Policy Gradient: Optimality

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CS 6789: Foundations of Reinforcement Learning

Slides courtesy of **Wen Sun**

Recap

Policy Gradient Deriviation

e.g., Reinforce, Natural Policy Gradient, TRPO, PPO:

(Williams 92, Kakade 02, Schulman et al 15, 17)

$$\pi_\theta(a \mid s) = \pi(a \mid s; \theta) \qquad J(\pi_\theta) = \mathbb{E}_{\pi_\theta}\left[\sum_{h=0}^{\infty} \gamma^h r_h\right]$$

$$\theta_{t+1} = \theta_t + \eta \nabla_\theta J(\pi_\theta) \mid_{\theta=\theta_t}$$

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$$\nabla_\theta J(\theta) := \frac{1}{1-\gamma} \mathbb{E}_{s,a \sim d^{\pi_\theta}} \left[\nabla_\theta \ln \pi_\theta(a \mid s) Q^{\pi_\theta}(s, a) \right]$$

Derivation of unbiased Stochastic Policy Gradient

$$\nabla_\theta J(\theta) := \frac{1}{1-\gamma}\mathbb{E}_{s,a\sim d^{\pi_\theta}}\left[\nabla_\theta \ln \pi_\theta(a \mid s) Q^{\pi_\theta}(s,a)\right]$$

Draw $h \propto \gamma^h$, **roll-in** π_θ to generate $s_h, a_h \sim \mathbb{P}_h^{\pi_\theta}$

Roll-out π_θ from (s_h, a_h) : terminate with prob $1-\gamma$, $\widetilde{Q}^{\pi_\theta}(s_h, a_h) = \sum_{\tau=h}^{t\geq h} r_\tau$

Unbiased estimate: $\nabla_\theta \ln \pi_\theta(a_h \mid s_h) \widetilde{Q}^{\pi_\theta}(s_h, a_h)$

Policy Gradient: Examples of Policy Parameterization (discrete actions)

1. Softmax Policy for Tabular MDPs:

$$\theta_{s,a} \in \mathbb{R}, \forall s, a \in S \times A$$

$$\pi_\theta(a \mid s) = \frac{\exp(\theta_{s,a})}{\sum_{a'} \exp(\theta_{s,a'})}$$

2. Softmax linear Policy (e.g., for linear MDPs):

Feature vector $\phi(s, a) \in \mathbb{R}^d$, and parameter $\theta \in \mathbb{R}^d$

$$\pi_\theta(a \mid s) = \frac{\exp(\theta^\top \phi(s, a))}{\sum_{a'} \exp(\theta^\top \phi(s, a'))}$$

3. Neural Policy:

Neural network $f_\theta : S \times A \mapsto \mathbb{R}$

$$\pi_\theta(a \mid s) = \frac{\exp(f_\theta(s, a))}{\sum_{a'} \exp(f_\theta(s, a'))}$$

Convergence to Stationary Point

$J(\pi_\theta)$ is non-convex (see example in the monograph)

Def of β-smooth:

$$\|\nabla_\theta J(\theta) - \nabla_\theta J(\theta_0)\|_2 \leq \beta\|\theta - \theta_0\|_2$$

$$\left| J(\theta) - J(\theta_0) - \nabla_\theta J(\theta_0)^\top(\theta - \theta_0) \right| \leq \frac{\beta}{2}\|\theta - \theta_0\|_2^2, \forall \theta, \theta_0$$

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[**Theorem**] If $J(\theta)$ is β-smooth, and we run SGA: $\theta_{t+1} = \theta_t + \eta \widetilde{\nabla}_\theta J(\theta_t)$

where $\mathbb{E}\left[\widetilde{\nabla}_\theta J(\theta_t)\right] = \nabla_\theta J(\theta_t), \quad \mathbb{E}\left[\|\widetilde{\nabla}_\theta J(\theta_t)\|_2^2\right] \leq \sigma^2,$

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then:

$$\mathbb{E}\left[\frac{1}{T}\sum_t \|\nabla_\theta J(\theta_t)\|_2^2\right] \leq O\left(\sqrt{\beta\sigma^2/T}\right)$$

Today (+future):

When do PG methods converge to a global optima?
(+ what about function approximation?)

Today:

- Let's consider using exact gradients.
  - This allows us to ignore estimation issues
  - Let's focus on "complete" parameterizations (e.g. the "tabular" case)
  - Π contains all stochastic policies (e.g. softmax)

- I: Landscape of the problem
  - As a general non-convex optimization problem:
    do small gradients imply good performance?
  - what about "exploration"?
- II: Global convergence results

PG as non-convex optimization

Convergence to Stationary Points of GD

$J(\pi_\theta)$ is non-convex (see example in the AJKS)

- Def of a β-smooth function F:
  $\|\nabla_\theta F(\theta) - \nabla_\theta F(\theta_0)\|_2 \leq \beta \|\theta - \theta_0\|_2$
  which implies:
  $$\left| F(\theta) - F(\theta_0) - \nabla_\theta F(\theta_0)^\top (\theta - \theta_0) \right| \leq \frac{\beta}{2} \|\theta - \theta_0\|_2^2$$

- Proposition: (stationary point convergence) Assume $F(\theta)$ is β-smooth.
  Suppose we run gradient ascent: $\theta_{t+1} = \theta_t + \eta \nabla_\theta F(\theta_t)$, with $\eta = 1/(2\beta)$. Then:
  $$\min_{t \leq T} \|\nabla_\theta F(\theta_t)\|_2^2 \leq \frac{2\beta \left(\max_\theta F(\theta) - F(\theta_0) \right)}{T}$$

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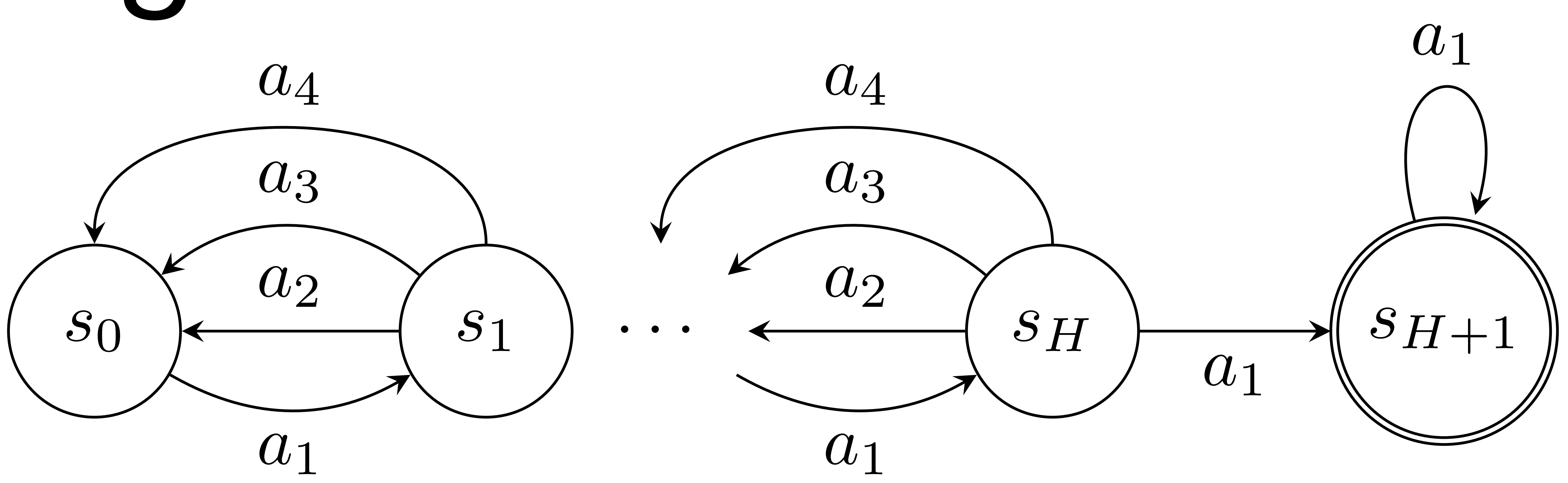
$$\Rightarrow \min_{t \leq T} \|\nabla_\theta F(\theta_t)\|^2 \leq \frac{1}{T} \sum_t \|\nabla_\theta F(\theta_t)\|^2 \leq \sum_t \frac{2\beta}{T} \big(F(\theta_{t+1}) - F(\theta_t)\big) \leq \frac{2\beta(F(\theta^\star) - F(\theta_0))}{T}$$

A “landscape” result

(and “exploration”)

Vanishing Gradients and Saddle Points



Set $\gamma = H/(H+1)$. Policy param:

for $a = a_1, a_2, a_3$, $\pi_\theta(a \mid s) = \theta_{s,a}$, and $\pi_\theta(a_4 \mid s) = 1 - \theta_{s,a_1} - \theta_{s,a_2} - \theta_{s,a_3}$

(this a "direct" param, which is valid inside the simplex)

Theorem: For $0 < \theta < 1$ (componentwise) and $\theta_{s,a_1} < 1/4$ (for all states s).

For all $k \leq O(H/\log(H))$, we have that

$$\|\nabla_\theta^k V^{\pi_\theta}(s_0)\| \leq (1/3)^{H/4}$$

(where $\|\nabla_\theta^k V^{\pi_\theta}(s_0)\|$ is the operator norm of the tensor $\nabla_\theta^k V^{\pi_\theta}(s_0)$).

Do small gradients imply global optimality?

Not in this case

“Vanilla” PG for the Softmax

Let’s consider having a staring state distribution with “coverage”

- Given our a starting distribution ρ over states, recall our objective is:
  $$\max_{\theta \in \Theta} V^{\pi_\theta}(\rho) \,.$$
  where $\{\pi_\theta \,|\, \theta \in \Theta \subset \mathbb{R}^d\}$ is some class of parametric policies.

- While we are interested in good performance under ρ, it is helpful to optimize under a different measure μ. Specifically, consider optimizing: $V^{\pi_\theta}(\mu)$, i.e.
  $$\max_{\theta \in \Theta} V^{\pi_\theta}(\mu) \,,$$
  even though our ultimate goal is performance under $V^{\pi_\theta}(\rho)$.

notation (+ overloading)

Today: we will use $d^{\pi}_{s_0}$ for a state distribution measure.

(it should be clear from context how we use it).

$$d^{\pi}_{s_0}(s) = (1-\gamma)\sum_{h=0}^{\infty}\gamma^h \mathbb{P}(s_h = s \mid s_0, \pi)$$

$$V^{\pi}(\mu) = E_{s\sim\mu}[V^{\pi}(s)]$$

$$d^{\pi}_{\mu}(s) = E_{s_0\sim\mu}[d^{\pi}_{s_0}(s)]$$

$$d^{\pi}_{s_0}(s,a) = (1-\gamma)\sum_{h=0}^{\infty}\gamma^h \mathbb{P}(s_h = s, a_h = a \mid s_0, \pi)$$

Advantage function: $A^{\pi}(s,a) = Q^{\pi}(s,a) - V^{\pi}(s)$

The Softmax Policy Class

- $$\pi_\theta(a \mid s) = \frac{\exp(\theta_{s,a})}{\sum_{a'} \exp(\theta_{s,a'})},$$
  (where the number of parameters is SA).

- We have that:
  $$\frac{\partial \log \pi_\theta(a \mid s)}{\partial \theta_{s',a'}} = \mathbf{1}\Big[s = s'\Big]\Big(\mathbf{1}\Big[a = a'\Big] - \pi_\theta(a' \mid s)\Big)$$
  where $\mathbf{1}[\,\cdot\,]$ is the indicator function.

- Lemma: For the softmax policy class, we have:
  $$\frac{\partial V^{\pi_\theta}(\mu)}{\partial \theta_{s,a}} = \frac{1}{1-\gamma} d_\mu^{\pi_\theta}(s)\pi_\theta(a \mid s)A^{\pi_\theta}(s, a)$$

Proof

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

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

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$$
\begin{aligned}
\frac{\partial V^{\pi_\theta}(\mu)}{\partial \theta_{s',a'}} &= \frac{1}{1-\gamma}\mathbb{E}_{s\sim d_\mu^{\pi_\theta}}\mathbb{E}_{a\sim\pi_\theta(\cdot|s)}\left[A^{\pi_\theta}(s,a)\frac{\partial \log \pi_\theta(a\,|\,s)}{\partial \theta_{s',a'}}\right] \\
&= \frac{1}{1-\gamma}\mathbb{E}_{s\sim d_\mu^{\pi_\theta}}\mathbb{E}_{a\sim\pi_\theta(\cdot|s)}\left[A^{\pi_\theta}(s,a)\mathbf{1}_{s=s'}\left(\mathbf{1}_{a=a'}-\pi_\theta(a'\,|\,s)\right)\right] \\
&= \frac{1}{1-\gamma}d_\mu^{\pi_\theta}(s')\mathbb{E}_{a\sim\pi_\theta(\cdot|s')}\left[A^{\pi_\theta}(s',a)\left(\mathbf{1}_{a=a'}-\pi_\theta(a'\,|\,s')\right)\right] \\
&= \frac{1}{1-\gamma}d_\mu^{\pi_\theta}(s')\left(\mathbb{E}_{a\sim\pi_\theta(\cdot|s')}\left[A^{\pi_\theta}(s',a)\right]\mathbf{1}_{a=a'}-\pi_\theta(a'\,|\,s')\mathbb{E}_{a\sim\pi_\theta(\cdot|s')}\left[A^{\pi_\theta}(s',a)\right]\right)
\end{aligned}
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&= \frac{1}{1-\gamma}d_\mu^{\pi_\theta}(s')\pi_\theta(a'\,|\,s')A^{\pi_\theta}(s',a')-0,
\end{aligned}
$$

Recall: The Performance Difference Lemma

For all π, π', s_0:

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

$$d^{\pi}_{s_0}(s) = (1-\gamma)\sum_{h=0}^{\infty}\gamma^h \mathbb{P}(s_h = s \mid s_0, \pi)$$

Global Convergence

- The update rule for gradient ascent is:
  $\theta^{(t+1)} = \theta^{(t)} + \eta \nabla_\theta V^{(t)}(\mu)$

- Concerns:
  - Non-convex
  - Flat gradients if $\theta_t \to \infty$
    (π_t becoming any deterministic policy implies θ_t approaches a stationary point)

- Theorem: Assume the μ is strictly positive i.e. $\mu(s) > 0$ for all states s. For $\eta \leq (1-\gamma)^3/8$, then we have that for all states s, $V^{(t)}(s) \to V^\star(s),$ as $t \to \infty$.

- Comments:
  - Rate could be exponentially slow in S, H.
  - $\mu > 0$ is *conjectured* to be a necessary condition

Do small gradients imply global optimality?

Yes, with

1) exponential complexity

2) μ necesssary

Recall

Lemma: For the softmax policy class, we have:

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

PG+Log Barrier Regularization

(for the softmax)

Log Barrier Regularization

- Relative-entropy for distributions p,q is: $\text{KL}(p, q) := E_{x\sim p}[-\log q(x)/p(x)]$.

- Consider the log barrier λ-regularized objective:
$$L_\lambda(\theta) := V^{\pi_\theta}(\mu) - \lambda\, E_{s\sim \text{Unif}_S}\Big[\text{KL}(\text{Unif}_A, \pi_\theta(\cdot\,|\,s))\Big]$$
$$= V^{\pi_\theta}(\mu) + \frac{\lambda}{SA}\sum_{s,a}\log \pi_\theta(a\,|\,s) + \lambda \log A$$

- Gradient Ascent:
$$\theta^{(t+1)} = \theta^{(t)} + \eta\, \nabla_\theta L_\lambda(\theta^{(t)})$$

- Do small gradients imply a globally optimal policy?

Stationarity and Optimality

- Log barrier regularized objective:

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

Stationarity and Optimality

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- Theorem: (Log barrier regularization) Suppose θ is such that:

$\|\nabla_\theta L_\lambda(\theta)\|_2 \le \epsilon_{opt}$ and $\epsilon_{opt} \le \lambda/(2SA)$

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then we have for all starting state distributions ρ:

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

Stationarity and Optimality

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

where the "distribution mismatch coefficient" is

$$\left\|\frac{d_\rho^{\pi^\star}}{\mu}\right\|_\infty = \max_s\left(\frac{d_\rho^{\pi^\star}(s)}{\mu(s)}\right)$$ (componentwise division notation)

Global Convergence with the Log Barrier

- The smoothness of $L_\lambda(\theta)$ is $\beta_\lambda := \frac{8\gamma}{(1-\gamma)^3} + \frac{2\lambda}{S}$

- Corollary: (Iteration complexity with log barrier regularization)
  Set $\lambda = \frac{\epsilon(1-\gamma)}{2\left\|\frac{d_\rho^{\pi^\star}}{\mu}\right\|_\infty}$ and $\eta = 1/\beta_\lambda$. Starting from any initial $\theta^{(0)}$,
  then for all starting state distributions ρ, we have
  $$\min_{t<T} \left\{V^\star(\rho) - V^{(t)}(\rho)\right\} \le \epsilon \quad \text{whenever} \quad T \ge c\frac{S^2A^2}{(1-\gamma)^6\,\epsilon^2}\left\|\frac{d_\rho^{\pi^\star}}{\mu}\right\|_\infty^2$$
  (for constant c).

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Yes, with

1) μ necesssary

2) log barrier regularization

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Proof, part 1

- The proof consists of showing that: $\max_a A^{\pi_\theta}(s, a) \leq 2\lambda/(\mu(s)S)$ for all states s.

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- To see that this is sufficient, observe that by the performance difference lemma:

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

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

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

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&\leq \frac{2\lambda}{1-\gamma}\max_s\left(\frac{d_\rho^{\pi^\star}(s)}{\mu(s)}\right).
\end{aligned}
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which would then complete the proof.

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$$\left\|\frac{d_\rho^{\pi^\star}}{\mu}\right\|_\infty = \max_s\left(\frac{d_\rho^{\pi^\star}(s)}{\mu(s)}\right)$$ (componentwise division notation)

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- need to show $A^{\pi_\theta}(s,a) \leq 2\lambda/(\mu(s)S)$ for all (s,a). consider (s,a) where that $A^{\pi_\theta}(s,a) \geq 0$ (else claim is true).

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

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&\le \frac{1-\gamma}{d_\mu^{\pi_\theta}(s)}\Big(\frac{1}{\pi_\theta(a\,|\,s)}\frac{\lambda}{2SA} + \frac{\lambda}{S}\Big) \\
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- Suppose we could show that $\pi_\theta(a\,|\,s) \geq 1/(2A)$, when $A^{\pi_\theta}(s,a) \geq 0$, then

$$\frac{1}{\mu(s)}\left(\frac{1}{\pi_\theta(a\,|\,s)}\frac{\lambda}{2SA} + \frac{\lambda}{S}\right) \leq \frac{1}{\mu(s)}\left(2A\frac{\lambda}{2SA} + \frac{\lambda}{S}\right) = \frac{2\lambda}{\mu(s)S}$$ and the proof is done!

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- Rearranging and using our assumption $\epsilon_{opt} \leq \lambda/(2SA)$,

$$\pi_\theta(a \mid s) \geq \frac{1}{A} - \frac{\epsilon_{opt} S}{\lambda} \geq \frac{1}{2A}.$$

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Summary

1. “Landscape” result: RL optimization is hard
2. “Vanilla” PG for Softmax with coverage
3. PG for Softmax with coverage and log barrier