# Reinforcement Learning

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#### Lecture 5: Policy Gradient 2

Laboratory for Information and Inference Systems (LIONS) École Polytechnique Fédérale de Lausanne (EPFL)

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## Recap: Policy optimization

o The objective of reinforcement learning in terms of the policy parameters is given by the following:

$$\max_{\theta} J(\pi_{\theta}) := \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^{t} r(s_{t}, a_{t}) | s_{0} \sim \mu, \pi_{\theta}\right] = \mathbb{E}_{s \sim \mu}[V^{\pi_{\theta}}(s)].$$

#### Tabular parametrization

Direct parameterization:

$$\pi_{\theta}(a|s) = \theta_{s,a}, \text{ with } \theta_{s,a} \geq 0, \sum_{a} \theta_{s,a} = 1.$$

Softmax parameterization:

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

# Non-tabular parametrization

Softmax parameterization:

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

Gaussian parameterization:

$$\pi_{\theta}(a|s) \sim \mathcal{N}\left(\mu_{\theta}(s), \sigma_{\theta}^{2}(s)\right).$$

### Recap: Policy gradient methods

o The exact policy gradient method is a special case of the stochastic policy gradient method.

### Stochastic policy gradient method

By stochastic policy gradient method, we mean the following update rule:

$$\theta_{t+1} \longleftarrow \theta_t + \alpha_t \hat{\nabla}_{\theta} J(\pi_{\theta_t}),$$

where  $\hat{\nabla}_{\theta}J(\pi_{\theta_t})$  is a stochastic estimate of the full gradient of the performance objective and is used in

- ► REINFORCE [18]
- ► REINFORCE with baseline [18]
- ► Actor-Critic [11]
- ▶ ..

#### **Previous lecture**

o In the previous lecture, we answered the following two questions.

# Question 1 (Non-concavity)

When do policy gradient methods converge to an optimal solution? If so, how fast?

### Question 2 (Vanishing gradient)

How to avoid vanishing gradients and further improve the convergence?

#### **Previous lecture**

o In the previous lecture, we answered the following two questions.

# Question 1 (Non-concavity)

When do policy gradient methods converge to an optimal solution? If so, how fast?

Remarks: o Optimization wisdom: GD/SGD can converge to the global optima for "convex-like" functions:

$$J(\pi^{\star}) - J(\pi) = \mathcal{O}(\|\nabla J(\pi)\|) \text{ or } \mathcal{O}(\|G(\pi)\|)$$

o Take-away: Despite nonconcavity, PG converges to the optimal policy, in a sublinear or linear rate.

# Question 2 (Vanishing gradient)

How to avoid vanishing gradients and further improve the convergence?

#### Previous lecture

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o Take-away: Despite nonconcavity, PG converges to the optimal policy, in a sublinear or linear rate.

## Question 2 (Vanishing gradient)

How to avoid vanishing gradients and further improve the convergence?

Remarks: Optimization wisdom: Use divergence with good curvature information.

o Take-away: Natural policy gradient achieves a faster convergence with better constants.

#### This lecture

o In this lecture, we will answer the following questions.

# Question 3 (theory)

- Why does NPG achieve a better convergence?
- o How can we further improve the algorithm?
- o To answer Question 3, we first revisit some optimization background (next few slides).

### Question 4 (practice)

- o How do we extend the algorithms to function approximation settings?
- o How do we extend the algorithms to online settings without computing exact gradient?
- o How do we extend the algorithms to off-policy settings?
- o To answer Question 4, we will have a look at recent papers (second part of this lecture).

## The algorithmic path towards an understanding

- o We will discover NPG and the two closely related algorithms: TRPO and OPPO.
- o We will study the implications of advantage estimation and exploration in their convergence.
- o We will further discuss the successful PPO algorithm.

Algorithm	Convergence rate	Unknown transitions	Hard environments
Vanilla PG [16]	$\mathcal{O}\left(\frac{16 \mathcal{S} \kappa^2}{c^2(1-\gamma)^5T}\right)$	×	×
Tabular NPG [2]	$\mathcal{O}\left(\frac{2}{(1-\gamma)^2T}\right)$	×	✓
Sample-based NPG	$\mathcal{O}\left(rac{1}{1-\gamma}\sqrt{rac{2\log \mathcal{A} }{T}}+\sqrt{\kappa\epsilon_{stat}} ight)$	<b>✓</b>	×
OPPO [5]	$\mathcal{O}\left(\frac{ \mathcal{S}  \mathcal{A} }{\sqrt{(1-\gamma)^3T}}\right)$	✓	<b>/</b>

#### Remarks:

- o Here are the key quantities in the table:
  - $c = [\min_{s,t} \pi_{\theta_t}(a^*(s)|s)]^{-1} > 0$
  - $\kappa = \left\| \frac{\lambda_{\mu}^{\pi^{\star}}}{\mu} \right\|$  is larger when it is harder to explore and is possibly  $\infty$ .
  - $ightharpoonup \epsilon_{\text{stat}}$  is the statistical error incurred in estimating the advantage function  $A^{\pi}$ .

### Revisiting gradient descent

- $\circ$  Consider the optimization problem  $\min_{\mathbf{x} \in \mathbb{R}^d} f(\mathbf{x})$ .
  - Gradient descent (GD):

$$\mathbf{x}_{t+1} = \mathbf{x}_t - \eta \nabla_{\mathbf{x}} f(\mathbf{x}_t).$$

Equivalent regularized form:

$$\mathbf{x}_{t+1} = \arg\min_{\mathbf{x}} \left\{ \nabla_{\mathbf{x}} f(\mathbf{x}_t)^{\top} (\mathbf{x} - \mathbf{x}_t) + \frac{1}{2\eta} \|\mathbf{x} - \mathbf{x}_t\|_2^2 \right\}.$$

Equivalent trust region form:

$$\mathbf{x}_{t+1} = \arg\min_{\mathbf{x}} \nabla_{\mathbf{x}} f(\mathbf{x}_t)^{\top} (\mathbf{x} - \mathbf{x}_t), \text{ s.t. } \|\mathbf{x} - \mathbf{x}_t\|_2 \le \eta \|\nabla_{\mathbf{x}} f(\mathbf{x}_t)\|.$$

**Question:**  $\circ$  Would GD give the same trajectory under invertible linear transformations  $(\mathbf{x} \to \mathbf{A}\mathbf{x})$ ?

# Revisiting gradient descent (cont'd)

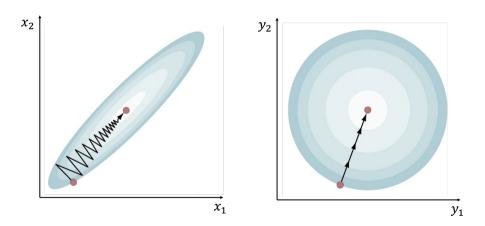


Figure: GD is not invariant w.r.t. linear transformations.

### **Recall Bregman divergences**

#### Bregman divergence

Let  $\omega: \mathcal{X} \to \mathbb{R}$  be continuously differentiable and 1-strongly convex w.r.t. some norm  $\|\cdot\|$  on  $\mathcal{X}$ . The Bregman divergence  $D_{\omega}$  associated to  $\omega$  is defined as

$$D_{\omega}(\mathbf{x}, \mathbf{y}) = \omega(\mathbf{x}) - \omega(\mathbf{y}) - \nabla \omega(\mathbf{y})^{T} (\mathbf{x} - \mathbf{y}),$$

for any  $\mathbf{x}, \mathbf{y} \in \mathcal{X}$ .

#### Examples:

- Euclidean distance:  $\omega(\mathbf{x}) = \frac{1}{2} ||\mathbf{x}||_2^2$ ,  $D_{\omega}(\mathbf{x}, \mathbf{y}) = \frac{1}{2} ||\mathbf{x} \mathbf{y}||_2^2$ .
- $\ \, \text{O Mahalanobis distance:} \ \, \omega(\mathbf{x}) = \tfrac{1}{2}\mathbf{x}^TQ\mathbf{x} \ \, \text{(where } Q \succeq I) \text{, } D_{\omega}(\mathbf{x},\mathbf{y}) = \tfrac{1}{2}(\mathbf{x}-\mathbf{y})^TQ(\mathbf{x}-\mathbf{y}).$
- o Kullback-Leibler divergence:  $\mathcal{X} = \{\mathbf{x} \in \mathbb{R}^d_+ : \sum_{i=1}^d x_i = 1\}$ ,  $\omega(\mathbf{x}) = \sum_{i=1}^d x_i \log x_i$

$$D_{\omega}(\mathbf{x}, \mathbf{y}) = \mathrm{KL}(\mathbf{x} \| \mathbf{y}) := \sum_{i=1}^{d} x_i \log \frac{x_i}{y_i}.$$

## **Background: Mirror descent**

### Mirror descent (Nemirovski & Yudin, 1983)

For a given strongly convex function  $\omega$  and initialization  $x_0$ , the iterates of mirror descent [3] are given by

$$\mathbf{x}_{t+1} = \underset{\mathbf{x} \in \mathcal{X}}{\arg\min} \{ \langle \nabla_{\mathbf{x}} f(\mathbf{x}_t), \mathbf{x} - \mathbf{x}_t \rangle + \frac{1}{\eta_t} D_{\omega}(\mathbf{x}, \mathbf{x}_t) \}.$$

#### Examples:

 $\circ \text{ Gradient descent: } \mathcal{X} \subseteq \mathbb{R}^d \text{, } \omega(\mathbf{x}) = \tfrac{1}{2} \|\mathbf{x}\|_2^2 \text{, } D_\omega(\mathbf{x},\mathbf{x}_t) = \tfrac{1}{2} \|\mathbf{x} - \mathbf{x}_t\|_2^2.$ 

$$\mathbf{x}_{t+1} = \Pi_{\mathcal{X}}(\mathbf{x}_t - \eta_t \nabla_{\mathbf{x}} f(\mathbf{x}_t)).$$

o Entropic mirror descent [3]:  $\mathcal{X} = \Delta_d$ ,  $\omega(\mathbf{x}) = \sum_{i=1}^d x_i \log x_i$ ,  $D_{\omega}(\mathbf{x}, \mathbf{x}_t) = \mathrm{KL}(\mathbf{x} \| \mathbf{x}_t)$ 

$$\mathbf{x}_{t+1} \propto \mathbf{x}_t \odot \exp(-\eta_t \nabla_{\mathbf{x}} f(\mathbf{x}_t)),$$

where  $\odot$  is element-wise multiplication and  $\exp(\cdot)$  is applied element-wise.

- o Entropic Mirror Descent attains nearly dimension-free convergence [3] (also see Chapter 4 [4]).
- o See Lecture 3 Supplementary Material for more details and examples.

### Background: Fisher information and KL divergence

#### Fisher Information Matrix

Consider a smooth parametrization of distributions  $heta\mapsto p_ heta(\cdot)$ , the Fisher information matrix is defined as

$$F_{\theta} = \mathbb{E}_{z \sim p_{\theta}} [\nabla_{\theta} \log p_{\theta}(z) \nabla_{\theta} \log p_{\theta}(z)^{\top}].$$

#### Remarks:

- o It is an invariant metric on the space of the parameters.
- o Fisher information matrix is the Hessian of KL divergence.

$$F_{\theta_0} = \frac{\partial^2}{\partial \theta^2} \left. \text{KL}(p_{\theta_0} \| p_{\theta}) \right|_{\theta = \theta_0}.$$

o The second-order Taylor expansion of KL divergence is given by

$$\mathrm{KL}(p_{\theta_0} \| p_{\theta}) \approx \frac{1}{2} (\theta - \theta_0)^{\top} F_{\theta_0} (\theta - \theta_0).$$

### Background: Natural gradient descent

- o Consider the optimization problem  $\min_{\mathbf{x} \in \Delta} f(\mathbf{x})$  and represent  $\mathbf{x}$  by  $p_{\theta}(\cdot)$ .
  - ▶ Natural gradient descent (Amari, 1998):

$$\theta_{t+1} = \theta_t - \eta(F_{\theta_t})^{\dagger} \nabla_{\theta} f(\theta_t).$$

Equivalent regularized form:

$$\theta_{t+1} = \arg\min_{\theta} \left\{ \nabla_{\theta} f(\theta_t)^{\top} (\theta - \theta_t) + \frac{1}{2\eta} (\theta - \theta_t)^{\top} F_{\theta_t} (\theta - \theta_t) \right\}.$$

Equivalent trust region form:

$$\theta_{t+1} = \arg\min_{\theta} \nabla_{\theta} f(\theta_t)^{\top} (\theta - \theta_t), \text{ s.t. } \frac{1}{2} (\theta - \theta_t)^{\top} F_{\theta_t} (\theta - \theta_t) \leq \frac{1}{2} \eta^2 \nabla_{\theta} f(\theta_t)^{\top} F_{\theta_t}^{\dagger} \nabla_{\theta} f(\theta_t).$$

# Natural Policy Gradient (NPG)

### Natural Policy Gradient (Kakade, 2002)[9]

Given the reinforcement learning objective  $\max_{\theta} J(\pi_{\theta}) := \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^{t} r(s_{t}, a_{t}) | s_{0} \sim \mu, \pi_{\theta}\right] = \mathbb{E}_{s \sim \mu}[V^{\pi_{\theta}}(s)]$ , the iterates of NPG are given by

$$\theta_{t+1} = \theta_t + \eta(F_{\theta_t})^{\dagger} \nabla_{\theta} J(\pi_{\theta_t}),$$

where  $\eta > 0$  is the step-size of the algorithm.

**Key elements:**  $\circ F_{\theta}$  is the Fisher Information Matrix:

$$F_{\theta} = \mathbb{E}_{s \sim \lambda_{u}^{\pi_{\theta}}, a \sim \pi_{\theta}(\cdot | s)} \left[ \nabla_{\theta} \log \pi_{\theta}(a | s) \nabla_{\theta} \log \pi_{\theta}(a | s)^{\top} \right].$$

o  $\nabla_{\theta} J(\pi_{\theta})$  is the policy gradient, which can be written as follows

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

 $\circ A^{\pi_{\theta}}(s, a)$  is the advantage function:

$$A^{\pi_{\theta}}(s, a) = Q^{\pi_{\theta}}(s, a) - V^{\pi_{\theta}}(s).$$

 $\circ$   $C^{\dagger}$  is the Moore-Penrose inverse of a matrix C.



#### Interpretation of NPG

o The update rule of NPG can be viewed as solving the quadratic approximation of the problem:

$$\theta_{t+1} \approx \mathop{\arg\max}_{\theta} \left\{ J(\pi_{\theta}), \text{ s.t. } \operatorname{KL}\left(p_{\theta_t}(\tau) \| p_{\theta}(\tau)\right) \leq \delta \right\},$$

where  $p_{\theta}(\tau)$  is the probability measure of the random trajectory  $\tau = (s_0, a_0, r_1, \dots, \dots)$ .

#### **Explanation:**

o Approximate the objective with the first-order Taylor expansion:

$$J(\pi_{\theta}) \approx J(\pi_{\theta_t}) + \nabla_{\theta} J(\pi_{\theta_t})^{\top} (\theta - \theta_t).$$

o Approximate the constraint with the second-order Taylor expansion (See Slide 11):

$$\mathrm{KL}\left(p_{\theta_t}(\tau) \| p_{\theta}(\tau)\right) \approx \frac{1}{2} (\theta - \theta_t)^{\top} F_{\theta_t}(\theta - \theta_t) \leq \delta$$

• Set 
$$\delta = \frac{1}{2} \eta^2 \nabla_{\theta} f(\theta_t)^{\top} F_{\theta_t}^{\dagger} \nabla_{\theta} f(\theta_t)$$
 and see Slide 13

#### Question:

o How can we compute the iterates of natural policy gradient efficiently?

### Computing natural policy gradient

 $\circ$  As opposed to naively computing  $(F_{\theta})^{\dagger} \nabla_{\theta} J(\pi_{\theta})$  in NPG, we will use a key identity.

# Equivalent form of NPG (Appendix C.3 [2])

Let  $w^*(\theta)$  be such that

$$(1 - \gamma)(F_{\theta})^{\dagger} \nabla_{\theta} J(\pi_{\theta}) = w^{\star}(\theta).$$

Then,  $w^*(\theta)$  is the solution to the following least squares minimization problem:

$$w^{\star}(\theta) \in \arg\min_{w} \mathbb{E}_{s \sim \lambda_{\mu}^{\pi_{\theta}}, a \sim \pi_{\theta}(\cdot | s)} \left[ \left( w^{\top} \nabla_{\theta} \log \pi_{\theta}(a | s) - A^{\pi_{\theta}}(s, a) \right)^{2} \right], \tag{1}$$

where  $A^{\pi_{\theta}}(s,a)$  is the advantage function  $A^{\pi_{\theta}}(s,a) = Q^{\pi_{\theta}}(s,a) - V^{\pi_{\theta}}(s)$ .

#### Proof:

$$\nabla_{w} \mathbb{E}_{s \sim \lambda_{\mu}^{\pi_{\theta}}, a \sim \pi_{\theta}(\cdot | s)} \left[ \left( w^{\top} \nabla_{\theta} \log \pi_{\theta}(a | s) - A^{\pi_{\theta}}(s, a) \right)^{2} \right] \Big|_{w^{\star}(\theta)} = 0$$

$$2w^{\star}(\theta)^{\top} \underbrace{\mathbb{E}_{s \sim \lambda_{\mu}^{\pi_{\theta}}, a \sim \pi_{\theta}(\cdot | s)} \left[ \nabla_{\theta} \log \pi_{\theta}(a | s) \nabla_{\theta} \log \pi_{\theta}(a | s)^{\top} \right]}_{F_{\theta}} - 2\underbrace{\mathbb{E}_{s \sim \lambda_{\mu}^{\pi_{\theta}}, a \sim \pi_{\theta}(\cdot | s)} \left[ A^{\pi_{\theta}}(s, a) \nabla_{\theta_{t}} \log \pi_{\theta}(a | s) \right]}_{(1 - \gamma)\nabla_{\theta} J(\pi_{\theta})} = 0$$

$$w^{\star}(\theta) = (1 - \gamma)(F_{\theta})^{\dagger} \nabla_{\theta} J(\pi_{\theta})$$

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where  $A^{\pi_{\theta}}(s, a)$  is the advantage function  $A^{\pi_{\theta}}(s, a) = Q^{\pi_{\theta}}(s, a) - V^{\pi_{\theta}}(s)$ .

**Remarks:** o Note that since the update rule of NPG is  $\theta_{t+1} = \theta_t + \eta(F_\theta)^\dagger \nabla_\theta J(\pi_\theta)$ , we can rewrite NPG as:

$$\theta_{t+1} = \theta_t + \frac{\eta}{1-\gamma} w^*(\theta_t).$$

 $\circ w^*(\theta_t)$  can be obtained by solving (1) via conjugate gradients, SGD, and other solvers.

#### Example 1: Tabular NPG under softmax parameterization

o With softmax parameterization, the NPG becomes the policy mirror descent algorithm (Slide 11)

#### NPG parameter update

Consider the softmax parameterization  $\pi_{\theta}(a|s) = \frac{\exp(\theta_{s,a})}{\sum_{a'} \exp(\theta_{s,a'})}$  and denote  $\pi_t = \pi_{\theta_t}$ , the NPG parameter update can be simplified to the following:

$$\theta_{t+1} = \theta_t + \frac{\eta}{1 - \gamma} A^{\pi_t}.$$

Proof available in the Supplementary material.

### NPG policy update + softmax parametrization = policy mirror descent

In policy space, the induced update corresponds to the following:

$$\pi_{t+1}(a|s) = \pi_t(a|s) \frac{\exp(\eta/(1-\gamma) \cdot A^{\pi_t}(s,a))}{Z_t(s)}, \text{ where } Z_t(s) = \frac{\sum_{a'} \exp(\theta_{t,s,a'})}{\sum_{a'} \exp(\theta_{t,s,a'} + \eta/(1-\gamma) \cdot A^{\pi_t}(s,a'))}.$$

## **Example 2: NPG with linear function approximation**

o In this case, we can also express the NPG update rule via a regression problem.

#### NPG parameter update

Consider  $\pi_{\theta}(a|s) = \frac{\exp(\theta^{\top}\phi(s,a))}{\sum_{t} \exp(\theta^{\top}\phi(s,a'))}$  and denote  $\pi_{t} = \pi_{\theta_{t}}$ . In this case we have that

 $\nabla_{\theta} \log(\pi_{\theta}(a|s)) = \phi(s,a) - \sum_{a'} \pi_{\theta}(a|s')\phi(s,a')$  and consequently:

$$w^{\star}(\theta) \in \arg\min_{w} \mathbb{E}_{s \sim \lambda_{\mu}^{\pi_{\theta}}, a \sim \pi_{\theta}(\cdot \mid s)} \left[ \left( w^{\top} \left( \phi(s, a) - \sum_{a'} \pi_{\theta}(a \mid s') \phi(s, a') \right) - A^{\pi_{\theta}}(s, a) \right)^{2} \right].$$

Finally, the induced NPG parameter update becomes:  $\theta_{t+1} = \theta_t + \frac{\eta}{1-\gamma} w^\star(\theta_t)$ 

### NPG policy update + softmax parametrization = policy mirror descent

Similarly, we can obtain a mirror descent update rule in the policy space.

$$\pi_{t+1}(a|s) = \pi_t(a|s) \frac{\exp\left(\frac{\eta}{(1-\gamma)} w^\star(\theta_t)^\top \phi(s,a)\right)}{Z_t(s)}, \text{ where } Z_t(s) = \frac{\sum_{a'} \exp(\theta_{t,s,a'})}{\sum_{a'} \exp\left(\theta_{t,s,a'} + \frac{\eta}{(1-\gamma)} w^\star(\theta_t)^\top \phi(s,a')\right)}$$

### Convergence of tabular NPG with softmax parametrization

o Question: In the case of NPG with softmax parametrization, how fast do we converge to the optimal solution?

#### NPG policy update

Remember that for the softmax parametrization we have:

$$\pi_{t+1}(a|s) = \pi_t(a|s) \frac{\exp(\eta/(1-\gamma) \cdot A^{\pi_t}(s,a))}{Z_t(s)}$$

#### Convergence of tabular NPG [2]

In the tabular setting, for any  $\eta \geq (1-\gamma)^2 \log |\mathcal{A}|$  and T>0, the tabular NPG satisfies

$$J(\pi^{\star}) - J(\pi_T) \le \frac{2}{(1-\gamma)^2 T}.$$

- **Remarks:**  $\circ$  Nearly dimension-free convergence, no dependence on  $|\mathcal{A}|, |\mathcal{S}|$ .
  - No dependence on distribution mismatch coefficient.
  - $\circ$  In the case of known environment,  $\eta = \infty$  recovers Policy Iteration (Supplementary material)
- Question: What is the computational cost of this (nearly) dimension-free method?

#### Sample-based NPG

o **Questions:** What if we do not know the environment? Can we estimate  $A^{\pi_t}(s,a)$ ?

# Sample-based NPG Initialize policy parameter $\theta_0 \in \mathbb{R}^d$ , step size n > 0. $\alpha > 0$ for t = 0, 1, ..., T - 1 do {NPG steps} Initialize $w_0$ , denote $\pi_t = \pi_\theta$ . for n = 0, 1, ..., N - 1 do {Gradient Descent steps for the regression problem} Sample $s \sim \lambda_{\mu}^{\pi_t}$ , $a \sim \pi_t(\cdot|s)$ Estimate $\hat{A}(s, a)$ {Unbiased estimator of $A^{\pi_t}(s, a)$ } Update $w_{n+1} \leftarrow w_n - \alpha(w^\top \nabla_\theta \log \pi_t(a|s) - \hat{A}(s,a)) \cdot \nabla_\theta \log \pi_t(a|s)$ {Gradient Descent step} end for Update $\theta_{t+1} = \theta_t + \frac{\eta}{1-\gamma} w_N$ {NPG step} end for

# Extra: How to sample from an occupancy measure and estimate $\hat{A}(s,a)$ ?

# Sampling routine for $\lambda_{\mu}^{\pi}$

**Input**: a policy  $\pi$ .

Sample  $T \sim \text{Geom}(1 - \gamma)$  and  $s_0 \sim \mu$ .

for  $t=0,1,\dots,T-1$  do

Sample  $a_t \sim \pi(\cdot|s_t)$ .

Sample  $s_{t+1} \sim P(\cdot|s_t, a_t)$ .

end for

Output :  $(s_T, a_T)$ .

# An estimation routine for $\hat{Q}(s,a)$

**Input:** a policy  $\pi$ .

Sample  $(s_T, a_T) \sim \lambda_{\mu}^{\pi}$ , Initialize  $\hat{Q} = 0$ .

while True do

Sample  $s_{T+1} \sim P(\cdot|s_T, a_T)$ .

Sample  $a_{T+1} \sim \pi(\cdot|s_T)$ .

Set  $\hat{Q} = \hat{Q} + r_{T+1}$ .

Set T = T + 1.

With probility  $1-\gamma$  terminate.

end while

Output :  $\hat{Q}$ .

#### Remarks:

- See Algorithm 1 in [2].
- $\circ$  We sample from the occupancy measure by generating  $(s_T,a_T)$  with  $T\sim {\sf Geometric}(1-\gamma).$
- $\circ \hat{Q}$  is an unbiased estimate of  $Q(s_T, a_T)$ .
- $\circ$  Unbiased estimates of  $V(s_T)$  and  $A(s_T, a_T)$  can be obtained from  $\hat{Q}(s, a)$ .

## Convergence of sample-based NPG with function approximation

o We provide convergence guarantees for sample-based NPG in the linear function approximation case.

# Convergence of sampled-based NPG (informal)

Let  $\pi_{\theta}(a|s) = \frac{\exp(\theta^{\top}\phi(s,a))}{\sum_{s} \exp(\theta^{\top}\phi(s,a'))}$  and  $\theta^{\star}$  be the parameters associated to the optimal policy.

$$\mathbb{E}\left[\min_{t \leq T} J(\pi_{\theta^\star}) - J(\pi_{\theta_t})\right] \leq \mathcal{O}\left(\frac{1}{1-\gamma} \sqrt{\frac{2\log|A|}{T}} + \sqrt{\kappa \epsilon_{\mathsf{stat}}} + \sqrt{\epsilon_{\mathsf{bias}}}\right),$$

where  $\epsilon_{\rm stat}$  is how close  $w_t$  is to a  $w^*(\theta_t)$  (statistical error) and  $\epsilon_{\rm bias}$  is how good the best policy in the class is (function approximation error).

Remarks:

 $\circ~\epsilon_{\rm bias}=0$  under the so called "realizability" assumption for the features i.e.,

$$\forall \pi \in \Pi, \quad \exists \theta \quad \text{s.t.} \quad Q^{\pi}(s, a) = \theta^{\top} \phi(s, a) \quad \forall s, a \in \mathcal{S} \times \mathcal{A}.$$

$$\circ \ \kappa = \left\| \frac{\lambda_{\mu}^{\pi^{\star}}}{\mu} \right\|_{\infty}$$
 quantifies how exploratory the initial distribution is and **might be unbounded**

Question:

 $\circ$  Can we obtain an algorithm that converges in hard to explore environments (unbounded  $\kappa$ )?

# Markov Decision Processes - Experts (MDP-E) [7]

## Markov Decision Processes - Experts (MDP-E)

Initialize policy  $\pi_0$ , learning rate  $\eta$ 

for t = 0, 1, ..., T - 1 do

Evaluate  $Q^{\pi_t}(s, a)$  for every state action pair.

$$\pi_{t+1}(a|s) \propto \pi_t(a|s) \exp \eta Q^{\pi_t}(s,a).$$

end for

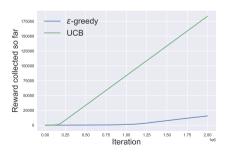
**Output :** A policy sampled uniformly at random from the sequence  $\pi_0, \ldots, \pi_{T-1}$ .

#### Remarks:

- o Check out the course Online Learning in Games!
- o MDP-E is a no-regret algorithm for adversarially changing rewards.
- o Therefore, it converges to the optimal policy for a fixed reward.

#### **Exploration in Policy Gradient methods**

- o When the transition dynamics of the agent are unknown the agent needs to explore the state space.
- $\circ$  Unless the initial state distribution is exploratory enough to guarantee  $\kappa$  small.
- $\circ$  Recall that  $\kappa$  is a constant appearing in the bound for sample based NPG.
- o Can we incorporate exploration techniques in policy gradient?
  - e.g.,  $\epsilon$ -greedy [17] and UCB [8] (we studied in the first coding exercise.)



#### Recall: Finite Horizon RL

- $\circ$  The agent interacts with the environment for K rounds with horizon H.
- $\circ$  The objective is to find the policy that maximizes  $\mathbb{E}_{\pi}\left[\sum_{h=1}^{H}r(s_{h},a_{h})\right]$ .
- o The optimal policy is non stationary.
- o A non stationary policy is a collection of H policies  $\pi_1, \ldots, \pi_H$ .
- o  $\pi_1$  is used for the first decision,  $\pi_2$  is used for the second decision and so on ....
- $\circ$  The value functions depend on the stage h, that is

$$Q_h^{\pi}(s,a) = \mathbb{E}_{\pi} \left[ \sum_{h'=h}^{H} r(s_{h'}, a_{h'}) | s_h = s, a_h = a \right], \quad V_h^{\pi}(s) = \mathbb{E}_{\pi} \left[ \sum_{h'=h}^{H} r(s_{h'}, a_{h'}) | s_h = s \right]$$

## Optimistic variant of the Proximal Policy Optimization (OPPO)

- o Key idea: Perform updates with optimistic estimates of the value function.
- o OPPO resambles NPG/MDP-E but with an optimistic evaluation step.

### OPPO [5] (simplified version)

Initialize policy parameter  $\theta_0 \in \mathbb{R}^d$ , step size  $\eta > 0$ ,  $\alpha > 0$  for  $t = 0, 1, \dots, T-1$  do

#### **Policy Evaluation**

Estimate bonus and transitions bonus<sub>h</sub>(s, a) and  $\hat{P}_h(s'|s, a)$ 

Compute optimistic value functions  $Q_h^t$ 

#### Policy Improvement

Update policies at every h, s, a with a NPG/MDP-E step

$$\pi_h^{t+1}(a|s) \propto \pi_h^t(a|s) \exp \eta Q_h^t(s,a)$$

end for

#### Estimate transition and bonuses

- o Compute the empirical average of the transition dynamics.
- $\circ$  Set the function bonus $_h^t(s,a)$  proportional to the square root of the inverse number of visits for s,a.
- o Intuition: The more often we visit a state, the more we expect the uncertainty to reduce.

### Estimating transitions and bonuses

```
\begin{aligned} &\text{for } t=0,1,\ldots,T-1 \text{ do} \\ &\text{for } h=0,1,\ldots,H-1 \text{ do} \\ &\text{Visit the state action pair } (s_h^t,a_h^t) \text{ and next state } s_{h+1}^t. \\ &\text{Update counts } N_h(s_h^t,a_h^t,s_{h+1}^t) \leftarrow N_h(s_h^t,a_h^t,s_{h+1}^t)+1,\ N(s_h^t,a_h^t) \leftarrow N(s_h^t,a_h^t)+1. \\ &\text{Estimate transtion } \hat{P}_h(s'|s,a) = \frac{N_h(s,a,s')}{N_h(s,a)+1} \text{ for all } s,a,s'. \\ &\text{Compute exploration bonuses } \mathrm{bonus}_h(s,a) \approx \sqrt{\frac{1}{N(s_h^t,a_h^t)}}. \\ &\text{end for end for } \end{aligned}
```

### Estimate optimistic value function

 $\circ$  Having estimated  $\hat{P}_h(s'|s,a)$  and the bonus  $\mathrm{bonus}_h^t(s,a)$ , we can compute  $Q_h^t(s,a)$  as follows.

### Backward induction to estimate $Q^t$ .

Initialize 
$$Q_{H+1}^t(s,a) = 0$$
.

for 
$$h = H, \dots, 1$$
 do

Recurse backward to compute  $Q_h^t$ 

$$Q_h^t(s, a) = r_h^t(s, a) + bonus_h^t(s, a) + \sum_{s', a'} \hat{P}_h(s'|s, a) \pi_{h+1}(a'|s') Q_{h+1}^t(s', a')$$

$$Q_h^t(s, a) = \text{clip}(Q_h^t(s, a); 0, H - h + 1)$$

end for

#### Remarks:

o If it holds that  $\left|\sum_{s'}(\hat{P}_h(s'|s,a)-P_h(s'|s,a))V(s')\right| \leq \mathrm{bonus}_h(s,a)$ , this construction ensures that Optimism and Bounded Optimism hold.

## Provable exploration in policy gradient

- $\circ$  Optimism means to overestimate the value of  $Q^{\pi_t}(s,a)$  at every state action pairs.
- $\circ$  Formally, it means that  $Q_h(s,a)$  satisfies

$$\begin{split} V_h^t(s) &= \mathbb{E}_{a \sim \pi(\cdot \mid s)}[Q_h^t(s, a)] \\ Q_h^t(s, a) &\geq r_h^t(s, a) + \sum_{s'} \mathsf{P}(s' \mid s, a) V_h^t(s') \end{split} \tag{Optimism}$$

- $\circ$  Notice that  $Q^{\pi_t}(s,a)$  would be the fixed point of the second expression.
- o At the same time we need an estimate that is not too optimistic.

$$r_h^t(s, a) + \sum_{s'} \mathsf{P}(s'|s, a) V_h^t(s') + 2\mathsf{bonus}_h^t(s, a) \ge Q_h^t(s, a)$$

(Bounded Optimism)

- $\circ$  bonus $_{b}^{t}(s,a)$  needs to be decreasing with the number of visits for (s,a).
- $\circ$  This ensures that  $Q_h^t(s,a) o Q_h^{\pi_t}(s,a)$

#### Benefit of OPPO

- $\text{o The regret bound of OPPO: } \sum\nolimits_{t=1}^{T} V^{\star}(s_1) V^{\pi_t}(s_1) \leq \mathcal{O}\bigg(\sum\nolimits_{h=1}^{H} \sum\nolimits_{t=1}^{T} \mathrm{bonus}_h^t(s_h^t, a_h^t)\bigg).$
- $\circ$  Next, one shows that  $\sum_{h=1}^{H}\sum_{t=1}^{T}\mathrm{bonus}_{h}^{t}(s_{h}^{t},a_{h}^{t})\leq\mathcal{O}(\sqrt{T}).$

#### Theorem

Let  $\pi^1, \pi^2, \dots, \pi^T$  the sequence of non stationary policies generated by OPPO. Then it holds that

$$\sum_{t=1}^{T} V^{\star}(s_1) - V^{\pi_t}(s_1) \le \mathcal{O}\left(\sqrt{T}\right)$$

This holds also when the reward function can change adversarially from episode to episode.

### Recall convergence of sampled-based NPG

$$\mathbb{E}\left[\min_{t \leq T} J(\pi_{\theta_t}) - J(\pi_{\theta_t})\right] \leq \mathcal{O}\left(\frac{1}{1-\gamma} \sqrt{\frac{2\log|A|}{T}} + \sqrt{\kappa \epsilon_{\mathsf{stat}}} + \sqrt{\epsilon_{\mathsf{bias}}}\right),$$

where  $\kappa$  depends on the initial distribution and the environment.

**Remarks:**  $\circ$  OPPO is much better because it removes the dependence on  $\kappa$ .

# **Revisiting baselines**

- The baselines can be used as a variance reduction mechanism.
- o Actually, one can prove which choice for the baseline guarantees minimum variance.

#### **Theorem**

Consider the gradient with baseline  $\widehat{\nabla}_{\theta}J(\pi_{\theta}) = \sum_{t=1}^{\infty} \left(Q^{\pi_{\theta}}(s_{t}, a_{t}) - b(s_{t})\right) \nabla \log \pi_{\theta}(a_{t}|s_{t})$  for a trajectory  $\tau \sim p_{\theta}$ . Then,  $b^{\star}(s) = \arg \min_{b:\mathcal{S} \to \mathbb{R}} \left[ \operatorname{Var} \left[ \widehat{\nabla}_{\theta}J(\pi_{\theta}) |s \right] \right]$  satisfies

$$b^{\star}(s) = \frac{\|Q^{\pi_{\theta}}(s, a) \log \pi_{\theta}(a|s)\|}{\|\nabla \log \pi_{\theta}(a|s)\|}.$$

#### Is it always good to minimize variance?

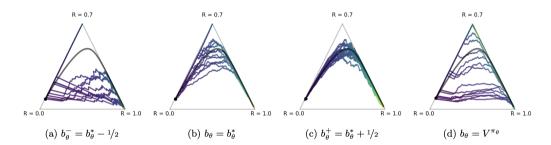
- o The answer is no. Because, reducing the variance of the baseline can hinder exploration.
- o As a result, the minimum variance baseline may lead to a suboptimal policy.
- o Here we describe the result in [6].

#### Theorem

Theorem 1 in [6] There exists a three-arm bandit where using the stochastic natural gradient on a softmax parameterized policy with the minimum-variance baseline can lead to convergence to a suboptimal policy with positive probability, and there is a different baseline (with larger variance) which results in convergence to the optimal policy with probability 1.

### Explore the baseline effect

o Three-arm bandit enviroment example:



- o The optimal policy plays the action in right corner.
- $\circ$  That is where the trajectories with baselines  $b_{\theta}^{+}$  and  $V^{\pi_{\theta}}$  converge to .
- o In the other cases, there are some trajectories converging to the top corner.
- o These results confirm the issue with the minimum variance baseline.

## Unbounded variance case [12]

- $\circ$  Consider a bandit experiment with stochastic rewards with an action dependent distribution R(a).
- o A common unbiased estimator is constructed using importance sampling.
- Using an action  $\hat{a} \sim \pi$  and observe  $r \sim R(\hat{a})$ .

$$\hat{r}(a) = \frac{r}{\pi(a)} \mathbf{1}(a = \hat{a})$$

o If we consider an additional baselines, we get the estimator

$$\hat{r}(a) = \frac{r - b}{\pi(a)} \mathbf{1}(a = \hat{a})$$

 $\circ$  The variance is unbounded no matter how b is chosen.

## **Popular Baselines**

### **Trust Region Policy Optimization**

John Schulman Sergey Levine Philipp Moritz Michael Jordan Pieter Abbeel JOSCHU @EECS.BERKELEY.EDU SLEVINE @EECS.BERKELEY.EDU PCMORITZ @EECS.BERKELEY.EDU JORDAN @CS.BERKELEY.EDU PABBEEL @CS.BERKELEY.EDU

University of California, Berkeley, Department of Electrical Engineering and Computer Sciences

TRPO (ICML, 2015)

## Proximal Policy Optimization Algorithms

John Schulman, Filip Wolski, Prafulla Dhariwal, Alec Radford, Oleg Klimov OpenAI

{joschu, filip, prafulla, alec, oleg}@openai.com

PPO (arXiv, 2017)

OpenAI implementation: https://github.com/openai/baselines

## Trust Region Policy Optimization (TRPO)

o How to choose the step-size of the stochastic policy gradient method? Trust region.

## TRPO (key idea) [14]

TRPO computes the marginal benefit of a new policy with respect to an old policy:

$$\theta_{t+1} = \underset{\theta}{\operatorname{arg\,max}} \quad \mathbb{E}_{s \sim \lambda_{\mu}^{\pi_{\theta_t}}, a \sim \pi_{\theta_t}(\cdot \mid s)} \left[ \frac{\pi_{\theta}(a \mid s)}{\pi_{\theta_t}(a \mid s)} A^{\pi_{\theta_t}}(s, a) \right],$$
s.t. 
$$\mathbb{E}_{s \sim \lambda_{\mu}^{\pi_{\theta_t}}} \left[ \operatorname{KL}(\pi_{\theta}(\cdot \mid s) || \pi_{\theta_t}(\cdot \mid s)) \right] \leq \delta.$$

where the constraint measures the distance between two policies.

### Remarks:

 $\circ$  The surrogate objective can be viewed as linear approximation in  $\pi$  of  $J(\pi_{\theta})$ :

$$J(\pi) = J(\pi_t) + \frac{1}{1 - \gamma} \mathbb{E}_{s \sim \lambda_{\mu}^{\pi}, a \sim \pi(a|s)} [A^{\pi_t}(s, a)].$$
 (PDL)

- o It can be approximated by a natural policy gradient step.
- o Line-search can ensure performance improvement and no constraint violation.

## TRPO: A detailed look at the implementation

- o Compute a search direction, which (almost) boils down to natural policy gradient.
  - ▶ The first order approximation of the objective.

$$\mathbb{E}_{s \sim \lambda_{\mu}^{\pi_{\theta_t}}, a \sim \pi_{\theta_t}(\cdot | s)} \left[ \frac{\pi_{\theta}(a | s)}{\pi_{\theta_t}(a | s)} A^{\pi_{\theta_t}}(s, a) \right] \approx \langle \nabla_{\theta} J(\theta_k), \theta - \theta_k \rangle$$

The second order expansion of the constraints

$$\mathbb{E}_{s \sim \lambda_{\mu}^{\pi_{\theta_t}}} \left[ \text{KL}(\pi_{\theta}(\cdot \mid s) || \pi_{\theta_t}(\cdot \mid s)) \right] \approx \frac{1}{2} (\theta - \theta_k)^T F(\theta_k) (\theta - \theta_k)$$

- $\circ$  Execute line seach along the direction  $F(\theta_k)^{\dagger} \nabla_{\theta} J(\theta_k)$ .
  - Approximations may result in a solution that does not satisfy the origin trust region.
  - $\blacktriangleright$  Select the largest possible step size  $\eta$  that  $x_{t+1} = x_t + \eta F(\theta_k)^{\dagger} \nabla_{\theta} J(\theta_k)$  satisfies the original constraints:

$$\eta = \sqrt{\frac{2\delta}{\nabla_{\theta} J(\theta_k)^{\top} F(\theta_k)^{\dagger} \nabla_{\theta} J(\theta_k)}}$$

## Equivalence between TRPO and MDP-E [7]

- o The previous result proves that TRPO produces a monotonically improving sequence of policies [14, Section 3].
- We can prove a stronger result noticing that TRPO is equivalent to MDP-E [13, Section B.3] and [7].

## **Proximal Policy Optimization (PPO2)**

- o Intuition: The main problem of TRPO lies in numerically computing the Quadratic Program.
- o Solution: Theoretical update equation is optimizing in a local region.

PPO uses no formal constraints and instead clips the distance between policies in the loss function.

## PPO (key idea) [15]

$$\max_{\theta} \quad \mathbb{E}_{s' \sim \lambda_{\mu}^{\pi_{\theta_t}}, a \sim \pi_{\theta_t}(\cdot \mid s)} \min \left\{ \frac{\pi_{\theta}(a \mid s)}{\pi_{\theta_t}(a \mid s)} A^{\pi_{\theta_t}}(s, a), \operatorname{clip}\left(\frac{\pi_{\theta}(a \mid s)}{\pi_{\theta_t}(a \mid s)}; 1 - \epsilon; 1 + \epsilon\right) A^{\pi_{\theta_t}}(s, a) \right\}$$

Remarks:

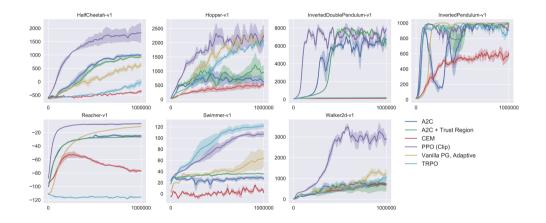
 $\circ$  PPO penalizes large deviation from the current policy directly inside the objective function through clipping the ratio  $\frac{\pi_{\theta}}{\pi_{\theta}}$ .

$$\operatorname{clip}(x;1-\epsilon;1+\epsilon) = \begin{cases} 1-\epsilon, \text{ if } x < 1-\epsilon \\ 1+\epsilon, \text{ if } x > 1+\epsilon \\ x, \text{ otherwise} \end{cases}$$

- o Run SGD. No need to deal with the KL divergence or trust region constraints.
- o Vastly adopted in practice but little is known about its theoretical properties.



## **Numerical Performance [15]**





## More Applications

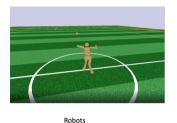






Figure: PPO performs well in many locomotion task and games.

- o Some links:
  - https://www.youtube.com/watch?v=hx\_bgoTF7bs
  - https://openai.com/blog/openai-baselines-ppo/

## Summary

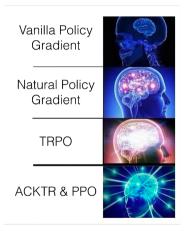




Figure from Schulman's slide on PPO in 2017.

## **Summary**

### Gradient Dominance Regularization



Vanilla Policy Gradient [16]	Gradient Descent
REINFORCE [18]	Stochastic Gradient Descent
Natural Policy Gradient [9]	
TRPO [1]	Mirror Descent
PPO [15]	
Conservative Policy Iteration [10]	Frank Wolfe

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# Supplementary Material



## Tabular NPG under softmax parametrization.

### Proof.

We need to show that  $w^*(\theta_t) = A^{\pi_t}$  in the case of softmax parametrization. To do so, we will first compute:

$$\nabla_{\theta} \log(\pi_{\theta}(a|s)) = \nabla_{\theta} \left( \theta_{s,a} - \log \left( \sum_{a'} \exp(\theta_{s,a'}) \right) \right) = e_{s,a} - \pi_{\theta}(\cdot|s).$$

In this case, we can check that  $A^{\pi_{\theta}} \in \arg\min_{w} \mathbb{E}_{s \sim \lambda_{\mu}^{\pi_{\theta}}, a \sim \pi_{\theta}(\cdot \mid s)} \left[ \left( w^{\top} \nabla_{\theta} \log \pi_{\theta}(a \mid s) - A^{\pi_{\theta}}(s, a) \right)^{2} \right]$  because:

$$\begin{split} \left(A^{\pi\theta}\,^\top\nabla_\theta\log\pi_\theta(a|s)-A^{\pi\theta}\,(s,a)\right) &= \left(A^{\pi\theta}\,^\top(e_{s,a}-\pi_\theta(\cdot|s))-A^{\pi\theta}\,(s,a)\right)\\ &= A^{\pi\theta}\,(s,a)-A^{\pi\theta}\,(s,a) + \sum_{a'}\pi_\theta(a'|s))A^{\pi\theta}\,(s,a')\\ & [\text{Def. of }A^{\pi\theta}\,(s,a)] = \sum_{a'}\pi_\theta(a'|s))(Q^{\pi\theta}\,(s,a')-V^{\pi\theta}\,(s))\\ & [\text{Def. of }V^{\pi\theta}\,(s)] = V^{\pi\theta}\,(s))-V^{\pi\theta}\,(s))\\ &= 0 \end{split}$$

## Proof of tabular NPG convergence

## Lemma (Policy Improvement)

For any policy  $\pi$  and  $\pi_{t+1}$  being obtained with NPG in the softmax parametrization setup, we can express the performance difference as:

$$J(\pi) - J(\pi_t) = \frac{1}{\eta} \mathbb{E}_{s \sim \lambda_{\mu}^{\pi}} \left[ \mathsf{KL}(\pi(\cdot|s) \| \pi_t(\cdot|s)) - \mathsf{KL}(\pi(\cdot|s) \| \pi_{t+1}(\cdot|s)) + \log Z_t(s) \right].$$

Proof sketch:

o Recall from Performance Difference Lemma:

$$J(\pi) - J(\pi_t) = \frac{1}{1 - \gamma} \mathbb{E}_{s \sim \lambda_{\mu}^{\pi}, a \sim \pi(a|s)} [A^{\pi_t}(s, a)].$$

o From the update rule  $\pi_{t+1}(a|s)=\pi_t(a|s)rac{\exp(\eta A^{\pi_t}(s,a)/(1-\gamma))}{Z_t(s)}$ , we have

$$A^{\pi_t}(s, a) = \frac{1 - \gamma}{\eta} \log \frac{\pi_{t+1}(a|s)Z_t(s)}{\pi_t(a|s)}.$$

o Combing these two equations, we have the above lemma.

## Proof of Tabular NPG convergence (cont'd)

### Proof (NPG):

 $\circ$  Setting  $\pi = \pi^*$  in the previous lemma and telescoping from  $t = 0, \dots, T-1$ 

$$\frac{1}{T} \sum_{t=0}^{T-1} J(\pi^*) - J(\pi_t) \le \frac{1}{\eta T} \mathbb{E}_{s \sim \lambda_{\mu}^{\pi^*}} \left[ KL(\pi^*(\cdot|s) \| \pi_0(\cdot|s)) \right] + \frac{1}{\eta T} \sum_{t=0}^{T} \mathbb{E}_{s \sim \lambda_{\mu}^{\pi^*}} \left[ \log Z_t(s) \right].$$

• Setting  $\pi = \pi_{t+1}$  in the previous lemma, we have

$$J(\pi_{t+1}) - J(\pi_t) \ge \frac{1}{\eta} \mathbb{E}_{s \sim \lambda_{\mu}^{\pi_{t+1}}} \left[ \log Z_t(s) \right] \ge \frac{1 - \gamma}{\eta} \mathbb{E}_{s \sim \mu} \left[ \log Z_t(s) \right] \ge 0, \forall \mu.$$

o Combining these two equations and the fact that  $J(\pi) \geq \frac{1}{1-\alpha}$  implies that

$$\frac{1}{T} \sum_{t=0}^{T-1} J(\pi^*) - J(\pi_t) \le \frac{\log |\mathcal{A}|}{\eta T} + \frac{1}{(1-\gamma)^2 T}.$$

## **NPG** in the $\eta = \infty$ setup.

In the case of being able to compute  $A^{\pi\theta}$ , and setting  $\eta=\infty$ , we can see that NPG is equivalent to Policy Iteration (Lecture 2). Taking the NPG update rule for the softmax parametrization to the limit:

$$\begin{split} \pi_{t+1}(a|s) &= \lim_{\eta \to \infty} \pi_t(a|s) \cdot \frac{\exp(\eta/(1-\gamma)A^{\pi_t}(s,a)) \cdot \sum_{a'} \exp(\theta_{t,s,a'})}{\sum_{a'} \exp(\theta_{t,s,a'} + \eta/(1-\gamma)A^{\pi_t}(s,a'))} \\ &= \lim_{\eta \to \infty} \frac{\pi_t(a|s)}{e^{\theta_{t,s,a}}} \cdot \frac{\exp(\theta_{t,s,a} + \eta/(1-\gamma)A^{\pi_t}(s,a)) \cdot \sum_{a'} \exp(\theta_{t,s,a'})}{\sum_{a'} \exp(\theta_{t,s,a'} + \eta/(1-\gamma)A^{\pi_t}(s,a'))} \\ &= \lim_{\eta \to \infty} \frac{\exp(\theta_{t,s,a} + \eta/(1-\gamma)A^{\pi_t}(s,a))}{\sum_{a'} \exp(\theta_{t,s,a'} + \eta/(1-\gamma)A^{\pi_t}(s,a'))} \\ &= \max x \}] = 1 \left\{ a = \max A^{\pi_t}(s,a') \right\}. \end{split}$$

$$[\lim_{\eta \to \infty} \operatorname{softmax}(\eta \cdot x)_i = \mathbbm{1}\{x_i = \max x\}] = \mathbbm{1}\left\{a = \max_{a'} A^{\pi_t}(s, a')\right\}\,.$$

This means under  $\eta = \infty$ , we have that NPG gives us a greedy policy, where the action taken is given by:

$$\arg \max_{a'} A^{\pi_t}(s, a') = \arg \max_{a'} Q^{\pi_t}(s, a') - V^{\pi_t}(s) = \arg \max_{a'} Q^{\pi_t}(s, a'),$$

which is precisely the update formula for Policy Iteration.

## Proof for the analytical expression with lowest variance.

### Proof.

Start noticing that

$$\operatorname{Var}\left[\widehat{\nabla}_{\theta}J(\pi_{\theta})|s\right] = \mathbb{E}\left[\left\|\widehat{\nabla}_{\theta}J(\pi_{\theta})\right\|^{2}|s\right] - \left\|\mathbb{E}\left[\widehat{\nabla}_{\theta}J(\pi_{\theta})|s\right]\right\|^{2}$$
$$= \mathbb{E}\left[\left\|\widehat{\nabla}_{\theta}J(\pi_{\theta})\right\|^{2}|s\right] - \left\|\mathbb{E}_{a \sim \pi_{\theta}(\cdot|s)}\left[Q^{\pi_{\theta}}(s, a)\nabla\log\pi_{\theta}(a|s)\right]\right\|^{2}$$

Therefore  $\nabla_b \mathrm{Var}\left[\widehat{\nabla}_\theta J(\pi_\theta)|s\right] = \nabla_b \mathbb{E}\left[\left\|\widehat{\nabla}_\theta J(\pi_\theta)\right\|^2|s\right]$ . Developing the norm squared and differentianting, we get

$$\nabla_{b} \mathbb{E}\left[\left\|\widehat{\nabla}_{\theta} J(\pi_{\theta})\right\|^{2} | s\right] = 2\left(b(s) \mathbb{E}_{a \sim \pi_{\theta}(\cdot \mid s)} \left[\left\|\nabla \log \pi_{\theta}(a \mid s)\right\|^{2}\right] - \mathbb{E}_{a \sim \pi_{\theta}(\cdot \mid s)} \left[Q^{\pi_{\theta}}(s, a) \left\|\nabla \log \pi_{\theta}(a \mid s)\right\|^{2}\right]\right)$$

Therefore, the proof is concluded setting  $b^*$  to minimize the latter expression.