Taming nonconvexity in policy optimization

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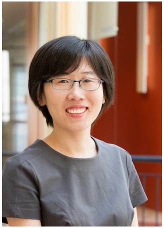

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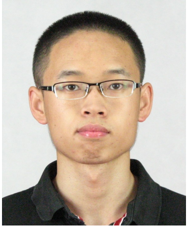
"Fast global convergence of natural policy gradient methods with entropy regularization," S. Cen, C. Cheng, Y. Chen, Y. Wei, Y. Chi, under revision, *Operations Research*, 2020



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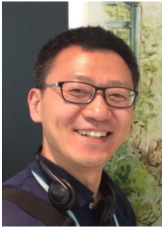

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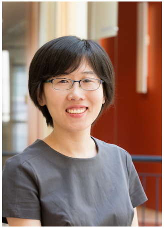

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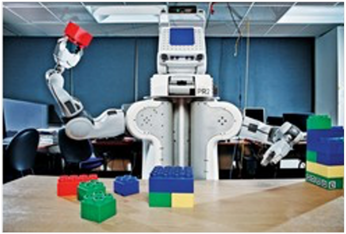
"Softmax policy gradient methods can take exponential time to converge,"
G. Li, Y. Wei, Y. Chi, Y. Gu, Y. Chen, arxiv:2102.11270, 2021

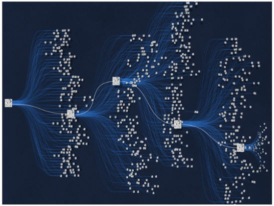
Reinforcement learning (RL)



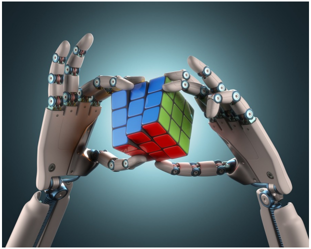
RL challenges

In RL, an agent learns by interacting with an environment

- unknown or changing environments
- delayed rewards or feedback
- enormous state and action space
- trial-and-error
- nonconvexity



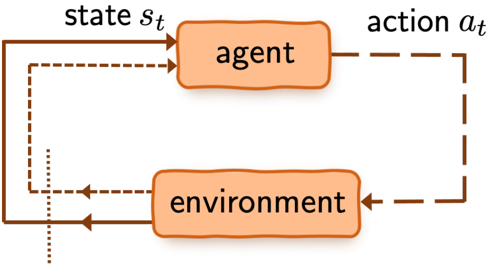
Recent successes in RL

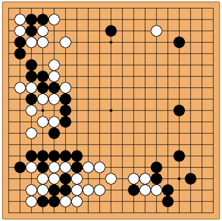


Policy optimization: a major contributor to these successes

Backgrounds: policy optimization for MDPs

Markov decision process (MDP)





- $\mathcal{S}$: state space
- $\mathcal{A}$: action space

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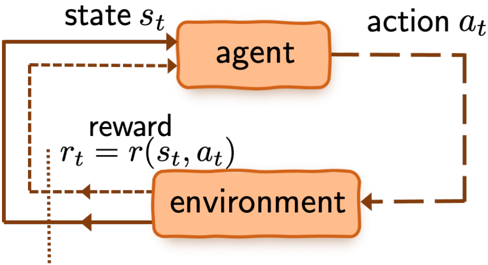

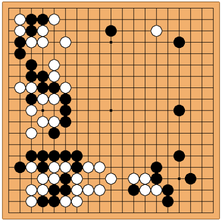

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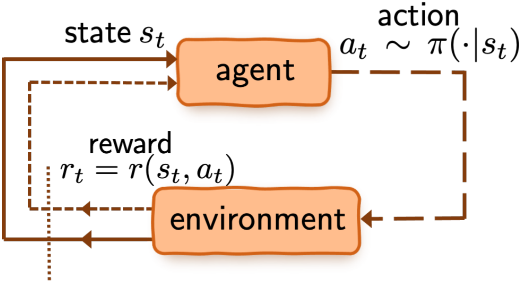

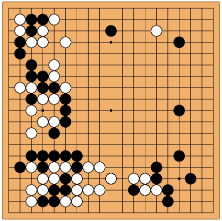

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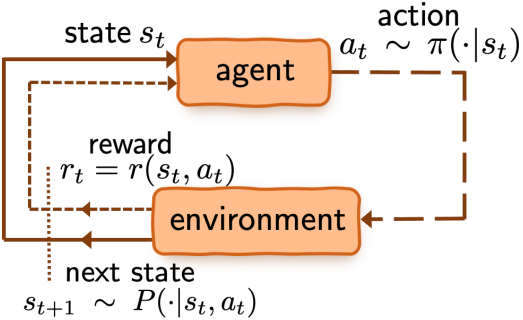

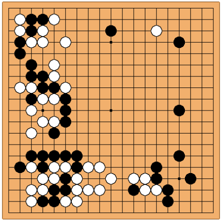

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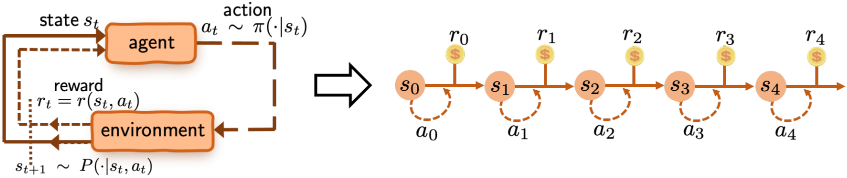
- $\pi(\cdot|s)$: policy (or action selection rule)
- $P(\cdot|s, a)$: transition probabilities

Value function and Q-function of policy π

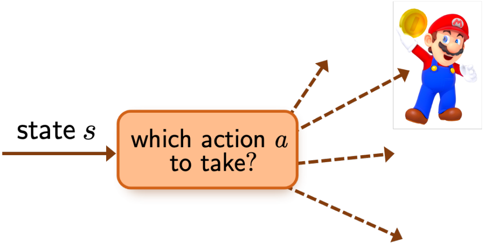


$$\forall s \in \mathcal{S} : \qquad V^\pi(s) := \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^t r_t \,\middle|\, s_0 = s\right]$$

$$\forall (s,a) \in \mathcal{S} \times \mathcal{A} : \quad Q^\pi(s,a) := \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^t r_t \,\middle|\, s_0 = s, a_0 = a\right]$$

- cumulative *discounted* reward; $\gamma \in [0,1)$: discount factor
  - **effective horizon**: $\frac{1}{1-\gamma}$
- sampled trajectory is generated under π

Optimal policy and optimal value



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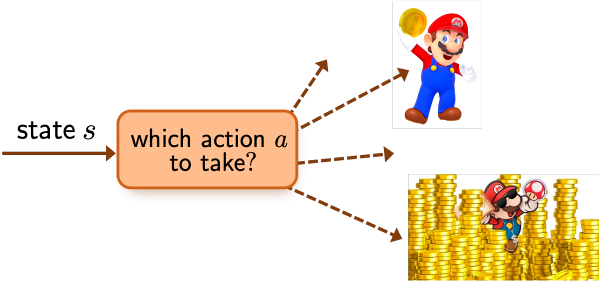

- **goal:** find optimal policy $\pi^\star$ that maximizes values
- optimal value / Q function: $V^\star := V^{\pi^\star}$, $Q^\star := Q^{\pi^\star}$

Policy optimization

Given state distribution $s \sim \rho$ (e.g. uniform)

$$\boxed{\max_{\pi} \; V^{\pi}(\rho) \coloneqq \mathbb{E}_{s\sim\rho}\left[V^{\pi}(s)\right]}$$

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$$\boxed{\max_{\pi}\ V^{\pi}(\rho) := \mathbb{E}_{s\sim\rho}\left[V^{\pi}(s)\right]} \quad \xrightarrow{\text{parameterize}} \quad \boxed{\max_{\theta}\ V^{\pi_\theta}(\rho) := \mathbb{E}_{s\sim\rho}\left[V^{\pi_\theta}(s)\right]}$$

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$$\pi_\theta(a|s) = \frac{\exp(\theta(s,a))}{\sum_a \exp(\theta(s,a))}$$

softmax parameterization

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parameterize $\Longrightarrow$

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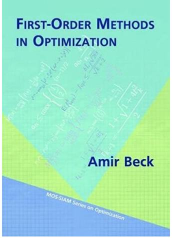
softmax parameterization

$\Downarrow$



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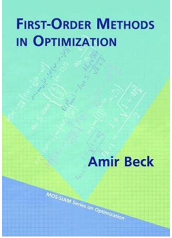
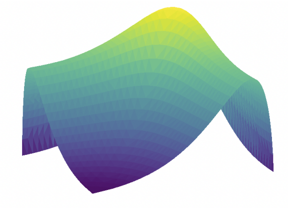


Policy gradient method (Sutton et al. '00)

$$\theta^{(t+1)} = \theta^{(t)} + \eta \nabla_\theta V^{(t)}(\rho), \qquad t = 0, 1, \cdots$$

- η: learning rate

Does policy gradient (PG) method converge?



- (Agarwal et al. '19) Softmax PG converges to global opt as $t \to \infty$

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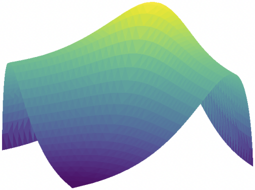

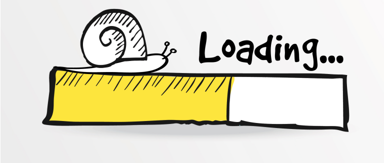

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However, "asymptotic convergence" might mean "taking forever"

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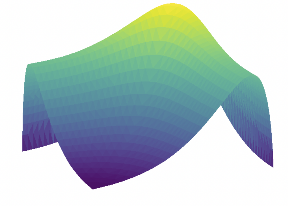

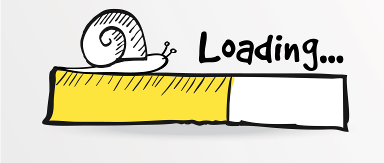

- (Agarwal et al. '19) Softmax PG converges to global opt as $t \to \infty$
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$O\left(\frac{1}{\varepsilon}\right)$ iterations

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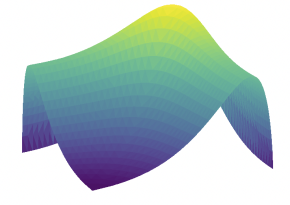

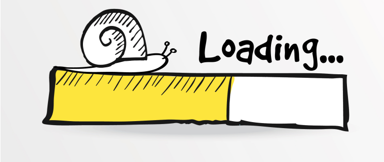

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$$\color{red}{c\left(|\mathcal{S}|, |\mathcal{A}|, \tfrac{1}{1-\gamma}, \cdots\right)} \color{blue}{O\left(\tfrac{1}{\varepsilon}\right)} \text{ iterations}$$

However, "asymptotic convergence" might mean "taking forever"

A negative message

Theorem 1 (Li, Wei, Chi, Gu, Chen '21)

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

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

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

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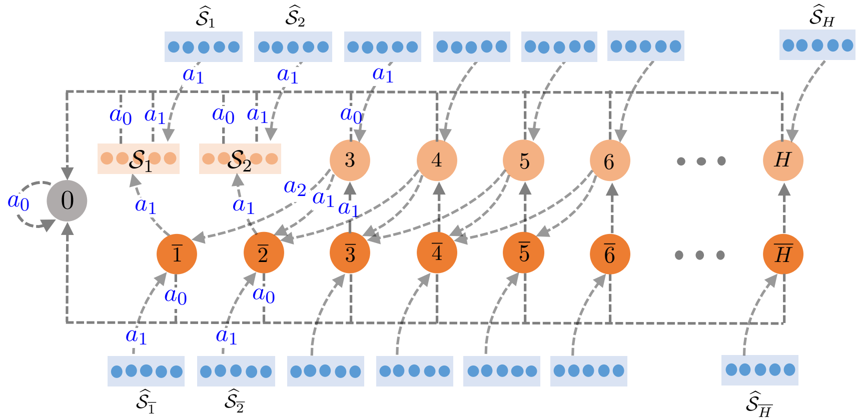
- Softmax PG can take (super)-exponential time to converge (in problems w/ large state space & long effective horizon)!

MDP construction for our lower bound



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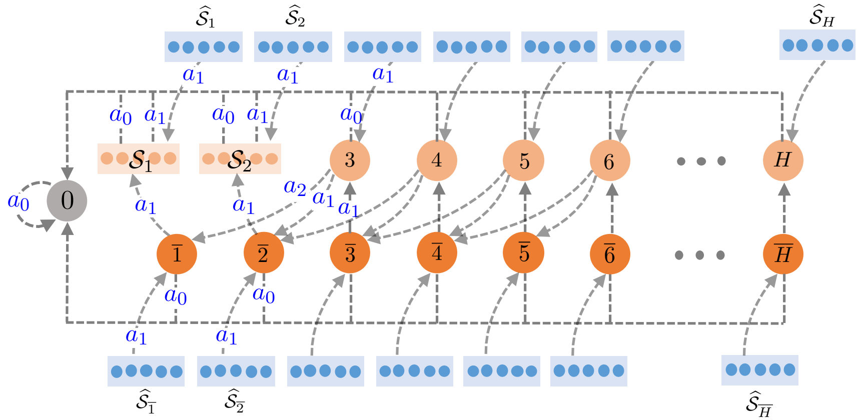

Key ingredients: for $3 \le s \le H \asymp \frac{1}{1-\gamma}$,

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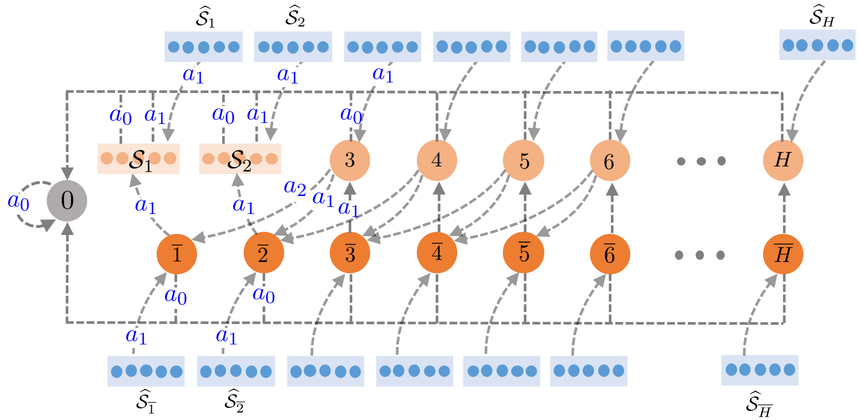
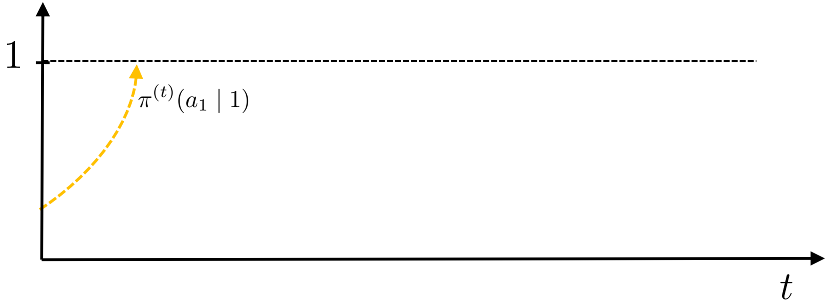


Key ingredients: for $3 \leq s \leq H \asymp \frac{1}{1-\gamma}$,

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

What is happening in our constructed MDP?



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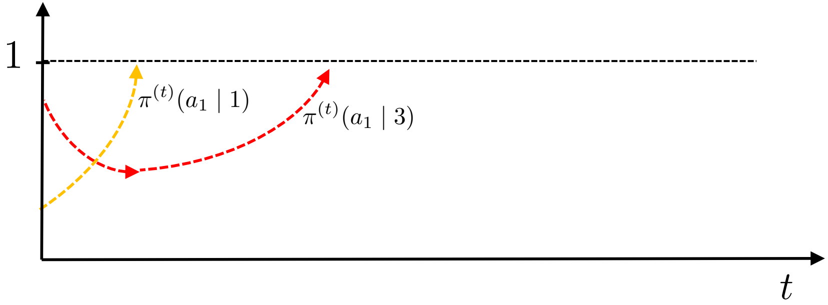

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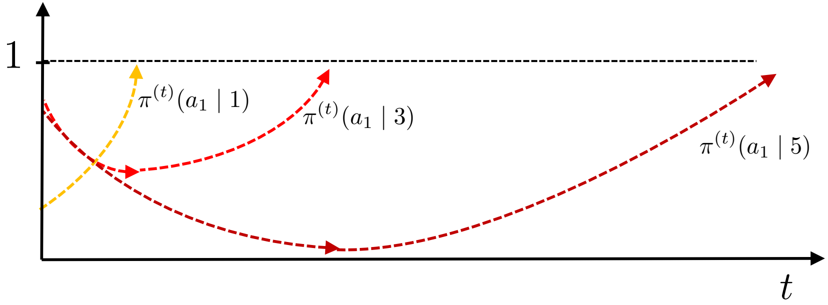

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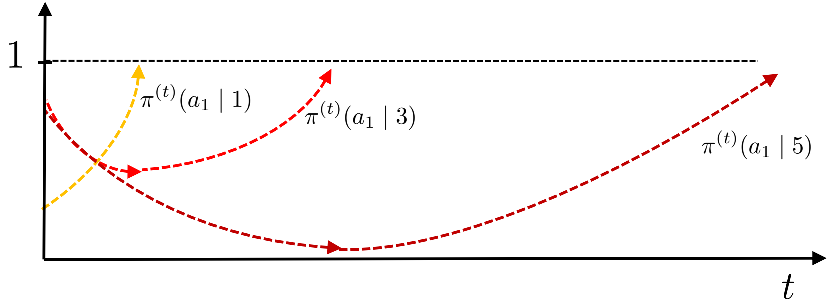

observation: convergence time for state s grows geometrically as $s \uparrow$

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

Booster 1: entropy regularization

accelerate convergence by regularizing value function

$$V_\tau^\pi(s) := \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^t \big(r_t - \tau \log \pi(a_t \mid s_t)\big) \,\Big|\, s_0 = s\right]$$

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\begin{aligned}
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&= V^\pi(s) + \frac{\tau}{1-\gamma} \mathop{\mathbb{E}}_{s \sim d_s^\pi} \Big[\underbrace{-\sum_a \pi(a|s) \log \pi(a \,|\, s)}_{\text{Shannon entropy}} \,\Big|\, s_0 = s\Big]
\end{aligned}
$$

- τ: regularization parameter
- d_s^π: certain marginal distribution

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entropy-regularized value maximization

$$\text{maximize}_\theta \quad V_\tau^{\pi_\theta}(\rho) := \mathbb{E}_{s\sim\rho}\big[V_\tau^{\pi_\theta}(s)\big]$$

Entropy-regularized PG remains slow ...

Theorem 2 (Li, Wei, Chi, Gu, Chen '21)

There is an MDP s.t. it takes entropy-regularized softmax PG at least

$$\min\left\{\exp\left(\Theta\left(\frac{1}{\varepsilon}\right)\right),\ \frac{1}{\eta}|\mathcal{S}|^{2^{\Theta(\frac{1}{1-\gamma})}}\right\}\ \textit{iterations}$$

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

- Softmax PG method with entropy regularization can still take exponential time to converge!

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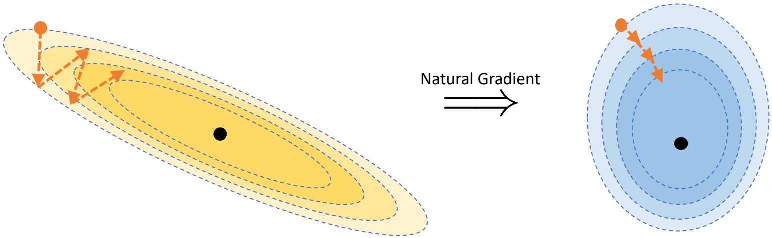
- Softmax PG method with entropy regularization can still take exponential time to converge!
- (Mei et al. '20) entropy-regularized softmax PG converges in

$$c\big(|\mathcal{S}|, |\mathcal{A}|, \tfrac{1}{1-\gamma}, \cdots\big)\, O\big(\tfrac{1}{\varepsilon}\big) \text{ iterations}$$

Booster 2: natural policy gradient (NPG)

precondition gradients to improve search directions ...



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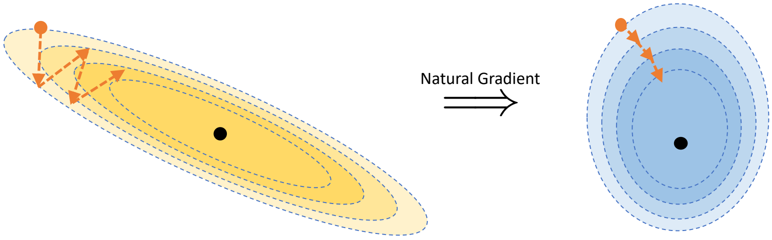


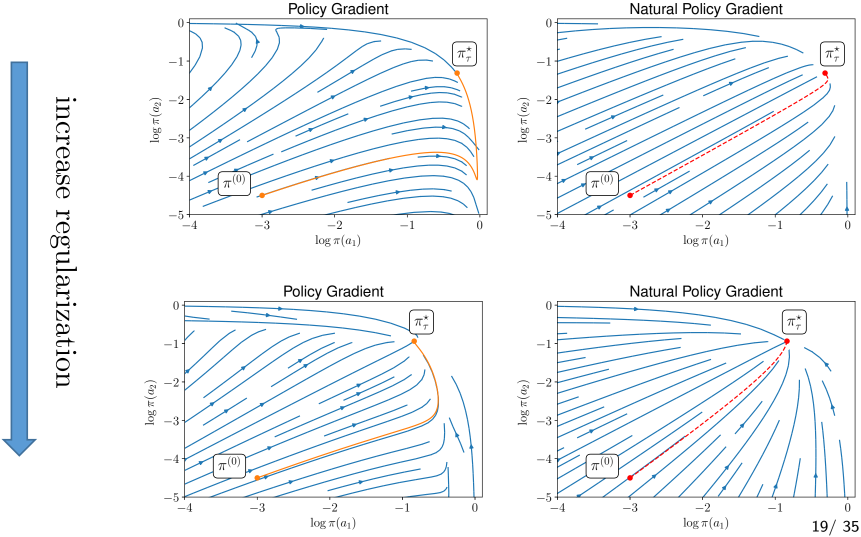
NPG method (Kakade '02)

$$\theta^{(t+1)} = \theta^{(t)} + \eta(\mathcal{F}_\rho^\theta)^\dagger \nabla_\theta V_\tau^{(t)}(\rho), \qquad t = 0, 1, \cdots$$

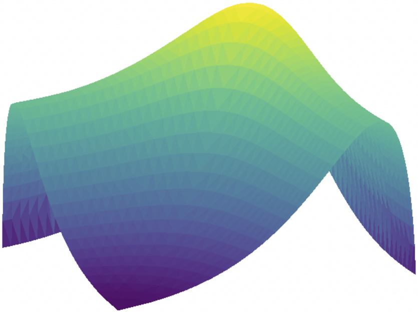
- $\mathcal{F}_\rho^\theta := \mathbb{E}\Big[\big(\nabla_\theta \log \pi_\theta(a \,|\, s)\big)\big(\nabla_\theta \log \pi_\theta(a \,|\, s)\big)^\top\Big]$: Fisher info

Entropy-regularized natural gradient helps!

A toy bandit example: 3 arms with rewards 1, 0.9 and 0.1



Challenge: non-concavity



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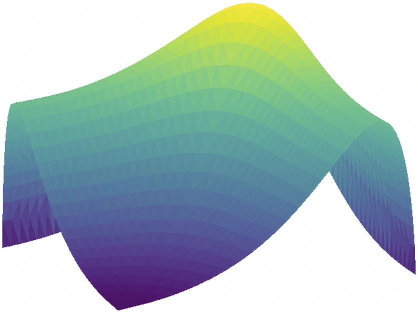
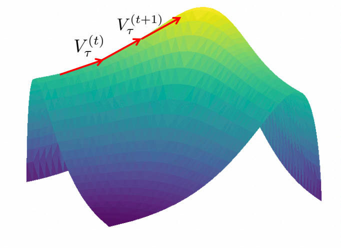


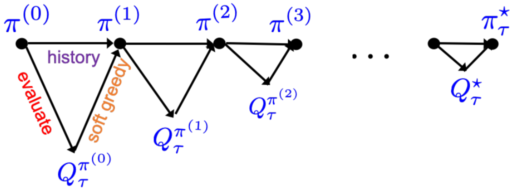
Recent advances

- PG for control (Fazel et al., 2018; Bhandari and Russo, 2019)
- PG for tabular MDPs (Agarwal et al. 19, Bhandari and Russo '19, Mei et al '20)
- unregularized NPG for tabular MDPs (Agarwal et al. '19, Bhandari and Russo '20)
- ...



How to characterize the efficiency of entropy-regularized NPG in tabular settings?

Entropy-regularized NPG in tabular settings



An alternative expression in policy space (tabular setting)

$$\pi^{(t+1)}(a|s) \propto \pi^{(t)}(a|s)^{1-\frac{\eta\tau}{1-\gamma}} \exp\left(\frac{\eta Q_\tau^{(t)}(s,a)}{1-\gamma}\right), \qquad t = 0, 1, \cdots$$

- $Q_\tau^{(t)}$: soft Q-function of $\pi^{(t)}$; $\quad 0 < \eta \leq \frac{1-\gamma}{\tau}$: learning rate

- invariant to the choice of initial state distribution ρ

Linear convergence with exact gradients

optimal policy: $\pi_\tau^\star$; *optimal "soft" Q function:* $Q_\tau^\star := Q_\tau^{\pi_\tau^\star}$

Exact oracle: perfect gradient evaluation

Theorem 3 (Cen, Cheng, Chen, Wei, Chi '20)

For any $0 < \eta \leq (1-\gamma)/\tau$, *entropy-regularized NPG achieves*

$$\|Q_\tau^\star - Q_\tau^{(t+1)}\|_\infty \leq C_1 \gamma \left(1 - \eta\tau\right)^t, \quad t = 0, 1, \cdots$$

- $C_1 = \|Q_\tau^\star - Q_\tau^{(0)}\|_\infty + 2\tau \left(1 - \frac{\eta\tau}{1-\gamma}\right) \|\log \pi_\tau^\star - \log \pi^{(0)}\|_\infty$

Implications: iteration complexity

$\#$ iterations needed to reach $\|Q_\tau^\star - Q_\tau^{(t+1)}\|_\infty \le \varepsilon$ is at most

- **General learning rates ($0 < \eta < \frac{1-\gamma}{\tau}$):**

$$\frac{1}{\eta\tau} \log\left(\frac{C_1\gamma}{\varepsilon}\right)$$

- **Soft policy iteration ($\eta = \frac{1-\gamma}{\tau}$):**

$$\frac{1}{1-\gamma} \log\left(\frac{\|Q_\tau^\star - Q_\tau^{(0)}\|_\infty \gamma}{\varepsilon}\right)$$

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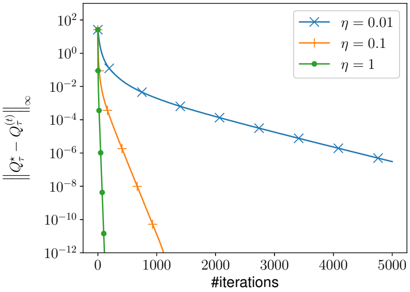
Nearly dimension-free global linear convergence!

Regularized NPG vs. unregularized NPG

regularized NPG

$\tau = 0.001$

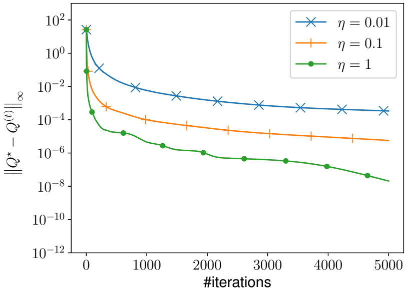


linear rate: $\frac{1}{\eta\tau}\log\left(\frac{1}{\varepsilon}\right)$

Ours

unregularized NPG

$\tau = 0$



sublinear rate: $\frac{1}{\min\{\eta,(1-\gamma)^2\}\varepsilon}$

(Agarwal et al. '19)

Regularized NPG vs. unregularized NPG

regularized NPG
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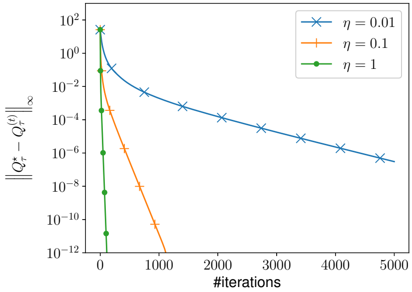

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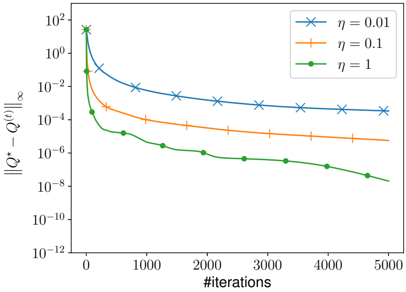

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(Agarwal et al. '19)

Entropy regularization enables faster convergence!

Entropy-regularized NPG with inexact gradients

Inexact oracle: inexact evaluation of $Q_\tau^{(t)}$, which returns $\widehat{Q}_\tau^{(t)}$ s.t.

$$\big\|\widehat{Q}_\tau^{(t)} - Q_\tau^{(t)}\big\|_\infty \le \delta,$$

e.g. using sample-based estimators

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Inexact entropy-regularized NPG:

$$\pi^{(t+1)}(a|s) \;\propto\; \big(\pi^{(t)}(a|s)\big)^{1-\frac{\eta\tau}{1-\gamma}} \exp\Big(\frac{\eta \widehat{Q}_\tau^{(t)}(s,a)}{1-\gamma}\Big)$$

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Question: stability vis-à-vis inexact gradient evaluation?

Linear convergence with inexact gradients

$$\big\|\widehat{Q}_\tau^{(t)} - Q_\tau^{(t)}\big\|_\infty \le \delta$$

Theorem 4 (Cen, Cheng, Chen, Wei, Chi '20)

For any stepsize $0 < \eta \le (1-\gamma)/\tau$, *entropy-regularized NPG attains*

$$\big\|Q_\tau^\star - Q_\tau^{(t+1)}\big\|_\infty \le \gamma(1-\eta\tau)^t C_1 + C_2$$

- $C_1 = \|Q_\tau^\star - Q_\tau^{(0)}\|_\infty + 2\tau\Big(1 - \dfrac{\eta\tau}{1-\gamma}\Big)\|\log \pi_\tau^\star - \log \pi^{(0)}\|_\infty$
- $C_2 = \dfrac{2\gamma\big(1 + \frac{\gamma}{\eta\tau}\big)}{1-\gamma}\delta$: error floor

- converges linearly at the same rate until an error floor is hit

Returning to the original MDP?

How to employ entropy-regularized NPG to find an ε-optimal policy for the original (unregularized) MDP?

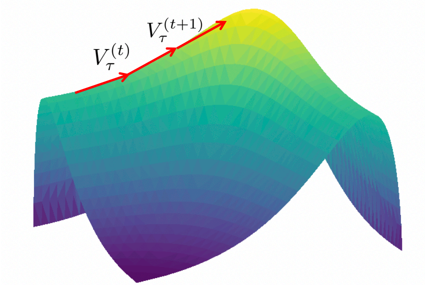
Returning to the original MDP?

How to employ entropy-regularized NPG to find an ε-optimal policy for the original (unregularized) MDP?

- suffices to find an $\frac{\varepsilon}{2}$-optimal policy of regularized MDP w/ regularization parameter $\tau = \frac{(1-\gamma)\varepsilon}{4 \log |\mathcal{A}|}$
- iteration complexity is the same as before (up to log factor)

A little analysis when $\eta = \frac{1-\gamma}{\tau}$

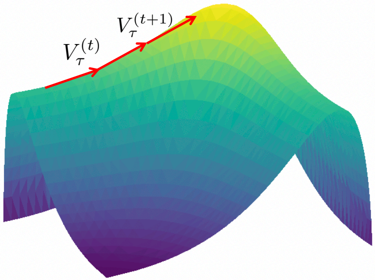
A key lemma: monotonic performance improvement



$$V_\tau^{(t+1)}(\rho) - V_\tau^{(t)}(\rho) = \mathop{\mathbb{E}}_{s\sim d_\rho^{(t+1)}} \Bigg[\left(\frac{1}{\eta} - \frac{\tau}{1-\gamma}\right) \underbrace{\mathsf{KL}\Big(\pi^{(t+1)}(\cdot|s) \,\Big\|\, \pi^{(t)}(\cdot|s)\Big)}_{\text{KL divergence}}$$

$$+ \frac{1}{\eta} \underbrace{\mathsf{KL}\left(\pi^{(t)}(\cdot|s) \,\Big\|\, \pi^{(t+1)}(\cdot|s)\right)}_{\text{KL divergence}} \Bigg]$$

A key lemma: monotonic performance improvement



$$V_\tau^{(t+1)}(\rho) - V_\tau^{(t)}(\rho) = \mathop{\mathbb{E}}_{s\sim d_\rho^{(t+1)}}\Bigg[\left(\frac{1}{\eta} - \frac{\tau}{1-\gamma}\right)\underbrace{\mathsf{KL}\Big(\pi^{(t+1)}(\cdot|s)\,\Big\|\,\pi^{(t)}(\cdot|s)\Big)}_{\text{KL divergence}}$$

$$+\frac{1}{\eta}\underbrace{\mathsf{KL}\left(\pi^{(t)}(\cdot|s)\,\Big\|\,\pi^{(t+1)}(\cdot|s)\right)}_{\text{KL divergence}}\Bigg]$$

$$\geq 0 \qquad \left(\text{if } 0 < \eta \leq \frac{1-\gamma}{\tau}\right)$$

Recall: Bellman's optimality principle

Bellman operator

$$\mathcal{T}(Q)(s,a) := \underbrace{r(s,a)}_{\text{immediate reward}} + \gamma \mathop{\mathbb{E}}_{s' \sim P(\cdot|s,a)} \underbrace{\left[\max_{a' \in \mathcal{A}} Q(s',a') \right]}_{\text{next state's value}}$$

- one-step look-ahead

Recall: Bellman's optimality principle

Bellman operator

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Bellman equation: $Q^\star$ is *unique* solution to

$$\mathcal{T}(Q) = Q$$

γ**-contraction of Bellman operator:**

$$\|\mathcal{T}(Q_1) - \mathcal{T}(Q_2)\|_\infty \le \gamma \|Q_1 - Q_2\|_\infty$$

Richard Bellman

Soft Bellman operator

$$\begin{aligned}\mathcal{T}_\tau(Q)(s,a) := & \underbrace{r(s,a)}_{\text{immediate reward}} \\ & + \gamma \mathop{\mathbb{E}}_{s' \sim P(\cdot|s,a)} \left[\max_{\pi(\cdot|s')} \mathop{\mathbb{E}}_{a' \sim \pi(\cdot|s')} \left[\underbrace{Q(s',a')}_{\text{next state's value}} - \underbrace{\tau \log \pi(a'|s')}_{\text{regularizer}} \right] \right]\end{aligned}$$

Soft Bellman operator

$$\mathcal{T}_\tau(Q)(s,a) := \underbrace{r(s,a)}_{\text{immediate reward}} + \gamma \mathop{\mathbb{E}}_{s' \sim P(\cdot|s,a)} \left[\max_{\pi(\cdot|s')} \mathop{\mathbb{E}}_{a' \sim \pi(\cdot|s')} \Big[\underbrace{Q(s',a')}_{\text{next state's value}} - \underbrace{\tau \log \pi(a'|s')}_{\text{regularizer}} \Big] \right]$$

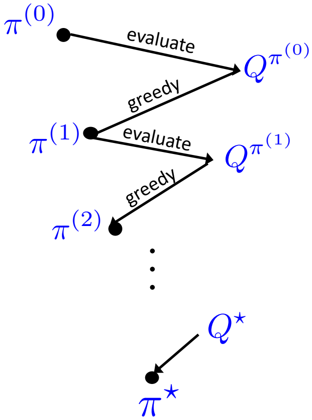
Soft Bellman equation: $Q^\star_\tau$ is *unique* solution to

$$\mathcal{T}_\tau(Q) = Q$$

γ-contraction of soft Bellman operator:

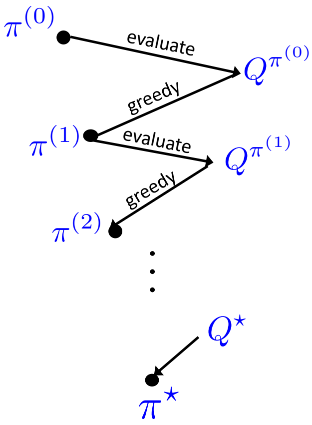
$$\|\mathcal{T}_\tau(Q_1) - \mathcal{T}_\tau(Q_2)\|_\infty \le \gamma \|Q_1 - Q_2\|_\infty$$

policy iteration



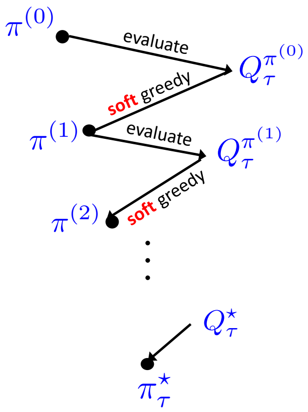
Bellman operator

policy iteration



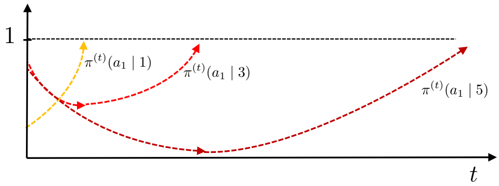
Bellman operator

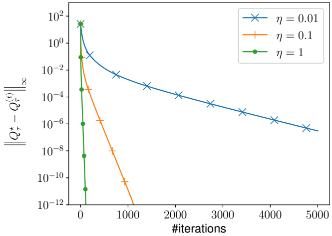
soft policy iteration ($\eta = \frac{1-\gamma}{\tau}$)



soft Bellman operator

Concluding remarks





- Softmax policy gradient can take exponential time to converge
- Entropy regularization & natural gradients help!

Papers:

"Fast global convergence of natural policy gradient methods with entropy regularization," S. Cen, C. Cheng, Y. Chen, Y. Wei, Y. Chi, arxiv:2007.06558, 2020

"Softmax policy gradient methods can take exponential time to converge," G. Li, Y. Wei, Y. Chi, Y. Gu, Y. Chen, arxiv:2102.11270, 2021