

# Policy Gradient: Optimality

**Sham Kakade and Wen Sun**

**CS 6789: Foundations of Reinforcement Learning**

Recap

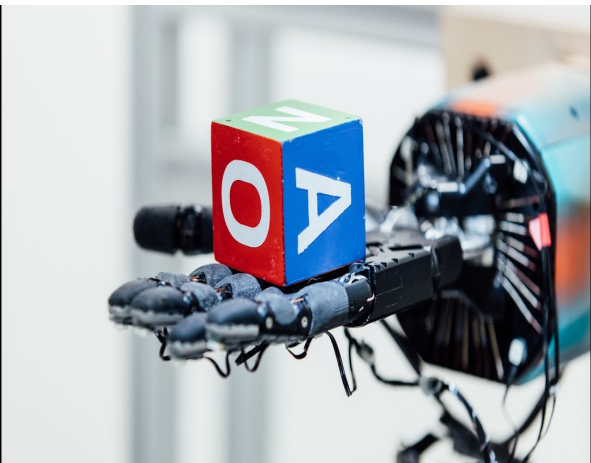
# Policy Optimization



[AlphaZero, Silver et.al, 17]



[OpenAI Five, 18]



[OpenAI,19]

# Today: Policy Gradient Derivation

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

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

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

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

Main question for today's lecture:  
how to compute the gradient?

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

## Derivation of unbiased Stochastic Policy Gradient

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

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

**Roll-out**  $\pi_{\theta}$  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:  $\nabla_{\theta} \ln \pi_{\theta}(a_h | s_h) \widetilde{Q}^{\pi_{\theta}}(s_h, a_h)$

# Policy Gradient: Examples of Policy Parameterization (discrete actions)

## 1. Softmax Policy for Tabular MDPs:

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

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

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

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

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

## 3. Neural Policy:

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

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

## Convergence to Stationary Point

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

Def of  $\beta$ -smooth:

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

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

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

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

then:

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

$\exists \epsilon$

$$\nabla_\theta J(\theta_\epsilon) \leq$$

# 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)  
 $\Pi$  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

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which implies:

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

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- **Proposition:** (stationary point convergence) Assume  $F(\theta)$  is  $\beta$ -smooth. Suppose we run gradient ascent:  $\theta_{t+1} = \theta_t + \eta \nabla_\theta F(\theta_t)$ , with  $\eta = 1/(2\beta)$ . Then:

$$\min_{t \leq T} \|\nabla_\theta F(\theta_t)\|_2^2 \leq \frac{2\beta (\max_\theta F(\theta) - F(\theta_0))}{T}$$

# Convergence to Stationary Point

**Proposition:** (stationary point convergence) Assume  $F(\theta)$  is  $\beta$ -smooth.

Suppose we run gradient ascent:  $\theta_{t+1} = \theta_t + \eta \nabla_{\theta} F(\theta_t)$ , with  $\eta = 1/(2\beta)$ . Then:

$$\min_{t \leq T} \|\nabla_{\theta} F(\theta_t)\|_2^2 \leq \frac{2\beta(F(\theta^*) - F(\theta_0))}{T}$$

see notes/  
slides  
for proof.

$$\left| F(\theta_{t+1}) - F(\theta_t) - \nabla_{\theta} F(\theta_t)^{\top} (\theta_{t+1} - \theta_t) \right| \leq \frac{\beta}{2} \|\theta_{t+1} - \theta_t\|^2$$

$$\Rightarrow \left| F(\theta_{t+1}) - F(\theta_t) - \eta \nabla_{\theta} F(\theta_t)^{\top} \nabla_{\theta} F(\theta_t) \right| \leq \frac{\beta}{2} \eta^2 \|\nabla_{\theta} F(\theta_t)\|^2$$

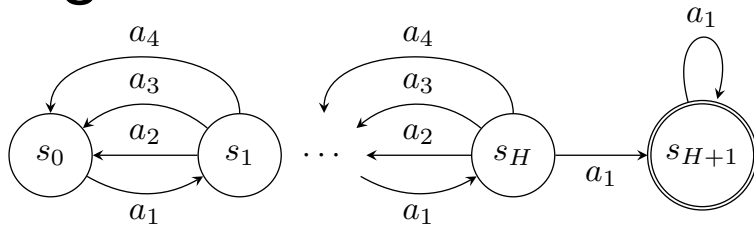
$$\Rightarrow \eta \|\nabla_{\theta} F(\theta_t)\|^2 \leq F(\theta_{t+1}) - F(\theta_t) + \frac{\beta}{2} \eta^2 \|\nabla_{\theta} F(\theta_t)\|^2$$

$$\Rightarrow \frac{1}{2\beta} \|\nabla_{\theta} F(\theta_t)\|^2 \leq F(\theta_{t+1}) - F(\theta_t) \quad \text{using } \eta \leq \frac{1}{\beta}$$

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

A “landscape” result  
(and “exploration”)

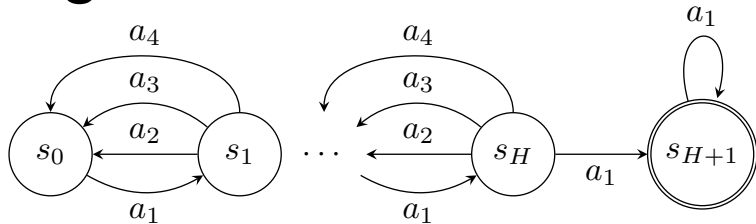
# Vanishing Gradients and Saddle Points



$$r = 1$$



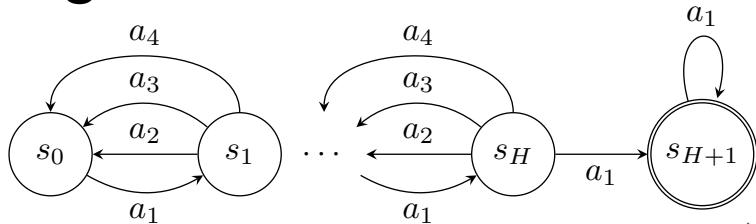
# Vanishing Gradients and Saddle Points



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

for  $a = a_1, a_2, a_3$ ,  $\pi_\theta(a | s) = \theta_{s,a}$ , and  $\pi_\theta(a_4 | s) = 1 - \theta_{s,a_1} - \theta_{s,a_2} - \theta_{s,a_3}$   
(this a “direct” param, which is valid inside the simplex)

# Vanishing Gradients and Saddle Points



$$|S| = H + 1$$

$$H \approx \frac{1}{1-\gamma} \text{ "not RL"}$$

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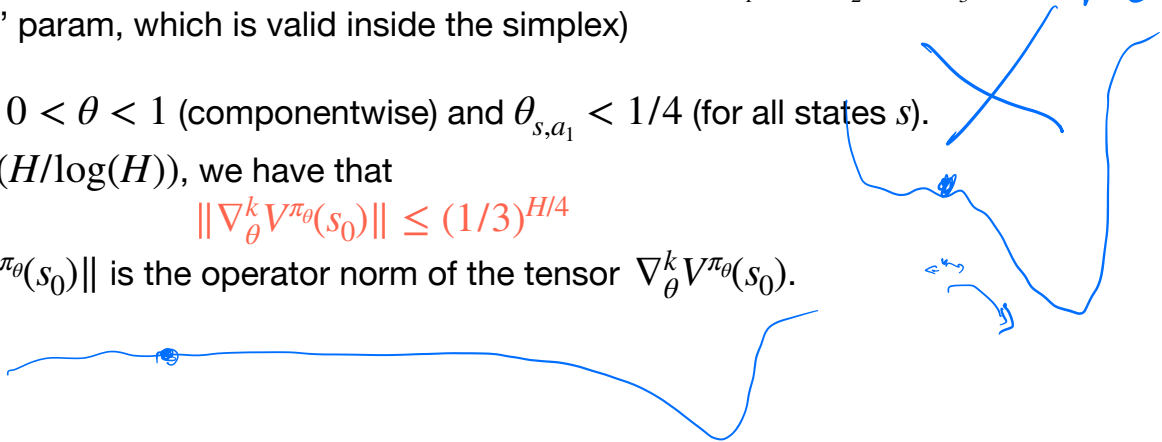
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**Theorem:** For  $0 < \theta < 1$  (componentwise) and  $\theta_{s,a_1} < 1/4$  (for all states  $s$ ).

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  $\nabla_\theta^k V^{\pi_\theta}(s_0)$ ).



“Vanilla” PG for the Softmax

Let's consider having a ataring state  
distribution with "coverage"

"Bad case"  
was starting  
at  $S_0$

# Let's consider having a ataring state distribution with “coverage”

- Given our a starting distribution  $\rho$  over states, recall our objective is:

$$\max_{\theta \in \Theta} V^{\pi_{\theta}}(\rho) . \quad = \quad \mathbb{E}_{s_0 \sim \rho} V^{\pi_{\theta}}(s_0)$$

where  $\{\pi_{\theta} \mid \theta \in \Theta \subset \mathbb{R}^d\}$  is some class of parametric policies.

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where  $\{\pi_{\theta} \mid \theta \in \Theta \subset \mathbb{R}^d\}$  is some class of parametric policies.

- While we are interested in good performance under  $\rho$ , it is helpful to optimize under a different measure  $\mu$ . 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  $V^{\pi_{\theta}}(\rho)$ .

$\rho \leftrightarrow$  what we care about  
say some  $s_0$

use some  $\mu$  which has "coverage"  
 $V^{\pi_{\theta}}(s_0)$

# notation (+ overloading)

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

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

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

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

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

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

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

# The Softmax Policy Class



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- We have that:

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

where  $\mathbf{1}[\cdot]$  is the indicator function.

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- **Lemma:** For the softmax policy class, we have:

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

# Proof

$$\begin{aligned}\frac{\partial V^{\pi_\theta}(\mu)}{\partial \theta_{s,a}} &= E_{\tau \sim \text{Pr}_\mu^{\pi_\theta}} \left[ \sum_{t=0}^{\infty} \gamma^t \nabla_\theta \ln \pi_\theta(a | s) A^{\pi_\theta}(s, a) \right] \\ &= E_{\tau \sim \text{Pr}_\mu^{\pi_\theta}} \left[ \sum_{t=0}^{\infty} \gamma^t \mathbf{1}[s_t = s] \left( \mathbf{1}[a_t = a] A^{\pi_\theta}(s, a) - \pi_\theta(a | s) A^{\pi_\theta}(s_t, a_t) \right) \right] \\ &= E_{\tau \sim \text{Pr}_\mu^{\pi_\theta}} \left[ \sum_{t=0}^{\infty} \gamma^t \mathbf{1}[(s_t, a_t) = (s, a)] A^{\pi_\theta}(s, a) \right] + \pi_\theta(a | s) \sum_{t=0}^{\infty} \gamma^t E_{\tau \sim \text{Pr}_\mu^{\pi_\theta}} \left[ \mathbf{1}[s_t = s] A^{\pi_\theta}(s_t, a_t) \right] \\ &= \frac{1}{1 - \gamma} E_{(s', a') \sim d^{\pi_\theta}} \left[ \mathbf{1}[(s', a') = (s, a)] A^{\pi_\theta}(s, a) \right] + 0 \\ &= \frac{1}{1 - \gamma} d^{\pi_\theta}(s, a) A^{\pi_\theta}(s, a),\end{aligned}$$

$d_\mu^{\pi_\theta}(s, a) = d_\mu^{\pi_\theta}(s) \pi_\theta(s, a)$

# Remember: The Performance Difference Lemma

For all  $\pi, \pi', s_0$ :

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

$d_{s_0}^{\pi}$        $\pi'$

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

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strictly by

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$$\mu^{\pi}(s) > 0$$

- **Theorem:** Assume the  $\mu$  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  $s$ ,  $V^{(t)}(s) \rightarrow V^*(s)$ , as  $t \rightarrow \infty$ .

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- Comments:

- rate could be exponentially slow in S, H.

- need  $\mu > 0$  is necessary.

$\implies d_{\mu}^{\pi}(s) > 0$

# PG+Log Barrier Regularization (for the softmax)

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$$L_\lambda(\theta) := V^{\pi_\theta}(\mu) - \lambda E_{s \sim \text{Unif}_S}[\text{KL}(\text{Unif}_A, \pi_\theta(\cdot | s))]$$

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

$$\begin{aligned} &= \frac{1}{2} \log \frac{1}{2} \\ &+ \frac{1}{2} \log \frac{0}{\frac{1}{2}} \end{aligned}$$

$$P_{\text{tails}} = \frac{1}{2} \quad P_{\text{heads}} = \frac{1}{2}$$

$$q_{\text{tails}} = 1 \quad q_{\text{heads}} = 0$$

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

- Do small gradients imply a globally optimal policy?



# Stationarity and Optimality

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# Stationarity and Optimality

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- **Theorem:** (Log barrier regularization) Suppose  $\theta$  is such that:

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

then we have for all starting state distributions  $\rho$ :

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

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

- where the “distribution mismatch coefficient” is

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

with  $\mu = U_{\gamma,0} f$   
 $\Rightarrow \left\| \cdot \right\|_\infty \leq S$

# Global Convergence with the Log Barrier

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- 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  $\lambda = \frac{\epsilon(1-\gamma)}{2\left\|\frac{d\rho^{\pi^*}}{\mu}\right\|_\infty}$  and  $\eta = 1/\beta_\lambda$ . Starting from any initial  $\theta^{(0)}$ ,

then for all starting state distributions  $\rho$ , we have

$$\min_{t < T} \{V^*(\rho) - V^{(t)}(\rho)\} \leq \epsilon \quad \text{whenever} \quad T \geq c \frac{S^2 A^2}{(1-\gamma)^6 \epsilon^2} \left\|\frac{d\rho^{\pi^*}}{\mu}\right\|_\infty^2$$

(for constant c).

*works*

$$\mathcal{P}(s) \approx \mathcal{I}(s = s_0)$$

*poly it. complexity*  
↓  
*(it  $\mu = V_{\text{inf}}$ )*

# Remember: The Performance Difference Lemma

For all  $\pi, \pi', s_0$ :

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

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



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~~XXX~~

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

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

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

$$\leq \frac{1}{1-\gamma} \sum_s 2d_\rho^{\pi^*}(s) \lambda/(\mu(s)S)$$

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

which would then complete the proof.

✓ by max  
 (  $\pi^*$  is a dist. )

✓ by ~~XXX~~

$\leq \frac{2\lambda}{1-\gamma} \frac{1}{S} \cdot \sum_s \left\| \frac{d_\rho^{\pi^*}}{\mu} \right\|_1$

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

# Proof, part 2

- 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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$$\leq \frac{1-\gamma}{d_\mu^{\pi_\theta}(s)} \left( \frac{1}{\pi_\theta(a|s)} \frac{\lambda}{2SA} + \frac{\lambda}{S} \right)$$

$$\leq \frac{1}{\mu(s)} \left( \frac{1}{\pi_\theta(a|s)} \frac{\lambda}{2SA} + \frac{\lambda}{S} \right)$$

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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

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



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

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