# Algorithmic and Theoretical Foundations of RL

## Policy Optimization

Ke Wei, School of Data Science, Fudan University

With help from Jie Feng and Jiacai Liu

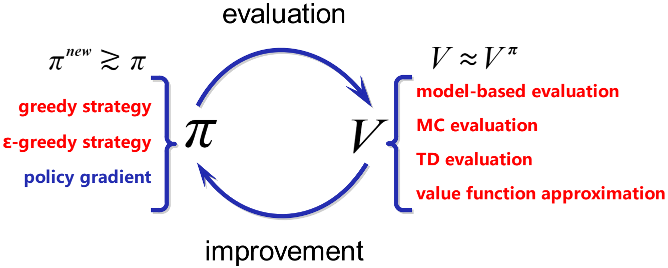
# Table of Contents

Introduction

REINFORCE

Actor-Critic Methods

# Value-Based vs Policy-Based RL



- Value-based RL: Learn (optimal) state/action values and policy is implicitly inferred (e.g., greedy or $\epsilon$-greedy);
- Policy-based RL: Directly parametrize the policy and search in the space of policies via optimization.

# Policy-Based RL

Consider a policy parameterization such that :

$$\pi_\theta(\cdot|s) \text{ defines a probability distribution on } \mathcal{A}.$$

Note that once $\theta$ is given, policy is determined.

**Goal:** Search for best $\theta$ subject to certain performance measure.

Typical advantages of policy-based methods include:

- Better convergence properties
- Effective in high dimensional or continuous action spaces
- Can learn stochastic policies.

However, since $J(\theta)$ can be highly non-concave, optimization methods tend to converge to a local optimum rather than a global optimum.

# Policy Parameterization: Softmax Policy

For discrete action space, a common choice is softmax policy (Boltzmann distribution):

$$\pi_\theta(a|s) = \frac{\exp(f_\theta(s,a))}{\sum_{a' \in \mathcal{A}} \exp(f_\theta(s,a'))}.$$

A special example is when

$$f_\theta(s,a) = \phi(s,a)^T \theta,$$

where $\phi(s,a)$ is a feature vector.

# Policy Parameterization: Gaussian Policy

For continuous action space, Gaussian distribution is natural:

$$\pi_\theta(\cdot|s) \text{ is the pdf of } \mathcal{N}(\mu_\theta(s), \sigma_\theta^2(s)).$$

A special example is

$$\pi_\theta(\cdot|s) \text{ is the pdf of } \mathcal{N}(\phi(s)^T\theta, \sigma^2),$$

where $\phi(s)$ is a feature vector.

# Policy Optimization

Consider average state value with initial distribution $\mu$ as performance measure:

$$J(\theta) = \mathbb{E}_{s_0 \sim \mu}\left[v_{\pi_\theta}(s_0)\right] = \mathbb{E}_{\tau \sim P_\mu^{\pi_\theta}}\left[r(\tau)\right],$$

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

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

It is natural to formulate the RL problem as

$$\theta^* = \underset{\theta}{\operatorname{argmax}}\ J(\theta).$$

- The initial state distribution can be for example Dirac delta distribution, uniform distribution, or stationary distribution under policy $\pi_\theta$. Here we assume $\mu$ is a fixed distribution .

For simplicity, we only discuss the case where sate and action spaces are discrete.

# Alternative Expression of State Value and Visitation Measure

Theorem 1 (Expression of State Value in Terms of Visitation Measure)

*For any policy $\pi$, there holds*

$$\mathbb{E}_{s_0 \sim \mu}\left[v_\pi(s_0)\right] = \frac{1}{1-\gamma} \mathbb{E}_{s \sim d_\mu^\pi} \mathbb{E}_{a \sim \pi(\cdot|s)} \mathbb{E}_{s' \sim P(\cdot|s,a)} \left[r(s,a,s')\right],$$

*where*

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

*is discounted state visitation measure under policy $\pi$ and initial distribution $\mu$.*

If $\pi = \pi_\theta$, then $\mathbb{E}_{s_0 \sim \mu}\left[v_\pi(s_0)\right] = J(\theta)$.

# Proof of Theorem 1

$$
\begin{aligned}
v_\pi(s_0) &= \mathbb{E}_{\tau\sim P^\pi_{s_0}}\left[\sum_{t=0}^{\infty}\gamma^t r(s_t,a_t,s_{t+1})\right] \\
&= \sum_{t=0}^{\infty}\mathbb{E}_{\tau\sim P^\pi_{s_0}}\left[\gamma^t r(s_t,a_t,s_{t+1})\right] \\
&= \sum_{t=0}^{\infty}\sum_{s}\sum_{a}\sum_{s'}\gamma^t\cdot P(s_t=s|s_0,\pi)\pi(a|s)P(s'|s,a)r(s,a,s') \\
&= \sum_{s}\sum_{a}\sum_{s'}\left(\sum_{t=0}^{\infty}\gamma^t\cdot P(s_t=s|s_0,\pi)\right)\pi(a|s)P(s'|s,a)r(s,a,s') \\
&= \frac{1}{1-\gamma}\sum_{s}\sum_{a}\sum_{s'}d^\pi_{s_0}(s)\pi(a|s)P(s'|s,a)r(s,a,s').
\end{aligned}
$$

Expression for $\mathbb{E}_{s_0\sim\mu}\left[v_\pi(s_0)\right]$ can be obtained directly by averaging over $s_0\sim\mu$.

# Visitation Measure in Matrix Form

Lemma 1

*The visitation measure can be expressed in the following matrix form*

$$d_\mu^\pi = (1-\gamma)(I-\gamma(P^\pi)^T)^{-1}\mu,$$

*where $P^\pi = (p^\pi_{ss'})$ is transition matrix induced by policy $\pi$ (see Lecture 1).*

**Proof.** This lemma can be proved by expanding $(I-\gamma(P^\pi)^T)^{-1}$.

# Optimization Methods

- Gradient free methods
  - Random search
  - Simulated annealing
  - Various evolutionary algorithms
- Gradient ascent methods
  - Compute gradient by finite difference
  - Compute gradient analytically

For gradient free methods, see for example Chapter 10 of “Algorithms for decision making” by Kochenderfer et al., 2022.

# Compute Policy Gradient

Theorem 2

*Suppose $\pi_\theta$ is differentiable for all states and actions. We have the following expressions for $\nabla J(\theta)$:*

- *Return expression:*

$$\nabla_\theta J(\theta) = \mathbb{E}_{\tau \sim P_\mu^{\pi_\theta}} \left[ r(\tau) \sum_{t=0}^{\infty} \nabla_\theta \log \pi_\theta(a_t|s_t) \right];$$

- *Action value expression:*

$$\nabla_\theta J(\theta) = \mathbb{E}_{\tau \sim P_\mu^{\pi_\theta}} \left[ \sum_{t=0}^{\infty} \gamma^t q_{\pi_\theta}(s_t, a_t) \nabla_\theta \log \pi_\theta(a_t|s_t) \right].$$

# Proof of Theorem 2

The following log derivative trick will be very useful in the proof:

$$\nabla f(x) = f(x)\nabla \log f(x).$$

By the definition of $J(\theta)$, we have

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

# Proof of Theorem 2 (Cont'd)

For the action value expression, we have

$$
\begin{aligned}
&\mathbb{E}_{\tau\sim P_\mu^{\pi_\theta}}\left[r(\tau)\sum_{t=0}^{\infty}\nabla_\theta \log \pi_\theta(a_t|s_t)\right] \\
&= \sum_{t=0}^{\infty}\mathbb{E}_{\tau\sim P_\mu^{\pi_\theta}}\left[r(\tau)\nabla_\theta \log \pi_\theta(a_t|s_t)\right] \\
&= \sum_{t=0}^{\infty}\mathbb{E}_{\tau\sim P_\mu^{\pi_\theta}}\left[\sum_{k=0}^{\infty}\gamma^k r(s_k, a_k, s_{k+1})\nabla_\theta \log \pi_\theta(a_t|s_t)\right] \\
&= \sum_{t=0}^{\infty}\mathbb{E}_{\tau\sim P_\mu^{\pi_\theta}}\left[\sum_{k=0}^{t-1}\gamma^k r(s_k, a_k, s_{k+1})\nabla_\theta \log \pi_\theta(a_t|s_t)\right] \\
&\quad + \sum_{t=0}^{\infty}\mathbb{E}_{\tau\sim P_\mu^{\pi_\theta}}\left[\sum_{k=t}^{\infty}\gamma^k r(s_k, a_k, s_{k+1})\nabla_\theta \log \pi_\theta(a_t|s_t)\right]
\end{aligned}
$$

The part can also be derived via the recursive relation $v_{\pi_\theta}(s_0) = \sum_{a_0} \pi_\theta(a_0|s_0) q_{\pi_\theta}(s_0, a_0)$ and the chain rule.

# Proof of Theorem 2 (Cont'd)

$$= \sum_{t=0}^{\infty} \mathbb{E}_{\tau \sim P_{\mu}^{\pi_\theta}} \left[ \sum_{k=t}^{\infty} \gamma^k r(s_k, a_k, s_{k+1}) \nabla_\theta \log \pi_\theta(a_t|s_t) \right]$$

$$= \sum_{t=0}^{\infty} \mathbb{E}_{\tau \sim P_{\mu}^{\pi_\theta}} \left[ \gamma^t q_{\pi_\theta}(s_t, a_t) \nabla_\theta \log \pi_\theta(a_t|s_t) \right],$$

where in the fourth equality we have used the fact

$$\mathbb{E}_{a_t \sim \pi_\theta(\cdot|s_t)} \left[ \nabla_\theta \log \pi_\theta(a_t|s_t) \right] = 0.$$

# Policy Gradient Theorem

The policy gradient theorem allows us to decompose the policy gradient into the expression of an expectation over state-action pairs.

**Theorem 3 (Policy Gradient Theorem)**

*Recalling the definition of visitation measure, we have*

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

**Proof.** The proof is overall similar to that of Theorem 1.

- Note that $\nabla_\theta \log \pi_\theta(a|s)$ is the direction that $\pi_\theta(a|s)$ increases (i.e., the probability of selecting $a$ at $s$ increases). The weight $q_{\pi_\theta}(s, a)$ demonstrates that if $q_{\pi_\theta}(s, a)$ is large, it should move more towards the direction that increases the probability of choosing $a$.

# Policy Gradient Ascent

$$\begin{aligned}\theta &\leftarrow \theta + \alpha \cdot \mathbb{E}_{s,a}\left[q_{\pi_\theta}(s,a)\nabla_\theta \log \pi_\theta(a|s)\right] \\ &= \theta + \alpha \cdot \mathbb{E}_{s,a}\left[\frac{q_{\pi_\theta}(s,a)}{\pi_\theta(a|s)}\nabla_\theta \pi_\theta(a|s)\right]\end{aligned}$$

- Large $q_{\pi_\theta}(s,a)$ means that weight in front of the direction $\nabla_\theta \pi_\theta(a|s)$ is large. Thus, the method attempts to exploit actions with large action values.
- Small $\pi_\theta(a|s)$ means that weight in front of the direction $\nabla_\theta \pi_\theta(a|s)$ is large. This reflects that the method attempts to explore actions with low probability.

# Table of Contents

Introduction

REINFORCE

Actor-Critic Methods

# MC Evaluation of Policy Gradient

From the proof of Theorem 2, we can see that the random variable in action value expression potentially has smaller variance than that in return version since some randomness is eliminated in the proof. Thus we consider MC evaluation of action value expression.

- Sample $N$ episodes:

$$\tau^{(i)} = (s_0^{(i)}, a_0^{(i)}, r_0^{(i)}, \cdots, s_{T-1}^{(i)}, a_{T-1}^{(i)}, r_{T-1}^{(i)}, s_T^{(i)}) \sim \pi_\theta;$$

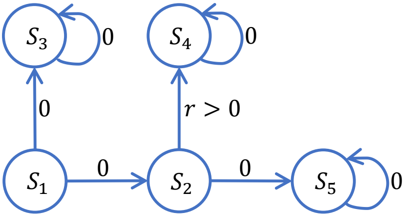
- Use return $G_t = \sum_{t'=t}^{T-1} \gamma^{t'-t} r_{t'}$ as an unbiased estimate of $q_{\pi_\theta}(s_t, a_t)$:

$$\nabla J(\theta) \approx \frac{1}{N} \sum_{i=1}^{N} \sum_{t=0}^{T-1} \gamma^t G_t^{(i)} \nabla_\theta \log \pi_\theta(a_t^{(i)} | s_t^{(i)}).$$

# REINFORCE

```
Algorithm 1: REINFORCE
Initialization: $\pi_\theta(a|s)$ and $\theta_0$.
for $k = 0, 1, 2, \ldots$ do
    Sample episodes $\mathcal{D}_k = \{\tau^{(i)}\}$:
        $$\tau^{(i)} = (s_0^{(i)}, a_0^{(i)}, r_0^{(i)}, \cdots, s_{T-1}^{(i)}, a_{T-1}^{(i)}, r_{T-1}^{(i)}, s_T^{(i)}) \sim \pi_{\theta_k}$$
    Policy gradient calculation:
        $$g_k = \frac{1}{|\mathcal{D}_k|} \sum_{i=1}^{|\mathcal{D}_k|} \sum_{t=0}^{T-1} \gamma^t G_t^{(i)} \nabla_\theta \log \pi_{\theta_k}(a_t^{(i)}|s_t^{(i)})$$
    Policy parameter update:
        $$\theta_{k+1} = \theta_k + \alpha_k g_k$$
end
```

# Illustrative Example



- Suffice to consider states $s_1$ and $s_2$ since $s_3, s_4$ and $s_5$ are terminal states.
- Denote the up ($\uparrow$) action by $a_1$ and the right ($\rightarrow$) action by $a_2$.
- Consider the softmax parameterization,

$$\pi_\theta(a|s) = \frac{\exp(\theta_{s,a})}{\sum_{a' \in \mathcal{A}} \exp(\theta_{s,a'})},$$

with parameters $\theta = (\theta_{s_1,a_1}, \theta_{s_1,a_2}, \theta_{s_2,a_1}, \theta_{s_2,a_2})^T$.

# Illustrative Example (Cont'd)

Assume $\gamma = 1$. Let $\theta_0 = (0,0,0,0)^\intercal$ and sample episode $\tau = (s_1, a_2, 0, s_2, a_1, r, s_4)$. First note that

$$\frac{\partial \log \pi_\theta(a|s)}{\partial \theta_{s',a'}} = 1[s = s'] \left(1[a = a'] - \pi_\theta(a'|s)\right) .$$

At timestep $t = 0$:

- ▶ Calculate the total rewards: $G_0 = 0 + r = r$;
- ▶ Calculate $\nabla_\theta \log \pi_\theta(a_2|s_1) = (-\frac{1}{2}, \frac{1}{2}, 0, 0)^\intercal$.

At timestep $t = 1$:

- ▶ Calculate the total rewards: $G_1 = r$;
- ▶ Calculate $\nabla_\theta \log \pi_\theta(a_1|s_2) = (0, 0, \frac{1}{2}, -\frac{1}{2})^\intercal$.

Parameter update:

$$\theta \leftarrow \theta + \nabla_\theta \log \pi_\theta(a_2|s_1)G_0 + \nabla_\theta \log \pi_\theta(a_1|s_2)G_1 = (-\frac{r}{2}, \frac{r}{2}, \frac{r}{2}, -\frac{r}{2})^T.$$

# Variance Reduction with Baseline

Recall the action value expression

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

Conditioned on $s$, we would like to find a baseline (control variate) $b(s)$ such that the variance of $(q_{\pi_\theta}(s,a) - b(s))\nabla_\theta \log \pi_\theta(a|s)$ can be reduced.

- The expectation is not changed by adding $b(s)$ since

$$\mathbb{E}_{a\sim\pi_\theta(\cdot|s)}\left[b(s)\nabla_\theta \log \pi_\theta(a|s)\right] = 0.$$

- The optimal $b(s)$ is given by

$$b(s) = \frac{\mathbb{E}_{a\sim\pi_\theta(\cdot|s)}\left[q_{\pi_\theta}(s,a)\|\nabla_\theta \log \pi_\theta(a|s)\|_2^2\right]}{\mathbb{E}_{a\sim\pi_\theta(\cdot|s)}\left[\|\nabla_\theta \log \pi_\theta(a|s)\|_2^2\right]}.$$

# Variance Reduction with Baseline (Cont'd)

- With the baseline, the action value expression for policy gradient becomes

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

$$= \mathbb{E}_{\tau \sim P_\mu^{\pi_\theta}} \left[ \sum_{t=0}^{\infty} \gamma^t \big( q_{\pi_\theta}(s_t, a_t) - b(s_t) \big) \nabla_\theta \log \pi_\theta(a_t|s_t) \right].$$

- Note that the optimal $b(s)$ can be viewed as the expected value of $q$-values, but weighted by gradient magnitudes. Thus, it is reasonable to take

$$b(s) = v_{\pi_\theta}(s),$$

which is a common baseline in practice. With this choice for $b(s)$, we have the advantage function expression for policy gradient

$$\nabla J(\theta) = \mathbb{E}_{\tau \sim P_\mu^{\pi_\theta}} \left[ \sum_{t=0}^{\infty} \gamma^t A_{\pi_\theta}(s_t, a_t) \nabla_\theta \log \pi_\theta(a_t|s_t) \right],$$

where $A_{\pi_\theta}(s_t, a_t) = q_{\pi_\theta(s_t, a_t)} - v_{\pi_\theta}(s_t)$ is the advantage function.
Since $v_{\pi_\theta}(s)$ is not directly accessible, we may estimate it via value function approximation $v_{\pi_\theta}(s) \approx v(s; \omega)$.

# REINFORCE with Baseline

```
Algorithm 2: REINFORCE with Baseline
Initialization: initial policy parameters $\theta_0$, initial value function parameters $\omega_0$ .
for $k = 0, 1, 2, \ldots$ do
    Sample a trajectories $\mathcal{D}_k = \{\tau_i\}$ following $\pi_{\theta_k}$.
    for $t = 0, 1, 2 \ldots T - 1$ of each trajectory $\tau_i$ do
        Compute the return: $G_t^{(i)} = \sum_{t'=t}^{T-1} \gamma^{t'-t} r_{t'}^{(i)}$.
        Compute advantage estimates: $\widehat{A}_t^{(i)} = G_t^{(i)} - V(s_t; \omega_k)$.
    end
    Estimate policy gradient:
        $$g_k = \frac{1}{|\mathcal{D}_k|} \sum_{i=1}^{|\mathcal{D}_k|} \sum_{t=0}^{T-1} \gamma^t \cdot \widehat{A}_t^{(i)} \nabla_\theta \log \pi_{\theta_k} \left( a_t^{(i)} | s_t^{(i)} \right).$$
    Policy parameter update:
        $$\theta_{k+1} = \theta_k + \alpha_k g_k.$$
    Fit value function by regression on mean-squared error (via e.g., GD/SGD):
        $$\omega_{k+1} = \operatorname*{argmin}_{\omega} \frac{1}{|\mathcal{D}_k| \, T} \sum_{i=1}^{|\mathcal{D}_k|} \sum_{t=0}^{T-1} \left( V(s_t; \omega) - G_t^{(i)} \right)^2$$
end
```

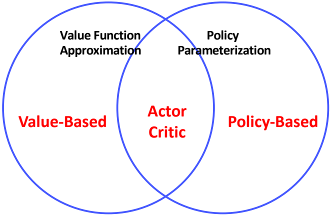
# Table of Contents

Introduction

REINFORCE

Actor-Critic Methods

# Overall Idea



- Value-based: Learn value function
- (Pure) Policy-based: Learn policy function
- Actor-critic: learn value and policy functions

# Actor-Critic Methods

**Motivation.** MC policy gradient evaluation is sample inefficient and has high variance. Similar to VFA in value-based RL, we can approximate values that appears in the policy gradient and update VFA parameters in learning process.

- Actor: learn parameterized policy $\pi_\theta(\cdot|\cdot)$ via policy gradient;
- Critic: learn value function $v(:;\omega)$ or $q(:;\omega)$ in $\nabla J(\theta)$ via policy evaluation.

Recall TD policy evaluation for state value and action value parameter as follows:

$$\text{(State value)} \quad \delta_t = r_t + \gamma \cdot v(s_{t+1};\omega) - v(s_t;\omega), \;\; \omega \leftarrow \omega + \alpha_t \delta_t \nabla_\omega v(s_t;\omega)$$

$$\text{(Action value)} \quad \delta_t = r_t + \gamma \cdot q(s_{t+1}, a_{t+1};\omega) - q(s_t, a_t;\omega)$$

$$\omega \leftarrow \omega + \alpha_t \delta_t \nabla_\omega q(s_t, a_t;\omega) - q(s_t, a_t;\omega)$$

Actor-critic (or policy gradient) methods fit into the framework of policy evaluation and policy improvement. Policy improvement is achieved by gradient ascent, hence is actor. The evaluation of policy (state/action/advantage) instructs the direction to improve the policy, hence is critic.

# Action-Value Actor-Critic

```
Algorithm 3: Action-Value Actor-Critic
Initialization: policy parameters $\theta_0$, action value function parameter $\omega_0$.
for $t = 0, 1, \cdots$ do
    Sample a tuple $(s_t, a_t, r_t, s_{t+1}, a_{t+1}) \sim \pi_\theta$
    Calculate $\delta_t \leftarrow r_t + \gamma \cdot q(s_{t+1}, a_{t+1}; \omega) - q(s_t, a_t; \omega)$
    Critic update: $\omega \leftarrow \omega + \beta_t \cdot \delta_t \nabla_\omega q(s_t, a_t; \omega)$
    Actor update: $\theta \leftarrow \theta + \alpha_t \cdot q(s_t, a_t; \omega) \nabla_\theta \log \pi_\theta (a_t | s_t)$
end
```

There are other versions of actor-critic, e.g., the parameters are only updated at the end of an episode by using all the episode data simultaneously.

# Advantage Actor-Critic Method (A2C)

In A2C, advantage function expression for policy gradient is used and value function approximation is applied to state values:

$$q(s_t, a_t) \approx r_t + \gamma v(s_{t+1}; \omega), \quad A(s_t, a_t) \approx \underbrace{r_t + \gamma v(s_{t+1}; \omega) - v(s_t; \omega)}_{\delta_t}$$

**Algorithm 4:** Advantage Actor-Critic (A2C)

```
Initialization: policy parameters $\theta_0$, state value function parameter $\omega_0$.
for $t = 0, 1, \cdots$ do
    Sample a tuple $(s_t, a_t, r_t, s_{t+1}) \sim \pi_\theta$
    Calculate $\delta_t \leftarrow r_t + \gamma v(s_{t+1}; \omega) - v(s_t; \omega)$
    Critic update: $\omega \leftarrow \omega + \beta_t \cdot \delta_t \nabla_\omega v(s_t; \omega)$
    Actor update: $\theta \leftarrow \theta + \alpha_t \cdot \delta_t \nabla_\theta \log \pi_\theta (a_t|s_t)$
end
```

Questions?