}})$*. Then the following statements hold:*

1. Well-posedness: *The Kakade gradient flow* (67) *admits a unique global solution* $(\pi_t)_{t\geq 0}$.

2. Central path property: *For all $t \geq 0$ it holds that*

$$\pi_t = \operatorname*{arg\,max}_{\pi \in \Delta_{\mathcal{A}}^{\mathcal{S}}} \Big\{ R(\pi) - t^{-1} D_{\mathrm{K}}(\pi, \pi_0) \Big\}. \tag{72}$$

3. Sublinear convergence: *For all $t \geq 0$ we have*

$$0 \leq R^\star - R(\pi_t) \leq \frac{\min_{\pi^\star \in \Pi^\star} D_{\mathrm{K}}(\pi^\star, \pi_0) - D_{\mathrm{K}}(\pi_t, \pi_0)}{t} \leq \frac{\min_{\pi^\star \in \Pi^\star} D_{\mathrm{K}}(\pi^\star, \pi_0)}{t}. \tag{73}$$

4. Implicit bias: *The gradient flow $(\pi_t)_{t \geq 0}$ convergence and it holds that*

$$\lim_{t \to +\infty} \pi_t = \pi^\star = \operatorname*{arg\,min}_{\pi \in \Pi^\star} D_{\mathrm{K}}(\pi, \pi_0). \tag{74}$$

Proof. First, note that both 2 and 3 hold on the maximal existence interval $[0, T_\infty)$ of the gradient flow, which is a direct consequence of Appendix A.3 and Theorem B.7. Further, 4 follows from Appendix A.3 and Theorem B.7 if $T_\infty = +\infty$, hence, it remains to show well posedness.

The well-posedness of the conditional Fisher-Rao gradient flow of linear programs has been established in (Müller, 2023), which can be carried over to the Kakade gradient flow using the isometry. Here, we offer a different proof that utilizes the central path property of the Kakade gradient flow. The local well-posedness of the gradient flow follows from the Picard-Lindelöf theorem and it remains to show that $T_\infty := \inf\{t > 0 : \inf_{s \in [0,t)} \operatorname{dist}(\pi_s, \partial \Delta_{\mathcal{A}}^{\mathcal{S}}) = 0\} = +\infty$. Assume that $T < +\infty$, then it is elementary to check that $\pi_t \to \pi_T$ for $t \nearrow T$, where π_T solves the entropy regularized problem with strength $\tau = T^{-1}$. Note that $\pi_T \in \operatorname{int}(\Delta_{\mathcal{A}}^{\mathcal{S}})$ contradicting $\inf_{t \in [0,T]} \operatorname{dist}(\pi_t, \partial \Delta_{\mathcal{A}}^{\mathcal{S}}) = 0$. □

Remark B.9 (Implicit and algorithmic bias). In the case of multiple optimal policies the Kakade gradient flow will converge towards the Kakade projection of the initial policy to the set of optimal policies. The selection of gradient schemes of a particular optimizer in the case of multiple optima is commoly referred to as the *implicit* or *algorithmic bias* of the method. In the context of reinforcement learning the implicit bias was studied for discrete time natural policy gradient and policy mirror descent methods. First, for a natural actor-critic scheme in linear Markov decision processes the Kakade divergence of the optimization trajectory $(\pi_k)_{k \in \mathbb{N}}$ to the maximum entropy policy $\pi^\star$ is bounded by $D_{\mathrm{K}}(\pi^\star, \pi_k) \leq \log k + (1-\gamma)^{-2}$ (Hu et al., 2021). This control on the Bregman divergence to the maximum entropy policy ensures that the probabily of selecting an optimal action $a \in A_s^\star$ decays at most like $\pi_k(a|s) \geq ck^{-1}$, but fails to identify the limiting policy.

On the other hand,policy mirror descent scheme with decaying entropy regularization strength τ_k was studied in (Li et al., 2023). Here, it is shown that for several choices of regularization strengths and stepsizes the resulting policies π_k converge to the maximum entropy optimal policy thereby characterizing the algorithmic bias of this approach. Whereas this analysis is able to characterize the limit of the optimization scheme it utilizes decaying explicit regularization.

In contrast, our implicit bias result works in continuous time and utilizes the correspondence between the gradient flows and regularized problems. This allows us to show convergence towards the (generalized) maximum entropy optimal policies without relying on explicit regularization.

We built on the correspondence between the solutions of entropy-regularized problems and Kakade gradient flows of unregularized problems in our analysis in multiple ways. First, this lets us transfer the sublinear estimate on the entropy regularization error. More importantly, this allows us to study the gradient flows, which we can do to provide a linear convergence result for both the gradient flow as well as the entropy regularization error.

Proposition B.10 (Sublinear convergence of value functions)**.** *Let Assumption B.2 hold, denote the set of optimal policies by $\Pi^\star := \{\pi \in \Delta_{\mathcal{A}}^{\mathcal{S}} : R(\pi) = R^\star\}$, and fix an initial policy $\pi_0 \in \Delta_{\mathcal{A}}^{\mathcal{S}}$ and denote the generalized maximum entropy optimal policy by $\pi^\star = \arg\min_{\pi \in \Pi^\star} D_{\mathrm{K}}(\pi, \pi_0)$. Then for all $t \geq 0$ it holds that*

$$0 \leq V^\star(s) - V^{\pi_t}(s) \leq \frac{D_{\mathrm{K}}(\pi^\star, \pi_0)}{t} \quad \textit{for all } s \in \mathcal{S}. \tag{75}$$

In particular, it holds that

$$\frac{\gamma \cdot D_{\mathrm{K}}(\pi^\star, \pi_0)}{t} \leq A^\star(s,a) - A^{\pi_t}(s,a) \leq \frac{D_{\mathrm{K}}(\pi^\star, \pi_0)}{t} \quad \textit{for all } s \in \mathcal{S}, a \in \mathcal{A}. \tag{76}$$

Proof. Let us fix $s \in \mathcal{S}$. By Theorem B.3 the Kakade gradient flow $(\pi_t)_{t\geq 0}$ is independent of the initial distribution μ, as long as it has full support. Let us pick some μ_n with full support and $\mu_n \to \nu_s$, then $R^{\mu_n}(\pi) \to V^\pi(s)$ for any π. By Corollary A.10 we have

$$0 \leq (R^{\mu_n})^\star - R^{\mu_n}(\pi_t) \leq \frac{D_{\mathrm{K}}(\pi^\star, \pi_0)}{t} \quad \text{for all } t \geq 0, n \in \mathbb{N},$$

which yields (75) for $n \to +\infty$. We use this to estimate

$$\begin{aligned} Q^\star(s,a) - Q^{\pi_t}(s,a) &= r(s,a) + \gamma \sum_{s'} V^\star(s') P(s'|s,a) - r(s,a) - \gamma \sum_{s'} V^{\pi_t}(s') P(s'|s,a) \\ &= \gamma \sum_{s'} (V^\star(s') - V^{\pi_t}(s')) P(s'|s,a) \\ &\leq \frac{\gamma D_{\mathrm{K}}(\pi^\star, \pi_0)}{t}. \end{aligned}$$

In particular, this implies

$$A^{\pi_t}(s,a) - A^\star(s,a) = V^\star(s) - V^{\pi_t}(s) + Q^{\pi_t}(s,a) - Q^\star(s,a) \leq V^\star(s) - V^{\pi_t}(s) \leq \frac{D_{\mathrm{K}}(\pi^\star, \pi_0)}{t}$$

and similarly

$$A^{\pi_t}(s,a) - A^\star(s,a) \geq Q^{\pi_t}(s,a) - Q^\star(s,a) \geq -\frac{\gamma D_{\mathrm{K}}(\pi^\star, \pi_0)}{t}.$$

□

C. Essentially Sharp Analysis of Entropy Regularization

We now improve the sublinear convergence rates and provide essentially matching upper and lower bounds showing exponential convergence in terms of value and of the the policies when measured in the Kakade divergence. To this end we work with the interpretation of the solutions of the regularized problems as solutions of the Kakade gradient flow and employ the explicit expression (68) and the sublinear convergence guarantee from Proposition B.10 to establish a linear convergence result for Kakade gradient flows. We complement this with a lower bound that matches the upper bound up to a polynomial factor. We work in the following setting.

Setting C.1. *Consider a finite discounted Markov decision process $(\mathcal{S}, \mathcal{A}, P, \gamma, r)$, an initial distribution $\mu \in \Delta_{\mathcal{S}}$ and fix a policy $\pi_0 \in \mathrm{int}(\Delta_{\mathcal{A}}^{\mathcal{S}})$ and let Assumption B.2 hold and denote the optimal reward by $R^\star := \max\{R(\pi) : \pi \in \Delta_{\mathcal{A}}^{\mathcal{S}}\}$. Further, let $(\pi_t)_{t\geq 0}$ be the unique global solution of the Kakade policy gradient flow (67) or equivalently the solutions of the entropy regularized problems*

$$\pi_t = \operatorname*{arg\,max}_{\pi \in \Delta_{\mathcal{A}}^{\mathcal{S}}} \Big\{ R(\pi) - t^{-1} D_{\mathrm{K}}(\pi, \pi_0) \Big\}. \tag{77}$$

We denote the generalized maximum entropy optimal policy $\pi^\star = \arg\min_{\pi \in \Pi^\star} D_{\mathrm{K}}(\pi, \pi_0)$ by, where $\Pi^\star := \{\pi \in \Delta_{\mathcal{A}}^{\mathcal{S}} : R(\pi) = R^\star\}$ denotes the set of optimal policies and set $c := D_{\mathrm{K}}(\pi^\star, \pi_0)$. Finally, we set

$$\Delta := -\max\left\{A^\star(s,a) : A^\star(s,a) \neq 0, s \in \mathcal{S}, a \in \mathcal{A}\right\}. \tag{78}$$

Note that $\Delta > 0$ unless every action is optimal in every state. We can interpret Δ as the minimal suboptimality of a suboptimal action under $A^\star$.

C.1. Convergence in value

The above result ensures that the probability $\pi_t(a|s)$ of selecting a suboptimal action a decays exponentially which implies exponential convergence of the reward $R(\pi_t)$ achieved by the policies.

Theorem C.2 (Convergence in value)**.** *Consider Setting C.1. For any $t \geq 1$ it holds that*

$$\frac{\Delta \cdot \min_{s\in\mathcal{S}} d^{\pi_t}(s) \sum_{a \notin A_s^\star} \pi_0(a|s)}{1-\gamma} \cdot e^{-\Delta(t-1) - c\log t - 2\|r\|_\infty} \leq R^\star - R(\pi_t) \leq \frac{2\|r\|_\infty}{1-\gamma} \cdot e^{-\Delta(t-1) + \gamma c \log t}. \tag{79}$$

Note that the coefficient of the lower bound depends on t. However, the coefficient does not become arbitrarily small as $\min_s d^{\pi_t}(s) \to \min_s d^\star(s) > 0$ for $t \to +\infty$. Further, the policies $(\pi_t)_{t\geq 0}$ do not depend on μ, where d^{π_t} does. If we choose μ to be the uniform distribution, then $d^\pi(s) \geq (1-\gamma)|\mathcal{S}|^{-1}$, which yields a lower bound of

$$R^\star - R(\pi_t) \geq \frac{\Delta \cdot \sum_{a \notin A_s^\star} \pi_0(a|s)}{|\mathcal{S}|} \cdot e^{-\Delta(t-1)-\gamma c \log t - 2\|r\|_\infty},$$

where the coefficient is independent of t.

We combine the explicit expression (68) as well as the sublinear convergence of the advantage function towards the optimal advantage function $A^\star$ to bound the individual entries of the policies along the gradient flow trajectory.

Lemma C.3. *Consider Setting C.1. Then for all $t \geq t_0 > 0$, $s \in \mathcal{S}$, and $a \in \mathcal{A}$ it holds that*

$$\pi_{t_0}(a|s) e^{A^\star(s,a)(t-t_0) - c\log(\frac{t}{t_0})} \leq \pi_t(a|s) \leq \pi_{t_0}(a|s) e^{A^\star(s,a)(t-t_0)+\gamma c \log(\frac{t}{t_0})} \tag{80}$$

and and further for $t \geq 1$ it holds that

$$\pi_0(a|s) e^{A^\star(s,a)(t-1) - c\log t - 2\|r\|_\infty} \leq \pi_t(a|s) \leq \pi_0(a|s) e^{A^\star(s,a)(t-1)+\gamma c \log t + 2\|r\|_\infty}. \tag{81}$$

Proof. As the policies $(\pi_t)_{t\geq 0}$ solve the Kakade policy gradient flow in $\Delta_{\mathcal{A}}^{\mathcal{S}}$ we have

$$\partial_t \pi_t(a|s) = A^{\pi_t}(s,a)\pi_t(a|s). \tag{82}$$

By Proposition B.10 it holds that

$$\left(A^\star(s,a) - \frac{c}{t}\right)\pi_t(a|s) \leq \partial_t \pi_t(a|s) \leq \left(A^\star(s,a) + \frac{\gamma c}{t}\right)\pi_t(a|s),$$

where $c = D(\pi^\star, \pi_0)$. Now, Grönwall's inequality yields

$$\pi_T(a|s) \leq \pi_{t_0}(a|s) \exp\left(A^\star(s,a)(T-t_0) + \gamma c \int_{t_0}^T t^{-1} \mathrm{d}t\right) = \pi_{t_0}(a|s) e^{A^\star(s,a)(T-t_0)+\gamma c \log T - \gamma c \log t_0}$$

as well as

$$\pi_T(a|s) \geq \pi_{t_0}(a|s) \exp\left(A^\star(s,a)(T-t_0) - c \int_{t_0}^T t^{-1} \mathrm{d}t\right) = \pi_{t_0}(a|s) e^{A^\star(s,a)(T-t_0) - c \log T + c \log t_0}.$$

Further, note that $\|A^\pi\|_\infty \leq \|Q^\pi\|_\infty + \|V^\pi\|_\infty \leq 2\|r\|_\infty$ and hence Grönwall yields

$$\pi_0(a|s) e^{-2\|r\|_\infty t_0} \leq \pi_{t_0}(a|s) \leq \pi_0(a|s) e^{2\|r\|_\infty t_0}$$

and choosing $t_0 = 1$ finishes the proof. □

Lemma C.4 (Sub-optimality gap)**.** *Consider a discrete discounted Markov decision process. Then for any policy $\pi \in \Delta_{\mathcal{A}}^{\mathcal{S}}$ it holds that*

$$\frac{\Delta}{1-\gamma} \cdot \sum_{s\in\mathcal{S}, a\notin A_s^\star} d^\pi(s)\pi(a|s) \leq R^\star - R(\pi) \leq \frac{2\|r\|_\infty}{1-\gamma} \sum_{s\in\mathcal{S}, a\notin A_s^\star} d^\pi(s)\pi(a|s). \tag{83}$$

Proof. By the performance difference Lemma A.7, we have

$$(1-\gamma)(R^\star - R(\pi)) = -\sum_{s\in\mathcal{S}, a\notin A_s^\star} d^\pi(s)\pi(a|s)A^\star(s,a) \leq \|A^\star\|_\infty \sum_{s\in\mathcal{S}, a\notin A_s^\star} d^\pi(s)\pi(a|s)$$

Further, note that $|A^\star(s,a)| \leq |Q^\star(s,a)| + |V^\star(s)| \leq 2\|r\|_\infty$. The lower bound follows with an analog argument as

$$(1-\gamma)(R^\star - R(\pi)) = -\sum_{s,a} d^\pi(s)\pi(a|s)A^\star(s,a) \geq \Delta \sum_{s,a} d^\pi(s)\pi(a|s).$$

□

Proof of Theorem C.2. We use Lemma C.4 together with Lemma C.3 and estimate

$$\sum_{s\in\mathcal{S},a\notin A_s^\star} d^{\pi_t}(s)\pi_t(a|s) \leq \sum_{s\in\mathcal{S},a\notin A_s^\star} d^{\pi_t}(s)\pi_1(a|s)e^{-\Delta(t-1)+\gamma c\log t} \leq e^{-\Delta(t-1)+\gamma c\log t}.$$

For the lower bound, we fix $s_0 \in \mathcal{S}$ and $a_0 \in \mathcal{A}$ with $A^\star(s,a) = -\Delta$ and estimate

$$\begin{aligned}\sum_{s\in\mathcal{S},a\notin A_s^\star} d^{\pi_t}(s)\pi_t(a|s) &\geq \sum_{s\in\mathcal{S},a\notin A_s^\star} d^{\pi_t}(s)\pi_0(a|s)e^{A^\star(s,a)(t-1)-c\log t-2\|r\|_\infty} \\ &\geq d^{\pi_t}(s_0)\sum_{a\notin A_{s_0}^\star}\pi_0(a|s_0)e^{-\Delta(t-1)-c\log t-2\|r\|_\infty} \\ &\geq \min_{s\in\mathcal{S}}\left\{d^{\pi_t}(s)\sum_{a\notin A_s^\star}\pi_0(a|s)\right\}\cdot e^{-\Delta(t-1)-c\log t-2\|r\|_\infty}\end{aligned}$$

□

C.2. Convergence of policies

Having studied the decay of the suboptimality gap $R^\star - R(\pi_t)$, we now give sharp bounds for convergence of the policies measured in the Kakade divergence.

Theorem C.5 (Convergence of policies)**.** *Consider Setting C.1. It holds that*

$$\min_{s\in\mathcal{S},a\notin A_s^\star} d^\star(s)\pi_0(a|s)\cdot e^{-\Delta(t-1)-c\log t-2\|r\|_\infty} \leq D_{\mathrm{K}}(\pi^\star,\pi_t) \leq \frac{e^{-\Delta(t-1)+\gamma c\log t}}{1-e^{-\Delta(t-1)+\gamma c\log t}}, \tag{84}$$

where the upper bound holds if $e^{-\Delta(t-1)+\gamma c\log t} < 1$ which is satisfied for $t > 0$ large enough.

Note that the denominator of the upper bound converges to 1 for $t \to +\infty$. We will use the following auxiliary result in the proof of Theorem C.5.

Lemma C.6. *Consider a finite set $\mathcal{X}$ and the face $F \coloneqq \{\mu \in \Delta_{\mathcal{X}} : \mu_x = 0 \text{ for all } x \notin X\}$ of the simplex $\Delta_{\mathcal{X}}$ for some $X \subseteq \mathcal{X}$. Then*

$$\min_{\mu\in F} D_{\mathrm{KL}}(\mu,\nu) = -\log\left(\sum_{x\in X}\nu_x\right). \tag{85}$$

In particular, for any $\mu,\nu \in \Delta_{\mathcal{X}}$ we have

$$D_{\mathrm{KL}}(\mu,\nu) \geq -\log\left(\sum_{x\in\mathrm{supp}(\mu)}\nu_x\right). \tag{86}$$

Proof. We set $g(\mu) \coloneqq D_{\mathrm{KL}}(\mu,\nu)$ and consider the information projection $\hat{\nu} = \arg\min_{\mu\in F} D_{\mathrm{KL}}(\mu,\nu)$ of $\nu \in \Delta_{\mathcal{X}}$ onto F, which is characterized by $v^\top\nabla g(\hat{\nu}) = 0$ for all $v \in TF = \mathrm{span}\{\nu_{x_1} - \nu_{x_2} : x_1, x_2 \in X\}$. As $\partial_x g(\mu) = \log(\frac{\mu_x}{\nu_x}) + 1$ this is equivalent to

$$\log\left(\frac{\hat{\nu}_{x_1}}{\nu_{x_1}}\right) = \log\left(\frac{\hat{\nu}_{x_2}}{\nu_{x_2}}\right) \quad \text{for all } x_1, x_2 \in X.$$

This implies $\frac{\hat{\nu}_x}{\hat{\nu}_x}$ is constant for $x \in X$ and hence we obtain

$$\hat{\nu}_x = \begin{cases}\frac{\nu_x}{\sum_{x'\in X}\nu_{x'}} & \text{for } x \in X \\ 0 & \text{for } x \notin X.\end{cases}$$

Setting $c^{-1} := \sum_{x\in X} \nu_x$ we obtain

$$\min_{\mu\in F} D_{\mathrm{KL}}(\mu,\nu) = D_{\mathrm{KL}}(\hat{\nu},\nu) = \sum_{x\in X} c\nu_x \log\left(\frac{c\nu_x}{\nu_x}\right) = \log c.$$

To show (86), we choose $X := \mathrm{supp}(\mu)$ and use $D_{\mathrm{KL}}(\mu,\nu) \geq \min_{\xi\in F} D_{\mathrm{KL}}(\xi,\nu)$. □

Lemma C.7. *Consider a finite MDP and let $\pi^\star \in \Pi^\star$ be the Kakade projection of $\pi \in \mathrm{int}(\Delta_{\mathcal{A}}^{\mathcal{S}})$ onto the set of optimal policies $\Pi^\star$. Then it holds that*

$$\sum_{s\in\mathcal{S}} d^\star(s) \sum_{a\notin A_s^\star} \pi(a|s) \leq D_{\mathrm{K}}(\pi^\star,\pi) \leq \frac{\max_{s\in\mathcal{S}} \sum_{a\notin A_s^\star} \pi(a|s)}{1-\max_{s\in\mathcal{S}} \sum_{a\notin A_s^\star} \pi(a|s)} \tag{87}$$

Proof. We first prove the upper bound. To this end, we consider the state-wise information projection

$$\hat{\pi}(\cdot|s) = \arg\min\left\{D_{\mathrm{KL}}(\mu,\pi(\cdot|s)) : \mu\in\Delta_{\mathcal{A}}, \mathrm{supp}(\mu)\subseteq A_s^\star\right\}$$

of the policy π_t to the set of optimal policies. By concavity we have $-\log(1-h) \leq \frac{h}{1-h}$ for $h<1$ and using Lemma C.6 we estimate

$$\begin{aligned}
D_{\mathrm{K}}(\pi^\star,\pi) &\leq D_{\mathrm{K}}(\hat{\pi},\pi) \\
&= -\sum_{s\in\mathcal{S}} d^{\hat{\pi}}(s) D_{\mathrm{KL}}(\hat{\pi}(\cdot|s),\pi_t(\cdot|s)) \\
&= -\sum_{s\in\mathcal{S}} d^{\hat{\pi}}(s) \log\left(\sum_{a\in A_s^\star} \pi(a|s)\right) \\
&= -\sum_{s\in\mathcal{S}} d^{\hat{\pi}}(s) \log\left(1-\sum_{a\notin A_s^\star} \pi(a|s)\right) \\
&\leq \sum_{s\in\mathcal{S}} d^{\hat{\pi}}(s) \cdot \frac{\sum_{a\notin A_s^\star} \pi(a|s)}{1-\sum_{a\notin A_s^\star} \pi(a|s)}. \\
&\leq \sum_{s\in\mathcal{S}} d^{\hat{\pi}}(s) \cdot \frac{\max_{s'\in\mathcal{S}} \sum_{a\notin A_{s'}^\star} \pi(a|s')}{1-\max_{s'\in\mathcal{S}} \sum_{a\notin A_{s'}^\star} \pi(a|s')}. \\
&= \frac{\max_{s\in\mathcal{S}} \sum_{a\notin A_s^\star} \pi(a|s)}{1-\max_{s\in\mathcal{S}} \sum_{a\notin A_s^\star} \pi(a|s)}.
\end{aligned}$$

Similar to the upper bound, we use $-\log(1-h) \geq -\log'(1)\cdot(-h) = h$ for $h<1$ and Lemma C.6 to estimate

$$\begin{aligned}
D_{\mathrm{K}}(\pi^\star,\pi) &= \sum_{s\in\mathcal{S}} d^\star(s) D_{\mathrm{KL}}(\pi^\star(\cdot|s),\pi(\cdot|s)) \\
&\geq -\sum_{s\in\mathcal{S}} d^\star(s) \log\left(\sum_{a\in A_s^\star} \pi(a|s)\right) \\
&= -\sum_{s\in\mathcal{S}} d^\star(s) \log\left(1-\sum_{a\notin A_s^\star} \pi(a|s)\right) \\
&\geq \sum_{s\in\mathcal{S}} d^\star(s) \sum_{a\notin A_s^\star} \pi(a|s)
\end{aligned}$$

□

Proof of Theorem C.5. As expected, we work with Lemma C.7. By Lemma C.3 we have

$$\sum_{a \notin A_s^\star} \pi_t(a|s) \leq \sum_{a \notin A_s^\star} \pi_1(a|s) e^{-\Delta(t-1)+\gamma c \log t} \leq e^{-\Delta(t-1)+\gamma c \log t}$$

and thus

$$\frac{\max_{s\in\mathcal{S}} \sum_{a\notin A_s^\star} \pi_t(a|s)}{1-\max_{s\in\mathcal{S}} \sum_{a\notin A_s^\star} \pi_t(a|s)} \leq \frac{e^{-\Delta(t-1)+\gamma c \log t}}{1-e^{-\Delta(t-1)+\gamma c \log t}}$$

if $e^{-\Delta(t-1)+c\log t} < 1$ and Lemma C.7 yields the upper bound. For the lower bound, we fix $s_0 \in \mathcal{S}$ and $a_0 \in \mathcal{A}$ with $A^\star(s,a) = -\Delta$ and estimate

$$\begin{aligned}\sum_{s\in\mathcal{S}} d^\star(s) \sum_{a\notin A_s^\star} \pi_t(a|s) &\geq \sum_{s\in\mathcal{S}} d^\star(s) \sum_{a\notin A_s^\star} \pi_0(a|a) e^{A^\star(s,a)(t-1)-c\log t - 2\|r\|_\infty} \\ &\geq d^\star(s_0)\pi_0(a_0|s_0) e^{-\Delta(t-1)-c\log t-2\|r\|_\infty} \\ &\geq \min_{s\in\mathcal{S}, a\notin A_s^\star} d^\star(s)\pi_0(a|s) \cdot e^{-\Delta(t-1)-c\log t-2\|r\|_\infty}.\end{aligned}$$

□

D. Overall Error Analysis for Regularized Natural Policy Gradients

Entropy regularization is commonly added to encourage exploration and accelerate the optimization process, however, the unregularized objective is still the objective criterion one wishes to optimize. Hence, it is a natural question to ask what accuracy one can achieve with a budget of k iteration loops with a method that aims to optimize the regularized reward. One way to approach this is to use the error decomposition

$$0 \leq R^\star - R(\pi_k) = R^\star - R(\pi_\tau^\star) + R(\pi_\tau^\star) - R_\tau(\pi_\tau^\star) + R_\tau(\pi_\tau^\star) - R_\tau(\pi_k) + R_\tau(\pi_k) - R(\pi_k), \tag{88}$$

Applying the $0 \leq R(\pi) - R_\tau(\pi) = O(\tau)$ bound on the entropy regularization error gives

$$0 \leq R^\star - R(\pi_k) = O(\tau) + R_\tau(\pi_\tau^\star) - R_\tau(\pi_k) = O(\tau + e^{-\tau\eta k}) \tag{89}$$

for entropy regularized natural policy gradients with stepsize $\eta > 0$, see (Çaycı et al., 2021; Cen et al., 2021). Choosing $\tau = \frac{\log k}{\eta k}$ yields the estimate $R^\star - R(\pi_k) = O(\frac{\log k}{\eta k})$ on the unregularized reward, see (Cen et al., 2021). We use our exponential estimate $R^\star - R(\pi_\tau^\star) = \tilde{O}(e^{-\Delta\tau^{-1}})$ to improve this to a $\tilde{O}(e^{-\sqrt{\Delta\eta k/2}})$ guarantee, where $\tilde{O}$ hides polynomial terms in ηk. Note that the $\tilde{O}(e^{-\Delta\tau^{-1}})$ estimate is only available for the optimal policy $\pi_\tau^\star$ and hence, we can not apply it to all terms in the error decomposition (88). Therefore, we employ the following stability result on the reward function.

Proposition D.1 (Lipschitz-continuity of the reward (Müller, 2023))**.** *It holds that*

$$|R(\pi_1) - R(\pi_2)| \leq \frac{\|r\|_\infty}{1-\gamma} \cdot \|\pi_1 - \pi_2\|_1 \quad \textit{for all } \pi_1, \pi_2 \in \Delta_{\mathcal{A}}^{\mathcal{S}}. \tag{90}$$

Now we can upper bound the suboptimality gap $R^\star - R(\pi)$ of a policy in terms of $R^\star - R(\pi_\tau^\star)$ and the distance between π and $\pi_\tau^\star$.

Lemma D.2. *For any policy $\pi \in \Delta_{\mathcal{A}}^{\mathcal{S}}$ we have*

$$0 \leq R^\star - R(\pi) \leq R^\star - R(\pi_\tau^\star) + \frac{\sqrt{2}\cdot|\mathcal{S}|\cdot\|r\|_\infty}{1-\gamma} \cdot \|\log \pi_\tau^\star - \log \pi\|_\infty^{\frac{1}{2}}. \tag{91}$$

Proof. First, note that $R^\star - R(\pi) = R^\star - R(\pi_\tau^\star) + R(\pi_\tau^\star) - R(\pi)$. Using the Lipschitz continuity of the reward from

Proposition D.1 as well as Pinsker's and Jensen's inequality we estimate

$$\begin{aligned}
R(\pi_\tau^\star) - R(\pi) &\leq \frac{\|r\|_\infty}{1-\gamma} \cdot \|\pi_\tau^\star - \pi\|_1 \\
&= \frac{\|r\|_\infty}{1-\gamma} \cdot \sum_{s\in\mathcal{S}} \|\pi_\tau^\star(\cdot|s) - \pi(\cdot|s)\|_1 \\
&\leq \frac{\sqrt{2}\cdot\|r\|_\infty}{1-\gamma} \cdot \sum_{s\in\mathcal{S}} D_{\mathrm{KL}}(\pi_\tau^\star(\cdot|s), \pi(\cdot|s))^{\frac{1}{2}} \\
&\leq \frac{\sqrt{2}\cdot\|r\|_\infty}{1-\gamma} \cdot \sum_{s\in\mathcal{S}} \left(\sum_{a\in\mathcal{A}} \pi_\tau^\star(a|s) \log \frac{\pi_\tau^\star(a|s)}{\pi(a|s)} \right)^{\frac{1}{2}} \\
&\leq \frac{\sqrt{2}\cdot\|r\|_\infty}{1-\gamma} \cdot \sum_{s\in\mathcal{S}} \left(\sum_{a\in\mathcal{A}} \pi_\tau^\star(a|s) \|\log \pi_\tau^\star - \log \pi\|_\infty \right)^{\frac{1}{2}} \\
&= \frac{\sqrt{2}\cdot|\mathcal{S}|\cdot\|r\|_\infty}{1-\gamma} \cdot \|\log \pi_\tau^\star - \log \pi\|_\infty^{\frac{1}{2}}.
\end{aligned}$$

□

Lemma D.2 can by used in combination with any result bounding $D_{\mathrm{K}}(\pi_\tau^\star, \pi_k)$ for a policy optimization technique. If only bounds on $R_\tau(\pi_\tau^\star) - R_\tau(\pi_k)$ are available, one can also use the local bound $D_{\mathrm{K}}(\pi_\tau^\star, \pi) \leq \omega\tau^{-1}(R_\tau(\pi_\tau^\star) - R_\tau(\pi))$, which holds in a neighborhood of $\pi_\tau^\star$ that depends on $\omega \in (0,1)$, see (Müller & Montúfar, 2024, Lemma 29). Here, we limit our discussion to entropy-regularized natural policy gradient methods, which are known to converge linearly.

Theorem D.3 (Convergence of entropy regularized NPG, (Cen et al., 2021))**.** *Consider natural policy gradient with a tabular softmax policy parametrization, fix a regularization strength $\tau > 0$ and stepsize $\eta > 0$ and denote the iterates of the natural policy gradient updates by $(\pi_k)_{k\in\mathbb{N}}$ and set $Q_\tau^{(k)} := Q_\tau^{\pi_k}$ and denote the optimal entropy regularized policy and Q-function by $\pi_\tau^\star$ and $Q_\tau^\star$. Then for any $k \in \mathbb{N}$ it holds that*

$$\|Q_\tau^\star - Q_\tau^{(k+1)}\|_\infty \leq C(1-\eta\tau)^k \quad \textit{and} \tag{92}$$

$$\|\log \pi_\tau^\star - \log \pi_{k+1}\|_\infty \leq 2C\tau^{-1}(1-\eta\tau)^k, \tag{93}$$

where

$$C = \|Q_\tau^\star - Q_\tau^{(0)}\|_\infty + 2\tau\left(1 - \frac{\eta\tau}{1-\gamma}\right)\|\log \pi_\tau^\star - \log \pi_0\|_\infty \tag{94}$$

Now we can provide the following estimate on the performance of entropy regularized natural policy gradients measured in the unregularized reward.

Theorem D.4 (Overall error analysis)**.** *Consider a regularization strength $\tau \in (0,1]$ and assume that $(\pi_k)_{k\in\mathbb{N}}$ be the iterates produced by natural policy ascent with a log-linear tabular policy parametrization with stepsize $\eta > 0$ and denote the optimal unregularized policy by $\pi^\star$. Then it holds that*

$$R^\star - R(\pi_{k+1}) \leq \frac{2\|r\|_\infty e^\Delta}{1-\gamma} \cdot \tau^{-c} e^{-\Delta\tau^{-1}} + \frac{2\cdot|\mathcal{S}|\cdot\|r\|_\infty C^{\frac{1}{2}}}{1-\gamma} \cdot \tau^{-\frac{1}{2}} e^{-\frac{\eta\tau k}{2}}, \tag{95}$$

where $c = D_{\mathrm{K}}(\pi^\star, \pi_0)$ and C is defined in (94). In particular, choosing $\tau = \sqrt{\frac{2\Delta}{\eta k}}$ yields

$$R^\star - R(\pi_t) = O\left(\left(k^{\frac{c}{2}} + k^{\frac{1}{4}}\right) \cdot e^{-\sqrt{\frac{\Delta\eta k}{2}}}\right). \tag{96}$$

Proof. A direct combination of Lemma D.2, Theorem C.2, and Theorem D.3 we obtain (95). □

Remark D.5.

- Recently, a sharp asymptotic analysis of entropy-regularized natural policy gradient methods has been conducted showing $R_\tau^\star - R(\pi_k) = O((1+\eta\tau)^{-2k})$ compared to the $O((1-\eta\tau)^k)$ convergence of Theorem D.3. However, in order to use this result in our overall analysis, an analogous estimate on the convergence of the policies as well as a control on the entry times after which the rate holds is missing.
- Where we consider a fixed regularization and step size, $O(\gamma^k)$-convergence was established when exponentially decreasing the regularization and increasing the step size (Li et al., 2023).
- For the small stepsize limit $\eta \to 0$ the updates of the regularized natural policy gradient scheme will follow the regularized Kakade gradient flow that was recently studied in (Kerimkulov et al., 2023). These results complement the discrete-time analysis and ensure that $D_{\mathrm{K}}(\pi_\tau^\star, \pi_t) \leq e^{-\tau t} D_{\mathrm{K}}(\pi_\tau^\star, \pi_0)$, see (Kerimkulov et al., 2023, Equation (61)). An analog treatment to the discrete-time case yields an overall estimate of $O(e^{-\sqrt{\Delta t/2}})$ for the regularized flow with strength $\tau = \sqrt{2\Delta t^{-1}}$.