Algorithmic and Theoretical Foundations of RL

Policy Optimization II

Ke Wei School of Data Science Fudan University

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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

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

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

$$\Delta \theta \propto \underset{\|\mathbf{d}\|_{2} \leq \alpha}{\operatorname{argmax}} \{ J(\theta) + \langle \nabla J(\theta), \mathbf{d} \rangle \}.$$

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 $F(\theta)$):

$$\Delta \theta \propto \underset{\mathrm{KL}(P_{\theta} \parallel P_{\theta+d}) \leq \alpha}{\operatorname{argmax}} \{ J(\theta) + \langle \nabla J(\theta), \mathbf{d} \rangle \}$$
$$\propto F(\theta)^{\dagger} \nabla J(\theta),$$

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

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

This leads to natural gradient method:

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

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

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

It follows that

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

Derivation of Natural Gradient Direction

For I_1 , one has

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

For I_2 , one has

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

and

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

It follows that

$$\Delta \theta = \underset{\mathrm{KL}\left(P_{\theta} \parallel P_{\theta+d}\right) \leq 2\alpha}{\operatorname{argmax}} \left\{ \textit{J}(\theta) + \langle \nabla \textit{J}(\theta), \textit{d} \rangle \right\} \approx \underset{\textit{d}^{\intercal} \textit{F}(\theta) \textit{d} \leq 2\alpha}{\operatorname{argmax}} \left\{ \textit{J}(\theta) + \langle \nabla \textit{J}(\theta), \textit{d} \rangle \right\} \propto \textit{F}(\theta)^{\dagger} \nabla \textit{J}(\theta).$$

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

Natural Policy Gradient (NPG)

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

$$\max_{\theta} \mathbf{V}^{\pi_{\theta}}(\mu) = \mathbb{E}_{\mathbf{s}_{0} \sim \mu} \left[\mathbf{V}^{\pi_{\theta}}(\mathbf{s}_{0}) \right] = \mathbb{E}_{\tau \sim \mathbf{p}_{\mu}^{\pi_{\theta}}} \left[\mathbf{r}(\tau) \right],$$

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

$$P_{\mu}^{\pi_{\theta}}(\tau) = \mu(\textbf{s}_0) \prod_{t=0}^{\infty} \pi_{\theta}(\textbf{a}_t|\textbf{s}_t) \textbf{P}(\textbf{s}_{t+1}|\textbf{s}_t,\textbf{a}_t) \quad \text{and} \quad \textbf{r}(\tau) = \sum_{t=0}^{\infty} \gamma^t \textbf{r}_t.$$

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),

$$\begin{split} F(\theta) = & \mathbb{E}_{\tau \sim p_{\mu}^{\pi_{\theta}}} \left[\left(\sum_{t=0}^{\infty} \nabla_{\theta} \log \pi_{\theta}(a_{t}|\mathbf{s}_{t}) \right) \left(\sum_{t=0}^{\infty} \nabla_{\theta} \log \pi_{\theta}(a_{t}|\mathbf{s}_{t}) \right)^{\mathsf{T}} \right] \\ = & \mathbb{E}_{\tau \sim p_{\mu}^{\pi_{\theta}}} \left[\sum_{t=0}^{\infty} \nabla_{\theta} \log \pi_{\theta}(a_{t}|\mathbf{s}_{t}) (\nabla_{\theta} \log \pi_{\theta}(a_{t}|\mathbf{s}_{t}))^{\mathsf{T}} \right]. \end{split}$$

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

Average case:

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

where $d^{\pi_{\theta}}(s) = \mathbb{E}_{s_0 \sim \mu} \left[\lim_{t \to \infty} P(s_t = s | s_0, \pi_{\theta}) \right]$ is state stationary distribution.

▶ Discounted case:

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

where $d_{\mu}^{\pi_{\theta}}(s) = \mathbb{E}_{s_0 \sim \mu}\left[(1-\gamma)\sum_{t=0}^{\infty} \gamma^t P(s_t = s|s_0, \pi_{\theta})\right]$ 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

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

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

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:

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

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

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

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

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

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Overall Idea

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

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

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

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

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

$$\textbf{V}^{\pi_{\theta}}(\mu) \geq \textbf{V}_{t}(\theta) - \frac{2\gamma\varepsilon_{t}}{(1-\gamma)^{2}} \max_{\textbf{s}} \mathrm{KL}(\pi_{\theta_{t}}(\cdot|\textbf{s}) \| \pi_{\theta}(\cdot|\textbf{s})),$$

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

See "Trust region policy optimization" by Schulman et al. 2017 for derivation of second fact.

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 :

$$\max_{\theta} \ \textit{V}_t(\theta) \quad \text{subject to} \quad \max_{s} \mathrm{KL}(\pi_{\theta_t}(\cdot|s) \| \pi_{\theta}(\cdot|s)) \leq \delta.$$

Moreover, replace constraint by the average version and instead solve

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

TRPO is Approximately NPG Plus Line Search

After linear approximation to $V_{t}(\theta)$ and quadratic approximation to KL at θ_{t} ,

$$V_{t}(\theta) \approx (\nabla_{\theta} V^{\pi_{\theta_{t}}}(\mu))^{\mathsf{T}}(\theta - \theta_{t}), \ \mathbb{E}_{\mathsf{s} \sim d_{\mu}^{\pi_{\theta_{t}}}} \left[\mathrm{KL}(\pi_{\theta_{t}}(\cdot|\mathsf{s}) \| \pi_{\theta}(\cdot|\mathsf{s})) \right] \approx \frac{1}{2} (\theta - \theta_{t})^{\mathsf{T}} \mathsf{F}(\theta_{t}) (\theta - \theta_{t}),$$

we arrive at the same problem as that for NPG,

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

► TRPO is NPG with adaptive line search in implementations.

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Proximal Policy Optimization (PPO)

Recall from last section that

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

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

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

where

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

- ▶ 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): $\theta_{t+1} = \operatorname{argmax}_{\theta} V_t^{\text{clip}}(\theta)$.
- ▶ 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.

See "Proximal policy optimization algorithms" by Schulman et al. 2017 for details.

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Deterministic Policy Parameterization

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

Average state value:

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

where given trajectory $au = (s_t, \pi_{\theta}(s_t), s_{t+1})_{t=0}^{\infty}$,

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

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

▶ It is worth noting that $V^{\pi_{\theta}}(s) = Q^{\pi_{\theta}}(s, \pi_{\theta}(s))$.

Deterministic Policy Parameterization

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

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

where $d_{\mu}^{\pi_{\theta}}(s) = \mathbb{E}_{s_0 \sim \mu}\left[(1 - \gamma) \sum_{t=0}^{\infty} \gamma^t p_t(s|s_0, \pi_{\theta})\right]$ is state visitation density, and $p_t(s|s_0, \pi_{\theta})$ is the density over state space after transitioning t time steps. Note there is no expectation over action space since $\pi_{\theta}(s)$ 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,

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

Proof of Theorem 1

First note that

$$\begin{split} V^{\pi_{\theta}}(s_0) &= Q^{\pi_{\theta}}(s_0, \pi_{\theta}(s_0)) \\ &= \int_{s} \big(\textit{r}(s_0, \pi_{\theta}(s_0), s_1) + \gamma \textit{V}^{\pi_{\theta}}(s_1) \big) \textit{p}(s_1|s_0, \pi_{\theta}(s_0)) \mathrm{d}s_1. \end{split}$$

Therefore, one has

$$\begin{split} \nabla_{\theta} V^{\pi_{\theta}}(s_0) &= \int_{\mathcal{S}} \left. \nabla_{a} r(s_0, a, s_1) \right|_{a=\pi_{\theta}(s_0)} \left. \nabla_{\theta} \pi_{\theta}(s_0) p(s_1 | s_0, \pi_{\theta}(s_0)) \mathrm{d}s_1 \right. \\ &+ \left. \int_{\mathcal{S}} \left. r(s_0, \pi_{\theta}(s_0), s_1) \left. \nabla p(s_1 | s_0, a) \right|_{a=\pi_{\theta}(s_0)} \left. \nabla_{\theta} \pi_{\theta}(s_0) \mathrm{d}s_1 \right. \\ &+ \gamma \int_{\mathcal{S}} \left. V^{\pi_{\theta}}(s_1) \left. \nabla p(s_1 | s_0, a) \right|_{a=\pi_{\theta}(s_0)} \left. \nabla_{\theta} \pi_{\theta}(s_0) \mathrm{d}s_1 \right. \\ &+ \gamma \int_{\mathcal{S}} \left. \nabla_{\theta} V^{\pi_{\theta}}(s_1) p(s_1 | s_0, \pi_{\theta}(s_0)) \mathrm{d}s_1 \right. \end{split}$$

Proof of Theorem 1 (Cont'd)

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

$$\nabla_{\theta}\pi_{\theta}(\mathsf{s}_0) \nabla_{a}Q^{\pi_{\theta}}(\mathsf{s},a)|_{a=\pi_{\theta}(\mathsf{s}_0)}$$
.

Therefore,

$$\begin{split} \nabla_{\theta} \textbf{\textit{V}}^{\pi_{\theta}}(\textbf{\textit{s}}_{0}) &= \nabla_{\theta} \pi_{\theta}(\textbf{\textit{s}}_{0}) \; \nabla_{a} \textbf{\textit{Q}}^{\pi_{\theta}}(\textbf{\textit{s}},\textbf{\textit{a}})|_{\textbf{\textit{a}} = \pi_{\theta}(\textbf{\textit{s}}_{0})} + \gamma \int_{\mathcal{S}} \nabla_{\theta} \textbf{\textit{V}}^{\pi_{\theta}}(\textbf{\textit{s}}_{1}) \textbf{\textit{p}}(\textbf{\textit{s}}_{1}|\textbf{\textit{s}}_{0}, \pi_{\theta}(\textbf{\textit{s}}_{0})) \mathrm{d}\textbf{\textit{s}}_{1} \\ &= \ldots \\ &= \mathbb{E} \Big[\sum_{t=0}^{\infty} \gamma^{t} \nabla_{\theta} \pi_{\theta}(\textbf{\textit{s}}_{t}) \nabla_{a} \textbf{\textit{Q}}^{\pi_{\theta}}(\textbf{\textit{s}}_{t},\textbf{\textit{a}})|_{\textbf{\textit{a}} = \pi_{\theta}(\textbf{\textit{s}}_{t})} |\textbf{\textit{s}}_{0}, \pi_{\theta} \Big] \\ &= \frac{1}{1-\gamma} \mathbb{E}_{\textbf{\textit{s}} \sim d_{\textbf{\textit{s}}_{0}}^{\pi_{\theta}}} \left[\nabla_{\theta} \pi_{\theta}(\textbf{\textit{s}}) \nabla_{a} \textbf{\textit{Q}}^{\pi_{\theta}}(\textbf{\textit{s}},\textbf{\textit{a}})|_{\textbf{\textit{a}} = \pi_{\theta}(\textbf{\textit{s}})} \right]. \end{split}$$

Averaging over all \mathbf{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.
- lacktriangle Update of ω for action value function is overall the same to Fitted Q-learning.

See "Continuous control with deep reinforcement learning" by Lillicrap et al. 2016 for details.

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Motivation: Enhance exploration by entropy regularization

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

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

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

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

We can rewrite $V^\pi_\lambda(\mu)$ in terms of state values based on a regularized reward

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

where $\emph{V}^\pi_\lambda(\emph{s}) = \mathbb{E}\left[\sum_{t=0}^\infty \gamma^t \emph{r}_\lambda(\emph{s}_t,\emph{a}_t,\emph{s}_{t+1})|\emph{s}_0 = \emph{s},\pi\right]$ 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

ightharpoonup Soft state value V^π_λ :

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

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

$$Q_{\lambda}^{\pi}(\mathsf{s}, a) = \mathbb{E}\left[\frac{r(\mathsf{s}_0, a_0, \mathsf{s}_1)}{r(\mathsf{s}_0, a_0, \mathsf{s}_1)} + \sum_{t=1}^{\infty} \gamma^t r_{\lambda}(\mathsf{s}_t, a_t, \mathsf{s}_{t+1}) | \mathsf{s}_0 = \mathsf{s}, a_0 = a, \pi\right].$$

▶ Relation between Q_{λ}^{π} and V_{λ}^{π} :

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

► Soft Bellman equation:

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

Soft Bellman Operator

▶ For state value, soft Bellman operator $\mathcal{T}^{\pi}_{\lambda}$ 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}^π_λ is γ -contraction with respect to ℓ_∞ -norm and V^π_λ is unique fixed point.
- lacktriangle For action value, soft Bellman operator \mathcal{F}^π_λ under a policy π is defined by

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

• \mathcal{F}^π_λ is γ -contraction with respect to ℓ_∞ -norm and \mathbf{Q}^π_λ is unique fixed point.

Soft Bellman Optimality Equation: State Value

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

$$\begin{split} [\mathcal{T}_{\lambda}V_{\lambda}](s) &= \max_{\pi} \mathbb{E}_{a \sim \pi(\cdot|s)} \mathbb{E}_{s' \sim P(\cdot|s,a)}[r_{\lambda}(s,a,s') + \gamma V_{\lambda}(s')] \\ &= \max_{\pi} \mathbb{E}_{a \sim \pi(\cdot|s)} \left[\underbrace{\mathbb{E}_{s' \sim P(\cdot|s,a)}[r(s,a,s') + \gamma V_{\lambda}(s')]}_{::=Q_{\lambda}(s,a)} - \lambda \log \pi(a|s) \right] \\ &= \lambda \log \left(\left\| \exp \left(Q_{\lambda}\left(s,\cdot\right)/\lambda \right) \right\|_{1} \right), \end{split}$$

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

$$\pi_{\lambda}(a|s) = \frac{\exp(Q_{\lambda}(s,a)/\lambda)}{\|\exp(Q_{\lambda}(s,\cdot)/\lambda)\|_{1}}$$
$$= \frac{\exp(Q_{\lambda}(s,a)/\lambda)}{\exp([\mathcal{T}_{\lambda}V_{\lambda}](s)/\lambda)},$$

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 $\boldsymbol{\pi}$ (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

$$\begin{split} [\mathcal{F}_{\lambda}Q_{\lambda}](s,a) &= \mathbb{E}_{s' \sim P(\cdot|s,a)} \left[r(s,a,s') + \gamma \max_{\pi} \mathbb{E}_{a' \sim \pi(\cdot|s')} \left[Q_{\lambda}(s',a') - \lambda \log \pi(a'|s') \right] \right] \\ &= \mathbb{E}_{s' \sim P(\cdot|s,a)} \left[r(s,a,s') + \gamma \left[\lambda \log \left(\left\| \exp \left(Q_{\lambda}\left(s', \cdot \right) / \lambda \right) \right\|_{1} \right) \right] \right], \end{split}$$

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

 $ightharpoonup \mathcal{F}_{\lambda}$ 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

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

The equality is achieved by the optimal policy given by

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

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

$$V_{\lambda}^{*}(\mathsf{s}) = \lambda \log \left(\left\| \exp \left(Q_{\lambda}^{*}\left(\mathsf{s}, \cdot \right) / \lambda \right) \right\|_{1} \right) = Q_{\lambda}^{*}(\mathsf{s}, \mathsf{a}) - \lambda \log \pi_{\lambda}^{*}(\mathsf{a}|\mathsf{s}), \quad \forall \mathsf{a}.$$

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 $\lambda \to 0$, $\pi_{\lambda}^*(a|s) \to 0$ for $a \notin \operatorname{argmax} Q^*(s, a)$.
- ► Since one has

$$\max_{a} \mathbf{Q}_{\lambda}^{*}(\mathbf{s}, a) \leq \lambda \log \left(\left\| \exp \left(\mathbf{Q}_{\lambda}^{*}\left(\mathbf{s}, \cdot \right) / \lambda \right) \right\|_{1} \right) \leq \lambda \log |\mathcal{A}| + \max_{a} \mathbf{Q}_{\lambda}^{*}(\mathbf{s}, a),$$

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

Soft Policy Iteration

Soft policy evaluation:

$$\mathbf{Q}_{\lambda}^{\pi_k} = \mathcal{F}_{\lambda}^{\pi} \mathbf{Q}_{\lambda}^{\pi_k} = \mathbb{E}_{\mathbf{S}' \sim \mathsf{P}(\cdot | \mathbf{S}, \mathbf{a})}[\mathbf{r}(\mathbf{S}, \mathbf{a}, \mathbf{S}') + \gamma \mathbf{V}_{\lambda}^{\pi_k}(\mathbf{S}')].$$

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

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

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

$$\max_{\boldsymbol{\theta}} \mathbf{V}_{\boldsymbol{\lambda}}^{\pi_{\boldsymbol{\theta}}}(\boldsymbol{\mu}) = \mathbb{E}_{\mathbf{S} \sim \boldsymbol{\mu}} \left[\mathbf{V}_{\boldsymbol{\lambda}}^{\pi_{\boldsymbol{\theta}}}(\mathbf{S}) \right].$$

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

- ► Reparametrizarion 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.

