Foundations of Reinforcement Learning

Policy optimization: REINFORCE, PG and NPG

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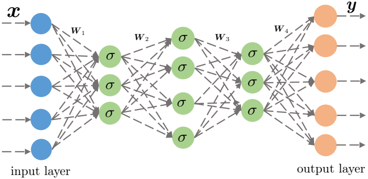
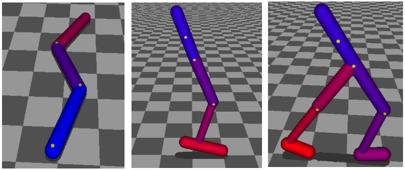
Outline

Policy optimization

$$\text{maximize}_\theta \quad \text{value}(\text{policy}(\theta))$$

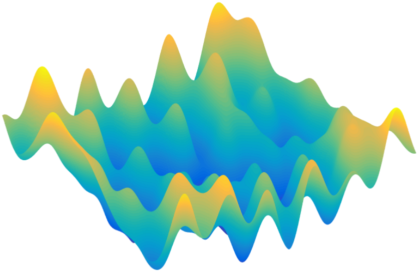
- directly optimize the policy, which is the quantity of interest;
- allow flexible differentiable parameterizations of the policy;
- work with both continuous and discrete problems.





Theoretical challenges: non-concavity

Little understanding on the global convergence of policy gradient methods until very recently, e.g. (Fazel et al., 2018; Bhandari and Russo, 2019; Agarwal et al., 2019; Mei et al. 2020), and many more.



Our goal:

- introduce the algorithmic framework of popular policy gradient methods
- understand finite-time convergence rates of popular heuristics

Introduction to policy gradient methods

Policy gradient methods

Given an initial state distribution $s \sim \rho$, find policy π such that

$$\text{maximize}_{\pi} \quad V^{\pi}(\rho) := \mathbb{E}_{s \sim \rho}\left[V^{\pi}(s)\right]$$

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Policy gradient method

For $t = 0, 1, \cdots$

$$\theta^{(t+1)} = \theta^{(t)} + \eta \nabla_\theta V^{\pi_\theta^{(t)}}(\rho)$$

where η *is the learning rate.*

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How to calculate the gradient?

Policy gradient derivation

- Assume π_θ is differentiable when it is non-zero with gradient $\nabla_\theta \pi_\theta$.

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The policy gradient can be decomposed as

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\begin{aligned}
&\nabla_\theta V^{\pi_\theta}(\rho) \\
&= \nabla_\theta \mathbb{E}_{s_0 \sim \rho}\left[V^{\pi_\theta}(s_0)\right] \\
&= \mathbb{E}_{s_0 \sim \rho}\left[\nabla_\theta\left(\sum_{a_0 \in \mathcal{A}} \pi_\theta(a_0|s_0) Q^{\pi_\theta}(s_0, a_0)\right)\right] \\
&= \mathbb{E}_{s_0 \sim \rho}\left[\sum_{a_0 \in \mathcal{A}} \nabla_\theta \pi_\theta(a_0|s_0) Q^{\pi_\theta}(s_0, a_0) + \sum_{a_0 \in \mathcal{A}} \pi_\theta(a_0|s_0) \nabla_\theta Q^{\pi_\theta}(s_0, a_0)\right]
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\end{aligned}
$$

We discuss the two terms separately.

Policy gradient derivation - first term

Note that

$$\nabla_\theta \pi_\theta(a|s) = \pi_\theta(a|s)\frac{\nabla_\theta \pi_\theta(a|s)}{\pi_\theta(a|s)} = \pi_\theta(a|s)\underbrace{\nabla_\theta \log \pi_\theta(a|s)}_{\text{score function}}.$$

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The first term in the policy gradient is expressed as

$$\begin{aligned} &\mathbb{E}_{s_0 \sim \rho} \left[\sum_{a_0 \in \mathcal{A}} \nabla_\theta \pi_\theta(a_0|s_0) Q^{\pi_\theta}(s_0, a_0) \right] \\ &= \mathbb{E}_{s_0 \sim \rho} \left[\sum_{a_0 \in \mathcal{A}} \pi_\theta(a_0|s_0) \nabla_\theta \log \pi_\theta(a_0|s_0) Q^{\pi_\theta}(s_0, a_0) \right] \\ &= \mathbb{E}_{s_0 \sim \rho, a_0 \sim \pi_\theta(\cdot|s_0)} \left[\nabla_\theta \log \pi_\theta(a_0|s_0) Q^{\pi_\theta}(s_0, a_0) \right] \end{aligned}$$

Policy gradient derivation - second term

The second term in the policy gradient is expressed as

$$\begin{aligned}
&\mathbb{E}_{s_0\sim\rho}\left[\sum_{a_0\in\mathcal{A}}\pi_\theta(a_0|s_0)\nabla_\theta Q^{\pi_\theta}(s_0,a_0)\right]\\
&=\mathbb{E}_{s_0\sim\rho,a_0\sim\pi_\theta(\cdot|s_0)}\big[\nabla_\theta Q^{\pi_\theta}(s_0,a_0)\big]\\
&=\mathbb{E}_{s_0\sim\rho,a_0\sim\pi_\theta(\cdot|s_0)}\left[\nabla_\theta\big(r(s_0,a_0)+\gamma\mathbb{E}_{s_1\sim P(\cdot|s_0,a_0)}V^{\pi_\theta}(s_1)\big)\right]\\
&=\gamma\mathbb{E}_{s_0\sim\rho,a_0\sim\pi_\theta(\cdot|s_0),s_1\sim P(\cdot|s_0,a_0)}\big[\nabla_\theta V^{\pi_\theta}(s_1)\big],
\end{aligned}$$

which is similar to what we want to bound, but a discounted one-step look-ahead.

Policy gradient derivation - recursion

Letting τ denote the trajectory following policy π_θ, by recursion,

$$\begin{aligned}\nabla_\theta V^{\pi_\theta}(\rho) = \mathbb{E}_{s_0\sim\rho, a_0\sim\pi_\theta(\cdot|s_0)}\left[\nabla_\theta \log \pi_\theta(a_0|s_0) Q^{\pi_\theta}(s_0, a_0)\right] \\ + \gamma \mathbb{E}_{s_0\sim\rho, a_0\sim\pi_\theta(\cdot|s_0), s_1\sim P(\cdot|s_0,a_0)}\left[\nabla_\theta V^{\pi_\theta}(s_1)\right]\end{aligned}$$

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&= \mathbb{E}_{(s_i, a_i)_{i \geq 0} \sim \tau} \left[\sum_{i=0}^{\infty} \gamma^t \nabla_\theta \log \pi_\theta(a_i|s_i) Q^{\pi_\theta}(s_i, a_i) \right]
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&= \frac{1}{1-\gamma} \mathbb{E}_{s\sim d_\rho^{\pi_\theta}, a\sim\pi_\theta(\cdot|s)}\Big[Q^{\pi_\theta}(s,a)\nabla \log \pi_\theta(a|s)\Big],
\end{aligned}$$

where $d_\rho^{\pi_\theta}$ is the **state visitation distribution:**

$$d_{s_0}^{\pi}(s) = (1-\gamma)\sum_{t=0}^{\infty}\gamma^t \mathbb{P}^{\pi}(s_t = s \mid s_0), \qquad d_\rho^\pi = \mathbb{E}_{s_0\sim\rho}[d_{s_0}^\pi(s)].$$

The policy gradient theorem

Theorem 1 (Policy gradient theorem [Sutton et al., 1999])

The policy gradient can be evaluated via

$$\nabla_\theta V^{\pi_\theta}(\rho) = \frac{1}{1-\gamma} \mathbb{E}_{s \sim d_\rho^{\pi_\theta}, a \sim \pi_\theta(\cdot|s)} \Big[Q^{\pi_\theta}(s,a) \nabla \log \pi_\theta(a|s) \Big],$$

where

- $d_\rho^{\pi_\theta}$ *is the state visitation distribution,*
- $\nabla \log \pi_\theta(a|s)$ *is the score function.*

Provides an effective scheme for policy gradient evaluation (e.g., REINFORCE):

- rolling out trajectory following π_θ
- evaluating the value function Q^{π_θ}

Examples of policy parameterization

Discrete action space: softmax parameterization with function approximation

$$\pi_\theta(a|s) \propto \exp(\phi(s,a)^\top \theta)$$

- $\phi(s,a)$ is the feature vector of each state-action pair;
- the score function $\nabla \log \pi_\theta(a|s) = \phi(s,a) - \mathbb{E}_{a\sim\pi_\theta(\cdot|s)}[\phi(s,\cdot)]$.

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Continuous action space: Gaussian policy

$$a \sim \mathcal{N}(\mu(s), \sigma^2), \quad \mu(s) = \phi(s)^\top \theta$$

- $\phi(s)$ is the feature of each state;
- σ^2 is the variance (kept constant for simplicity);
- the score function $\nabla \log \pi_\theta(a|s) = \frac{(a-\mu(s))\phi(s)}{\sigma^2}$.

Baseline

The policy gradient can have high variance with limited samples.

Variance reduction: introducing a baseline

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

to help minimize the variance:

$$\begin{aligned}
\mathbb{E}_{a\sim\pi_\theta(\cdot|s)}\Big[\nabla \log \pi_\theta(a|s)\Big] &= \sum_a \pi_\theta(a|s)\frac{\nabla_\theta \pi_\theta(a|s)}{\pi_\theta(a|s)} \\
&= \sum_a \nabla_\theta \pi_\theta(a|s) \\
&= \nabla_\theta \sum_a \pi_\theta(a|s) = 0
\end{aligned}$$

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- In practice, choose $b(s) = V^{\pi_\theta}(s)$, leading to

$$\nabla_\theta V^{\pi_\theta}(\rho) = \frac{1}{1-\gamma}\mathbb{E}_{s\sim d_\rho^{\pi_\theta}, a\sim\pi_\theta(\cdot|s)}\Big[A^{\pi_\theta}(s,a)\nabla \log \pi_\theta(a|s)\Big]$$

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- $A^\pi(s,a) = Q^\pi(s,a) - V^\pi(s)$ is the advantage function.
- Instead of estimating $Q^\pi(s,a)$, directly estimate $A^\pi(s,a)$.

Global convergence of softmax policy gradient methods

Softmax policy gradient methods

Given an initial state distribution $s \sim \rho$, find policy π such that

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softmax parameterization:

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where η *is the learning rate.*

Global convergence of the PG method

Exact gradient evaluation: suppose we can perfectly evaluate the gradient

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Theorem 2 ([Agarwal et al., 2021])

Assume ρ is strictly positive, i.e., $\rho(s) > 0$ for all states s. For $\eta \leq (1-\gamma)^3/8$, then we have that for all states s,

$$V^{(t)}(s) = V^{\pi_\theta^{(t)}}(s) \to V^\star(s), \qquad t \to \infty.$$

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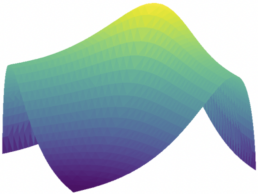
- Softmax policy gradient finds the global optimal policy despite nonconcavity!

How fast does softmax PG converge?



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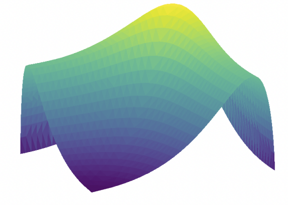

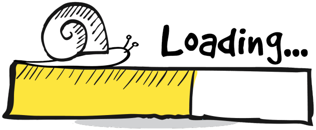

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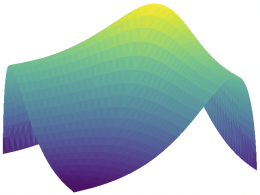

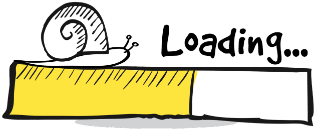

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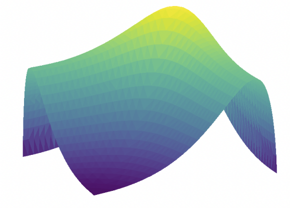

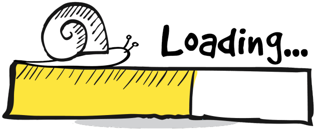

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Is the rate of PG good, bad or ugly?

A negative message

Theorem 3 ([Li et al., 2023])

There exists an MDP s.t. it takes softmax PG at least

$$\frac{1}{\eta}\,|\mathcal{S}|^{2^{\Theta(\frac{1}{1-\gamma})}} \text{ iterations}$$

to achieve $\|V^{(t)} - V^{\star}\|_{\infty} \leq 0.15$.

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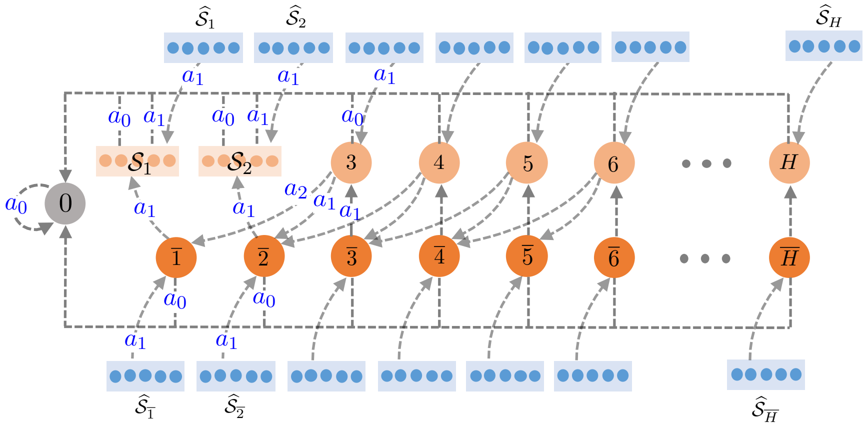
- Softmax PG can take (super)-exponential time to converge (in problems w/ large state space $\&$ long effective horizon)!
- Also hold for average sub-opt gap $\frac{1}{|\mathcal{S}|}\sum_{s\in\mathcal{S}}\left[V^{(t)}(s) - V^{\star}(s)\right]$.

MDP construction for our lower bound



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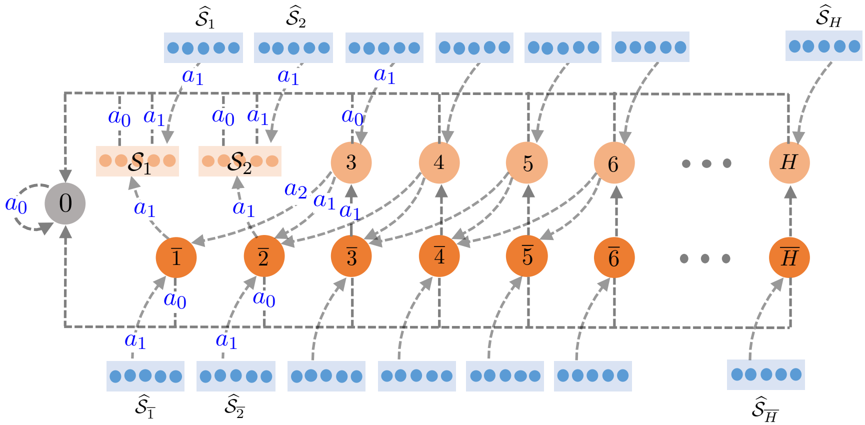

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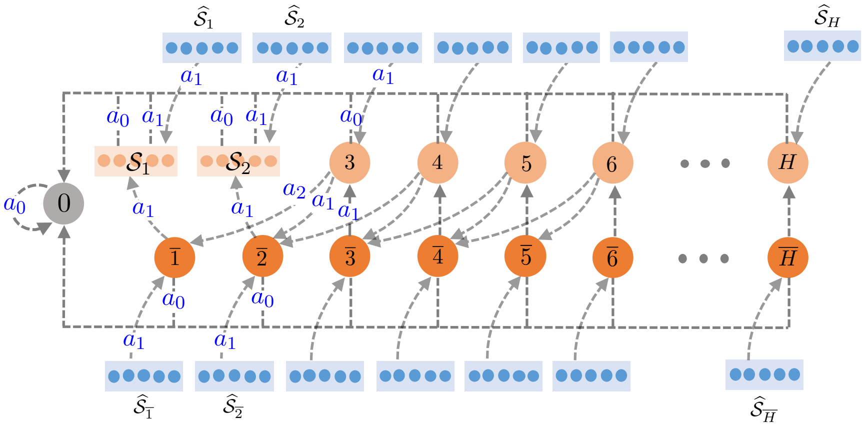
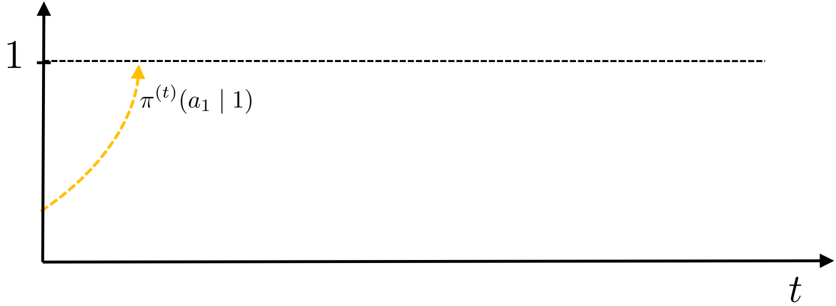


Key ingredients: for $3 \leq s \leq H \asymp \frac{1}{1-\gamma}$,

- $\pi^{(t)}(a_{\mathsf{opt}} \mid s)$ keeps decreasing until $\pi^{(t)}(a_{\mathsf{opt}} \mid s-2) \approx 1$

What is happening in our constructed MDP?



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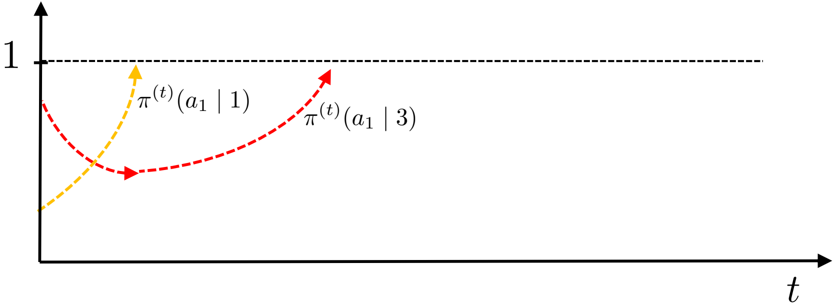

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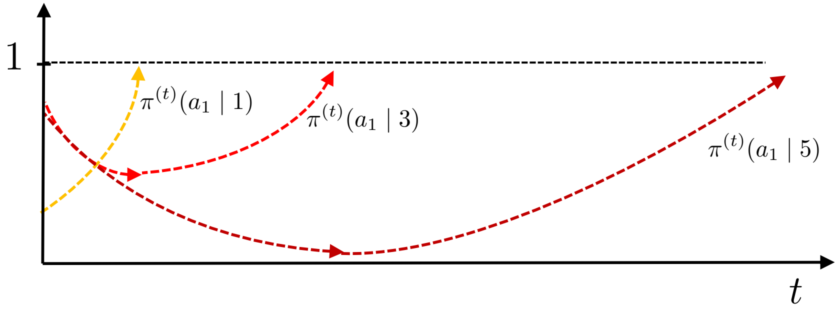

Convergence time for state s grows geometrically as s increases

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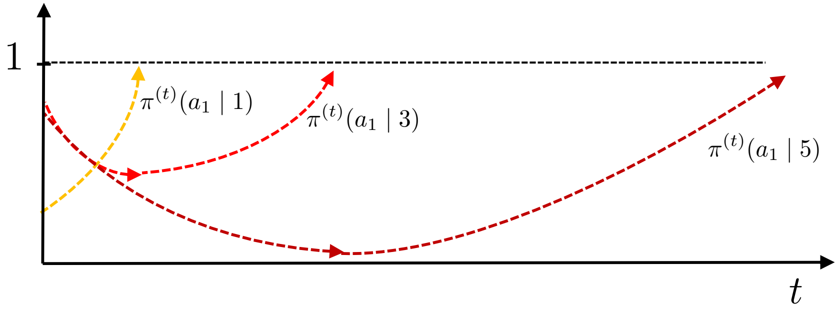
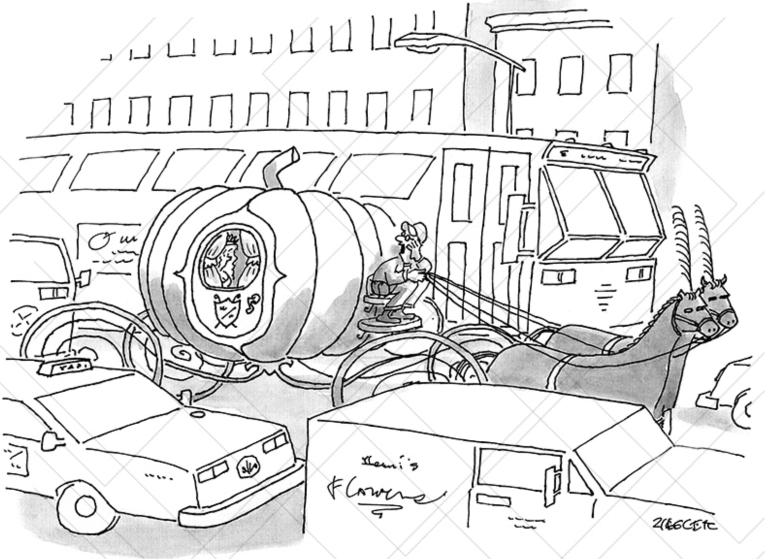


Convergence time for state s grows geometrically as s increases

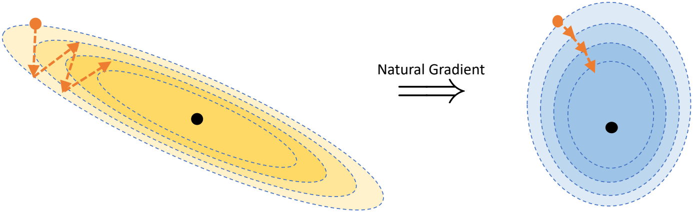
$$\text{convergence-time}(s) \gtrsim \big(\text{convergence-time}(s-2)\big)^{1.5}$$



"Seriously, lady, at this hour you'd make a lot better time taking the subway."

Natural policy gradient methods

Natural policy gradient



Natural policy gradient (NPG) method [Kakade, 2001]

For $t = 0, 1, \cdots$

$$\theta^{(t+1)} = \theta^{(t)} + \eta (\mathcal{F}_\rho^\theta)^\dagger \nabla_\theta V^{\pi_\theta^{(t)}}(\rho)$$

where η is the learning rate and $\mathcal{F}_\rho^\theta$ is the Fisher information matrix:

$$\mathcal{F}_\rho^\theta := \mathbb{E}\left[\big(\nabla_\theta \log \pi_\theta(a|s)\big) \big(\nabla_\theta \log \pi_\theta(a|s)\big)^\top \right].$$

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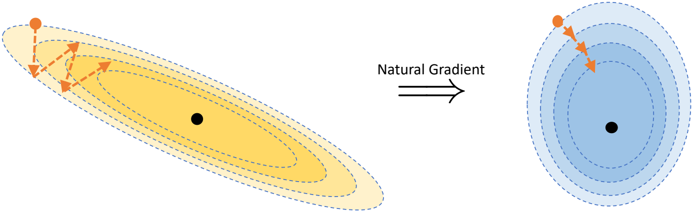

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Connection with TRPO/PPO

TRPO/PPO (Schulman et al., 2015; 2017) are popular heuristics in training RL algorithms, with **KL regularization**

$$\mathsf{KL}(\pi_\theta^{(t)} \| \pi_\theta) \approx \frac{1}{2}(\theta - \theta^{(t)})^\top \mathcal{F}_\rho^\theta (\theta - \theta^{(t)})$$

via constrained or proximal terms:

$$\begin{aligned} \theta^{(t+1)} &= \operatorname*{argmax}_\theta V^{\pi_\theta^{(t)}}(\rho) + (\theta - \theta^{(t)})^\top \nabla_\theta V^{\pi_\theta^{(t)}}(\rho) - \eta \mathsf{KL}(\pi_\theta^{(t)} \| \pi_\theta) \\ &\approx \theta^{(t)} + \eta (\mathcal{F}_\rho^\theta)^\dagger \nabla_\theta V^{\pi_\theta^{(t)}}(\rho), \end{aligned}$$

leading to exactly NPG!

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NPG $\approx$ TRPO/PPO!

NPG in the tabular setting

Natural policy gradient (NPG) method (Tabular setting)

For $t = 0, 1, \cdots,$ *NPG updates the policy via*

$$\pi^{(t+1)}(\cdot|s) \propto \underbrace{\pi^{(t)}(\cdot|s)}_{\text{current policy}} \underbrace{\exp\left(\frac{\eta Q^{(t)}(s,\cdot)}{1-\gamma}\right)}_{\text{soft greedy}} \propto \pi^{(t)}(\cdot|s) \exp\left(\frac{\eta A^{(t)}(s,\cdot)}{1-\gamma}\right)$$

where $Q^{(t)} := Q^{\pi^{(t)}}$ *and* $A^{(t)} := A^{\pi^{(t)}}$ *is the Q/advantage function of* $\pi^{(t)}$*, and* $\eta > 0$ *is the learning rate.*

- the derivation is left as an exercise; see [Agarwal et al., 2019].

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- invariant with the choice of ρ
- Reduces to policy iteration (PI) when $\eta = \infty$.

Global convergence of NPG

Theorem 4 ([Agarwal et al., 2021])

Set $\pi^{(0)}$ *as a uniform policy. For all* $t \geq 0$, *we have*

$$V^{(t)}(\rho) \geq V^{\star}(\rho) - \left(\frac{\log |\mathcal{A}|}{\eta} + \frac{1}{(1-\gamma)^2} \right) \frac{1}{t}.$$

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Implication: set $\eta \geq (1-\gamma)^2 \log |\mathcal{A}|$, we find an ϵ-optimal policy within at most

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Global convergence at a sublinear rate independent of $|\mathcal{S}|$, $|\mathcal{A}|$!

Key ingredients of the proof

Lemma 5 (Performance difference lemma)

For all policies π, π' and distributions ρ over $\mathcal{S}$,

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

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- measures the performance difference for any pairs of policies

Lemma 6 (Policy improvement of NPG)

$$V^{(t+1)}(\rho) - V^{(t)}(\rho) \geq \frac{(1-\gamma)}{\eta}\mathbb{E}_{s \sim \rho} \log Z_t(s) \geq 0$$

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

- monotonic performance improvement of NPG

Step 1: bounding the optimality gap

Denote $d^\star := d^\star_\rho$, and $\pi_s := \pi(\cdot|s)$. By the performance difference lemma,

$$
\begin{aligned}
& V^\star(\rho) - V^{(t)}(\rho) \\
&= \frac{1}{1-\gamma}\mathbb{E}_{s\sim d^\star} \sum_a \pi^\star(a|s) A^{(t)}(s,a) \\
&= \frac{1}{\eta}\mathbb{E}_{s\sim d^\star} \sum_a \pi^\star(a|s) \log \frac{\pi^{(t+1)}(a|s) Z_t(s)}{\pi^{(t)}(a|s)} \\
&= \frac{1}{\eta}\mathbb{E}_{s\sim d^\star} \left(\mathsf{KL}(\pi_s^\star \| \pi_s^{(t)}) - \mathsf{KL}(\pi_s^\star \| \pi_s^{(t+1)}) + \sum_a \pi^\star(a|s) \log Z_t(s) \right) \\
&= \frac{1}{\eta}\mathbb{E}_{s\sim d^\star} \Big(\mathsf{KL}(\pi_s^\star \| \pi_s^{(t)}) - \mathsf{KL}(\pi_s^\star \| \pi_s^{(t+1)}) + \log Z_t(s) \Big).
\end{aligned}
$$

Step 2: telescoping

By the improvement lemma $V^{(t+1)}(\rho) \geq V^{(t)}(\rho)$,

$$
\begin{aligned}
V^\star(\rho) - V^{(T-1)}(\rho) &\leq \frac{1}{T}\sum_{t=0}^{T-1}\Big(V^\star(\rho) - V^{(t)}(\rho)\Big) \\
&= \frac{1}{\eta T}\sum_{t=0}^{T-1}\mathbb{E}_{s\sim d^\star}\Big(\mathsf{KL}(\pi_s^\star \| \pi_s^{(t)}) - \mathsf{KL}(\pi_s^\star \| \pi_s^{(t+1)}) + \log Z_t(s)\Big) \\
&\leq \frac{1}{\eta T}\mathbb{E}_{s\sim d^\star}\mathsf{KL}(\pi_s^\star \| \pi_s^{(0)}) + \frac{1}{\eta T}\sum_{t=0}^{T-1}\mathbb{E}_{s\sim d^\star}\log Z_t(s),
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&\leq \frac{1}{\eta T}\mathbb{E}_{s\sim d^\star}\mathsf{KL}(\pi_s^\star \| \pi_s^{(0)}) + \frac{1}{\eta T}\sum_{t=0}^{T-1}\mathbb{E}_{s\sim d^\star}\log Z_t(s),
\end{aligned}$$

where the second term is bounded by the policy improvement lemma

$$\begin{aligned}
\frac{1}{\eta}\sum_{t=0}^{T-1}\mathbb{E}_{s\sim d^\star}\log Z_t(s) &\leq \frac{1}{1-\gamma}\sum_{t=0}^{T-1}\Big(V^{(t+1)}(d^\star) - V^{(t)}(d^\star)\Big) \\
&\leq \frac{1}{1-\gamma}\Big(V^{(T)}(d^\star) - V^{(0)}(d^\star)\Big)
\end{aligned}$$

Step 3: finishing up

Putting the above together,

$$\begin{aligned} & V^\star(\rho) - V^{(T-1)}(\rho) \\ & \leq \frac{1}{\eta T}\mathbb{E}_{s\sim d^\star}\mathsf{KL}(\pi_s^\star \| \pi_s^{(0)}) + \frac{1}{(1-\gamma)T}\Big(V^{(T)}(d^\star) - V^{(0)}(d^\star)\Big) \\ & \leq \frac{\log|\mathcal{A}|}{\eta T} + \frac{1}{(1-\gamma)^2 T}, \end{aligned}$$

where we used $\mathsf{KL}(\pi_s^\star \| \pi_s^{(0)}) \leq \log|\mathcal{A}|$ and $V \leq \frac{1}{1-\gamma}$.

Proof of Lemma 6

Proof of $\log Z_t(s) \geq 0$**:**

$$\begin{aligned}
\log Z_t(s) &= \log \sum_a \pi^{(t)}(a|s) \exp\left(\eta A^{(t)}(s,a)/(1-\gamma)\right) \\
&\geq \sum_a \pi^{(t)}(a|s) \log \exp\left(\eta A^{(t)}(s,a)/(1-\gamma)\right) \qquad \text{(Jensen's inequality)} \\
&= \frac{\eta}{1-\gamma} \sum_a \pi^{(t)}(a|s) A^{(t)}(s,a) \\
&= \frac{\eta}{1-\gamma} \sum_a \pi^{(t)}(a|s) (Q^{\pi^{(t)}}(s,a) - V^{\pi^{(t)}}(s)) \\
&= 0
\end{aligned}$$

Proof of Lemma 6

Bounding $V^{(t+1)}(\rho) - V^{(t)}(\rho)$: by the performance difference lemma,

$$
\begin{aligned}
V^{(t+1)}(\rho) - V^{(t)}(\rho) &= \frac{1}{1-\gamma}\mathbb{E}_{s\sim d_\rho^{(t+1)}} \sum_a \pi^{(t+1)}(a|s) A^{(t)}(s,a) \\
&= \frac{1}{\eta}\mathbb{E}_{s\sim d_\rho^{(t+1)}} \sum_a \pi^{(t+1)}(a|s) \log \frac{\pi^{(t+1)}(a|s) Z_t(s)}{\pi^{(t)}(a|s)} \\
&= \frac{1}{\eta}\mathbb{E}_{s\sim d_\rho^{(t+1)}} \mathsf{KL}(\pi^{(t+1)}(s) \| \pi^{(t)}(s)) + \frac{1}{\eta}\mathbb{E}_{s\sim d_\rho^{(t+1)}} \log Z_t(s) \\
&\geq \frac{(1-\gamma)}{\eta}\mathbb{E}_{s\sim\rho} \log Z_t(s),
\end{aligned}
$$

where we use $d_\rho^{(t+1)} \geq (1-\gamma)\rho$ and $\log Z_t(s) \geq 0$.

References I

Agarwal, A., Jiang, N., Kakade, S. M., and Sun, W. (2019).
Reinforcement learning: Theory and algorithms.

Agarwal, A., Kakade, S. M., Lee, J. D., and Mahajan, G. (2021).
On the theory of policy gradient methods: Optimality, approximation, and distribution shift.
The Journal of Machine Learning Research, 22(1):4431–4506.

Kakade, S. M. (2001).
A natural policy gradient.
Advances in Neural Information Processing Systems, 14.

Li, G., Wei, Y., Chi, Y., and Chen, Y. (2023).
Softmax policy gradient methods can take exponential time to converge.
Mathematical Programming.

Mei, J., Xiao, C., Szepesvari, C., and Schuurmans, D. (2020).
On the global convergence rates of softmax policy gradient methods.
In *International Conference on Machine Learning*, pages 6820–6829. PMLR.

Sutton, R. S., McAllester, D., Singh, S., and Mansour, Y. (1999).
Policy gradient methods for reinforcement learning with function approximation.
Advances in neural information processing systems, 12.