

Algorithmic and Theoretical Foundations of RL

Policy Optimization II

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Gradient Method over Distributions

It is clear that policy optimization for RL is a special case of optimization over probability distributions:

$$\max_{\theta} J(\theta) = \mathbb{E}_{X \sim P_{\theta}} [f(X)].$$

The gradient ascent method for this problem is given by

$$\theta^+ = \theta + \eta \cdot \nabla J(\theta),$$

where the search direction $\Delta\theta = \nabla J(\theta)$ satisfies

$$\Delta\theta \propto \operatorname{argmax}_{\|d\|_2 \leq \alpha} \{J(\theta) + \langle \nabla J(\theta), d \rangle\}.$$

Question: Is it more natural to search over probability distribution space since $J(\theta)$ essentially relies on P_{θ} ? **YES → Natural gradient method.**

Natural Gradient over Distributions

Natural gradient method conducts search based on KL divergence between probability distributions ($F(\theta)^\dagger$ is pseudoinverse of $F(\theta)$):

$$\begin{aligned}\Delta\theta &\propto \operatorname{argmax}_{\text{KL}(P_\theta \| P_{\theta+d}) \leq \alpha} \{J(\theta) + \langle \nabla J(\theta), d \rangle\} \\ &\propto F(\theta)^\dagger \nabla J(\theta),\end{aligned}$$

where $F(\theta)$ is the Fisher information matrix at θ , defined by

$$F(\theta) = \mathbb{E}_{X \sim P_\theta} \left[\nabla_\theta \log p_\theta(X) (\nabla_\theta \log p_\theta(X))^T \right].$$

This leads to natural gradient method:

$$\theta^+ = \theta + \eta \cdot F(\theta)^\dagger \nabla J(\theta),$$

which can also be viewed as preconditioned gradient method.

Derivation of Natural Gradient Direction

Given two probability distributions P and Q with pdf $p(x)$ and $q(x)$ respectively, the KL divergence is defined by

$$\text{KL}(P||Q) = \mathbb{E}_P \left[\log \frac{dP}{dQ} \right] = \mathbb{E}_P \left[\log \frac{p(X)}{q(X)} \right].$$

It follows that

$$\begin{aligned} \text{KL}(P_\theta || P_{\theta+d}) &= \mathbb{E}_{P_\theta} \left[\log \frac{p_\theta(X)}{p_{\theta+d}(X)} \right] \\ &= -\mathbb{E}_{P_\theta} [\log p_{\theta+d}(X) - \log p_\theta(X)] \\ &\approx -d^T \underbrace{\mathbb{E}_{P_\theta} \left[\frac{\nabla_\theta p_\theta(X)}{p_\theta(X)} \right]}_{I_1 = \mathbb{E}_{P_\theta} [\nabla_\theta \log p_\theta(X)]} - \frac{1}{2} d^T \underbrace{\mathbb{E}_{P_\theta} \left[\frac{\nabla_\theta^2 p_\theta(X)}{p_\theta(X)} - \frac{\nabla_\theta p_\theta(X) (\nabla_\theta p_\theta(X))^T}{p_\theta(X)^2} \right]}_{I_2 = \mathbb{E}_{P_\theta} [\nabla_\theta^2 \log p_\theta(X)]} d. \end{aligned}$$

Derivation of Natural Gradient Direction

For l_1 , one has

$$\mathbb{E}_{p_\theta} \left[\frac{\nabla_\theta p_\theta(X)}{p_\theta(X)} \right] = \int \nabla_\theta p_\theta(X) dx = 0.$$

For l_2 , one has

$$\mathbb{E}_{p_\theta} \left[\frac{\nabla_\theta^2 p_\theta(X)}{p_\theta(X)} \right] = \int \nabla_\theta^2 p_\theta(X) dx = 0$$

and

$$\mathbb{E}_{p_\theta} \left[\frac{\nabla_\theta p_\theta(X) (\nabla_\theta p_\theta(X))^T}{p_\theta(X)^2} \right] = \mathbb{E}_{p_\theta} \left[\nabla_\theta \log p_\theta(X) (\nabla_\theta \log p_\theta(X))^T \right] = F(\theta).$$

It follows that

$$\Delta\theta = \underset{\text{KL}(p_\theta \| p_{\theta+d}) \leq 2\alpha}{\operatorname{argmax}} \{J(\theta) + \langle \nabla J(\theta), d \rangle\} \approx \underset{d^T F(\theta) d \leq 2\alpha}{\operatorname{argmax}} \{J(\theta) + \langle \nabla J(\theta), d \rangle\} \propto F(\theta)^\dagger \nabla J(\theta).$$

The pseudoinverse basically means that we won't consider the direction such $F(\theta)d = 0$ since in this case one has $\text{KL}(p_\theta \| p_{\theta+d}) \approx d^T F(\theta) d = 0$ and the objective function roughly remains unchanged.

Natural Policy Gradient (NPG)

Natural policy gradient is natural gradient applied to RL optimization problem:

$$\max_{\theta} V^{\pi_{\theta}}(\mu) = \mathbb{E}_{s_0 \sim \mu} [V^{\pi_{\theta}}(s_0)] = \mathbb{E}_{\tau \sim P_{\mu}^{\pi_{\theta}}} [r(\tau)],$$

where given $\tau = (s_t, a_t, r_t)_{t=0}^{\infty}$,

$$P_{\mu}^{\pi_{\theta}}(\tau) = \mu(s_0) \prod_{t=0}^{\infty} \pi_{\theta}(a_t | s_t) P(s_{t+1} | s_t, a_t) \quad \text{and} \quad r(\tau) = \sum_{t=0}^{\infty} \gamma^t r_t.$$

Natural gradient search direction can be incorporated into different policy optimization methods (including REINFORCE, actor-critic) after MC evaluation of $F(\theta)$ (e.g., using data from an episode). We only focus on expression for $F(\theta)$.

By the definition of $F(\theta)$ and expression for $P_{\mu}^{\pi_{\theta}}$ (assuming $\pi_{\theta}(a|s) = 1$ for any θ),

$$\begin{aligned} F(\theta) &= \mathbb{E}_{\tau \sim P_{\mu}^{\pi_{\theta}}} \left[\left(\sum_{t=0}^{\infty} \nabla_{\theta} \log \pi_{\theta}(a_t | s_t) \right) \left(\sum_{t=0}^{\infty} \nabla_{\theta} \log \pi_{\theta}(a_t | s_t) \right)^{\top} \right] \\ &= \mathbb{E}_{\tau \sim P_{\mu}^{\pi_{\theta}}} \left[\sum_{t=0}^{\infty} \nabla_{\theta} \log \pi_{\theta}(a_t | s_t) (\nabla_{\theta} \log \pi_{\theta}(a_t | s_t))^{\top} \right]. \end{aligned}$$

Two Common Expressions of $F(\theta)$ to Avoid Divergence

- Average case:

$$\begin{aligned} F(\theta) &= \lim_{T \rightarrow \infty} \frac{1}{T} \mathbb{E}_{\tau \sim P_{\mu}^{\pi_{\theta}}} \left[\sum_{t=0}^{T-1} \nabla_{\theta} \log \pi_{\theta}(\mathbf{a}_t | \mathbf{s}_t) (\nabla_{\theta} \log \pi_{\theta}(\mathbf{a}_t | \mathbf{s}_t))^T \right] \\ &= \mathbb{E}_{\mathbf{s} \sim d^{\pi_{\theta}}, \mathbf{a} \sim \pi_{\theta}(\cdot | \mathbf{s})} \left[\nabla_{\theta} \log \pi_{\theta}(\mathbf{a} | \mathbf{s}) (\nabla_{\theta} \log \pi_{\theta}(\mathbf{a} | \mathbf{s}))^T \right], \end{aligned}$$

where $d^{\pi_{\theta}}(\mathbf{s}) = \mathbb{E}_{\mathbf{s}_0 \sim \mu} [\lim_{t \rightarrow \infty} P(\mathbf{s}_t = \mathbf{s} | \mathbf{s}_0, \pi_{\theta})]$ is state stationary distribution.

- Discounted case:

$$\begin{aligned} F(\theta) &= (1 - \gamma) \mathbb{E}_{\tau \sim P_{\mu}^{\pi_{\theta}}} \left[\sum_{t=0}^{+\infty} \gamma^t \nabla_{\theta} \log \pi_{\theta}(\mathbf{a}_t | \mathbf{s}_t) (\nabla_{\theta} \log \pi_{\theta}(\mathbf{a}_t | \mathbf{s}_t))^T \right] \\ &= \mathbb{E}_{\mathbf{s} \sim d_{\mu}^{\pi_{\theta}}, \mathbf{a} \sim \pi_{\theta}(\cdot | \mathbf{s})} \left[\nabla_{\theta} \log \pi_{\theta}(\mathbf{a} | \mathbf{s}) (\nabla_{\theta} \log \pi_{\theta}(\mathbf{a} | \mathbf{s}))^T \right], \end{aligned}$$

where $d_{\mu}^{\pi_{\theta}}(\mathbf{s}) = \mathbb{E}_{\mathbf{s}_0 \sim \mu} [(1 - \gamma) \sum_{t=0}^{\infty} \gamma^t P(\mathbf{s}_t = \mathbf{s} | \mathbf{s}_0, \pi_{\theta})]$ is discounted state visitation measure.

Remark

- For the discounted case, it is not difficult to verify that the natural gradient direction $F(\theta)^\dagger \nabla_\theta V^{\pi_\theta}(\mu)$ satisfies

$$F(\theta)^\dagger \nabla_\theta V^{\pi_\theta}(\mu) = \frac{1}{1-\gamma} \omega^*,$$

where ω^* is the (ℓ_2 -minimal) solution to

$$\min_{\omega} L(\omega) = \mathbb{E}_{s \sim d_\mu^{\pi_\theta}, a \sim \pi_\theta(\cdot|s)} \left[\left((\nabla_\theta \log \pi_\theta(a|s))^T \omega - A^{\pi_\theta}(s, a) \right)^2 \right].$$

See “On the theory of policy gradient methods: Optimality, approximation, and distribution shift” by Agarwal et al. 2021 for details.

Remark

- For the softmax parameterization (i.e., $\pi_\theta(a|s) = \exp(\theta_{s,a}) / (\sum_{a'} \exp(\theta_{s,a'}))$), it can be verified all the solutions to $\min_\omega L(\omega)$ has the following general form:

$$\omega_{s,a}^* = A^{\pi_\theta}(s, a) + c_s,$$

where c_s is a constant relying on s . Thus NPG in policy space is given by

$$\pi_{s,a}^+ = \frac{\pi_{s,a} \cdot \exp\left(\frac{\eta}{1-\gamma} A^{\pi_\theta}(s, a)\right)}{\sum_{a'} \pi_{s,a'} \cdot \exp\left(\frac{\eta}{1-\gamma} A^{\pi_\theta}(s, a')\right)},$$

which coincides with EQA in Lecture 7 (a policy mirror ascent method).

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Overall Idea

Given a policy π_{θ_t} , by performance difference lemma, we can rewrite $V^{\pi_{\theta}}(\mu)$ as

$$V^{\pi_{\theta}}(\mu) = V^{\pi_{\theta_t}}(\mu) + \frac{1}{1-\gamma} \mathbb{E}_{s \sim d_{\mu}^{\pi_{\theta}}} \mathbb{E}_{a \sim \pi_{\theta}(\cdot|s)} [A^{\pi_{\theta_t}}(s, a)] .$$

Since we do not have access to $d_{\mu}^{\pi_{\theta}}$, instead maximize the approximation:

$$\max_{\theta} V_t(\theta) = V^{\pi_{\theta_t}}(\mu) + \frac{1}{1-\gamma} \mathbb{E}_{s \sim d_{\mu}^{\pi_{\theta_t}}} \mathbb{E}_{a \sim \pi_{\theta}(\cdot|s)} [A^{\pi_{\theta_t}}(s, a)] .$$

Trust Region Policy Optimization (TRPO)

Two Facts

- ▶ Assume $\sum_a \pi_\theta(a|s) = 1$ for any θ . It is easy to see that $V^{\pi_\theta}(\mu)$ and $V_t(\theta)$ match at θ_t up to first derivative.
- ▶ It can be shown that

$$V^{\pi_\theta}(\mu) \geq V_t(\theta) - \frac{2\gamma\varepsilon_t}{(1-\gamma)^2} \max_s \text{KL}(\pi_{\theta_t}(\cdot|s) \parallel \pi_\theta(\cdot|s)),$$

where $\varepsilon_t = \max_{s,a} |A^{\pi_{\theta_t}}(s, a)|$.

Trust Region Policy Optimization (TRPO)

TRPO is Approximately NPG Plus Line Search

The second fact suggests that we may seek a new estimator by maximizing $V_t(\theta)$ in a small neighborhood of θ_t :

$$\max_{\theta} V_t(\theta) \quad \text{subject to} \quad \max_s \text{KL}(\pi_{\theta_t}(\cdot|s) \parallel \pi_{\theta}(\cdot|s)) \leq \delta.$$

Moreover, replace constraint by the average version and instead solve

$$\max_{\theta} V_t(\theta) \quad \text{subject to} \quad \mathbb{E}_{s \sim d_{\mu}^{\pi_{\theta_t}}} [\text{KL}(\pi_{\theta_t}(\cdot|s) \parallel \pi_{\theta}(\cdot|s))] \leq \delta.$$

Trust Region Policy Optimization (TRPO)

TRPO is Approximately NPG Plus Line Search

After linear approximation to $V_t(\theta)$ and quadratic approximation to KL at θ_t ,

$$V_t(\theta) \approx (\nabla_{\theta} V^{\pi_{\theta_t}}(\mu))^T (\theta - \theta_t), \quad \mathbb{E}_{s \sim d_{\mu}^{\pi_{\theta_t}}} [\text{KL}(\pi_{\theta_t}(\cdot|s) \parallel \pi_{\theta}(\cdot|s))] \approx \frac{1}{2} (\theta - \theta_t)^T F(\theta_t) (\theta - \theta_t),$$

we arrive at the same problem as that for NPG,

$$\max_{\theta} (\nabla_{\theta} V^{\pi_{\theta_t}}(\mu))^T (\theta - \theta_t) \quad \text{subject to} \quad \frac{1}{2} (\theta - \theta_t)^T F(\theta_t) (\theta - \theta_t) \leq \delta.$$

- TRPO is NPG with adaptive line search in implementations.

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Recall from last section that

$$\begin{aligned} V_t(\theta) &\propto \mathbb{E}_{s \sim d_{\mu}^{\pi_{\theta_t}}} \mathbb{E}_{a \sim \pi_{\theta}(\cdot|s)} [A^{\pi_{\theta_t}}(s, a)] \\ &= \mathbb{E}_{s \sim d_{\mu}^{\pi_{\theta_t}}} \mathbb{E}_{a \sim \pi_{\theta_t}(\cdot|s)} \left[\frac{\pi_{\theta}(a|s)}{\pi_{\theta_t}(a|s)} A^{\pi_{\theta_t}}(s, a) \right], \end{aligned}$$

serves as a surrogate function of true target in small region around θ_t .

PPO keeps new policy close to old one through clipped objective.

PPO with Clipped Objective

Let $r(\theta) = \frac{\pi_{\theta}(a|s)}{\pi_{\theta_t}(a|s)}$. Then $r(\theta_t) = 1$. The clipped objective function is given by

$$V_t^{\text{clip}}(\theta) = \mathbb{E}_{s \sim d_{\mu}^{\pi_{\theta_t}}} \mathbb{E}_{a \sim \pi_{\theta_t}(\cdot|s)} \left[\min \left(r(\theta) A^{\pi_{\theta_t}}(s, a), \text{clip}(r(\theta), 1 - \epsilon, 1 + \epsilon) A^{\pi_{\theta_t}}(s, a) \right) \right],$$

where

$$\text{clip}(r(\theta), 1 - \epsilon, 1 + \epsilon) = \begin{cases} 1 + \epsilon, & r(\theta) > 1 + \epsilon, \\ r(\theta), & r(\theta) \in [1 - \epsilon, 1 + \epsilon], \\ 1 - \epsilon, & r(\theta) < 1 - \epsilon. \end{cases}$$

- ▶ The \min operation ensure $V_t^{\text{clip}}(\theta)$ provides a lower bound. Since a maximal point will be computed subsequently, \min will not cancel the effect of clip .
- ▶ PPO policy update (in expectation): $\theta_{t+1} = \text{argmax}_{\theta} V_t^{\text{clip}}(\theta)$.
- ▶ In flat region, gradient of $V_t^{\text{clip}}(\theta)$ is zero, thus won't move far from θ_t is using policy gradient type method to solve the sub-problem.

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Deterministic Policy Parameterization

Consider the case where \mathcal{S} and \mathcal{A} are continuous, and use π_θ to denote a deterministic policy: $\mathbf{a} = \pi_\theta(\mathbf{s})$ is an action.

► Average state value:

$$V^{\pi_\theta}(\mu) = \int_{\mathcal{S}} V^{\pi_\theta}(\mathbf{s}_0) \mu(\mathbf{s}_0) d\mathbf{s}_0 = \mathbb{E}_{\tau \sim p_\mu^{\pi_\theta}} \left[\sum_{t=0}^{\infty} \gamma^t r(\mathbf{s}_t, \pi_\theta(\mathbf{s}_t), \mathbf{s}_{t+1}) \right],$$

where given trajectory $\tau = (\mathbf{s}_t, \pi_\theta(\mathbf{s}_t), \mathbf{s}_{t+1})_{t=0}^{\infty}$,

$$p_\mu^{\pi_\theta}(\tau) = \mu(\mathbf{s}_0) \prod_{t=0}^{\infty} p(\mathbf{s}_{t+1} | \mathbf{s}_t, \pi_\theta(\mathbf{s}_t))$$

is the probability density over τ . Note that there is no probability over action space since $\pi_\theta(\mathbf{s})$ selects a deterministic action.

Deterministic Policy Parameterization

- Similarly, we can express $V^{\pi_\theta}(\mu)$ over state space

$$\begin{aligned} V^{\pi_\theta}(\mu) &= \frac{1}{1-\gamma} \int_{\mathcal{S}} d_{\mu}^{\pi_\theta}(\mathbf{s}) d\mathbf{s} \int_{\mathcal{S}} p(\mathbf{s}'|\mathbf{s}, \pi_\theta(\mathbf{s})) r(\mathbf{s}, \pi_\theta(\mathbf{s}), \mathbf{s}') d\mathbf{s}' \\ &= \frac{1}{1-\gamma} \mathbb{E}_{\mathbf{s} \sim d_{\mu}^{\pi_\theta}} \mathbb{E}_{\mathbf{s}' \sim p(\cdot|\mathbf{s}, \pi_\theta(\mathbf{s}))} [r(\mathbf{s}, \pi_\theta(\mathbf{s}), \mathbf{s}')] , \end{aligned}$$

where $d_{\mu}^{\pi_\theta}(\mathbf{s}) = \mathbb{E}_{\mathbf{s}_0 \sim \mu} [(1-\gamma) \sum_{t=0}^{\infty} \gamma^t p_t(\mathbf{s}|\mathbf{s}_0, \pi_\theta)]$ is state visitation **density**, and $p_t(\mathbf{s}|\mathbf{s}_0, \pi_\theta)$ is the density over state space after transitioning t time steps. Note there is no expectation over action space since $\pi_\theta(\mathbf{s})$ is deterministic.

Deterministic Policy Gradient Theorem

Theorem 1 (Deterministic Policy Gradient Theorem)

Suppose that $\nabla_{\theta} \pi_{\theta}(s)$ and $\nabla_a Q^{\pi_{\theta}}(s, a)$ exist. Then,

$$\nabla_{\theta} V^{\pi_{\theta}}(\mu) = \frac{1}{1 - \gamma} \mathbb{E}_{s \sim d_{\mu}^{\pi_{\theta}}(s)} [\nabla_{\theta} \pi_{\theta}(s) \nabla_a Q^{\pi_{\theta}}(s, a)|_{a=\pi_{\theta}(s)}] .$$

Proof of Theorem 1

First note that

$$\begin{aligned} V^{\pi_\theta}(s_0) &= Q^{\pi_\theta}(s_0, \pi_\theta(s_0)) \\ &= \int_{\mathcal{S}} (r(s_0, \pi_\theta(s_0), s_1) + \gamma V^{\pi_\theta}(s_1)) p(s_1 | s_0, \pi_\theta(s_0)) ds_1. \end{aligned}$$

Therefore, one has

$$\begin{aligned} \nabla_\theta V^{\pi_\theta}(s_0) &= \int_{\mathcal{S}} \nabla_a r(s_0, a, s_0)|_{a=\pi_\theta(s_0)} \nabla_\theta \pi_\theta(s_0) p(s_1 | s_0, \pi_\theta(s_0)) ds_1 \\ &\quad + \int_{\mathcal{S}} r(s_0, \pi_\theta(s_0), s_1) \nabla p(s_1 | s_0, a)|_{a=\pi_\theta(s_0)} \nabla_\theta \pi_\theta(s_0) ds_1 \\ &\quad + \gamma \int_{\mathcal{S}} V^{\pi_\theta}(s_1) \nabla p(s_1 | s_0, a)|_{a=\pi_\theta(s_0)} \nabla_\theta \pi_\theta(s_0) ds_1 \\ &\quad + \gamma \int_{\mathcal{S}} \nabla_\theta V^{\pi_\theta}(s_1) p(s_1 | s_0, \pi_\theta(s_0)) ds_1. \end{aligned}$$

Proof of Theorem 1 (Cont'd)

Moreover, it is easy to verify that the sum of the first three terms is equal to

$$\nabla_{\theta} \pi_{\theta}(s_0) \nabla_a Q^{\pi_{\theta}}(s, a)|_{a=\pi_{\theta}(s_0)}.$$

Therefore,

$$\begin{aligned} \nabla_{\theta} V^{\pi_{\theta}}(s_0) &= \nabla_{\theta} \pi_{\theta}(s_0) \nabla_a Q^{\pi_{\theta}}(s, a)|_{a=\pi_{\theta}(s_0)} + \gamma \int_{\mathcal{S}} \nabla_{\theta} V^{\pi_{\theta}}(s_1) p(s_1 | s_0, \pi_{\theta}(s_0)) ds_1 \\ &= \dots \\ &= \mathbb{E} \left[\sum_{t=0}^{\infty} \gamma^t \nabla_{\theta} \pi_{\theta}(s_t) \nabla_a Q^{\pi_{\theta}}(s_t, a)|_{a=\pi_{\theta}(s_t)} | s_0, \pi_{\theta} \right] \\ &= \frac{1}{1-\gamma} \mathbb{E}_{s \sim d_{s_0}^{\pi_{\theta}}} [\nabla_{\theta} \pi_{\theta}(s) \nabla_a Q^{\pi_{\theta}}(s, a)|_{a=\pi_{\theta}(s)}]. \end{aligned}$$

Averaging over all s_0 completes the proof of Theorem 1.

Deep Deterministic Policy Gradient (DDPG)

- ▶ DDPG is a policy gradient method which learns a deterministic policy π_θ and an action value function $Q^\omega(s, a) \approx Q^{\pi_\theta}(s, a)$. It is an actor-critic algorithm.
- ▶ Policy of DDPG is deterministic, need to add random noisy when collecting data; experience replay buffer is also used to break statistical dependence.
- ▶ Update of ω for action value function is overall the same to Fitted Q-learning.

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Entropy Regularization

Motivation: Enhance exploration by entropy regularization

Given a policy π , entropy regularized objective function is define by

$$\begin{aligned} V_{\lambda}^{\pi}(\mu) &= \frac{1}{1-\gamma} \mathbb{E}_{s \sim d_{\mu}^{\pi}} \left[\mathbb{E}_{a \sim \pi(\cdot|s)} \mathbb{E}_{s' \sim P(\cdot|s,a)} [r(s, a, s')] + \lambda H(\pi(\cdot|s)) \right] \\ &= \frac{1}{1-\gamma} \mathbb{E}_{s \sim d_{\mu}^{\pi}} \mathbb{E}_{a \sim \pi(\cdot|s)} \mathbb{E}_{s' \sim P(\cdot|s,a)} [r(s, a, s') - \lambda \log \pi(a|s)] , \end{aligned}$$

where $H(\pi(\cdot|s))$ denotes the entropy of the probability distribution $\pi(\cdot|s)$:

$$H(\pi(\cdot|s)) = \mathbb{E}_{a \sim \pi(\cdot|s)} \left[\log \frac{1}{\pi(a|s)} \right] .$$

We can rewrite $V_{\lambda}^{\pi}(\mu)$ in terms of state values based on a regularized reward

$$V_{\lambda}^{\pi}(\mu) = \mathbb{E}_{s \sim \mu} [V_{\lambda}^{\pi}(s)] ,$$

where $V_{\lambda}^{\pi}(s) = \mathbb{E} [\sum_{t=0}^{\infty} \gamma^t r_{\lambda}(s_t, a_t, s_{t+1}) | s_0 = s, \pi]$ with

$$r_{\lambda}(s, a, s') = r(s, a, s') - \lambda \log \pi(a|s) .$$

► Note that $r_{\lambda}(s, a, s')$ is not a fixed reward but varies from π to π .

Soft Bellman Equation

- Soft state value V_λ^π :

$$V_\lambda^\pi(s) = \mathbb{E} \left[\sum_{t=0}^{\infty} \gamma^t r_\lambda(s_t, a_t, s_{t+1}) | s_0 = s, \pi \right].$$

- Soft action value $Q_\lambda^\pi(s, a)$: [a_0 is chosen, thus entropy equal to 0]

$$Q_\lambda^\pi(s, a) = \mathbb{E} \left[r(s_0, a_0, s_1) + \sum_{t=1}^{\infty} \gamma^t r_\lambda(s_t, a_t, s_{t+1}) | s_0 = s, a_0 = a, \pi \right].$$

- Relation between Q_λ^π and V_λ^π :

$$\begin{aligned} Q_\lambda^\pi(s, a) &= \mathbb{E}_{s' \sim P(\cdot | s, a)} [r(s, a, s') + \gamma V_\lambda^\pi(s')], \\ V_\lambda^\pi(s) &= \mathbb{E}_{a \sim \pi(\cdot | s)} [-\lambda \log \pi(a | s) + Q_\lambda^\pi(s, a)]. \end{aligned}$$

- Soft Bellman equation:

$$\begin{aligned} V_\lambda^\pi(s) &= \mathbb{E}_{a \sim \pi(\cdot | s)} \mathbb{E}_{s' \sim P(\cdot | s, a)} [r_\lambda(s, a, s') + \gamma V_\lambda^\pi(s')], \\ Q_\lambda^\pi(s, a) &= \mathbb{E}_{s' \sim P(\cdot | s, a)} [r(s, a, s') + \gamma \mathbb{E}_{a' \sim \pi(\cdot | s')} [Q_\lambda^\pi(s', a') - \lambda \log \pi(a' | s')]]. \end{aligned}$$

Soft Bellman Operator

- For state value, soft Bellman operator \mathcal{T}_λ^π under a policy π is defined by

$$[\mathcal{T}_\lambda^\pi V_\lambda](s) = \mathbb{E}_{a \sim \pi(\cdot|s)} \mathbb{E}_{s' \sim P(\cdot|s,a)} [r_\lambda(s, a, s') + \gamma V_\lambda(s')].$$

- \mathcal{T}_λ^π is γ -contraction with respect to ℓ_∞ -norm and V_λ^π is unique fixed point.
- For action value, soft Bellman operator \mathcal{F}_λ^π under a policy π is defined by

$$[\mathcal{F}_\lambda^\pi Q_\lambda](s, a) = \mathbb{E}_{s' \sim P(\cdot|s,a)} [r(s, a, s') + \gamma \mathbb{E}_{a' \sim \pi(\cdot|s')} [Q_\lambda(s', a') - \lambda \log \pi(a'|s')]] ,$$

- \mathcal{F}_λ^π is γ -contraction with respect to ℓ_∞ -norm and Q_λ^π is unique fixed point.

Soft Bellman Optimality Equation: State Value

For any $V_\lambda \in \mathbb{R}^{|S|}$, the soft Bellman optimality operator \mathcal{T}_λ is defined by

$$\begin{aligned} [\mathcal{T}_\lambda V_\lambda](s) &= \max_{\pi} \mathbb{E}_{a \sim \pi(\cdot|s)} \mathbb{E}_{s' \sim P(\cdot|s,a)} [r_\lambda(s, a, s') + \gamma V(s')] \\ &= \max_{\pi} \mathbb{E}_{a \sim \pi(\cdot|s)} \left[\underbrace{\mathbb{E}_{s' \sim P(\cdot|s,a)} [r(s, a, s') + \gamma V(s')]}_{:= Q_\lambda(s, a)} - \lambda \log \pi(a|s) \right] \\ &= \lambda \log \left(\|\exp(Q_\lambda(s, \cdot) / \lambda)\|_1 \right), \end{aligned}$$

where maximum value is attained at (i.e, extracted policy)

$$\begin{aligned} \pi_\lambda(a|s) &= \frac{\exp(Q_\lambda(s, a) / \lambda)}{\|\exp(Q_\lambda(s, \cdot) / \lambda)\|_1} \\ &= \frac{\exp(Q_\lambda(s, a) / \lambda)}{\exp([\mathcal{T}_\lambda V_\lambda](s) / \lambda)}. \end{aligned}$$

following Lemma 5 of Lecture 7.

Remark

- Entropy regularization moves the maxima to the interior so that it has an explicit solution in terms of softmax representation.
- Also by Lemma 5 of Lecture 7, one has for any $a \neq a'$,

$$Q_\lambda(s, a) - \lambda \log \pi_\lambda(a|s) = Q_\lambda(s, a') - \lambda \log \pi_\lambda(a'|s)$$

at optimal π (adding entropy tends to average something). Thus,

$$[\mathcal{T}_\lambda V_\lambda](s) = Q_\lambda(s, a) - \lambda \log \pi_\lambda(a|s), \quad \forall a.$$

- \mathcal{T}_λ is γ -contraction with respect to ℓ_∞ -norm.

Soft Bellman Optimality Equation: Action Value

For $Q_\lambda \in \mathbb{R}^{|\mathcal{S}| \times |\mathcal{A}|}$, the soft Bellman optimality operator \mathcal{F}_λ is defined by

$$\begin{aligned} [\mathcal{F}_\lambda Q_\lambda](s, a) &= \mathbb{E}_{s' \sim P(\cdot | s, a)} \left[r(s, a, s') + \gamma \max_{\pi} \mathbb{E}_{a' \sim \pi(\cdot | s')} [Q_\lambda(s', a') - \lambda \log \pi(a' | s')] \right] \\ &= \mathbb{E}_{s' \sim P(\cdot | s, a)} \left[r(s, a, s') + \gamma \left[\lambda \log \left(\left\| \exp(Q_\lambda(s', \cdot) / \lambda) \right\|_1 \right) \right] \right], \end{aligned}$$

where maximum value is attained at $\pi_\lambda(\cdot | s') \propto \exp(Q_\lambda(s', \cdot) / \lambda)$.

► \mathcal{F}_λ is γ -contraction with respect to ℓ_∞ -norm.

Optimal Policy

Theorem 2

Let V_λ^* and Q_λ^* be the fixed points of \mathcal{T}_λ and \mathcal{F}_λ , respectively. One has

$$V_\lambda^*(s) = \max_{\pi} V_\lambda^\pi(s), \quad \forall s \quad \text{and} \quad Q_\lambda^*(s, a) = \max_{\pi} Q_\lambda^\pi(s, a), \quad \forall s, a.$$

The equality is achieved by the optimal policy given by

$$\pi_\lambda^*(a|s) = \frac{\exp(Q_\lambda^*(s, a)/\lambda)}{\|\exp(Q_\lambda^*(s, \cdot)/\lambda)\|_1}.$$

Moreover, $Q_\lambda^*(s, a) = \mathbb{E}_{s' \sim P(\cdot|s, a)}[r(s, a, s') + \gamma V_\lambda^*(s')] \text{ and}$

$$V_\lambda^* = \lambda \log (\|\exp (Q_\lambda^*(s, \cdot) / \lambda)\|_1) = Q_\lambda^*(s, a) - \lambda \log \pi_\lambda^*(a|s), \quad \forall a.$$

See “Bridging the gap between value and policy based reinforcement learning” by Nachum et al. 2017 for details.

Remark

- ▶ Theorem 2 implies that optimal policy is unique with entropy regularization.
- ▶ It is evident that as $\lambda \rightarrow 0$, $\pi_\lambda^*(a|s) \rightarrow 0$ for $a \notin \operatorname{argmax} Q^*(s, a)$.
- ▶ Since one has

$$\max_a Q_\lambda^*(s, a) \leq \lambda \log (\|\exp (Q_\lambda^*(s, \cdot) / \lambda)\|_1) \leq \lambda \log |\mathcal{A}| + \max_a Q_\lambda^*(s, a),$$

it is easy to see that $V_\lambda^*(s) \rightarrow \max_a Q^*(s, a) = V^*(s)$ as $\lambda \rightarrow 0$.

Soft Policy Iteration

- Soft policy evaluation:

$$Q_{\lambda}^{\pi_k} = \mathcal{F}_{\lambda}^{\pi} Q_{\lambda}^{\pi_k} = \mathbb{E}_{s' \sim P(\cdot | s, a)} [r(s, a, s') + \gamma V_{\lambda}^{\pi_k}(s')].$$

- Soft policy improvement (soft greedy, use softmax to approximate max):

$$\pi_{k+1} = \frac{\exp(Q_{\lambda}^{\pi_k}(s, \cdot)/\lambda)}{\|\exp(Q_{\lambda}^{\pi_k}(s, \cdot)/\lambda)\|_1}.$$

Theorem 3 (Informal)

It can be shown that π_{k+1} is an improved policy compared to π_k and the γ -rate convergence of soft PI can also be established.

See “Soft actor-critic: Off-policy maximum entropy deep reinforcement learning with a stochastic actor” by Haarnoja et al. 2018 for details.

Soft Actor Critic (SAC)

SAC is a policy based or actor-critic method for solving

$$\max_{\theta} V_{\lambda}^{\pi_{\theta}}(\mu) = \mathbb{E}_{s \sim \mu} [V_{\lambda}^{\pi_{\theta}}(s)] .$$

In addition to typical ways for updating value function and policy parameters,

- ▶ Reparametrization trick is used in the computation of policy gradient;
- ▶ Both state and action values have been parametrized for stable training.

See “Soft actor-critic: Off-policy maximum entropy deep reinforcement learning with a stochastic actor” by Haarnoja et al. 2018 for details.

Questions?