7. Optimal Control and Policy Based Reinforcement Learning

# **Optimal Control**

## Discrete-Time Optimal Control

- ✓ Dynamic Programming
- ✓ Affine Quadratic Problem
- ✓ Infinite Horizon Linear Quadratic Problem

## Continuous-Time Optimal Control

- ✓ Dynamic Programming (Hamilton-Jacobi-Bellman Equation)
- ✓ Minimum Principle
- ✓ Affine Quadratic Problem
- ✓ Infinite Horizon Linear Quadratic Problem

## **Basic Principle to Analyze Dynamic Games**

### **Equilibrium concept:**

-Nash; Zero-sum; Stackelberg; Correlated

	Single Agent	Multi Agent
Static	Static optimization	Static Game
Dynamic	Dynamic Optimization	Dynamic Game

## **Dynamic optimization as a static optimization concept:**

- -Minimum principle (necessary condition)
- -Dynamic programming principle (sufficient condition)
- -Need to specify information structure

$$L^{1*} \triangleq L^{1}(\mathbf{u}^{1*}; u^{2*}; ...; u^{N*}) \leq L^{1}(\mathbf{u}^{1}; u^{2*}; ...; u^{N*}),$$

$$L^{2*} \triangleq L^{2}(u^{1*}; \mathbf{u}^{2*}; ...; u^{N*}) \leq L^{2}(u^{1*}; \mathbf{u}^{2}; ...; u^{N*}),$$

$$...$$

$$L^{N*} \triangleq L^{N}(u^{1*}; u^{2*}; ...; \mathbf{u}^{N*}) \leq L^{N}(u^{1*}; u^{2*}; ...; \mathbf{u}^{N*})$$

(Think in normal form game setting)

	Single Agent	Multi Agent
Static	Static optimization	Static Game
Dynamic	Dynamic Optimization	Dynamic Game

## **Action space**

	Model based	Finite	Infinite
space	Discrete	Discrete time MDP $P(s_{t+1} s_t, a_t)$	Discrete-time dynamic system $x_{t+1} = f(x_t, u_t)$
Ime	Continuous	Continuous time MDP $P(s_{t+h} s_t, a_t)$	Continuous-time dynamic system $\dot{x}_t = f(x_t, u_t)$

	Single Agent	Multi Agent
Static	Static optimization	Static Game
Dynamic	Dynamic Optimization	Dynamic Game

## **Action space**

pace	Model free	Finite	Infinite
	Discrete	Value-based Reinforcement Learning	Policy-based Reinforcement Learning
	Continuous		

Time space

	Single Agent	Multi Agent
Static	Static optimization	Static Game
Dynamic	Dynamic Optimization	Dynamic Game

## **Action space**

I ime space	Model based	Finite	Infinite
	Discrete	Markov Game (Stochastic Game)	DT Infinite dynamic game (Stochastic Game)
	Continuous	Continuous time Markov Game	CT-time Infinite dynamic game (differential game)

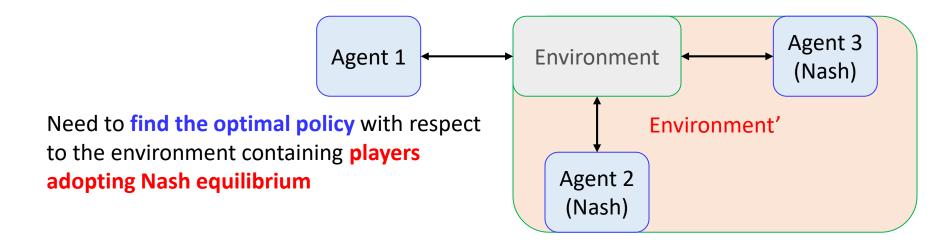
	Single Agent	Multi Agent
Static	Static optimization	Static Game
Dynamic	Dynamic Optimization	Dynamic Game

## **Action space**

	Model free	Finite	Infinite
space	Discrete	Multi-Agent Value-based RL	Multi-Agent Policy-based RL
Ime	Continuous		

### Why We Learn Optimal Control Theory?

- Optimal control problems constitute a special class of infinite dynamic games with one player and one criterion
  - > The mathematical tools available for such problems are useful in dynamic game theory
- If the players adopt the non-cooperative Nash equilibrium solution concept, in which case each player is faced with a single criterion optimization problem (i.e., optimal control problem) with the strategies of the remaining players taken to be fixed at their equilibrium values.
  - ➤ Hence, in order to verify whether a given set of strategies is in Nash equilibrium, we inevitably have to utilize the tools of optimal control theory.



## **Discrete-Time Optimal Control Problems**

Want to find a control sequence  $u = \{u_k, k \in \mathbf{K}\}$  which minimizes

$$L(u) = \sum_{k=0}^{K-1} g_k(x_k, u_k) + g_K(x_K)$$
 (1)

where the state variable  $x_k$  satisfies discrete-time system constraints:

$$x_{k+1} = f_k(x_k, u_k), \qquad u_k \in U_k, \qquad k \in \mathbf{K}$$
 (2)

on time steps  $k \in \mathbf{K} = \{0, 1, ..., K - 1\}$ 

•  $u = \{u_k, k \in \mathbf{K}\}, u_k = \gamma_k(x_k)$ 

 $\checkmark \gamma_k(\cdot)$  is a permissible control strategy at stage  $k \in \mathbf{K}$ 

### **Dynamic Programming for Discrete-Time Optimal Control Problems**

• In order to determine the minimizing control strategy, we define the expression for the minimum cost from any staring point x at any initial time k, which is so called value function

$$V(k,x) = \min_{\gamma_k,\dots,\gamma_K} \left[ \sum_{i=k}^K g_i(x_{i+1},u_i,x_i) \right]$$
 with  $u_i = \gamma_i(x_i) \in U_i$  and  $x_k = x$  (3)

A direct application of the principle of optimality now readily leads to the recursive relation

$$V(k,x) = \min_{u_k} \left[ g_k(f_k(x, u_k), u_k, x) + V(k+1, f_k(x, u_k)) \right]$$
(4)

- If the optimal control problem admits a solution  $u^* = \{\gamma_k^*, k \in \mathbf{K}\}$ , then the solution V(1, x) of Eq.(4) should be equal to  $L(u^*)$
- Each  $u_k^*$  should be determined as an argument of the RHS of Eq.(4)(single-shot optimization)

An optimal policy has the property that whatever the initial state and initial decision are, the remaining decisions must constitute an optimal policy with regard to the state resulting from the first decision.

- discrete-time system  $x_{t+1} = Ax_t + Bu_t$ ,  $x_0 = x^{init}$
- problem: choose  $u_0$ ,  $u_1$ , ... to minimize

$$J = \sum_{\tau=0}^{\infty} (x_{\tau}^T Q x_{\tau} + u_{\tau}^T R u_{\tau})$$

with given constant state and input weight matrices

$$Q = Q^T \ge 0, \qquad R = R^T > 0$$

✓ this is an infinite dimensional problem

• **Problem**: it's possible that  $J = \infty$  for all input sequences  $u_0, \dots$ 

$$x_{t+1} = 2x_t + 0u_t, \qquad x^{init} = 1$$

- Let's assume (A, B) is controllable
- then for any  $x^{init}$  there's an input sequence

$$u_0, \dots, u_{n-1}, 0, 0, \dots$$

that steers x to zero at t = n, and keeps it there

- ✓ For this  $u, J < \infty$
- ✓ And therefore,  $\min_{u} J < \infty$  for any  $x^{init}$

• To apply dynamic programming approach define value function  $V: \mathbf{R}^n o \mathbf{R}$ 

$$V(z) = \min_{u_0, \dots} \sum_{\tau=0}^{\infty} (x_{\tau}^T Q x_{\tau} + u_{\tau}^T R u_{\tau})$$

subject to 
$$x_0 = z$$
,  $x_{\tau+1} = Ax_{\tau} + Bu_{\tau}$ 

- V(z) is the minimum LQR cost-to-go, starting from state z
- doesn't depend on time-to-to, which is always ∞; infinite horizon problem is shift invariant

- Fact: V is quadratic, i.e.,  $V(z) = z^T P z$ , where  $P = P^T \ge 0$
- Applying Bellman minimum principle (or HJB equation for discrete system)

$$V(z) = \min_{w} \left( z^{T} Q z + w^{T} R w + V (A z + B w) \right)$$

or

$$z^{T}Pz = \min_{w} \left( z^{T}Qz + w^{T}Rw + (Az + Bw)^{T}P(Az + Bw) \right)$$

- minimizing  $w^* = -(R + B^T P B)^{-1} B^T P A z$
- so HJB equation is

$$z^{T}Pz = z^{T}Qz + w^{*T}Rw^{*} + (Az + Bw^{*})^{T}P(Az + Bw^{*})$$
$$= z^{T}(Q + A^{T}PA - A^{T}PB(R + B^{T}PB)^{-1}B^{T}PA)z$$

 $\checkmark$  This must hold for all z, so we can conclude that P satisfies the **ARE** 

$$P = Q + A^T P A - A^T P B (R + B^T P B)^{-1} B^T P A$$

• The optimal input is constant state feedback  $u_t = Kx_t$ 

$$K = -(R + B^T P B)^{-1} B^T P A$$

- Fact: the ARE has only one positive semidefinite solution P
  - ✓ ARE plus  $P = P^T \ge 0$  uniquely characterizes value function
- Consequence: The Riccati recursion

$$P_{k+1} = Q + A^T P_k A - A^T P_k B (R + B^T P_k B)^{-1} B^T P_k A, \qquad P_1 = Q$$

converges to the unique PSD solution of the ARE (when (A,B) controllable)

Infinite-horizon LQR optimal control is same as steady-state finite horizon optimal control

## **Continuous-Time Optimal Control Problems**

Consider the following optimal control problem defined by

$$L(u) = \int_0^T g(t, x(t), u(t)) dt + q(T, x(T))$$
 (5)

where the state variable x(t) satisfies the differential equation:

$$\dot{x}(t) = f(t, x(t), u(t)), \qquad x(0) = x_0, \qquad t \ge 0$$
 (6)

- $u(t) = \gamma(t, x(t)) \in U$ ,
  - $\checkmark \gamma \in \Gamma$  is the class of all admissible feedback strategies

## **Dynamic Programming for Continuous-Time Optimal Control Problems**

• The minimum cost-to-go from any initial state x and any initial time t is described by the so-called **value function** defined by

$$V(t,x) = \min_{u(s), t \le s \le T} \left[ \int_t^T g(s,x(s),u(s)) ds + q(T,x(T)) \right]$$
 (7)

Satisfying the boundary condition

$$V(T,x) = q(T,x(T))$$
(8)

## Hamilton-Jacobi-Bellman (HJB) equation

- The dynamic programming approach, when applied to optimal control problems defined in continuous time, leads to a partial differential equation (PDE) which is know as the *Hamilton-Jacobi-Bellman (HJB) equation*.
- A direct application of *the principle of optimality* on Eq. (7), under the assumption of continuous differentiability of V, leads to the HJB equation

$$-\frac{\partial V(t,x)}{\partial t} = \min_{u} \left[ \frac{\partial V(t,x)}{\partial x} f(t,x,u) + g(t,x,u) \right]$$
(9)

with V(T,x) = q(T,x(T)) boundary condition

- In general, it is not easy to compute V(t,x) and the continuous differentiability assumption is rather restrictive.
- If V(t,x) exists, the HJB equation provides a means of obtaining the optimal control strategy (sufficient condition)

### Proof of Hamilton-Jacobi-Bellman (HJB) equation

#### **Proof:**

According to Bellman's optimality principle, the following identity holds for small  $\delta$ 

$$V(t,x(t)) = \min_{u \in U} [g(t,x,u)\delta + V(t+\delta,x(t+\delta))]$$

where 
$$V(t + \delta, x(t + \delta)) = V(t + \delta, x(t) + f(t, x, u) \cdot \delta)$$

$$= V(t, x(t)) + \frac{\partial V(t, x)}{\partial t} \delta + \frac{\partial V(t, x)}{\partial x} f(t, x, u) \cdot \delta + o(\delta)$$

Substituting into (3) gives

$$V(t,x(t)) = \min_{u \in U} \left[ g(t,x,u) \cdot \delta + V(t,x(t)) + \frac{\partial V(t,x)}{\partial x} f(t,x,u) \cdot \delta + \frac{\partial V(t,x)}{\partial t} \delta + o(\delta) \right]$$

Canceling V(t, x(t)) both side and divide by  $\delta$  gives:

$$-\frac{\partial V(t,x)}{\partial t} = \min_{u} \left[ \frac{\partial V(t,x)}{\partial x} f(t,x,u) + g(t,x,u) \right]$$

## Obtaining the optimal control strategy from HJB equation

#### Theorem

If a continuously differentiable function V(t,x) can be found that satisfies the HJB equation (9), then it generate the optimal strategy through the static (pointwise) minimization problem defined by the RHS of (9)

$$-\frac{\partial V(t,x)}{\partial t} = \min_{u \in U} \left[ \frac{\partial V(t,x)}{\partial x} f(t,x,u) + g(t,x,u) \right]$$
(9)

$$u^{*}(t) = \underset{u \in U}{\operatorname{argmin}} \left[ \frac{\partial V(t, x)}{\partial x} f(t, x, u) + g(t, x, u) \right]$$
 (10)

## Obtaining the optimal control strategy from HJB equation

#### **Proof:**

• If we are given two strategies,  $\gamma^* \in \Gamma$  (the optimal one) and  $\gamma \in \Gamma$  (an arbitrary one), with the corresponding terminating trajectories  $x^*$  and x, and terminal times  $T^*$  and T, respectively, then Eq. (9) reads

$$g(t,x,u) + \frac{\partial V(t,x)}{\partial x} f(t,x,u) + \frac{\partial V(t,x)}{\partial t} \ge 0$$
 (11)

$$g(t, x^*, u^*) + \frac{\partial V(t, x^*)}{\partial x} f(t, x^*, u^*) + \frac{\partial V(t, x^*)}{\partial t} \equiv 0$$
 (12)

where  $\gamma^*$  and  $\gamma$  have been replaced by the corresponding controls  $u^*$  and u, respectively.

• Integrating Eq.(11) from 0 to T and Eq.(12) from 0 to  $T^*$  leads to

$$\int_{0}^{T} g(t, x, u) + V(T, x(T)) - V(0, x_{0}) \ge 0$$

$$\int_{0}^{T^{*}} g(t, x^{*}, u^{*}) + V(T, x^{*}(T^{*})) - V(0, x_{0}) = 0$$

• Elimination of  $V(0, x_0)$  yields

$$\int_0^T g(t, x, u) + q(T, x(T)) \ge \int_0^{T^*} g(t, x^*, u^*) + q(T^*, x^*(T^*)) \ge 0$$

 $\succ u^*$  is the optimal control (sequence of actions), and therefore  $\gamma^*$  is the optimal strategy

- continuous-time system  $\dot{x}(t) = Ax(t) + Bu(t)$
- problem: choose u(t) to minimize

$$J(u) = \int_0^T (x(t)^T Q x(t) + u(t)^T R u(t)) dt + x(T)^T Q_f x(T)$$

- $\checkmark g = x^T Q x + u^T R u$
- $\checkmark f = Ax + Bu$
- ✓ Let's assume  $V(t,x) = x^T P_t x$
- HJB equation is employed

$$-\frac{\partial V(t,x)}{\partial t} = \min_{u \in U} \left[ \frac{\partial V(t,x)}{\partial x} f(t,x,u) + g(t,x,u) \right]$$
  
$$\Rightarrow -x\dot{P}_t x = \min_{u \in U} \left[ 2P_t x (Ax + Bu) + x^T Qx + u^T Ru \right]$$

• minimizing over u yields  $u^* = -R^{-1}B^TP_t$ , and substitute to HJB;

$$-\dot{P}_{t} = A^{T} P_{t} + P_{t} A - P_{t} B R^{-1} B^{T} P_{t} + Q$$

which is called as *Riccati differential equation* in optimal control.

## The Minimum Principle

- Dynamic optimization using Dynamic Programming approach → HJB equation
  - Handy to use
  - Easy to extend to stochastic feedback control
- Dynamic optimization using the Lagrangian Method→ Minimum Principle
  - Intuitively show how dynamic optimization is solved using static optimization technique
  - Will be used to state the equilibrium condition (necessary conditions) for various dynamic game

### From Static Optimization to Dynamic Optimization

• We derive the first-order necessary conditions for the basic dynamic optimization problem to find a control function  $u(\cdot)$  that minimizes the cost functional

$$J(u) = \int_0^T g(t, x(t), u(t)) dt + h(x(T)) \text{ where } h(x(T)) = q(T, x(T))$$

where the state variable x(t) satisfies the differential equation:

$$\dot{x}(t) = f(t, x(t), u(t)), \qquad x(0) = x_0$$

- $\checkmark x(t) \in \mathbf{R}^n, u(t) = \mathbf{R}^m$
- ✓ It is assumed that the dynamic process starts from t=0 and ends at the fixed terminal time T>0.
- $\checkmark f(t,x,u)$  and g(t,x,u) are continuous functions on  $\mathbb{R}^{n+m+1}$
- ✓ The set of admissible control functions  $u(t) \in U$  consists of the set of functions that are continuous on [0, T].

• Inspired by the theory of static optimization we introduce for each t in the interval [0,T] the quantity  $\lambda(t)[f(t,x(t),u(T))-\dot{x}(t)]$  that satisfies

$$\int_0^T \lambda(t) [f(t, x(t), u(t)) - \dot{x}(t)] dt = 0$$

- $\checkmark$  the Lagrange multiplier  $\lambda(t)$  (or costate variable) is an arbitrarily chosen row vector
- Define the new cost function  $\bar{J}$  which coincides with the original cost function J if the dynamic constraint,  $\dot{x}(t) = f(t, x(t), u(t))$ , is satisfied as

$$\bar{J} := \int_0^T \{g(t, x, u) + \lambda(t)f(t, x, u) - \lambda(t)\dot{x}(t)\}dt + h(x(T))$$

$$= \int_0^T \{H(t, x, u, \lambda) - \lambda(t)\dot{x}(t)\}dt + h(x(T))$$

- ✓ Where the Hamiltonian function  $H(t, x, u, \lambda) = g(t, x, u) + \lambda(t)f(t, x, u)$
- Conducting integration by parts,  $\bar{J}$  can be rewritten as

$$\bar{J} := \int_0^T \{H(t, x, u, \lambda) + \dot{\lambda}(t)x(t)\}dt + h(x(T)) - \lambda(T)x(T) + \lambda(0)x_0$$

$$\bar{J}_1$$

$$\bar{J}_2$$

$$\bar{J}_3$$

- Assume that  $u^*(t) \in U$  is an optimal control path generating the minimum value of  $\bar{J}$  and  $x^*(t)$  is the corresponding optimal state trajectory
- If we perturb this optimal  $u^*(t)$  path with a continuous perturbing curve p(t), we can generate 'neighboring' control paths

$$u(t) = u^*(t) + \epsilon p(t)$$

- $\checkmark \epsilon$  is small scalar
- $\checkmark u(t)$  induces a corresponding 'neighboring' state trajectory  $x(t, \epsilon, p)$  with  $t \in [0, T]$
- The cost function associated with the perturbation becomes

$$\bar{J}(\epsilon) := \int_0^T \{H(t, x(t, \epsilon, p), \mathbf{u}(t), \lambda(t)) + \dot{\lambda}(t)x(t, \epsilon, p), \}dt + h(x(T, \epsilon, p), ) - \lambda(T)x(T, \epsilon, p) + \lambda(0)x_0$$

• By assumption  $\bar{J}(\epsilon)$  has a minimum at  $\epsilon=0 \to \frac{d\bar{J}(\epsilon)}{d\epsilon}=0$  at  $\epsilon=0$ 

$$\bar{J}(\epsilon) \coloneqq \int_0^T \{H(t, x(t, \epsilon, p), \mathbf{u}(t), \lambda(t)) + \dot{\lambda}(t)x(t, \epsilon, p), \}dt + h(x(T, \epsilon, p), ) - \lambda(T)x(T, \epsilon, p) + \lambda(0)x_0$$

• Evaluating the derivative of  $\bar{I}(\epsilon)$  yields

$$\frac{d\bar{J}(\epsilon)}{d\epsilon} = \int_0^T \left\{ \frac{\partial H}{\partial x} \frac{dx(t,\epsilon,p)}{d\epsilon} + \frac{\partial H}{\partial u} p(t) + \dot{\lambda}(t) \frac{dx(t,\epsilon,p)}{d\epsilon} \right\} dt + \frac{\partial h(x(T))}{\partial x} \frac{dx(T,\epsilon,p)}{d\epsilon} - \lambda(t) \frac{dx(T,\epsilon,p)}{d\epsilon}$$

$$\frac{d\bar{J}(\epsilon)}{d\epsilon} = \int_0^T \left\{ \left( \frac{\partial H}{\partial x} + \dot{\lambda}(t) \right) \frac{dx(t,\epsilon,p)}{d\epsilon} + \frac{\partial H}{\partial u} p(t) \right\} dt + \left( \frac{\partial h(x(T))}{\partial x} - \lambda(T) \right) \frac{dx(T,\epsilon,p)}{d\epsilon}$$

$$\checkmark \frac{d\bar{J}(\epsilon)}{d\epsilon} = 0 \text{ at } \epsilon = 0 \text{ if we choose } \lambda(t)$$

$$\frac{\partial H(t,x^*,u^*,\lambda)}{\partial x} + \dot{\lambda}(t) = 0 \text{ with } \frac{\partial h(x(T))}{\partial x} - \lambda(T)$$

$$\checkmark \frac{d\bar{J}(\epsilon)}{d\epsilon} = 0 \text{ at } \epsilon = 0 \text{ if and only if}$$

$$\int_0^T \frac{\partial H(t,x^*,u^*,\lambda)}{\partial u} p(t) dt = 0$$

This should hold for any continuous function p(t) on [0,T]. Choosing  $p(t) = \frac{\partial H^T(t,x^*,u^*,\lambda)}{\partial u}$  shows that another necessary condition

$$\frac{\partial H(t, x^*, u^*, \lambda)}{\partial u} = 0$$

• We derive the first-order necessary conditions for the basic dynamic optimization problem to find a control function  $u(\cdot)$  that minimizes the cost functional

$$J(u) = \int_0^T g(t, x(t), u(t)) dt + h(x(T)) \text{ where } h(x(T)) = q(T, x(T))$$

where the state variable x(t) satisfies the differential equation:

$$\dot{x}(t) = f(t, x(t), u(t)), \qquad x(0) = x_0$$

#### **Theorem**

If  $u^*(t) \in U$  is a control that yields a local minimum for the cost function above and  $x^*(t)$  and  $\lambda^*(t)$  are the corresponding state and costate, then it is necessary that

$$\dot{x}(t) = f(t, x^*, u^*) \left( = \frac{\partial H(t, x^*, u^*, \lambda)}{\partial \lambda} \right), \qquad x^*(0) = x_0$$

$$\dot{\lambda}^*(t) = \frac{\partial H(t, x^*, u^*, \lambda^*)}{\partial x}; \lambda^*(T) = \frac{\partial h(x^*(T))}{\partial x}$$

$$\frac{\partial H(t, x^*, u^*, \lambda^*)}{\partial u} = 0$$

• The dynamic optimization problem has been reduced to a static optimization problem which should hold at every single instant of time

## From the Euler Lagrange to Minimum Principle (Generalization)

- **Euler-Lagrange method** assumes that
  - $\checkmark u(t)$  could (in principle) to be chosen arbitrarily in  $R^m$
  - ✓ u(t) is continuous for all  $t \in [0, T]$
- However, these assumptions are too restrictive, thus a more general problem setting is required
- Pontryagin Minimum principle assumes that
  - ✓ There is a subset  $U \subset R^m$  such that for all  $t \in [0, T], u(t) \in U$
  - ✓ This is the next generalization of the Euler-Lagrange method

### **The Minimum Principle**

Consider the following optimal control problem defined by

$$L(u) = \int_0^T g(t, x(t), u(t)) dt + q(T, x(T))$$

where the state variable x(t) satisfies the differential equation:

$$\dot{x}(t) = f(t, x(t), u(t)), \qquad x(0) = x_0, \qquad t \ge 0$$

## Theorem (The minimum principle)

In the continuous time dynamic system defined by equation (1) and (2), optimal control  $u^*(t)$  and corresponding trajectory  $x^*(t)$  satisfy following equations:

$$H(t,\lambda,x,u) := g(t,x,u) + \lambda(t)f(t,x,u)$$

$$\dot{x}^*(t) = f(t,x^*,u^*) \left( = \frac{\partial H(t,x^*,u^*,\lambda)}{\partial \lambda} \right), x^*(0) = x_0;$$

$$\dot{\lambda}^*(t) = -\frac{\partial H(t,\lambda,x^*,u^*)}{\partial x}; \lambda^*(T) = \frac{\partial h(x^*(T))}{\partial x}$$

$$u^*(t) = \underset{u \in U}{\operatorname{argmin}} H(t,\lambda^*,x^*,u)$$

## **Proof of The Minimum Principle**

### Proof)

We start with Hamilton-Jacobi-Bellman equation,

$$\nabla_t V(t, x) + \min_{u \in U} [\nabla_x V(t, x) f(t, x, u) + g(t, x, u)] = 0$$

Let 
$$u^* = \underset{u \in U}{\operatorname{argmin}} [\nabla_{\!x} V(t, x) \cdot f(t, x, u) + g(t, x, u)]$$
 then

$$0 = \nabla_{x}V(t,x)f(t,x,u^{*}) + g(t,x,u^{*}) + \nabla_{t}V(t,x)$$

Derivatives w.r.t. x and t yields

$$0 = \nabla_{xx}^2 V(t, x) f(t, x, u^*) + \nabla_x V(t, x) \nabla_x f(t, x, u^*) + \nabla_x g(t, x, u^*) + \nabla_{xt}^2 V(t, x) \cdots (*)$$

$$0 = \nabla_{xt}^2 V(t, x) \cdot f(t, x, u^*) + \nabla_{tt}^2 V(t, x) \cdots (**)$$

(\*) and (\*\*) holds for all (t, x).

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## **Proof of The Minimum Principle**

## **Proof)**

$$0 = \nabla_{xx}^{2} V(t, x) f(t, x, u^{*}) + \nabla_{x} V(t, x) \nabla_{x} f(t, x, u^{*}) + \nabla_{x} g(t, x, u^{*}) + \nabla_{xt}^{2} V(t, x) \cdots (*)$$

$$0 = \nabla_{xt}^{2} V(t, x) \cdot f(t, x, u^{*}) + \nabla_{tt}^{2} V(t, x) \cdots (**)$$

the term  $\nabla^2_{xx}V(t,x^*)f(t,x^*,u^*) + \nabla^2_{xt}V(t,x^*)$  in (\*) is equal the following total derivative w.r.t. t

$$\frac{d}{dt}(\nabla_{\!x}V(t,x^*)), \qquad \left(\operatorname{let}\nabla_{\!x}V(t,x^*) \coloneqq p(t)\right)$$

(\*) becomes 
$$\dot{p}(t) = -\nabla_{x} f(x^{*}, u^{*}) p(t) - \nabla_{x} g(x^{*}, u^{*})$$

Similarly, the term  $\nabla_{xt}^2 V(t, x^*) f(t, x^*, u^*) + \nabla_{tt}^2 V(t, x^*)$  In (\*\*) is equal the total derivative

$$\frac{d}{dt}(\nabla_t V(t, x^*)), \qquad \left( \operatorname{let} \nabla_t V(t, x^*) \coloneqq p_0(t) \right)$$

and (\*\*) becomes  $\dot{p_0}(t) = 0 \rightarrow p_0(t) = \text{constant}$ 

We have boundary condition

$$p(T) = \nabla_{x}V(T(x^*), x^*) = \nabla_{x}q(T(x^*), x^*)$$

## **Proof of The Minimum Principle**

## **Proof)**

So, the original HJB 
$$u^* = \underset{u}{\operatorname{argmin}} [\nabla_{\!x} V(t,x) f(t,x,u) + g(t,x,u)]$$
 become

$$u^* = \underset{u \in U}{\operatorname{argmin}}[p(t) \cdot f(t, x, u) + g(t, x, u)]$$

Define H(x, u, p) := p(t)f(t, x, u) + g(t, x, u), then system and adjoint equations can be written in terms of Hamiltonian

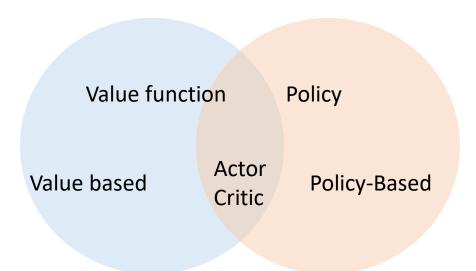
$$\dot{x}^*(t) = \nabla_p H(x^*, u^*, p), \qquad \dot{p}(t) = -\nabla_x H(x^*, u^*, p)$$

## Comments (Minimum principle v.s. HJB)

- When satisfied along a trajectory, Pontryagin's minimum principle is a *necessary* condition, not sufficient contrition, for an optimum.
- The Hamilton–Jacobi–Bellman equation provides a *necessary and sufficient* condition for an optimum, but this condition must be satisfied over the whole of the state space.
- While the Hamilton-Jacobi-Bellman equation admits a straightforward extension to stochastic optimal control problems, the minimum principle does not
  - > DP not only solves the original optimization problem, but tells us even at arbitrary times and arbitrary states what the best action is
  - ➤ Having the optimal policy available as a function of times and state ("feedback") is often viewed as even better than having it available only as a function of time ("open-loop form")
- The Minimum Principle requires solving an ODE with split boundary conditions. It is not trivial to solve, but easier than solving a PDE in the HJB.

# **Policy Gradient Based Reinforcement Learning**

# Overview



#### **Motivation**

- One of the primary goals of the field of artificial intelligence is to solve complex tasks from unprocessed, high-dimensional, sensory input.
- Recent progresses in RL have shown the possibilities
  - ✓ Deep Q Network for Atari games and
  - ✓ AlphaGo
- Although DQN solves problems with high-dimensional observation spaces, it can only handle discrete and low-dimensional action spaces

#### **Policy Gradient**

- Policy Gradient methods learn the policy directly with a parameterized function respect to  $\theta$ ,  $\pi_{\theta}(a|s)$ .
- The reward function can be defined as (in continuous case):

$$J(\theta) = \sum_{s \in \mathcal{S}} d^{\pi}(s) V^{\pi}(s) = \sum_{s \in \mathcal{S}} d^{\pi}(s) \sum_{a \in \mathcal{A}} \pi_{\theta}(a|s) Q^{\pi}(s,a)$$

 $\checkmark$  where  $d^{\pi}(s)$  is stationary distribution of Markov chain for  $\pi_{\theta}$  (on-policy state distribution under  $\pi$ )

$$d^{\pi}(s) = \lim_{t \to \infty} P(s_t = s | s_0, \pi_{\theta})$$

$$\checkmark d^{\pi} = d^{\pi_{\theta}}$$
;  $V^{\pi} = V^{\pi_{\theta}}$ ;  $Q^{\pi} = Q^{\pi_{\theta}}$  for simplicity

• We can find the best  $\theta^*$  using gradient ascent such that

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

- It is natural to expect policy-based methods are more useful in the continuous space
  - ✓ There is an infinite number of actions and (or) states to estimate the values
  - ✓ Difficult to compute  $\underset{a \in \mathcal{A}}{\operatorname{argmax}} Q^{\pi}(s, a)$  requiring full scan of the action space

# How to compute the gradient $\nabla J(\theta)$ ?

• Gradient can be computed by perturbing  $\theta$  by a small amount  $\epsilon$  in the k-th dimension.

$$\frac{\partial J(\theta)}{\partial \theta_k} \approx \frac{J(\theta + \epsilon u_k) - J(\theta)}{\epsilon}$$

- ✓ It works even when  $J(\theta)$  is not differentiable, but very slow
- Is there more efficient method?

#### **Policy Gradient Theorem**

The reward function is

$$J(\theta) = \sum_{s \in \mathcal{S}} d^{\pi}(s) V^{\pi}(s) = \sum_{s \in \mathcal{S}} d^{\pi}(s) \sum_{a \in \mathcal{A}} \pi_{\theta}(a|s) Q^{\pi}(s,a)$$

- Computing the gradient  $\nabla J(\theta)$  is tricky because it depends on both the action selection and the stationary distribution of states following the target selection behavior
- The policy gradient theorem makes the computation of  $\nabla I(\theta)$  simple

$$\begin{split} \nabla_{\theta} J(\theta) &= \nabla_{\theta} \sum_{s \in \mathcal{S}} d^{\pi}(s) \sum_{a \in \mathcal{A}} \pi_{\theta}(a|s) Q^{\pi}(s,a) \\ &\propto \sum_{s \in \mathcal{S}} d^{\pi}(s) \sum_{a \in \mathcal{A}} \nabla_{\theta} \pi_{\theta}(a|s) Q^{\pi}(s,a) \qquad \text{gradient does not depends on } Q^{\pi} \text{ (will be proved)} \\ &= \sum_{s \in \mathcal{S}} d^{\pi}(s) \sum_{a \in \mathcal{A}} \pi_{\theta}(a|s) \frac{\nabla_{\theta} \pi_{\theta}(a|s)}{\pi_{\theta}(a|s)} Q^{\pi}(s,a) \\ &= \sum_{s} d^{\pi}(s) \sum_{a \in \mathcal{A}} \pi_{\theta}(a|s) \nabla \ln \pi_{\theta}(a|s) Q^{\pi}(s,a) \qquad \because (\ln x)' = 1/x \\ &= \mathbb{E}_{\pi} [\nabla \ln \pi_{\theta}(a|s) Q^{\pi}(s,a)] \end{split}$$

 $\checkmark$  where  $\mathbb{E}_{\pi}$  refers to  $\mathbb{E}_{s \sim d^{\pi}, a \sim \pi_{\theta}}$  when both state and action distributions follow the policy  $\pi_{\theta}$  (on-policy)

# **Policy Gradient Theorem Proof**

$$\begin{split} \nabla_{\theta}V^{\pi}(s) &= \nabla_{\theta} \left( \sum_{a \in \mathcal{A}} \pi_{\theta}(a|s) Q^{\pi}(s,a) \right) \\ &= \sum_{a \in \mathcal{A}} \left( \nabla_{\theta} \pi_{\theta}(a|s) Q^{\pi}(s,a) + \pi_{\theta}(a|s) \nabla_{\theta} Q^{\pi}(s,a) \right) & \text{$:$ derivative product rule} \\ &= \sum_{a \in \mathcal{A}} \left( \nabla_{\theta} \pi_{\theta}(a|s) Q^{\pi}(s,a) + \pi_{\theta}(a|s) \nabla_{\theta} \sum_{s',r} P(s',r|s,a) (r + V^{\pi}(s')) \right) & \text{$:$ Extend $Q^{\pi}$ with further state value} \\ &= \sum_{a \in \mathcal{A}} \left( \nabla_{\theta} \pi_{\theta}(a|s) Q^{\pi}(s,a) + \pi_{\theta}(a|s) \sum_{s',r} P(s',r|s,a) \nabla_{\theta} V^{\pi}(s') \right) & \text{$:$ P(s',r|s,a)$ is not a function of $\theta$} \\ &= \sum_{a \in \mathcal{A}} \left( \nabla_{\theta} \pi_{\theta}(a|s) Q^{\pi}(s,a) + \pi_{\theta}(a|s) \sum_{s',r} P(s'|s,a) \nabla_{\theta} V^{\pi}(s') \right) & \text{$:$ P(s',r|s,a)$} \end{aligned}$$

$$\nabla_{\theta} V^{\pi}(s) = \sum_{a \in \mathcal{A}} \left( \nabla_{\theta} \pi_{\theta}(a|s) Q^{\pi}(s,a) + \pi_{\theta}(a|s) \sum_{s'} P(s'|s,a) \nabla_{\theta} V^{\pi}(s') \right)$$

 $\checkmark$  a nice recursive form and the future state value function  $V^{\pi}(s')$  can be repeated unrolled as will be shown next slide

# **Policy Gradient Theorem Proof**

$$\begin{split} \overline{V_{\theta}V^{\pi}(s)} &= \sum_{a \in \mathcal{A}} \left( \overline{V_{\theta}} \pi_{\theta}(a|s) Q^{\pi}(s,a) + \pi_{\theta}(a|s) \sum_{s'} P(s'|s,a) \overline{V_{\theta}} V^{\pi}(s') \right) \\ &= \phi(s) + \sum_{a \in \mathcal{A}} \pi_{\theta}(a|s) \sum_{s'} P(s'|s,a) \overline{V_{\theta}} V^{\pi}(s') \\ &= \phi(s) + \sum_{s'} \sum_{a} \pi_{\theta}(a|s) P(s'|s,a) \overline{V_{\theta}} V^{\pi}(s') \\ &= \phi(s) + \sum_{s'} \rho^{\pi}(s \to s',1) \overline{V_{\theta}} V^{\pi}(s') \\ &= \phi(s) + \sum_{s'} \rho^{\pi}(s \to s',1) \left[ \phi(s') + \sum_{s''} \rho^{\pi}(s' \to s'',1) \overline{V_{\theta}} V^{\pi}(s'') \right] \\ &= \phi(s) + \sum_{s'} \rho^{\pi}(s \to s',1) \phi(s') + \sum_{s''} \rho^{\pi}(s \to s'',2) \overline{V_{\theta}} V^{\pi}(s'') \\ &= \phi(s) + \sum_{s'} \rho^{\pi}(s \to s',1) \phi(s') + \sum_{s''} \rho^{\pi}(s \to s'',2) \overline{V_{\theta}} V^{\pi}(s'') \\ &= \phi(s) + \sum_{s'} \rho^{\pi}(s \to s',1) \phi(s') + \sum_{s''} \rho^{\pi}(s \to s'',2) \overline{V_{\theta}} V^{\pi}(s'') + \sum_{s'''} \rho^{\pi}(s \to s''',3) \overline{V_{\theta}} V^{\pi}(s''') \\ &= \cdots; \text{repeatedly unrolling the part of } \overline{V_{\theta}} V^{\pi}(\cdot) \\ &= \sum_{s''} \sum_{a} \rho^{\pi}(s \to x, k) \phi(x) \end{split}$$

# **Policy Gradient Theorem Proof**

$$\nabla_{\theta}J(\theta) = \nabla_{\theta}V^{\pi}(s_{0})$$

$$= \sum_{s} \sum_{k} \rho^{\pi}(s_{0} \to s, k)\phi(s)$$

$$= \sum_{s} \eta(s)\phi(s)$$

$$= \left(\sum_{s} \eta(s)\right) \sum_{s} \frac{\eta(s)}{(\sum_{s} \eta(s))}\phi(s)$$

$$\propto \sum_{s} \frac{\eta(s)}{(\sum_{s} \eta(s))}\phi(s)$$

$$= \sum_{s} d^{\pi}(s) \sum_{a \in \mathcal{A}} \nabla_{\theta}\pi_{\theta}(a|s)Q^{\pi}(s, a)$$

$$= \sum_{s} d^{\pi}(s) \sum_{a \in \mathcal{A}} \pi_{\theta}(a|s) \frac{\nabla_{\theta}\pi_{\theta}(a|s)}{\pi_{\theta}(a|s)}Q^{\pi}(s, a)$$

$$= \sum_{s} d^{\pi}(s) \sum_{a \in \mathcal{A}} \pi_{\theta}(a|s)\nabla_{\theta} \ln \pi_{\theta}(a|s)Q^{\pi}(s, a)$$

$$= \mathbb{E}_{\pi}[\nabla_{\theta} \ln \pi_{\theta}(a|s)O^{\pi}(s, a)]$$

$$: \eta(s) = \sum_{k=0}^{\infty} \rho^{\pi}(s_0 \to s, k)$$

: Normalize  $\eta(s), s \in \mathcal{S}$  to be a probability dist.

 $: \sum_{s} \eta(s)$  is a constant

$$: \phi(s) = \sum_{a \in \mathcal{A}} \nabla_{\theta} \pi_{\theta}(a|s) Q^{\pi}(s,a)$$

 $\mathbb{E}_{\pi}$  refers to  $\mathbb{E}_{s\sim d^{\pi},a\sim\pi_{\theta}}$  (on-policy)

# Generalized Advantage Estimation (GAE) (Schulman et al., 2016)

$$\nabla_{\theta} J(\theta) = \mathbb{E}_{\pi} [\nabla_{\theta} \ln \pi_{\theta}(a|s) Q^{\pi}(s,a)]$$

- The policy gradient theorem lays the theoretical foundation for various policy gradient algorithms.
- This vanilla policy gradient update has no bias but high variance. Many following algorithms were proposed to reduce the variance while keeping the bias unchanged.
  - ✓ Reinforce
  - ✓ Actor-Critic
  - ✓ Off-Policy Policy Gradient
  - ✓ High-dimensional Continuous Control Using Generalized Advantage Estimation (Schulman, et al., 2016)
  - ✓ Asynchronous Advantage Actor Critic (Miih et al., 2016)
  - ✓ Deterministic Policy Gradient (DPG)
  - ✓ Deep Deterministic Policy Gradient (DDPG) (Lillicrap, et al., 2015)
  - ✓ Addressing Function Approximation Error in Actor-Critic Methods (TD3) (Fujimoto, et al., 2018)
  - ✓ Trust region policy optimization (TRPO) (Schulman, et al., 2015)
  - ✓ Proximal Policy Optimization (PPO) (Schulman, et al., 2017)
  - ✓ Soft Actor Critic (SAC) (Haarnoja et al., 2018)
  - ✓ Multi-Agent Deep Deterministic Policy Gradient (MADDPG) (Lowe et al., 2017)

#### REINFORCE Algorithm

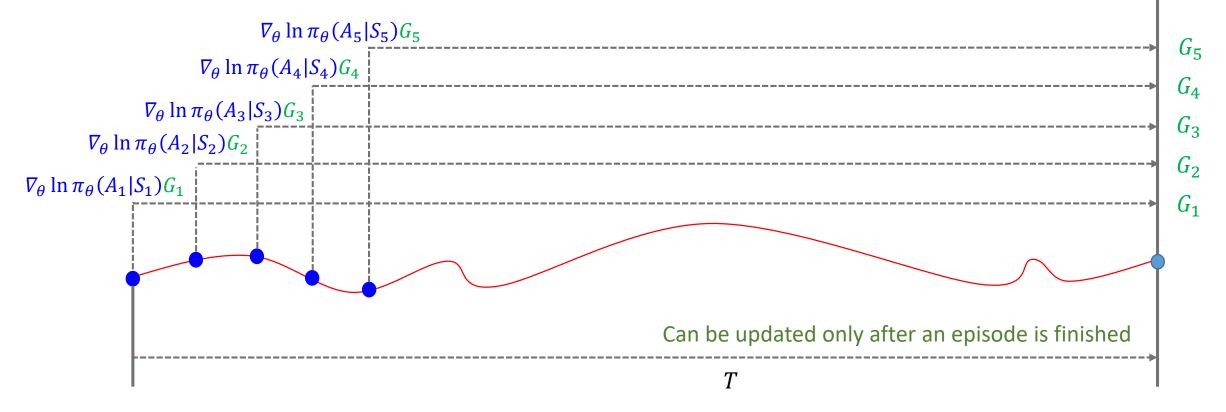
- REINFORCE (Monte-Carlo policy gradient) relies on an estimated return by Monte-Carlo methods using episode samples to update the policy parameter  $\theta$
- REINFORCE works because the expectation of the sample gradient is equal to the actual gradient:

$$\nabla_{\theta} J(\theta) = \mathbb{E}_{\pi} [\nabla_{\theta} \ln \pi_{\theta}(a|s) Q^{\pi}(s,a)]$$

$$= \mathbb{E}_{\pi} [\nabla_{\theta} \ln \pi_{\theta}(A_t|S_t) G_t] \qquad \qquad : Q^{\pi}(s,a) = \mathbb{E}_{\pi} [G_t|S_t, A_t]$$

- $\checkmark$  Measure  $G_t$  from real sample trajectories and use that to update policy gradient
- ✓ It relies on a full trajectory and that's why it is a Monte-Carlo method
  - 1. Initialize the policy parameter  $\theta$  at random.
  - 2. Generate one trajectory on policy  $\pi_{\theta}$ :  $S_1, A_1, R_2, S_2, A_2, \ldots, S_T$ .
  - 3. For t=1, 2, ..., T:
    - 1. Estimate the the return  $G_t$ ;
    - 2. Update policy parameters:  $heta \leftarrow heta + lpha \gamma^t G_t 
      abla_{ heta} \ln \pi_{ heta}(A_t | S_t)$
- A widely used variation of REINFORCE is to subtract a baseline value from the return  $G_t$  to reduce the variance of gradient estimation while keeping the bias unchanged

#### **REINFORCE** Algorithm



- Update per every action
- Update per every episode
- Update per episode & batch

$$\theta \leftarrow \theta + \alpha \gamma^t \nabla_{\theta} \ln \pi_{\theta}(A_t | S_t) G_t$$

$$\theta \leftarrow \theta + \alpha \left[ \sum_{t=1}^{T} \gamma^{t} \nabla_{\theta} \ln \pi_{\theta}(A_{t}|S_{t}) G_{t} \right]$$

$$\theta \leftarrow \theta + \alpha \left[ \frac{1}{N} \sum_{i=1}^{N} \sum_{t=1}^{T} \gamma^{t} \nabla_{\theta} \ln \pi_{\theta} \left( A_{t}^{(i)} \middle| S_{t}^{(i)} \right) G_{t}^{(i)} \right]$$

#### **Actor-Critic**

- It makes a lot of sense to learn the value function in addition to the policy, since knowing the value function can assist the policy update, such as by reducing gradient variance in vanilla policy gradients
- Two main components in policy gradient are the policy model and the value function.

 $w \leftarrow w + \alpha_w \delta_t \nabla_w Q_w(s, a)$ 

5. Update  $a \leftarrow a'$  and  $s \leftarrow s'$ .

- Critic updates the value function parameters w and depending on the algorithm it could be action value  $Q_w(s,a)$  or state-value  $V_w(s)$
- Actor updates the policy parameters  $\theta$  for  $\pi_{\theta}(a|s)$ , in the direction suggested by the critic

```
1. Initialize s, \theta, w at random; sample a \sim \pi_{\theta}(a|s).
2. For t=1\dots T:
1. Sample reward r_t \sim R(s,a) and next state s' \sim P(s'|s,a);
2. Then sample the next action a' \sim \pi_{\theta}(a'|s');
3. Update the policy parameters: \theta \leftarrow \theta + \alpha_{\theta}Q_w(s,a)\nabla_{\theta}\ln\pi_{\theta}(a|s);
4. Compute the correction (TD error) for action-value at time t: \delta_t = r_t + \gamma Q_w(s',a') - Q_w(s,a)
```

and use it to update the parameters of action-value function:

(on-policy learning)

## Off-Policy Policy Gradient (Degris, White & Sutton, 2012).

- Both REINFORCE and the vanilla version of actor-critic method are on-policy:
  - ✓ training samples are collected according to the target policy the very same policy that we try to optimize for.
- Off policy methods, however, result in several additional advantages:
  - ✓ The off-policy approach does not require full trajectories and can reuse any past episodes (experience replay) for much better sample efficiency.
  - ✓ The sample collection follows a behavior policy different from the target policy, bringing better exploration

## **Off-Policy Policy Gradient**

$$J(\theta) = \sum_{s \in \mathcal{S}} d^{\beta}(s) \sum_{a \in \mathcal{A}} \pi_{\theta}(a|s) Q^{\pi}(s, a) = \mathbb{E}_{s \sim d^{\beta}} \left[ \sum_{a \in \mathcal{A}} \pi_{\theta}(a|s) Q^{\pi}(s, a) \right]$$

$$\nabla_{\theta} J(\theta) = \nabla_{\theta} \mathbb{E}_{s \sim d^{\beta}} \left[ \sum_{a \in \mathcal{A}} \pi_{\theta}(a|s) Q^{\pi}(s, a) \right]$$

$$= \mathbb{E}_{s \sim d^{\beta}} \left[ \sum_{a \in \mathcal{A}} (\nabla_{\theta} \pi_{\theta}(a|s) Q^{\pi}(s, a) + \pi_{\theta}(a|s) \nabla_{\theta} Q^{\pi}(s, a)) \right]$$

$$pprox \mathbb{E}_{s \sim d^{\beta}} \left[ \sum_{a \in \mathcal{A}} \nabla_{\theta} \pi_{\theta}(a|s) Q^{\pi}(s,a) \right]$$

$$= \mathbb{E}_{s \sim d^{\beta}} \left[ \sum_{a \in \mathcal{A}} \beta(a|s) \frac{\pi_{\theta}(a|s)}{\beta(a|s)} \frac{\nabla_{\theta} \pi_{\theta}(a|s)}{\pi_{\theta}(a|s)} Q^{\pi}(s, a) \right]$$

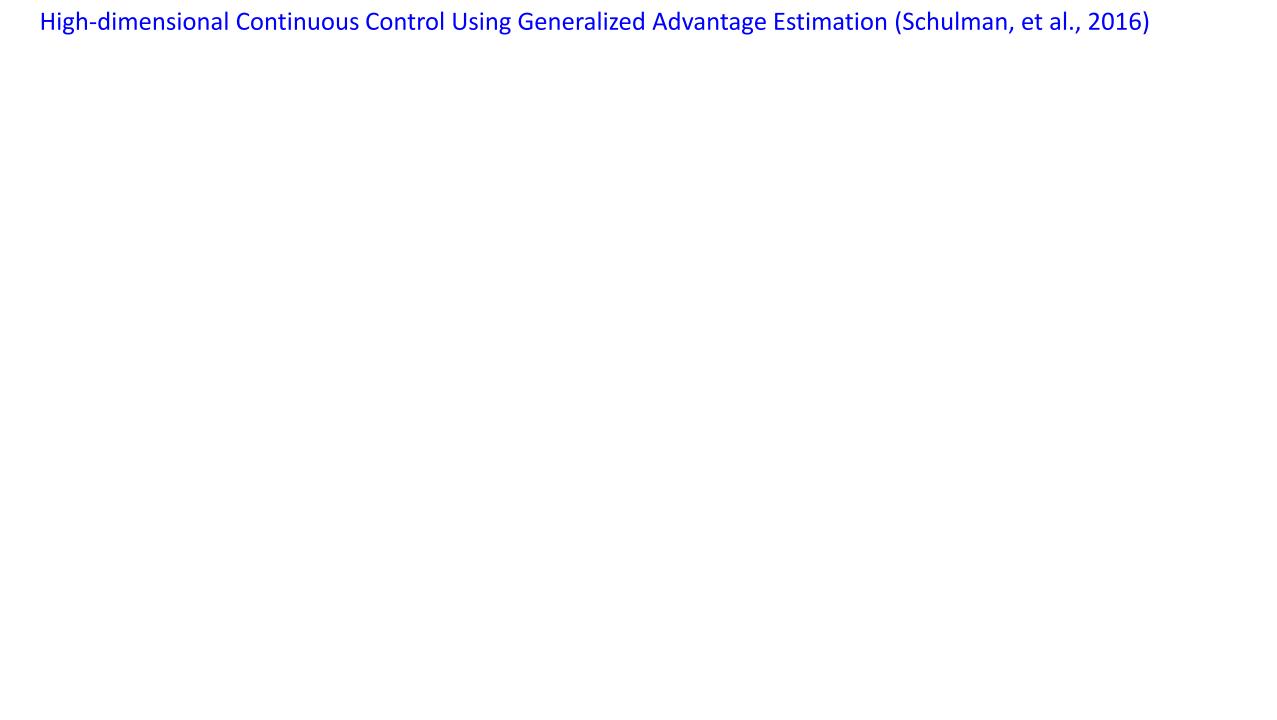
$$= \mathbb{E}_{\beta} \left[ \frac{\pi_{\theta}(a|s)}{\beta(a|s)} \nabla_{\theta} \ln \pi_{\theta}(a|s) Q^{\pi}(s,a) \right]$$

#### Importance weight

Derivative product rule

Ignore  $\pi_{\theta}(a|s)\nabla_{\theta}Q^{\pi}(s,a)$ 

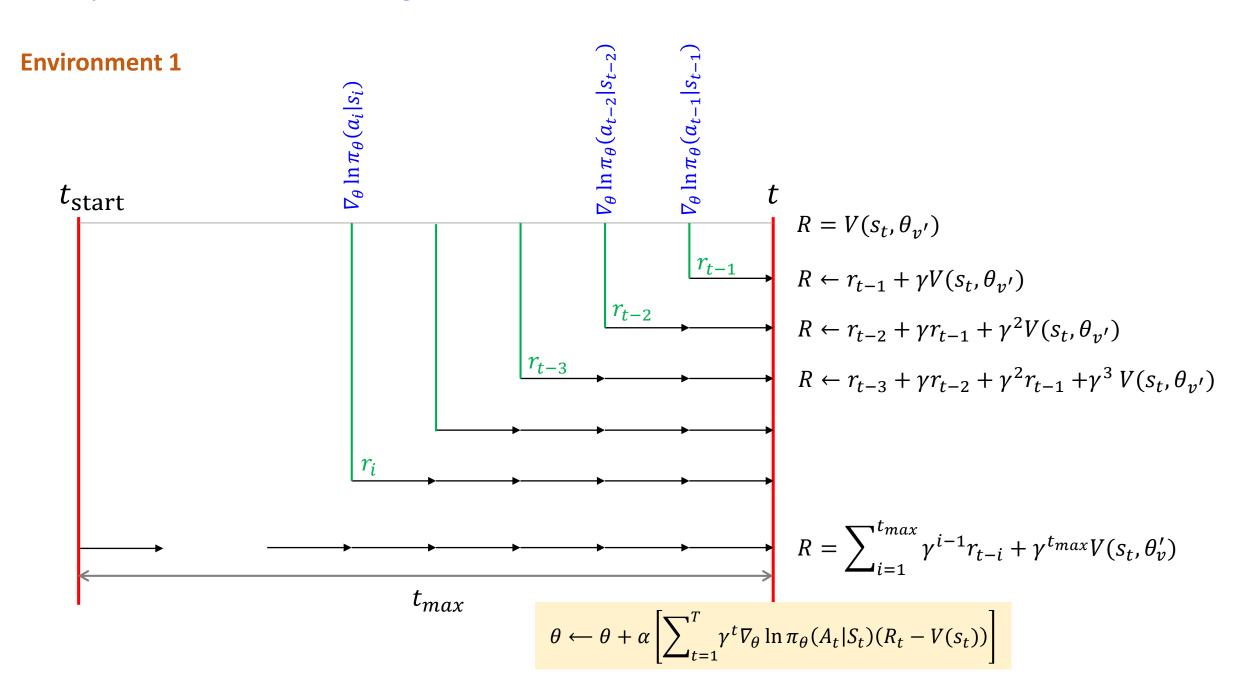
- if we use an approximated gradient with the gradient of Q ignored, we still guarantee the policy improvement and eventually achieve the true local minimum (Degris, White & Sutton, 2012).
- In summary, when applying policy gradient in the off-policy setting, we can simple adjust it with a weighted sum and the weight is the ratio of the target policy to the behavior policy,



- Deep RL algorithms based on experience replay have achieved unprecedented success in challenging domains such as Atari 2600. However, experience replay has several drawbacks:
  - It uses more memory and commutation per real interaction
  - It requires off-policy learning algorithms that can update from data generated by an older policy
- Instead of experience replay, A3C asynchronously executes multiple gents in parallel, on multiple instances of the environment
  - Parallelism decorrelates the agents' data input a more stationary processes, since at any given time step the parallel agents will be experiencing a variety of different states.
  - Parallelism stabilizes learning, playing a role of experience replay buffer
- Make the observation that multiple actor-learners running in parallel are likely to be exploring different parts of the environment
  - One can explicitly use different exploration policies in each actor-learners to maximize the diversity
  - Make samples less correlated

```
Algorithm S3 Asynchronous advantage actor-critic - pseudocode for each actor-learner thread.
   // Assume global shared parameter vectors \theta and \theta_v and global shared counter T=0
   // Assume thread-specific parameter vectors \theta' and \theta'_v
   Initialize thread step counter t \leftarrow 1
   repeat
        Reset gradients: d\theta \leftarrow 0 and d\theta_v \leftarrow 0.
        Synchronize thread-specific parameters \theta' = \theta and \theta'_v = \theta_v
        t_{start} = t
        Get state s_t
        repeat
             Perform a_t according to policy \pi(a_t|s_t;\theta')
             Receive reward r_t and new state s_{t+1}
             t \leftarrow t + 1
             T \leftarrow T + 1
        until terminal s_t or t - t_{start} == t_{max}
       R = \begin{cases} 0 & \text{for terminal } s_t \\ V(s_t, \theta'_v) & \text{for non-terminal } s_t \text{// Bootstrap from last state} \end{cases}
        for i \in \{t - 1, ..., t_{start}\} do
             R \leftarrow r_i + \gamma R
             Accumulate gradients wrt \theta': d\theta \leftarrow d\theta + \nabla_{\theta'} \log \pi(a_i|s_i;\theta')(R - V(s_i;\theta'_v))
             Accumulate gradients wrt \theta'_v: d\theta_v \leftarrow d\theta_v + \partial (R - V(s_i; \theta'_v))^2 / \partial \theta'_v
        end for
        Perform asynchronous update of \theta using d\theta and of \theta_v using d\theta_v.
   until T > T_{max}
```

• The gradient accumulation step can be considered as a parallelized reformation of mini-batch-based stochastic gradient update



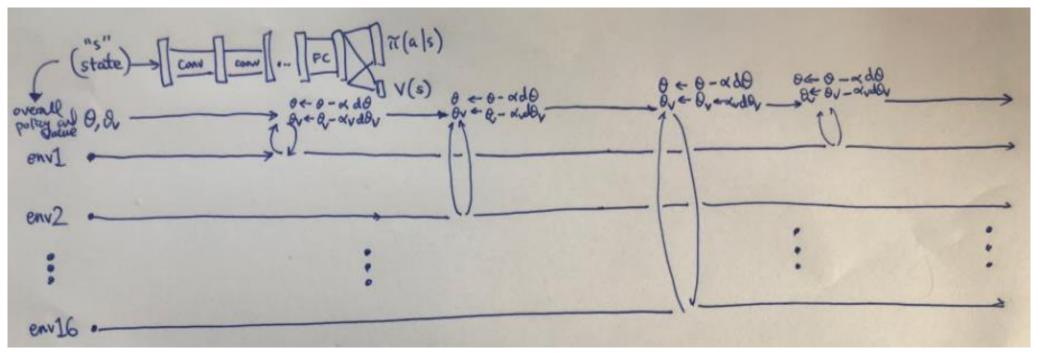


Figure from: <a href="https://danieltakeshi.github.io/2018/06/28/a2c-a3c/">https://danieltakeshi.github.io/2018/06/28/a2c-a3c/</a>

- So far, the policy function  $\pi(.|s)$  is always modeled as a probability distribution over actions a given the current state s and thus it is stochastic.
- Deterministic policy gradient (DPG) instead models the policy as a deterministic decision:  $a = \mu(s)$ .
- How can you calculate the gradient of the policy function when it outputs a single action?
- Let's define few notations to facilitate the discussion:
  - $\rho_0(s)$ : The initial distribution over states
  - $\rho^{\mu}(s \to s', k)$ : Starting from state s, the visitation probability density at state s' after moving k steps  $\rho^{\mu}(s') = \int_{S} \sum_{k=1}^{\infty} \gamma^{k-1} \rho_{0}(s) \rho^{\mu}(s \to s', k) ds$  Discounted state distribution, defined as

The objective function to optimize for is listed as follows:

$$J(\theta) = \int_{S} \rho^{\mu}(s) Q(s, \mu_{\theta}(s)) ds$$

• Deterministic policy gradient theorem:

$$\nabla_{\theta} J(\theta) = \int_{S} \rho^{\mu}(s) \nabla_{a} Q^{\mu}(s, a) \nabla_{\theta} \mu_{\theta}(s) \Big|_{a = \mu_{\theta}(s)} ds$$
$$= \mathbb{E}_{s \sim \rho^{\mu}} \left[ \nabla_{a} Q^{\mu}(s, a) \nabla_{\theta} \mu_{\theta}(s) \Big|_{a = \mu_{\theta}(s)} \right]$$

- We can consider the deterministic policy as a special case of the stochastic one, when the probability distribution contains only one extreme non-zero value over one action.
- We expect the stochastic policy to require more samples as it integrates the data over the whole state and action space.

The deterministic policy gradient theorem can be plugged into common policy gradient frameworks.

$$J(\theta) = \int_{S} \rho^{\mu}(s) Q(s, \mu_{\theta}(s)) ds$$

• on-policy actor-critic algorithm with deterministic policy  $a = \mu_{\theta}(s)$ 

$$\delta_{t} = R_{t} + \gamma Q_{w}(s_{t+1}, a_{t+1}) - Q_{w}(s_{t}, a_{t})$$

$$w_{t+1} = w_{t} + \alpha_{w} \delta_{t} \nabla_{w} Q_{w}(s_{t}, a_{t})$$

$$\theta_{t+1} = \theta_{t} + \alpha_{\theta} \nabla_{a} Q_{w}(s_{t}, a_{t}) \nabla_{\theta} \mu_{\theta}(s)$$

$$a_{t} = \mu_{\theta}(s_{t})$$

- However, unless there is sufficient noise in the environment, it is very hard to guarantee enough
  exploration due to the determinacy of the policy.
  - We can either add noise into the policy (ironically this makes it nondeterministic!) or
  - learn it off-policy way by following a different stochastic behavior policy to collect samples.

- Let's consider the off-policy approach.
- The training trajectories are generated by a stochastic policy  $\beta(a|s)$ 
  - $\checkmark$  the state distribution follows the corresponding discounted state density  $\rho^{\beta}$
- The objective function and the gradient of it can be computed as:

$$J(\theta) = \int_{S} \rho^{\beta}(s) Q^{\mu}(s, \mu_{\theta}(s)) ds$$

$$\nabla_{\theta} J(\theta) = \int_{S} \rho^{\beta}(s) \nabla_{a} Q^{\mu}(s, a) \nabla_{\theta} \mu_{\theta}(s) \Big|_{a = \mu_{\theta}(s)} ds$$

$$= \mathbb{E}_{s \sim \rho^{\beta}} \Big[ \nabla_{a} Q^{\mu}(s, a) \nabla_{\theta} \mu_{\theta}(s) \Big|_{a = \mu_{\theta}(s)} \Big]$$

- Because the policy is deterministic, we only need  $Q^{\mu}(s, \mu_{\theta}(s))$  rather than  $\sum_{a} \pi(a|s)Q^{\pi}(s, a)$  as the estimated reward of a given state s.
  - ✓ Because the deterministic policy gradient removes the integral over actions, we can avoid importance sampling even when using off-policy approach.
  - ✓ We expect the deterministic policy requires less samples than stochastic policy as it integrates the data over only state space.

# Deep Deterministic Policy Gradient (DDPG) (Lillicrap, et al., 2015)

- Deep Deterministic Policy Gradient (DDPG), is a model-free off-policy actor-critic algorithm, combining DPG with DQN.
  - Recall that DQN (Deep Q-Network) stabilizes the learning of Q-function by experience replay and the frozen target network.
- The original DQN works in discrete action space, and DDPG extends it to continuous space with the actor-critic framework while learning a deterministic policy.
- In order to do better exploration, an exploration policy  $\mu'$  is constructed by adding noise  $\mathcal{N}$ :

$$\mu'(s) = \mu_{\theta}(s) + \mathcal{N}$$

• In addition, DDPG does soft updates ("conservative policy iteration") on the parameters of both actor and critic, with  $au\ll 1$ 

$$\theta' \leftarrow \tau\theta + (1-\tau)\theta'$$

✓ In this way, the target network values are constrained to change slowly, different from the design in DQN that the target network stays frozen for some period of time.

# Deep Deterministic Policy Gradient (DDPG) (Lillicrap, et al., 2015)

#### Algorithm 1 DDPG algorithm

Randomly initialize critic network  $Q(s, a|\theta^Q)$  and actor  $\mu(s|\theta^\mu)$  with weights  $\theta^Q$  and  $\theta^\mu$ .

Initialize target network Q' and  $\mu'$  with weights  $\theta^{Q'} \leftarrow \theta^{Q}$ ,  $\theta^{\mu'} \leftarrow \theta^{\mu}$ 

Initialize replay buffer R

for episode = 1, M do

Initialize a random process  $\mathcal{N}$  for action exploration

Receive initial observation state  $s_1$ 

for t = 1, T do

Select action  $a_t = \mu(s_t|\theta^{\mu}) + \mathcal{N}_t$  according to the current policy and exploration noise

Execute action  $a_t$  and observe reward  $r_t$  and observe new state  $s_{t+1}$ 

Store transition  $(s_t, a_t, r_t, s_{t+1})$  in R

Sample a random minibatch of N transitions  $(s_i, a_i, r_i, s_{i+1})$  from R

Set  $y_i = r_i + \gamma Q'(s_{i+1}, \mu'(s_{i+1}|\theta^{\mu'})|\theta^{Q'})$ 

Update critic by minimizing the loss:  $L = \frac{1}{N} \sum_{i} (y_i - Q(s_i, a_i | \theta^Q))^2$ 

Update the actor policy using the sampled policy gradient:

$$\nabla_{\theta^{\mu}} J \approx \frac{1}{N} \sum_{i} \nabla_{a} Q(s, a | \theta^{Q})|_{s=s_{i}, a=\mu(s_{i})} \nabla_{\theta^{\mu}} \mu(s | \theta^{\mu})|_{s_{i}}$$

Update the target networks:

$$\theta^{Q'} \leftarrow \tau \theta^{Q} + (1 - \tau)\theta^{Q'}$$
$$\theta^{\mu'} \leftarrow \tau \theta^{\mu} + (1 - \tau)\theta^{\mu'}$$

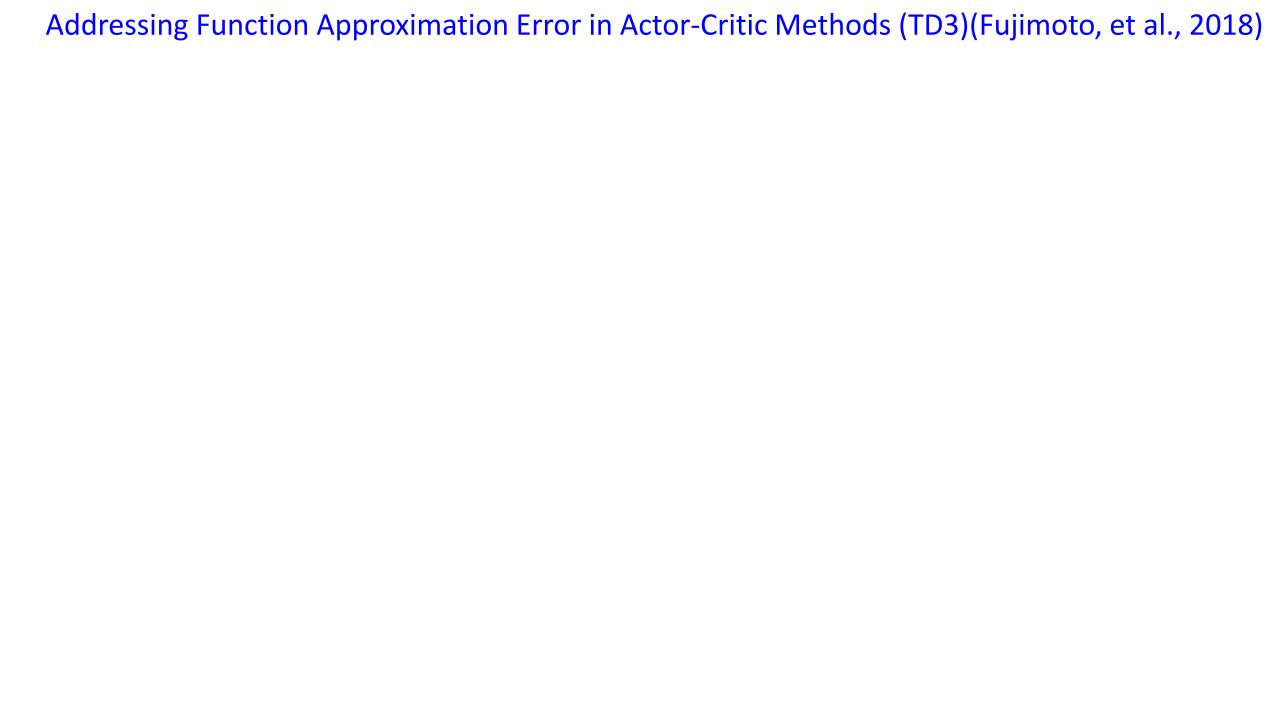
$$\nabla_{\theta} J(\theta) = \mathbb{E}_{s \sim \rho^{\beta}} \left[ \nabla_{a} Q^{\mu}(s, a) \nabla_{\theta} \mu_{\theta}(s) \Big|_{a = \mu_{\theta}(s)} \right]$$

Approximate it using minibatch samples

end for end for

Gradually changing target networks

for every transition



- Multi-agent DDPG (MADDPG) extends DDPG to an environment where multiple agents are coordinating to complete tasks with only local information.
- In the viewpoint of one agent, the environment is non-stationary as policies of other agents are quickly upgraded and remain unknown.
  - MADDPG is an actor-critic model redesigned particularly for handling such a non-stationary environment and interactions between agents.
- The problem can be formalized in the multi-agent version of MDP, also known as Markov games

```
\mathcal{N}: set of agents \mathcal{S}: set of joint states \mathcal{A}_i: set of possible action for agent i; \mathcal{A} = \mathcal{A}_1 \times \cdots \times \mathcal{A}_N set of joint action \mathcal{O}_i: set of observation for agent i; \mathcal{O} = \mathcal{O}_1 \times \cdots \times \mathcal{O}_N: set of joint observation \mathcal{T}: \mathcal{S} \times \mathcal{A}_1 \times \cdots \times \mathcal{A}_N \mapsto \mathcal{S} transition function \pi_{\theta_i}: \mathcal{O}_i \times \mathcal{A}_i \mapsto [0,1] stochastic policy of agent i \mu_{\theta_i}: \mathcal{O}_i \mapsto \mathcal{A}_i deterministic policy of agent i
```

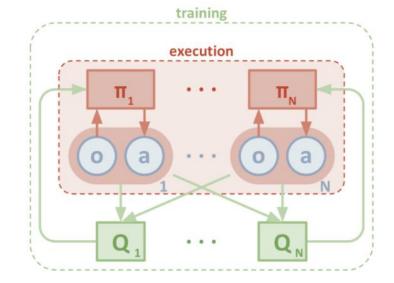
The critic in MADDPG learns a centralized action-value function for agent i

$$Q_i^{\vec{\mu}}(\vec{o}, a_1, \dots, a_N)$$

- $\checkmark$   $\vec{\mu} = \mu_1, ..., \mu_N$  :joint policies
- $\checkmark \vec{o} = o_1, ..., o_N$  :joint observations
- $\checkmark$   $\vec{a} = a_1, ..., a_N$  : joint actions
- Each  $Q_i^{\vec{\mu}}$  is learned separately for  $i=1,\ldots,N$  and therefore multiple agents can have arbitrary reward structures, including conflicting rewards in a competitive setting.

• Meanwhile multiple actors, one for each agent, are exploring and upgrading the policy parameters  $heta_i$  on

their own.



#### Actor update:

$$\nabla_{\theta_i} J(\theta_i) = \mathbb{E}_{(\vec{o}, a) \sim D} \left[ \nabla_{a_i} Q_i^{\vec{\mu}}(\vec{o}, a_1, \dots, a_N) \nabla_{\theta_i} \mu_{\theta_i}(o_i) \Big|_{a_i = \mu_{\theta_i}(o_i)} \right]$$

 $\checkmark$  D is the memory buffer for experience reply, containing multiple episode samples  $(\vec{o}, a_1, ..., a_N, r_1, ..., r_N, \vec{o}')$ : given current observation  $\vec{o}$ , agents take joint actions  $a_1, ..., a_N$  and get rewards  $r_1, ..., r_N$ , leading to the new observation  $\vec{o}'$ 

#### Critic update:

$$\mathcal{L}(\theta_i) = \mathbb{E}_{(\vec{o}, a_1, \dots, a_N, r_1, \dots, r_N, \vec{o}') \sim D} \left[ \left( Q_i^{\vec{\mu}}(\vec{o}, a_1, \dots, a_N) - y \right)^2 \right]$$

where 
$$y = r_i + \gamma Q_i^{\overrightarrow{\mu}'}(\overrightarrow{o}', a_1', \dots, a_N')\Big|_{a_i' = \mu_{\theta_i}'(o_i)}$$

- $\checkmark$   $\vec{\mu}'$  are the target policies with delayed softly-updated parameters.
- $\checkmark$  For each agent need to have  $\vec{\mu}=\mu_1,...,\mu_N$  to compute the joint actions at the next observation  $\vec{o}'$
- ✓ Each agent learns other agents policy its own during the learning process.
- ✓ Using the approximated policies, MADDPG still can learn efficiently although the inferred policies might not be accurate.

- To mitigate the high variance triggered by the interaction between competing or collaborating agents in the environment, MADDPG proposed one more element policy ensembles:
  - ✓ Train K policies for one agent;
  - ✓ Pick a random policy for episode rollouts;
  - ✓ Take an ensemble of these K policies to do gradient update.
- In summary, MADDPG added three additional ingredients on top of DDPG to make it adapt to the multi-agent environment:
  - ✓ Centralized critic + decentralized actors;
  - ✓ Actors are able to use estimated policies of other agents for learning;
  - ✓ Policy ensembling is good for reducing variance.

# Trust region policy optimization (TRPO) (Schulman, et al., 2015)

- To improve training stability, we should avoid parameter updates that change the policy too much at one step.
- Trust region policy optimization (TRPO) carries out this idea by enforcing a KL divergence constraint on the size of policy update at each iteration.
- If off policy, the objective function measures the total advantage over the state visitation distribution and actions, while the rollout is following a different behavior policy  $\beta(a|s)$ :

$$J(\theta) = \sum_{s \in \mathcal{S}} \rho^{\pi_{\theta}} \text{old} \sum_{a \in \mathcal{A}} \pi_{\theta}(a|s) \hat{A}_{\theta} \text{old}(s, a)$$

$$= \sum_{s \in \mathcal{S}} \rho^{\pi_{\theta}} \text{old} \sum_{a \in \mathcal{A}} \beta(a|s) \frac{\pi_{\theta}(a|s)}{\beta(a|s)} \hat{A}_{\theta} \text{old}(s, a)$$

$$= \mathbb{E}_{s \sim \rho^{\pi_{\theta}} \text{old}, a \sim \beta} \left[ \frac{\pi_{\theta}(a|s)}{\beta(a|s)} \hat{A}_{\theta} \text{old}(s, a) \right]$$

- $\checkmark$   $\theta_{\rm old}$  is the policy parameters before the update and thus known to us.  $\rho^{\pi_{\theta_{\rm old}}}$  is defined similary.
- $\checkmark \beta(a|s)$  is the behavior policy for collecting trajectories

## Trust region policy optimization (TRPO) (Schulman, et al., 2015)

• If on policy, the behavior policy is  $\pi_{\theta}(a|s)$ :

$$J(\theta) = \mathbb{E}_{s \sim \rho^{\pi_{\theta}} \text{old}, a \sim \beta} \left[ \frac{\pi_{\theta}(a|s)}{\beta(a|s)} \hat{A}_{\theta_{\text{old}}}(s, a) \right]$$
$$= \mathbb{E}_{s \sim \rho^{\pi_{\theta}} \text{old}, a \sim \pi_{\theta}} \left[ \frac{\pi_{\theta}(a|s)}{\pi_{\theta} \text{old}} \hat{A}_{\theta_{\text{old}}}(s, a) \right]$$

• TRPO aims to maximize the objective function  $J(\theta)$  subject to, trust region constraint which enforces the distance between old and new policies measured by KL-divergence to be small enough, within a parameter  $\delta$ 

$$\mathbb{E}_{s \sim \rho^{\pi_{\theta}} \text{old}} \left[ D_{KL} \left( \pi_{\theta} \text{old} (\cdot | s) \| \pi_{\theta} (\cdot | s) \right) \right] \leq \delta$$

- In this way, the old and new policies would not diverge too much when this hard constraint is met.
  - While still, TRPO can guarantee a monotonic improvement over policy iteration (why?)

## Proximal Policy Optimization (PPO) (Schulman, et al., 2017)

- Given that TRPO is relatively complicated and we still want to implement a similar constraint, proximal
  policy optimization (PPO) simplifies it by using a clipped surrogate objective while retaining similar
  performance.
- Denote the probability ratio between old and new policies as:

$$r(\theta) = \frac{\pi_{\theta}(a|s)}{\pi_{\theta \text{ old}}(a|s)}$$

Then, the objective function of TRPO (on policy) becomes:

$$J^{\text{TRPO}}(\theta) = \mathbb{E}\left[\frac{\pi_{\theta}(a|s)}{\pi_{\theta \text{ old}}(a|s)}\hat{A}_{\theta \text{ old}}(s,a)\right] = \mathbb{E}\left[r(\theta)\hat{A}_{\theta \text{ old}}(s,a)\right]$$

- Without a limitation on the distance between  $\theta_{\rm old}$  and  $\theta$ , to maximize  $J^{\rm TRPO}(\theta)$  would lead to instability with extremely large parameter updates and big policy ratios.
- PPO imposes the constraint by forcing  $r(\theta)$  to be within a small interval around 1, precisely  $[1-\epsilon,1+\epsilon]$

$$J^{\text{CLIP}}(\theta) = \mathbb{E}\left[\min\left(r(\theta)\hat{A}_{\theta_{\text{old}}}(s, a), \text{clip}(r(\theta), 1 - \epsilon, 1 + \epsilon)\hat{A}_{\theta_{\text{old}}}(s, a)\right)\right]$$

✓ The function clip  $(r(\theta), 1 - \epsilon, 1 + \epsilon)$  clips the ratio  $r(\theta)$  within  $[1 - \epsilon, 1 + \epsilon]$ .

## Proximal Policy Optimization (PPO) (Schulman, et al., 2017)

- When applying PPO on the network architecture with shared parameters for both policy (actor) and value (critic) functions, the objective function is augmented composed of
  - ✓ the clipped reward
  - ✓ an error term on the value estimation
  - ✓ an entropy term to encourage sufficient exploration.

$$J^{\text{CLIP}'}(\theta) = \mathbb{E}\left[J^{\text{CLIP}}(\theta) - c_1(V_{\theta}(s) - V_{target})^2 + c_2H(s, \pi_{\theta}(\cdot))\right]$$

 $c_1$  and  $c_2$  are two hyperparameters constants.

## Actor-critic with experience replay (ACER) (Wang, et al., 2017)

- ACER is an off-policy actor-critic model with experience replay,
  - ✓ greatly increasing the sample efficiency and decreasing the data correlation.
- ACER is A3C's off-policy counterpart.
- The major obstacle to making A3C off policy is how to control the stability of the off-policy estimator.
   ACER proposes three designs to overcome it:
  - ✓ Use Retrace Q-value estimation;
  - ✓ Truncate the importance weights with bias correction;
  - ✓ Apply efficient TRPO.

Will be updated later

## Actor-critic with experience replay (ACER) (Wang, et al., 2017)

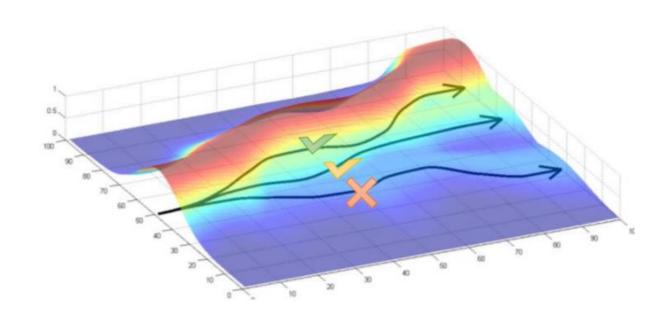
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   ACER proposes three designs to overcome it:
  - ✓ Use Retrace Q-value estimation;
  - ✓ Truncate the importance weights with bias correction;
  - ✓ Apply efficient TRPO.

Will be updated later

Soft Actor Critic (SAC) (Haarnoja et al., 2018)



- We derived Policy Gradient Theorem using the concept of state value function to employ recursive formula on the basis of dynamic programming (Bellman equation)
- Not let's derive similar result without using DP approach but using episodic approach where agent engages in multiple trajectories in its environment



• Let's define a trajectory  $\tau$  of length T as

$$\tau = (s_0, a_0, r_0, s_1, a_1, r_1, \dots, s_{T-1}, a_{T-1}, s_T)$$

- $\checkmark$   $s_0$  comes from the starting distribution of states
- $\checkmark a_i \sim \pi_{\theta}(a_i | s_i)$  with  $\pi_{\theta}$  parameterized **policy**
- $\checkmark s_i \sim P(s_i | s_{i-1}, a_{i-1})$  with P dynamic model describing how **environment** changes
- The probability of trajectory  $\tau = (s_0, a_0, r_0, s_1, a_1, r_1, \dots, s_{T-1}, a_{T-1}, s_T)$  can be expressed as

$$p(\tau) = \mu(s_0) \prod_{t=0}^{T-1} \pi_{\theta}(a_t|s_t) P(s_{t+1}|s_t, a_t)$$

We can compute

$$\begin{split} \nabla_{\theta} \log p(\tau) &= \nabla_{\theta} \log \left( \mu(s_0) \prod_{t=0}^{T-1} \pi_{\theta}(a_t | s_t) P(s_{t+1} | s_t, a_t) \right) \\ &= \nabla_{\theta} \left[ \log \mu(s_0) + \sum_{t=0}^{T-1} (\log \pi_{\theta}(a_t | s_t) + \log P(s_{t+1} | s_t, a_t)) \right] \\ &= \sum_{t=0}^{T-1} \nabla_{\theta} \log \pi_{\theta}(a_t | s_t) \end{split}$$

We want to maximize

$$\mathbb{E}_{\pi_{\theta}}\left[\sum_{t=0}^{T-1} r_{t}\right] = \mathbb{E}_{\tau \sim p_{\theta}}[R(\tau)]$$

 $\because$  we know au is influenced by  $\pi_{ heta}$ 

The gradient of objective is computed as

$$\begin{split} \nabla_{\theta} \mathbb{E}_{\tau \sim p_{\theta}}[R(\tau)] &= \nabla_{\theta} \int p_{\theta}(\tau) R(\tau) d\tau \\ &= \int \frac{p_{\theta}(\tau)}{p_{\theta}(\tau)} \nabla_{\theta} p_{\theta}(\tau) R(\tau) d\tau \\ &= \int p_{\theta}(\tau) \nabla_{\theta} \ln p_{\theta}(\tau) R(\tau) d\tau \\ &= \mathbb{E}_{\tau \sim p_{\theta}}[\nabla_{\theta} \ln p_{\theta}(\tau) R(\tau)] \\ &= \mathbb{E}_{\tau \sim \pi_{\theta}} \left[ \sum_{t=0}^{T-1} \nabla_{\theta} \log \pi_{\theta}(a_{t}|s_{t}) R(\tau) \right] \\ &= \mathbb{E}_{\tau \sim \pi_{\theta}} \left[ \sum_{t=0}^{T-1} \nabla_{\theta} \log \pi_{\theta}(a_{t}|s_{t}) \left( \sum_{t=0}^{T-1} r_{t} \right) \right] \end{split}$$

$$: \nabla_{\theta} \log p(\tau) = \sum_{t=0}^{T-1} \nabla_{\theta} \log \pi_{\theta}(a_t|s_t)$$

We have

$$\nabla_{\theta} \mathbb{E}_{\tau \sim \pi_{\theta}}[R(\tau)] = \mathbb{E}_{\tau \sim \pi_{\theta}} \left[ \sum_{t=0}^{T-1} \nabla_{\theta} \log \pi_{\theta}(a_t | s_t) \left( \sum_{t=0}^{T-1} r_t \right) \right]$$

- $\checkmark$  The expectation is with respect to the policy function, so we can think  $\tau \sim \pi_{\theta}$
- We need trajectories to get an empirical expectation, which estimates the actual expectation. The naïve way is to run the agent on batch of episodes

$$\theta \leftarrow \theta + \alpha \nabla_{\theta} \mathbb{E}_{\tau \in \mathcal{T}}[R(\tau)]$$

 $\checkmark$  where T is a set of trajectories sampled

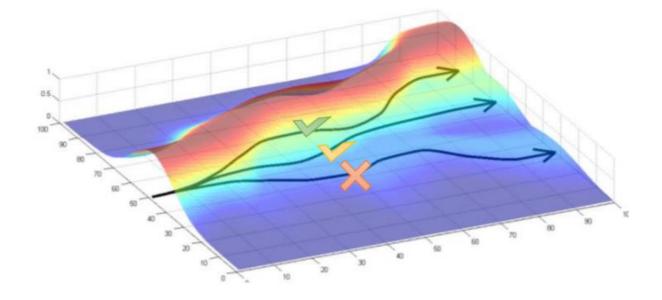
$$\nabla_{\theta} \mathbb{E}_{\tau \in \mathcal{T}}[R(\tau)] \approx \frac{1}{N} \sum_{i=1}^{N} \sum_{t=0}^{T-1} \nabla_{\theta} \log \pi_{\theta} \left( a_{t}^{(i)} \middle| s_{t}^{(i)} \right) \left( \sum_{t=0}^{T-1} r_{t}^{(i)} \right)$$

- $\tau^{(i)} = \left(s_0^{(i)}, a_0^{(i)}, r_0^{(i)}, s_1^{(i)}, a_1^{(i)}, r_1^{(i)}, \dots, s_{T-1}^{(i)}, a_{T-1}^{(i)}, r_{T-1}^{(i)}, s_T^{(i)}\right) \text{ is the } i\text{-th trajectory.}$
- ✓ This approach will be too slow and unreliable due to high variance on the gradient estimate
- ✓ We need various variance reduction techniques.

### **Interpreting Policy Gradient**

$$\nabla_{\theta} \mathbb{E}_{\tau \sim \pi_{\theta}}[R(\tau)] = \mathbb{E}_{\tau \sim \pi_{\theta}} \left[ \left( \sum_{t=0}^{T-1} \nabla_{\theta} \log \pi_{\theta}(a_{t}|s_{t}) \right) \left( \sum_{t=0}^{T-1} r_{t} \right) \right] \approx \frac{1}{N} \sum_{i=1}^{N} \left( \sum_{t=0}^{T-1} \nabla_{\theta} \log \pi_{\theta} \left( a_{t}^{(i)} \middle| s_{t}^{(i)} \right) \right) \left( \sum_{t=0}^{T-1} r_{t}^{(i)} \right)$$
probability of trajectory

Reward of trajectory



- Increase the likelihood for the trajectory with large accumulated reward
- Decrease the likelihood for the trajectories with small accumulated reward

### Variance Reduction (Imposing Causality)

$$\nabla_{\theta} \mathbb{E}_{\tau \sim \pi_{\theta}}[R(\tau)] = \mathbb{E}_{\tau \sim \pi_{\theta}} \left[ \left( \sum_{t=0}^{T-1} \nabla_{\theta} \log \pi_{\theta}(a_{t}|s_{t}) \right) \left( \sum_{t=0}^{T-1} r_{t} \right) \right] \approx \frac{1}{N} \sum_{i=1}^{N} \left( \sum_{t=0}^{T-1} \nabla_{\theta} \log \pi_{\theta}\left(a_{t}^{(i)} \middle| s_{t}^{(i)}\right) \right) \left( \sum_{t=0}^{T-1} r_{t}^{(i)} \right)$$

• Apply causality: policy at time t' cannot affect reward at time t when t < t'

$$(f_0 + f_1 + \dots + f_t + \dots f_T)(f_0 + f_1 + \dots + f_t + \dots f_T)$$

$$= f_0(f_0 + f_1 + \dots + f_t + \dots f_T) +$$

$$f_1(f_0 + f_1 + \dots + f_t + \dots f_T) +$$

$$\vdots$$

$$f_t(f_0 + f_1 + \dots + f_t + \dots f_T) +$$

$$\vdots$$

$$f_T(f_0 + f_1 + \dots + f_t + \dots f_T) +$$

## Variance Reduction (Subtracting Baseline)

$$\nabla_{\theta} \mathbb{E}_{\tau \sim \pi_{\theta}}[R(\tau)] = \mathbb{E}_{\tau \sim \pi_{\theta}} \left[ \sum_{t=0}^{T-1} \nabla_{\theta} \log \pi_{\theta} \left( a_{t}^{(i)} \middle| s_{t}^{(i)} \right) \sum_{t'=t}^{T-1} r_{t'}^{(i)} \right] \approx \frac{1}{N} \sum_{i=1}^{N} \sum_{t=0}^{T-1} \nabla_{\theta} \log \pi_{\theta} \left( a_{t}^{(i)} \middle| s_{t}^{(i)} \right) \sum_{t'=t}^{T-1} r_{t'}^{(i)}$$

Subtract baseline term to reduce variance

$$\nabla_{\theta} \mathbb{E}_{\tau \sim \pi_{\theta}}[R(\tau)] = \mathbb{E}_{\tau \sim \pi_{\theta}} \left[ \sum_{t=0}^{T-1} \nabla_{\theta} \log \pi_{\theta}(a_t | s_t) \left( \sum_{t'=t}^{T-1} r_{t'} - b(s_t) \right) \right]$$

- We need to verify the things:
  - 1) Inserting baseline does not make the gradient estimate biased
  - 2) Baseline reduce actually variance
  - > Staying unbiased and reducing variance is always good!

### Variance Reduction (Subtracting Baseline)

(1) Inserting baseline does not make the gradient estimate biased

$$\begin{aligned} \nabla_{\theta} \mathbb{E}_{\tau \sim \pi_{\theta}} [R(\tau)] &= \mathbb{E}_{\tau \sim \pi_{\theta}} \left[ \sum_{t=0}^{T-1} \nabla_{\theta} \log \pi_{\theta}(a_{t}|s_{t}) \left( \sum_{t'=t}^{T-1} r_{t'} - b(s_{t}) \right) \right] \\ &= \mathbb{E}_{\tau \sim \pi_{\theta}} \left[ \sum_{t=0}^{T-1} \nabla_{\theta} \log \pi_{\theta}(a_{t}|s_{t}) \left( \sum_{t'=t}^{T-1} r_{t'} \right) - \sum_{t=0}^{T-1} \nabla_{\theta} \log \pi_{\theta}(a_{t}|s_{t}) b(s_{t}) \right] \end{aligned}$$

• All we need to show is that for any single time t, the gradient of  $\log \pi_{\theta}(a_t|s_t)$  multiplied with  $b(s_t)$  is zero:

$$\begin{split} \mathbb{E}_{\tau \sim \pi_{\theta}} [\nabla_{\theta} \log \pi_{\theta}(a_{t}|s_{t}) \, b(s_{t})] &= \mathbb{E}_{s_{0:t,a_{0:t-1}}} \left[ \mathbb{E}_{s_{t+1:T,a_{t:T-1}}} [\nabla_{\theta} \log \pi_{\theta}(a_{t}|s_{t}) \, b(s_{t})] \right] \\ &= \mathbb{E}_{s_{0:t,a_{0:t-1}}} \left[ b(s_{t}) \cdot \mathbb{E}_{s_{t+1:T,a_{t:T-1}}} [\nabla_{\theta} \log \pi_{\theta}(a_{t}|s_{t})] \right] \\ &= \mathbb{E}_{s_{0:t,a_{0:t-1}}} \left[ b(s_{t}) \cdot \mathbb{E}_{a_{t}} [\nabla_{\theta} \log \pi_{\theta}(a_{t}|s_{t})] \right] \\ &= \mathbb{E}_{s_{0:t,a_{0:t-1}}} [b(s_{t}) \cdot 0] = 0 \end{split}$$

$$: \mathbb{E}_{a_t}[\nabla_{\theta} \log \pi_{\theta}(a_t|s_t)] = \int \frac{\nabla_{\theta} \pi_{\theta}(a_t|s_t)}{\pi_{\theta}(a_t|s_t)} \pi_{\theta}(a_t|s_t) da_t = \nabla_{\theta} \int \pi_{\theta}(a_t|s_t) da_t = \nabla_{\theta} \cdot 1 = 0$$

### Variance Reduction (Subtracting Baseline)

#### (1) Inserting Baseline reduce actually variance

$$\begin{aligned} \nabla_{\theta} \mathbb{E}_{\tau \sim \pi_{\theta}} [R(\tau)] &= \mathbb{E}_{\tau \sim \pi_{\theta}} \left[ \sum_{t=0}^{T-1} \nabla_{\theta} \log \pi_{\theta}(a_{t}|s_{t}) \left( \sum_{t'=t}^{T-1} r_{t'} - b(s_{t}) \right) \right] \\ &= \mathbb{E}_{\tau \sim \pi_{\theta}} \left[ \sum_{t=0}^{T-1} \nabla_{\theta} \log \pi_{\theta}(a_{t}|s_{t}) \left( \sum_{t'=t}^{T-1} r_{t'} \right) - \sum_{t=0}^{T-1} \nabla_{\theta} \log \pi_{\theta}(a_{t}|s_{t}) b(s_{t}) \right] \end{aligned}$$

Why subtracting baseline reduces variance?

$$\operatorname{Var}\left(\sum_{t=0}^{T-1} \nabla_{\theta} \log \pi_{\theta}(a_{t}|s_{t}) \left(R_{t}(\tau) - b(s_{t})\right)\right) \approx \sum_{t=0}^{T-1} \mathbb{E}_{\tau \sim \pi_{\theta}} \left[\left(\nabla_{\theta} \log \pi_{\theta}(a_{t}|s_{t}) \left(R_{t}(\tau) - b(s_{t})\right)\right)^{2}\right] \qquad \operatorname{Var}\left(\sum_{i=1} X_{i}\right) \approx \sum_{i=1}^{T-1} \operatorname{Var}(X_{i})$$

$$\left(R_{t}(\tau) = \sum_{t'=t}^{T-1} r_{t'}\right) \approx \sum_{t=0}^{T-1} \mathbb{E}_{\tau \sim \pi_{\theta}} \left[\left(\nabla_{\theta} \log \pi_{\theta}(a_{t}|s_{t})\right)^{2}\right] \mathbb{E}_{\tau \sim \pi_{\theta}} \left[\left(\left(R_{t}(\tau) - b(s_{t})\right)^{2}\right)\right] \qquad E[AB] = E[A]E[B]$$

• We can optimally choose  $b(s_t)$  to minimize variance as

$$\min_{b(s_t)} \mathbb{E}_{\tau \sim \pi_{\theta}} \left[ \left( \left( R_t(\tau) - b(s_t) \right)^2 \right) \right]$$

- $\checkmark$  Which gives the least square solution  $b(s_t) = \mathbb{E}_{\tau \sim \pi_\theta}[R_t(\tau)]$ 
  - > have to re-fit the baseline estimate each time to make it as close to the expected return

# Variance Reduction (Advantage Function)

$$\begin{split} \nabla_{\theta} \mathbb{E}_{\tau \sim \pi_{\theta}}[R(\tau)] &= \mathbb{E}_{\tau \sim \pi_{\theta}} \left[ \sum_{t=0}^{T-1} \nabla_{\theta} \log \pi_{\theta}(a_{t}|s_{t}) \left( \sum_{t'=t}^{T-1} r_{t'} - b(s_{t}) \right) \right] \\ &= \mathbb{E}_{\tau \sim \pi_{\theta}} \left[ \sum_{t=0}^{T-1} \nabla_{\theta} \log \pi_{\theta}(a_{t}|s_{t}) \left( Q^{\pi}(s_{t}, a_{t}) - V^{\pi}(s_{t}) \right) \right] \\ &= \mathbb{E}_{\tau \sim \pi_{\theta}} \left[ \sum_{t=0}^{T-1} \nabla_{\theta} \log \pi_{\theta}(a_{t}|s_{t}) A^{\pi}(s_{t}, a_{t}) \right] \\ &= \mathbb{E}_{\tau \sim \pi_{\theta}} \left[ \sum_{t=0}^{T-1} \nabla_{\theta} \log \pi_{\theta}(a_{t}|s_{t}) \Psi_{t} \right] \end{split}$$

• The problem of policy gradient is reduces to finding good estimates  $\Psi_t$ , a topic of *Generalized Advantage Estimation* (Schulman et al., 2016)

where  $\Psi_t$  may be one of the following:

- 1.  $\sum_{t=0}^{\infty} r_t$ : total reward of the trajectory.
- 4.  $Q^{\pi}(s_t, a_t)$ : state-action value function.
- 2.  $\sum_{t'=t}^{\infty} r_{t'}$ : reward following action  $a_t$ .
- 5.  $A^{\pi}(s_t, a_t)$ : advantage function.
- 3.  $\sum_{t'=t}^{\infty} r_{t'} b(s_t)$ : baselined version of previous formula.
- 6.  $r_t + V^{\pi}(s_{t+1}) V^{\pi}(s_t)$ : TD residual.

## Variance Reduction (Off Policy learning)

$$\theta^* = \underset{\theta}{\operatorname{argmax}} \mathbb{E}_{\tau \sim \pi_{\theta}}[R(\tau)]$$

$$\nabla_{\theta} \mathbb{E}_{\tau \sim \pi_{\theta}}[R(\tau)] = \mathbb{E}_{\tau \sim \pi_{\theta}}[\nabla_{\theta} \log \pi_{\theta}(\tau) R(\tau)]$$

- Neural networks change only a little bit with each gradient step
- On-policy learning can be extremely inefficient!

$$\mathbb{E}_{\boldsymbol{\tau} \sim \boldsymbol{\pi}_{\boldsymbol{\theta}}}[R(\boldsymbol{\tau})] = \nabla_{\boldsymbol{\theta}} \mathbb{E}_{\boldsymbol{\tau} \sim \overline{\boldsymbol{\pi}}} \left[ \frac{\pi_{\boldsymbol{\theta}}(\boldsymbol{\tau})}{\overline{\boldsymbol{\pi}}(\boldsymbol{\tau})} R(\boldsymbol{\tau}) \right]$$

$$\frac{\pi_{\theta}(\tau)}{\bar{\pi}_{\theta}(\tau)} = \frac{p(s_0) \prod_{t=0}^{T-1} \pi_{\theta}(a_t|s_t) P(s_{t+1}|s_t, a_t)}{p(s_0) \prod_{t=0}^{T-1} \bar{\pi}(a_t|s_t) P(s_{t+1}|s_t, a_t)} = \frac{\prod_{t=0}^{T-1} \pi_{\theta}(a_t|s_t)}{\prod_{t=0}^{T-1} \bar{\pi}(a_t|s_t)}$$

importance sampling

$$E_{x \sim p(x)}[f(x)] = \int p(x)f(x)dx$$

$$= \int \frac{q(x)}{q(x)}p(x)f(x)dx$$

$$= \int q(x)\frac{p(x)}{q(x)}f(x)dx$$

$$= E_{x \sim q(x)}\left[\frac{p(x)}{q(x)}f(x)\right]$$

# Variance Reduction (Off Policy learning)

$$\begin{split} J(\theta) &= \mathbb{E}_{\tau \sim \pi_{\theta}}[R(\tau)] = \nabla_{\theta} \mathbb{E}_{\tau \sim \overline{\pi}} \left[ \frac{\pi_{\theta}(\tau)}{\overline{\pi}(\tau)} R(\tau) \right] \\ \nabla_{\theta'} J(\theta') &= \mathbb{E}_{\tau \sim \pi_{\theta}} \left[ \frac{\pi_{\theta'}(\tau)}{\pi_{\theta}(\tau)} \nabla_{\theta'} \log \pi_{\theta'}(\tau) R(\tau) \right] \\ &= \mathbb{E}_{\tau \sim \pi_{\theta}} \left[ \left( \prod_{t=1}^{T} \frac{\pi_{\theta'}(a_{t}|s_{t})}{\pi_{\theta}(a_{t}|s_{t})} \right) \left( \sum_{t=1}^{T} \nabla_{\theta'} \log \pi_{\theta'}(a_{t}|s_{t}) \right) \left( \sum_{t=1}^{T} r_{t} \right) \right] & \text{Ignore} \\ &= \mathbb{E}_{\tau \sim \pi_{\theta}} \left[ \sum_{t=1}^{T} \nabla_{\theta'} \log \pi_{\theta'}(a_{t}|s_{t}) \left( \prod_{t'=1}^{t} \frac{\pi_{\theta'}(a_{t'}|s_{t'})}{\pi_{\theta}(a_{t'}|s_{t'})} \right) \left( \sum_{t'=t}^{T} r_{t} \left( \prod_{t''=1}^{T} \frac{\pi_{\theta'}(a_{t''}|s_{t''})}{\pi_{\theta}(a_{t''}|s_{t''})} \right) \right) \right] & \text{Causality} \\ &\approx \mathbb{E}_{\tau \sim \pi_{\theta}} \left[ \sum_{t=1}^{T} \nabla_{\theta'} \log \pi_{\theta'}(a_{t}|s_{t}) \left( \prod_{t'=1}^{t} \frac{\pi_{\theta'}(a_{t'}|s_{t'})}{\pi_{\theta}(a_{t'}|s_{t'})} \right) \left( \sum_{t'=t}^{T} r_{t} \right) \right] \end{split}$$