On the Effectiveness of Nonconvex Optimization in Reinforcement Learning

Yuxin Chen

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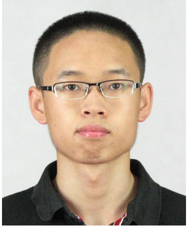
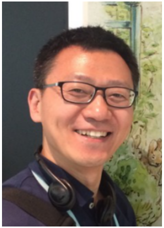
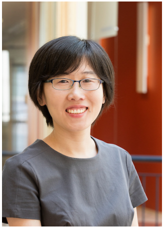


Gen Li
Tsinghua

Yuting Wei
UPenn

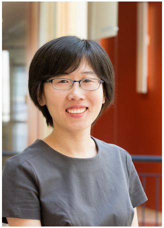


Yuantao Gu
Tsinghua



Yuejie Chi
CMU

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



Shicong Cen
CMU

Chen Cheng
Stanford

Yuting Wei
UPenn

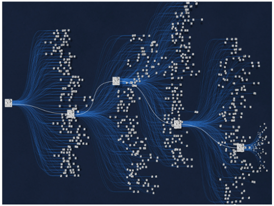
Yuejie Chi
CMU

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

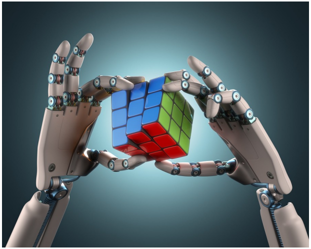
Reinforcement Learning (RL)

In RL, an agent learns by interacting with an environment

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

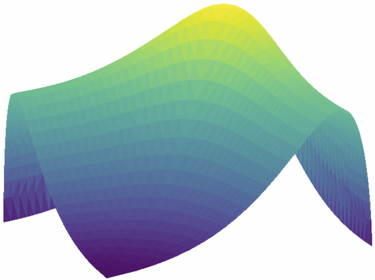


Recent successes in RL



Policy optimization: a major contributor to these successes

Challenges: large dimensionality and non-concavity



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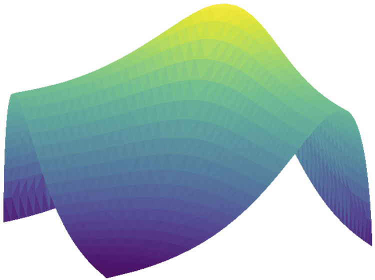
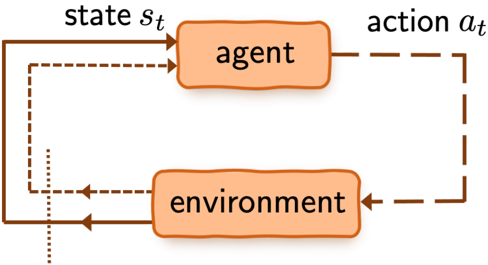


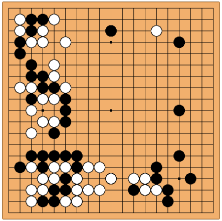
Recent advances towards understanding policy optimization

- finite-state MDPs (Agarwal et al. 19, Bhandari and Russo '19, Shani et al. '19, Mei et al. '20, Cen et al. '20, Zhang et al. '20, Lan '21, Zhan et al. '21, Cen et al. '21, Cayci et al. '21, Khodadadian et al. '21, ...)
- control (Fazel et al., 2018; Bhandari and Russo, 2019, ...)

Backgrounds: policy optimization for MDPs

Markov decision process (MDP)





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

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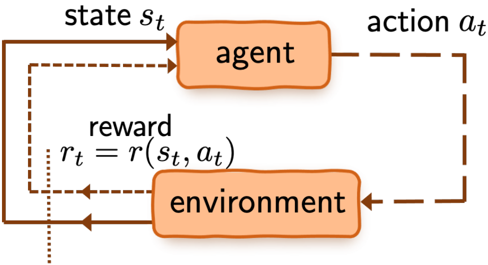

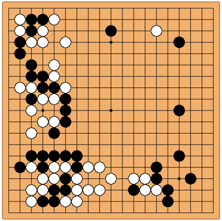

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- $r(s, a) \in [0, 1]$: immediate reward

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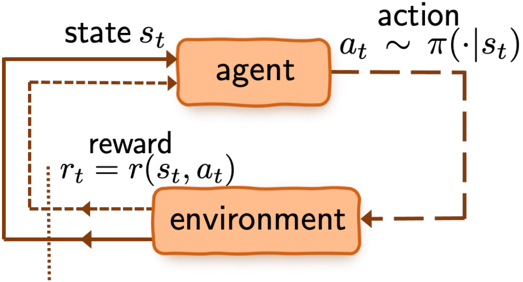

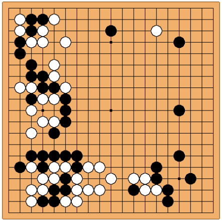

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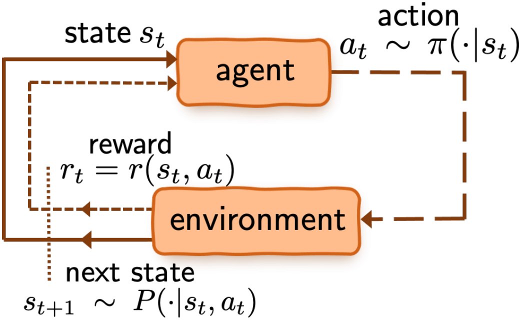

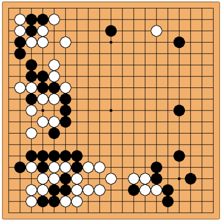

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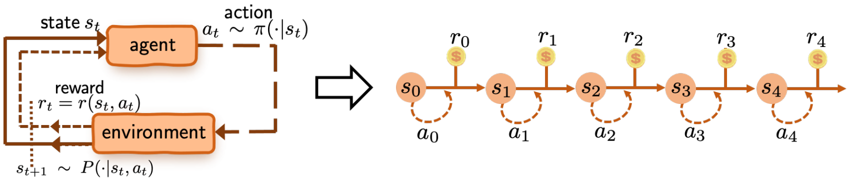
- $P(\cdot|s, a)$: transition probabilities

Value function and Q-function of policy π

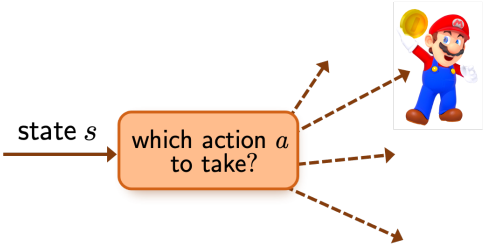


$$\forall s \in \mathcal{S}: \qquad V^\pi(s) := \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^t r_t \,\middle|\, s_0 = s\right]$$

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

- 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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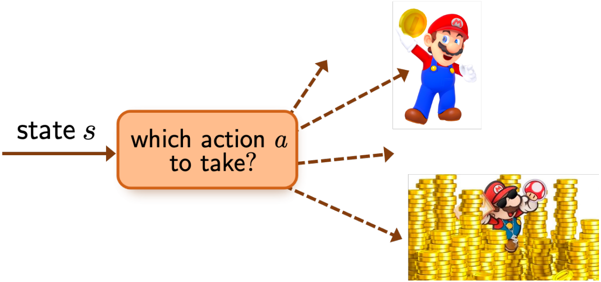

- **goal:** find optimal policy $\pi^\star$ that maximizes values
- optimal value / Q function: $V^\star := V^{\pi^\star}$, $Q^\star := Q^{\pi^\star}$

Policy optimization

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

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

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parameterize ⟹

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parameterize $\Longrightarrow$

$$\max_{\theta} \; V^{\pi_\theta}(\rho) := \mathop{\mathbb{E}}_{s\sim\rho}\left[V^{\pi_\theta}(s)\right]$$

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

softmax parameterization

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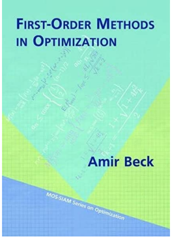

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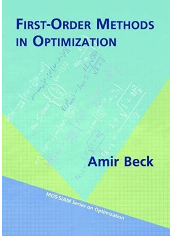
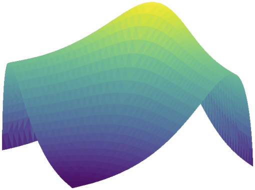


Policy gradient method (Sutton et al. '00)

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

- η: learning rate

Does policy gradient (PG) method converge?



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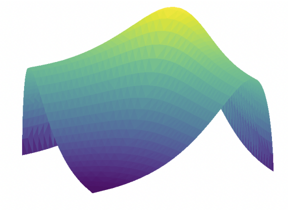

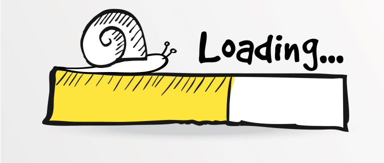

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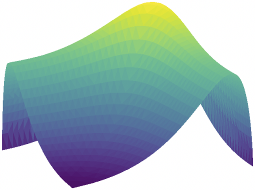

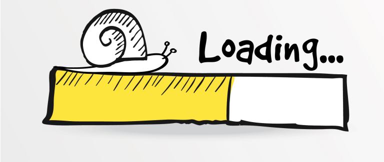

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$O\left(\frac{1}{\varepsilon}\right)$ iterations

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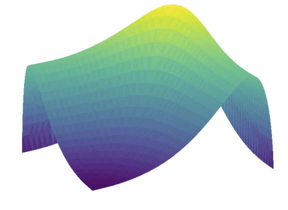

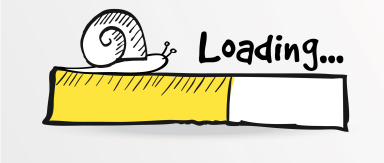

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$$c(|\mathcal{S}|, |\mathcal{A}|, \frac{1}{1-\gamma}, \cdots)\ O(\frac{1}{\varepsilon}) \text{ iterations}$$

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

A negative message

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

Suppose the learning rate obeys $0 < \eta < (1-\gamma)^2/5$. *There exists an MDP with* $|\mathcal{S}|$ *states and 3 actions s.t. it takes softmax PG at least*

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

to achieve $\frac{1}{|\mathcal{S}|}\sum_{s\in\mathcal{S}}|V^{(t)}(s) - V^{\star}(s)| \le 0.07$.

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

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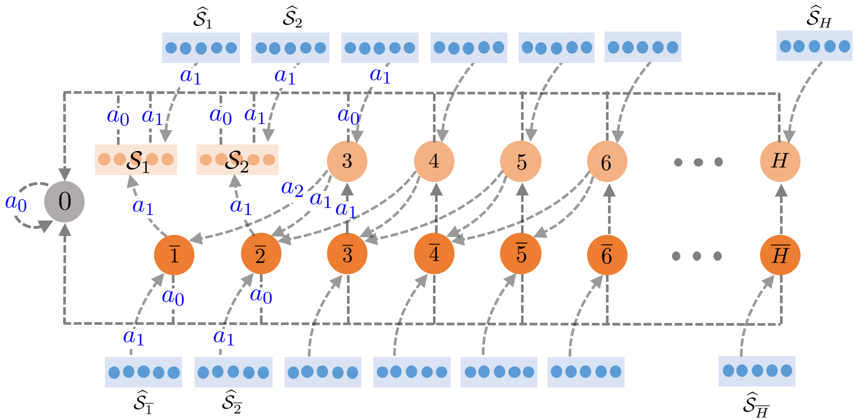
- This (super)-exponential lower bound arises even with
  - uniform initial state distribution
    $\longrightarrow$ benign distribution mismatch $\left\|\frac{d_\rho^\pi}{\rho}\right\|_\infty \leq |\mathcal{S}|$
  - uniform policy initialization

MDP construction for our lower bound



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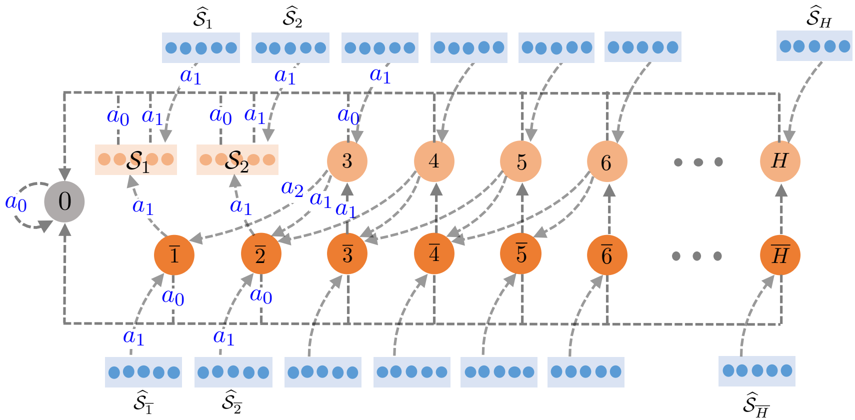

Key ingredients: for $3 \leq s \leq H \asymp \frac{1}{1-\gamma}$

- augmented chain-like structure

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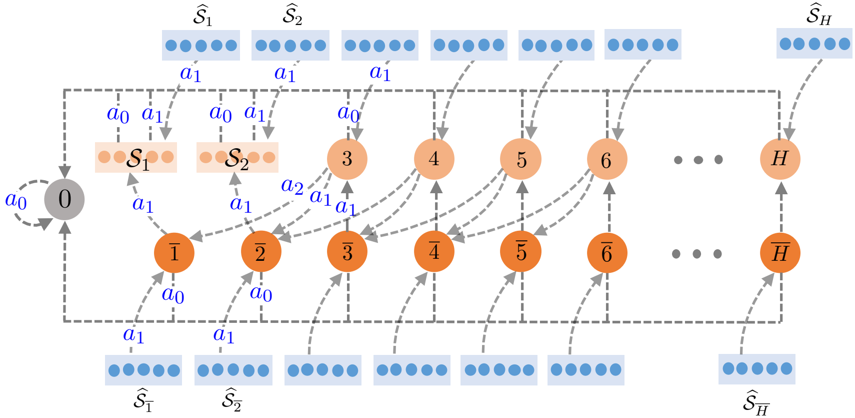
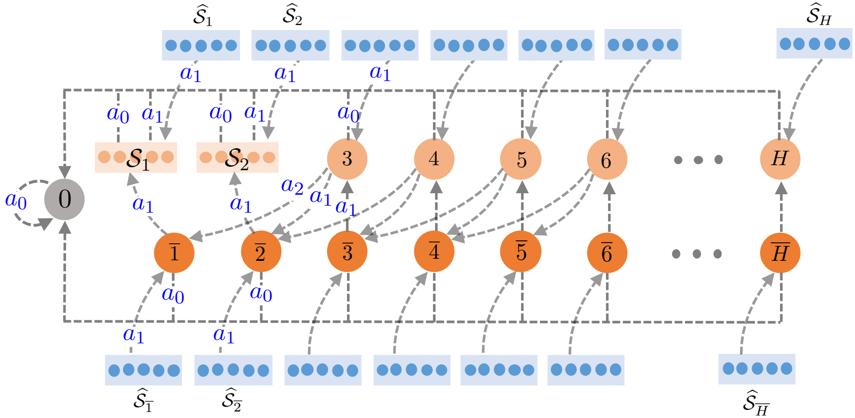


Key ingredients: for $3 \le s \le H \asymp \frac{1}{1-\gamma}$

- augmented chain-like structure
- $V^{(t)}(s)$ relies on $V^{(t)}(s-1)$, $V^{(t)}(s-2)$, $\cdots$ (delayed impacts)

MDP construction for our lower bound



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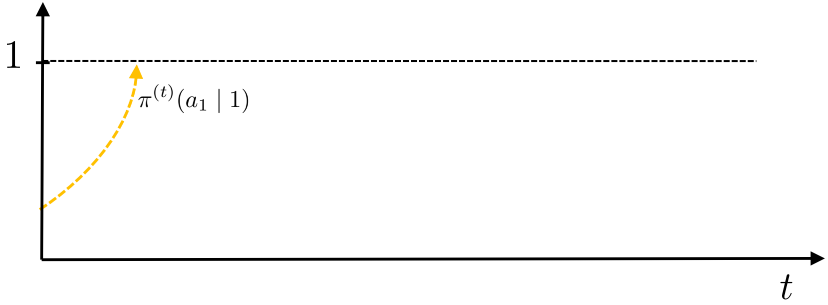
- $\pi^{(t)}(a_{\text{opt}} \,|\, s)$ keeps decreasing until $\pi^{(t)}(a_{\text{opt}} \,|\, s-2) \approx 1$

What is happening in our constructed MDP?



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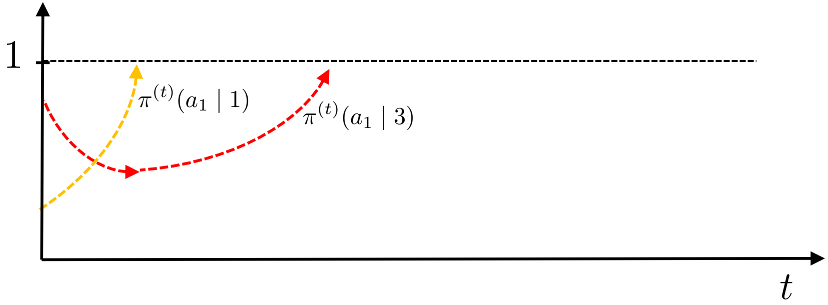

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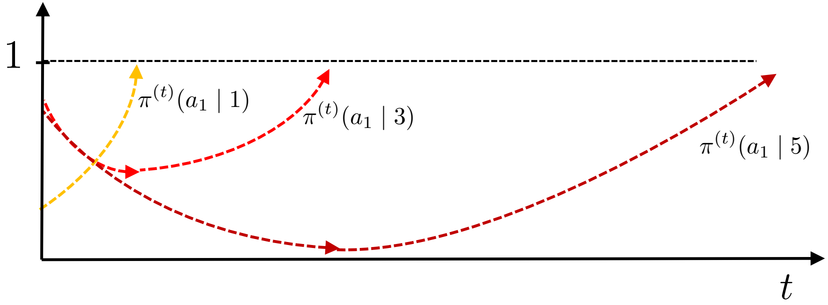

observation: convergence time for state s grows geometrically as $s \uparrow$

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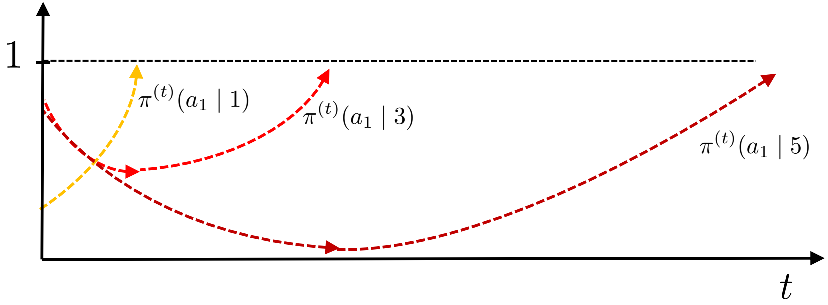

observation: convergence time for state s grows geometrically as $s \uparrow$

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

How to accelerate policy optimization?

Booster 1: entropy regularization

accelerate convergence by regularizing value function

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

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

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

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entropy-regularized value maximization

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

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

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

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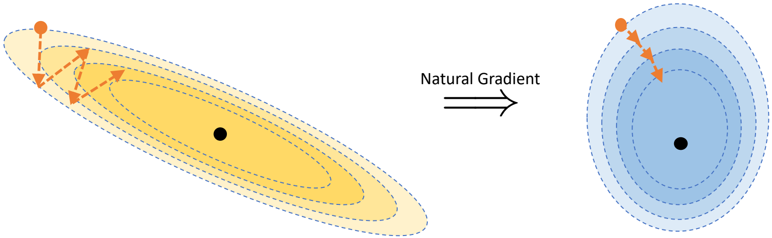
- Softmax PG method with entropy regularization can still take exponential time to converge!
- (Mei et al. '20) entropy-regularized softmax PG converges in

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

Booster 2: natural policy gradient (NPG)

precondition gradients to improve search directions ...



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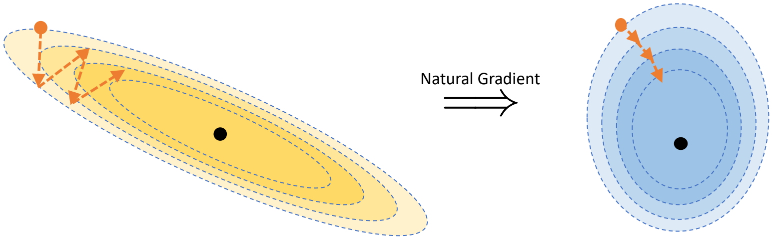


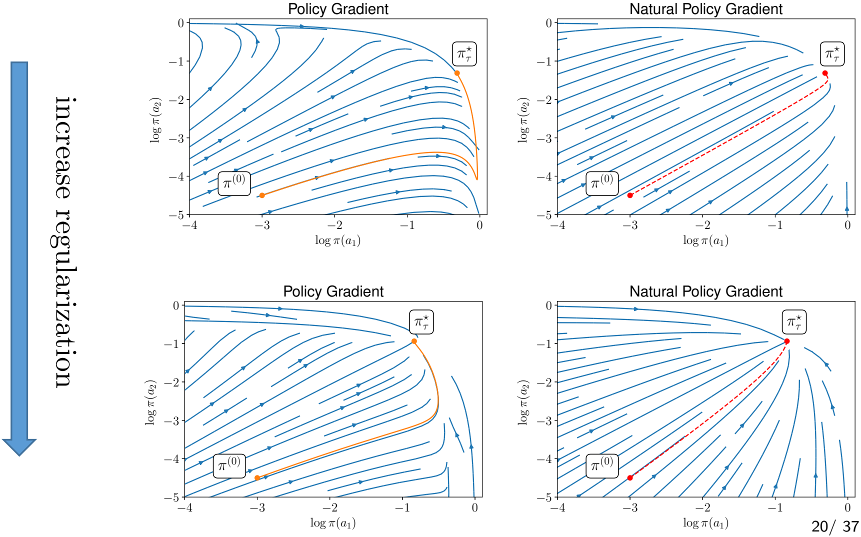
NPG method (Kakade '02)

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

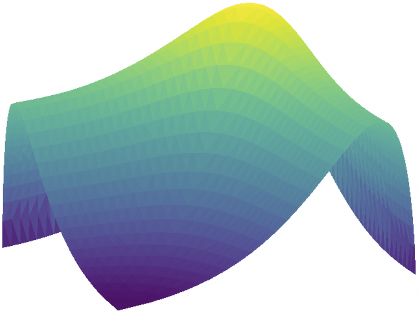
- $\mathcal{F}_\rho^\theta := \mathbb{E}\left[\left(\nabla_\theta \log \pi_\theta(a\,|\,s)\right)\left(\nabla_\theta \log \pi_\theta(a\,|\,s)\right)^\top\right]$: Fisher info

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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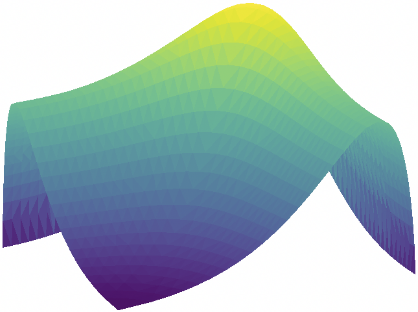
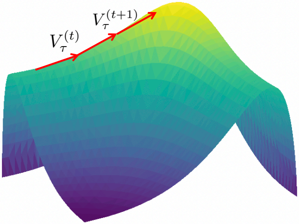


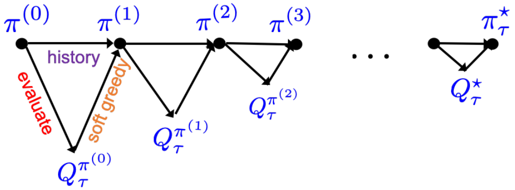
Recent advances

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

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

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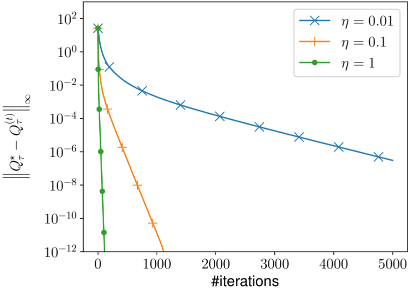
Nearly dimension-free global linear convergence!

Regularized NPG vs. unregularized NPG

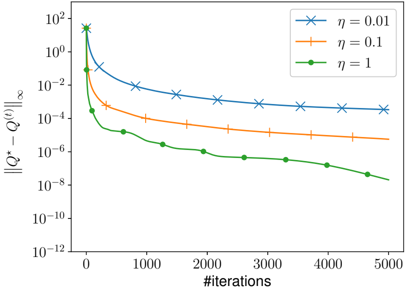
regularized NPG
$\tau = 0.001$



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

Ours

unregularized NPG
$\tau = 0$



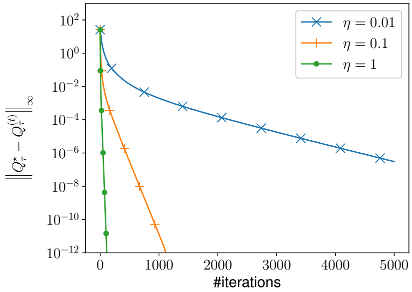
sublinear rate: $\frac{1}{\min\{\eta,(1-\gamma)^2\}\varepsilon}$

(Agarwal et al. '19)

Regularized NPG vs. unregularized NPG

regularized NPG

$\tau = 0.001$



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

Ours

unregularized NPG

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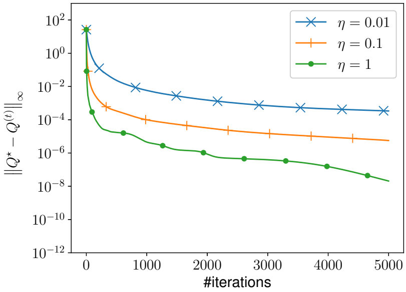

sublinear rate: $\frac{1}{\min\{\eta,(1-\gamma)^2\}\varepsilon}$

(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.

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

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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Inexact entropy-regularized NPG:

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

Linear convergence with inexact gradients

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

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

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

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

- $C_1 = \|Q_\tau^\star - Q_\tau^{(0)}\|_\infty + 2\tau\left(1 - \frac{\eta\tau}{1-\gamma}\right)\|\log\pi_\tau^\star - \log\pi^{(0)}\|_\infty$
- $C_2 = \frac{2\gamma\left(1+\frac{\gamma}{\eta\tau}\right)}{1-\gamma}\delta$: 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?

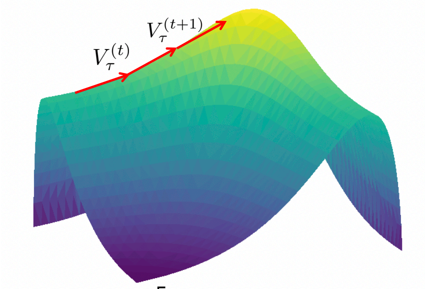
Returning to the original MDP?

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)

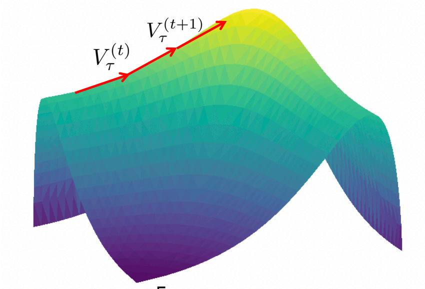
A little analysis when $\eta = \frac{1-\gamma}{\tau}$

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

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

- one-step look-ahead

Recall: Bellman's optimality principle

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- one-step look-ahead

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

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

γ**-contraction of Bellman operator:**

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

Richard Bellman

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 operator

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

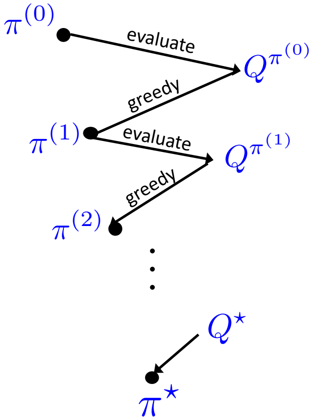
Soft Bellman equation: $Q_\tau^\star$ is *unique* solution to

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

γ-contraction of soft Bellman operator:

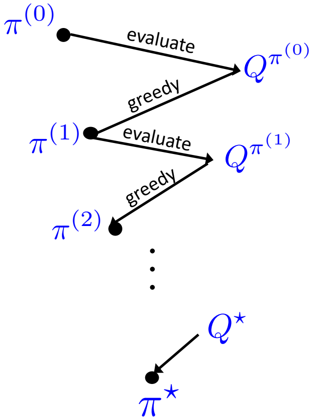
$$\|\mathcal{T}_\tau(Q_1) - \mathcal{T}_\tau(Q_2)\|_\infty \le \gamma \|Q_1 - Q_2\|_\infty$$

policy iteration



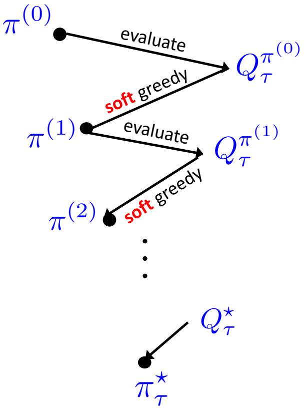
Bellman operator

policy iteration



Bellman operator

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



soft Bellman operator

A key linear system: general learning rates

Let $x_t := \begin{bmatrix} \|Q_\tau^\star - Q_\tau^{(t)}\|_\infty \\ \|Q_\tau^\star - \tau \log \xi^{(t)}\|_\infty \end{bmatrix}$ and $y := \begin{bmatrix} \|Q_\tau^{(0)} - \tau \log \xi^{(0)}\|_\infty \\ 0 \end{bmatrix}$,

where $\xi^{(t)} \propto \pi^{(t)}$ is some auxiliary sequence. Then

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where $\xi^{(t)} \propto \pi^{(t)}$ is some auxiliary sequence. Then

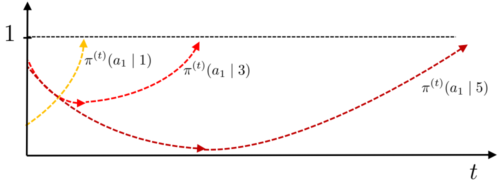
$$x_{t+1} \leq A x_t + \gamma \left(1 - \frac{\eta\tau}{1-\gamma}\right)^{t+1} y,$$

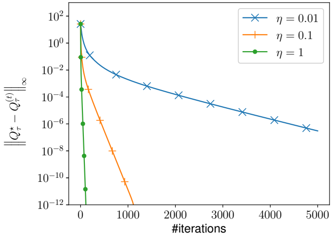
where

$$A := \begin{bmatrix} \gamma \\ 1 \end{bmatrix} \cdot \begin{bmatrix} \frac{\eta\tau}{1-\gamma} & 1 - \frac{\eta\tau}{1-\gamma} \end{bmatrix}$$

is a rank-1 matrix with a non-zero eigenvalue $\underbrace{1 - \eta\tau}_{\text{contraction rate!}}$.

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, accepted to *Operations Research*, 2020

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