# Deep Reinforcement Learning

Jubayer Ibn Hamid

## **Preface**

This document is a combination of notes from CS 224R taught by Prof. Chelsea Finn at Stanford University, CS 234 taught by Prof. Emma Brunskill at Stanford University, and CS 285 taught by Prof. Sergey Levine at UC Berkeley, as well as reading notes from various papers (in particular, Richard Sutton and Andrew Barto's "Reinforcement Learning: An Introduction" [1]).

Although these are reading notes, there may be various errors throughout, both minor and major, which almost certaintly did not appear in the original works that I was reading. If you find any, please let me know by sending me an email at <code>jubayer@stanford.edu</code>. I have also not been able to stick to the same notation throughout these notes and I apologize for that - in my defence, reinforcement learning is notorious for a lack of universal notation. Hopefully, the inconsistencies are not too troublesome.

## Contents

1	Markov Decision Processes		4
	1.1	Framework	4
	1.2	Values	5
	1.3	Optimal Values and Policies	7
	1.4	State Distributions	8
	1.5	Partially Observed MDPs	8
	1.6	Oversimplified Overview	8
2	Policy Gradient Methods		10
	2.1	Deriving the Policy Gradient	11
	2.2	Policy Gradient Theorem	12
	2.3	REINFORCE	15
	2.4	REINFORCE using causality	16
	2.5	REINFORCE with baseline	18
	2.6	On-Policy Actor-Critic Methods	20
	2.7	Making inroads to off-policy policy gradient	22
	2.8	Off-Policy Actor-Critic (OffPAC)	23
	2.9	Performance Difference Lemma	23
	2.10	Covariant/natural policy gradient	26
	2.11	Trust Region Policy Optimization (TRPO)	27
	2.12	Proximal Policy Optimization (PPO)	32
	2.13	Soft Actor-Critic (SAC)	36
	2.14	Deterministic Policy Gradient Methods (DPG)	39
A	Probability		41
	A.1	Total Variation Distance	41
		A.1.1 Defintions and Properties	42
		A.1.2 Coupling	43

## 1 Markov Decision Processes

#### 1.1 Framework

For the majority of these notes, we will consider the framework of a Markov Decision Process (MDP), represented as  $\langle \mathcal{S}, \mathcal{A}, p, r, \rho_0, \gamma, H \rangle$ , where  $\mathcal{S}$  is the state space,  $\mathcal{A}$  is the action space, p is the transition dynamics,  $r(s, a) \in \mathcal{R}$  is the reward function,  $\rho_0$  is the initial state distribution,  $\gamma \in [0, 1]$  is the discount factor and H is the task horizon (which could be positive infinity).

In this setting, the agent interacts with the environments continually which results in observed rewards. We say that the agent interacts with the environment at time steps  $t \in \mathbb{Z}^+$  (the set of positive integers).

The reward function is  $r(s_t, a_t) = \mathbb{E}[r|S_t = s_t, A_t = a_t]$  i.e., the expected reward from taking an action from the current state. Here we are assuming that the reward after taking action  $a_t$  from state  $s_t$  has a distribution and  $r(s_t, a_t)$  is the mean of that distribution. However, the reward could also be deterministic in which case the mean would collapse to the deterministic value. Eitherways, we will use the shorthand  $r_t := r(s_t, a_t)$ .

A finite MDP is an MDP such that S, A and R are finite sets. In finite MDPs, the transition probabilities and the distribution over rewards are discrete distributions.

The MDP framework is a neat abstraction of sequential decision-making. As [1] describes, the action can be low-level (e.g. voltages applies to the motors of a robot arm) or high-level decisions (e.g. spend more money on a book or not). The states can be low-level sensations (e.g. direct sensory readings) or high-level information (e.g. symbolic descriptions of objects in a room or even images).

**Definition 1.** (Policy). A policy refers to an agent's distribution over actions at each state i.e.,

$$\pi(a|s) := P(A_t = a|S_t = s).$$

Note that a policy can be deterministic too, in which case  $\pi(a|s)$  can be written as a Dirac-delta distribution.

An episode refers to "one play of the game" i.e., our agent ends up in the terminal state or the agent has taken H actions after which the environment is reset. For example, a game of Chess is an episodic task - even if the agent plays multiple games, the next episode begins independently of how the previous episode went. We sometimes denote the set of all terminal states as  $S^+$ .

Goal of reinforcement learning: Our agent seeks to maximize the expected discounted sum of rewards i.e.

$$\max_{\pi} \mathbb{E}\left[\sum_{t=0}^{H} \gamma^{t} r_{t} \mid \pi\right].$$

Note, the expectation is taken over the distribution of the random variables  $s_t, a_t, s_{t+1}, a_{t+1}, \ldots$  induced by transition dynamics  $p(s_{t'+1} \mid s_{t'}, a_{t'})$  and the policy  $\pi(a_{t'} | s_{t'})$  for all  $t' \in [0, H]$ . Also

note that the goal is not to maximize immediate reward but the cumulative reward in the long run.

#### 1.2 Values

**Definition 2.** (Return). The total return from a trajectory from time t ownards is

$$G_t = r_t + r_{t+1} + \dots + r_H$$

if H is finite. When we use the *discounted* sum of rewards (especially for non-episodic/continuing tasks), one can define the total discounted return even for infinite horizon tasks

$$G_t = r_t + \gamma r_{t+1} + \gamma^2 r_{t+2} + \dots = \sum_{k=0}^{\infty} \gamma^k r_{t+k}.$$

Then, we see that the goal of reinforcement learning is to maximize the expected total return from a trajectory. For most of these notes, I will try to be consistent and assume that H is infinite for the sake of simplicity.

**Note**: if  $\gamma < 1$ , then  $G_t$  is finite as long as the rewards  $r_{t'}, \forall t'$ , are boounded. We either require horizon H to be finite (episodic tasks) or, if  $H = \infty$  (continuing tasks), we require  $\gamma < 1$ . Otherwise, the value  $V_{\pi}(s)$  could blow up.

Note that we also have the following:  $G_t = r_t + \gamma G_{t+1}$ .

**Definition 3.** (Optimal Policy). The optimal policy is defined as:

$$\pi^*(a|s) = \arg\max_{\pi} \mathbb{E}_{\pi} \left[ \sum_{t} \gamma^t r_t \mid \pi, s \right]$$

Now, we introduce some more constructions that help express the goal of reinforcement learning - maximizing the expected (discounted) sum of rewards. To do so, we define the following:

**Definition 4.** Value function. Given a policy  $\pi$ , the value function of  $\pi$  refers to the expected sum of (discounted) rewards when starting from a given state s and acting according to  $\pi$ . For generality, suppose  $H = \infty$ , then this can be written as:

$$V_{\pi}(s) = \mathbb{E}_{\pi} \left[ \sum_{t=0}^{\infty} \gamma^{t} R_{t} \middle| \pi, S_{0} = s \right].$$

Note that the expectation is taken over trajectories  $s_0, a_0, r_0, s_1, a_1, r_1, \cdots$  where  $a_{t'} \sim \pi(\cdot \mid s_{t'})$  and  $s_{t'+1} \sim p(\cdot \mid s_{t'}, a_{t'})$  for all t'. Furthermore, note that the value of the terminal state is always zero (since no action is taken at the terminal state and, therefore, no reward is observed).

(This notation is not universal; sometimes people write  $V^{\pi}(s), v_{\pi}(s)$  or  $V(s; \pi)$  to mean the same thing.)

**Lemma 1.** We have the following recursive relationship for the value function:

$$V_{\pi}(s) = \mathbb{E}_{\substack{a \sim \pi(a|s) \\ s', r \sim P(s', r|s, a)}} [r + \gamma V_{\pi}(s') \mid S_0 = s].$$

This is called the Bellman equation for  $V^{\pi}$ .

*Proof.* The derivation is as follows:

$$\begin{split} V_{\pi}(s) &= \mathbb{E}_{\pi} \left[ \sum_{t=0}^{\infty} \gamma^{t} r_{t} | s_{0} = s \right]. \\ &= \mathbb{E}_{\pi} \left[ r_{0} + \sum_{t=1}^{\infty} \gamma^{t} r_{t} | s_{0} = s \right]. \\ &= \mathbb{E}_{\pi} \left[ r_{0} \right] + \mathbb{E}_{\pi} \left[ \gamma \cdot \sum_{t=1}^{\infty} \gamma^{t-1} r_{t} | s_{0} = s \right]. \\ &= \sum_{a} \pi(a | s_{0} = s) \sum_{s', r} P(s', r | s, a) \left[ r \right] + \sum_{a} \pi(a | s_{0} = s) \sum_{s', r} P(s', r | s, a) \left[ \gamma \mathbb{E}_{\pi} \left[ G_{t+1} | S_{1} = s' \right] \right] \\ &= \sum_{a} \pi(a | s) \sum_{s', r} P(s', r | s, a) \left[ r + \gamma V_{\pi}(s') \right] \\ &= \mathbb{E}_{\substack{a \sim \pi(a | s) \\ s', r \sim P(s', r | s, a)}} \left[ r + \gamma V_{\pi}(s') \right] \end{split}$$

We then see that the goal of RL is to find the optimal policy defined by  $\pi(a \mid s) = \arg \max_{\pi} V^{\pi}(s)$ .

Intuitively,  $V^{\pi}(s)$  is telling us, on average, how "good" we are when we start from state s and follow policy  $\pi$  (here "good" refers to the expected total return).

However, sometimes we might be interested in the following question - instead of following policy  $\pi$  from state s, what if we take a specific action a and then follow policy  $\pi$ . In other words, we are trying to understand the value of taking a specific action a over the trajectory induced by our policy  $\pi$ .

**Definition 5.** (State-action value function/action-value function/Q function.) The Q-value of an action from a state or the state-action value function is defined to be

$$Q_{\pi}(s, a) = \mathbb{E}_{\pi} \left[ \sum_{t=0}^{\infty} \gamma^{t} r_{t} \middle| S_{0} = s, A_{0} = a \right].$$

Intuitively,  $Q_{\pi}(s, a)$  refers to the expected sum of discounted rewards from taking action a from state s and then following policy  $\pi$  from then on.

**Lemma 2.** We have the following alternative expression of the action-value function in terms of the state-value function:

$$Q_{\pi}(s, a) = \mathbb{E}_{s', r \sim P(s', r | s, a)} [r + \gamma V_{\pi}(s') | S_0 = s, A_0 = a].$$

**Lemma 3.** We can express the state-value function in terms of the action-value function as follows:

$$V_{\pi}(s) = \mathbb{E}_{a \sim \pi(\cdot|s)} \left[ Q_{\pi}(s, a) | s \right].$$

## 1.3 Optimal Values and Policies

**Definition 6.** Optimal value function and optimal action-value function. The optimal value function is the expected sum of discounted rewards when starting from a given state s and acting optimally:

$$V^*(s) = \max_{\pi} \mathbb{E}_{\pi} \left[ \sum_{t=0}^{H} \gamma^t r_t | \pi, s_0 = s \right]$$
$$= \max_{\pi} V_{\pi}(s).$$

Similarly, we define

$$Q_*(s, a) = \max_{\pi} Q_{\pi}(s, a).$$

In other words,  $Q_*(s, a)$  is the value of taking action a and then acting optimally. We have the following relations

$$V_*(s) = \max_a Q_*(s, a)$$

and

$$Q_*(s_t, a_t) = \mathbb{E}[r_t + \gamma V_*(s_{t+1}) \mid s_t, a_t].$$

**Definition 7.** Optimal policy. We say  $\pi \geq \pi'$  if and only if  $V_{\pi}(s) \geq V_{\pi'}(s)$  for all  $s \in \mathcal{S}$ . The optimal policy  $\pi_*(s)$  is

$$\pi_*(s) = \arg\max_{\pi} V_{\pi}(s).$$

Note that  $\pi_*$  need not be unique.

**Lemma 4.** For an infinite horizon problem i.e  $H = \infty$ , the optimal policy is deterministic, stationary (i.e action distribution at a given state does not depend on the time) and not necessarily unique.

Why do we care about value functions and action-value functions? This is because knowing these would help us find the optimal policy fairly easily. Here are two ways you can do it:

1. If we have a policy  $\pi$  and we know  $q_{\pi}(s,a)$ , we can set the optimal policy to be

$$\pi^*(a \mid s) = 1\{a = \arg\max_{a'} q_{\pi}(s, a')\}. \tag{1}$$

In other words, the optimal policy could just take the optimal action in terms of  $q_{\pi}(s, a)$ . If we define this for every state, then we could get an optimal policy regardless of what  $\pi$  we use in equation 1. Note that this would make a deterministic policy.

2. if policy  $\pi_{\theta}(a \mid s)$  is parametrized by parameters  $\theta$ , we could update these parameters such that  $\pi_{\theta}(a \mid s)$  for any good action a is maximized. In other words, if action a is such that  $q_{\pi}(s, a) > V_{\pi}(s)$ , we maximize  $\pi_{\theta}(a \mid s)$  (increase probability of that action being taken).

#### 1.4 State Distributions

We will often require some notion of the distribution of states visited or distribution of states we might start from.

•  $\mathbb{P}(s_0 \to s, k, \pi_\theta)$  is the probability of reaching state s from  $s_0$  in k time-steps under policy  $\pi$ . We can calculate this as follows:

$$\mathbb{P}(s_0 \to s, k, \pi) = P(s_0) \prod_{t=0}^{k-2} \left( \sum_{a_t, s_{t+1}} \pi(a_t \mid s_t) P(s_{t+1} \mid s_t, a_t) \right) \sum_{a_{k-1}} \pi(a_{k-1} \mid s_{k-1}) P(s_k = s \mid s_{k-1}, a_{k-1}).$$

- $p^{\pi}(s) = \sum_{k=0}^{\infty} \gamma^k \mathbb{P}(s_0 \to s, k, \pi)$  is the improper discounted state distribution. This is called improper because this does not sum to 1.
- $d^{\pi}(s) := (1 \gamma) \sum_{t=0}^{\infty} \gamma^{t} \mathbb{P}(s_{0} \to s, t, \pi)$  is the distribution over all states induced by  $\pi$ . This is called the stationary distribution of Markov chain for  $\pi$ . The factor  $(1 \gamma)$  is a normalization constant and this distribution simply discounts states visited later in time.

#### 1.5 Partially Observed MDPs

We frequently find ourselves working with partially observed MDPs (POMDPs). In this setting, the agent has access to *observations* and not the states. These observations contain noisy and/or incomplete information about the state. In these settings, the agent's action depends on a *history* of observations and not just the most recent observation. In other words,  $a_t \sim \pi(\cdot \mid h_t)$  where  $h_t = (o_0, a_0, o_1, a_1, \dots, a_{t-1}, o_t)$  (here  $o_{t'}$  is the observation at time step t').

#### 1.6 Oversimplified Overview

With this, we can now give an overview of various methods discussed in these notes:

- 1. value-based methods: here we first try to estimate either the value function or the actionvalue function of a policy by interacting with the environment and collecting rewards. Once we have estimated the value of the policy, we update the policy and then we repeat. While this works for relatively small state and action spaces, for larger ones, we would requite value function approximation methods.
- 2. policy gradient methods: directly learn the optimal policy  $\pi_{\theta}$  parametrized by  $\theta$ . We learn this by updating  $\theta$  so as to maximize the expected value. For these methods, we would still require some estimation of the value of the policy or, at the very least, returns from a policy.
- 3. model-based reinforcement learning: learn the transition model i.e. the transition dynamics of the environment. Once we have this transition model, we can use it for planning or improving a policy.

Generally, the algorithms we consider will be characterized as one of two things:

- 1. off-policy: these algorithms can collect experiences (experiences are lists like  $s_t, a_t, r_t, s_{t+1}, a_{t+1}, r_{t+1}, \dots, s_{t+H}$ ) using a policy  $\pi_{\beta}$  and use that to update a different policy  $\pi_{\theta}$ .
- 2. on-policy: to update any policy  $\pi$ , we require experiences collected using policy  $\pi$ . In other words, we cannot use experiences from other policies to update this policy.

While on-policy methods can give us more reliable signals to help us update our policy, off-policy methods are more sample efficient.

## 2 Policy Gradient Methods

In policy gradient methods, we directly parametrise the policy to be  $\pi_{\theta}(a|s)$ . Our goal is then to find  $\pi_{\theta}$  that maximizes expected returns. In the other algorithms we have seen so far, we tried to estimate the value of a policy and then improved it, whereas, in the case of policy gradients, we will directly aim to learn the optimal policy. We may still learn a value function in order to help learn our parametrized optimal policy, but the value function will not be required for our action selection (in the sense that, when selecting which action to take, we will not query the value function - the value function is only used to help us update our policy  $\pi_{\theta}$ ). Methods that incorporate both a parametrized policy and a parametrized learned value function are often called actor-critic methods. For policy-based methods, we have no value function, but only a learned policy.

Policy gradient methods are useful for generating stochastic policies. A useful example of a parametrized policy to keep in mind is a Gaussian policy (especially for continuous action spaces) that is parametrized as  $a \sim \mathcal{N}(\mu_{\theta}(s), \Sigma) =: \pi_{\theta}(\cdot \mid s)$  (we usually set  $\Sigma$  to be a diagonal matrix). The policy can be parametrized in any way as long as it is differentiable with respect to its parameters. More complex parameterizations can be used; the choice of policy parameterization is sometimes a good way to inject prior knowledge about the desired form of the policy into the reinforcement learning system. In any case, we generally want to encourage the policy to explore and, to do so, we usually require that the policy never becomes deterministic i.e.  $\pi_{\theta}(a \mid s) \in (0, 1), \forall s, a$ .

Policy gradient methods are usually suitable for continuous action spaces and for high-dimensional action spaces. However, a common phenomenon with policy gradient methods is that these policies tend to be hard to evaluate and can have a high variance.

**Recall:** we will require the following notions of distributions over states that we introduced before in section 1.4:

- $\mathbb{P}(s_0 \to s, k, \pi_\theta)$  is the probability of reaching state s from  $s_0$  in k time-steps under policy  $\pi_\theta$ .
- $p^{\pi}(s) = \sum_{k=0}^{\infty} \gamma^k \mathbb{P}(s_0 \to s, k, \pi_{\theta})$  is the improper discounted state distribution.
- $d^{\pi_{\theta}}(s) := (1 \gamma) \sum_{t=0}^{\infty} \gamma^{t} \mathbb{P}(s_{0} \to s, t, \pi_{\theta})$  is the distribution over all states induced by  $\pi_{\theta}$  be. The factor  $(1 \gamma)$  is a normalization constant and this distribution simply discounts states visited later in time.

#### Overview:

- On-policy algorithms: REINFORCE, REINFORCE with baseline and actor-critic algorithms. These algorithms require sampling trajectories with the parameters at each iteration and *then* making updates to the policy.
- Off-policy algorithms: Off-policy actor-critic, SAC, etc. These algorithms collect trajectories using a behavior policy which are then used to update potentially different policies.

## 2.1 Deriving the Policy Gradient

In this note, we will cover episodic tasks. Let  $V(\theta) = V_{\pi_{\theta}}(s_0)$ , where  $s_0$  is the starting state (which we consider to be fixed for simplicity) and the dependency on  $\theta$  specifies that the value depends on the policy  $\pi_{\theta}$ . Policy  $\pi_{\theta}$  can be any distribution. For example, we may use a Gaussian policy and write  $\pi_{\theta}(a|s) = \mathcal{N}(f_{\text{neural network}}^{\theta}(s), \Sigma)$ .

Now, we want to maximize  $V(\theta)$ :

$$V(\theta) = V_{\pi_{\theta}}(s_0)$$

$$= \sum_{a} \pi_{\theta}(a|s_0) Q_{\pi_{\theta}}(s_0, a)$$

$$= \sum_{\tau} P_{\theta}(\tau) R(\tau)$$

where  $Q_{\pi_{\theta}}(s_0, a)$  is the expected reward attained under the policy  $\pi_{\theta}$  after taking action a from state  $s_0$ .  $P_{\theta}(\tau)$  is the probability of trajectory  $\tau = (s_0, a_0, r_0, s_1, ..., s_{T-1}, a_{T-1}, r_{T-1}, s_T)$  under policy  $\pi_{\theta}$  and  $R(\tau)$  is the total reward from trajectory  $\tau$ .

**Lemma 5.**  $\nabla_{\theta}V(\theta) = \sum_{\tau} R(\tau)P_{\theta}(\tau)\nabla_{\theta}\log(P_{\theta}(\tau))$ 

Proof.

$$\begin{split} \nabla_{\theta} V(\theta) &= \nabla_{\theta} \sum_{\tau} P_{\theta}(\tau) R(\tau) \\ &= \sum_{\tau} R(\tau) \nabla_{\theta} P_{\theta}(\tau) \\ &= \sum_{\tau} R(\tau) \frac{P_{\theta}(\tau)}{P_{\theta}(\tau)} \nabla_{\theta} P_{\theta}(\tau) \\ &= \sum_{\tau} R(\tau) \frac{P_{\theta}(\tau)}{P_{\theta}(\tau)} \nabla_{\theta} P_{\theta}(\tau) \\ &= \sum_{\tau} R(\tau) P_{\theta}(\tau) \nabla_{\theta} \log(P_{\theta}(\tau)) \end{split}$$

Now, using Lemma 5, we see that

$$\nabla_{\theta} V(\theta) = \mathbb{E}_{P_{\theta}}[R(\tau)\nabla_{\theta}\log(P_{\theta}(\tau))].$$

We can also get an approximation for our update rule:

$$\nabla_{\theta} V(\theta) \approx \frac{1}{m} \sum_{i=1}^{m} R(\tau^{(i)}) \nabla_{\theta} \log(P_{\theta}(\tau^{(i)})).$$

However, we still don't know how to compute the gradient of the log-probability. For that, we need the following lemma:

Lemma 6. 
$$\nabla_{\theta} \log(P_{\theta}(\tau)) = \sum_{t=0}^{T-1} \nabla_{\theta} \log \pi_{\theta}(a_t|s_t)$$

Proof.

$$\nabla_{\theta} \log (P_{\theta}(\tau)) = \nabla_{\theta} \log \left( \rho(s_0) \prod_{t=0}^{T-1} \pi_{\theta}(a_t | s_t) P(s_{t+1} | s_t, a_t) \right)$$

$$= \nabla_{\theta} \log (\rho(s_0)) + \sum_{t=0}^{T-1} \log \pi_{\theta}(a_t | s_t) + \log P(s_{t+1} | s_t, a_t)$$

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

With Lemma 6, we get the following tractable update rule:

$$\nabla_{\theta} V(\theta) = \mathbb{E}_{\tau \sim P_{\theta}(\tau)} \left[ \left( \sum_{t=0}^{T} \nabla_{\theta} \log \pi_{\theta}(a_{t}|s_{t}) \right) \left( \sum_{t=0}^{T} r(s_{t}, a_{t}) \right) \right].$$

We can easily compute this as long as we can take the derivative of  $\log \pi_{\theta}(a \mid s)$ .

### 2.2 Policy Gradient Theorem

We generalize this approach through the policy gradient theorem [1]. First, we consider an episodic task.

**Theorem 7.** (Policy Gradient Theorem (episodic case)) Suppose, our task is episodic. Furthermore, suppose, our start state is  $s_0$  for all trajectories. Then,

$$\nabla_{\theta} V(\theta) = \sum_{s} p^{\pi_{\theta}}(s) \sum_{a} Q_{\pi_{\theta}}(s, a) \nabla_{\theta} \pi_{\theta}(a|s)$$
$$= \mathbb{E}_{s \sim p^{\pi_{\theta}}(s), a \sim \pi_{\theta}(a|s)} \left[ Q_{\pi_{\theta}}(s, a) \nabla_{\theta} \log \pi_{\theta}(a|s) \right]$$

Proof.

$$\begin{split} \nabla_{\theta}V(\theta) &= \nabla_{\theta} \left( \sum_{a} \pi_{\theta}(a|s) q_{\pi_{\theta}}(s,a) \right) \\ &= \sum_{a} \left( \nabla_{\theta} \pi_{\theta}(a|s) \right) q_{\pi_{\theta}}(s,a) + \pi_{\theta}(a|s) \nabla_{\theta} q_{\pi_{\theta}}(a,s) \\ &= \sum_{a} \left( \nabla_{\theta} \pi_{\theta}(a|s) \right) q_{\pi_{\theta}}(s,a) + \pi_{\theta}(a|s) \nabla_{\theta} \left( \sum_{s',r} p(s',r|s,a) \left( r + \gamma V_{\pi_{\theta}}(s') \right) \right) \\ &= \sum_{a} \left( \nabla_{\theta} \pi_{\theta}(a|s) \right) q_{\pi_{\theta}}(s,a) + \pi_{\theta}(a|s) \left( \sum_{s',r} p(s',r|s,a) \gamma \cdot \nabla_{\theta} \left( V_{\pi_{\theta}}(s') \right) \right) \\ &= \sum_{a} \nabla_{\theta} \pi_{\theta}(a|s) q_{\pi_{\theta}}(s,a) + \\ \pi_{\theta}(a|s) \sum_{s'} p(s'|s,a) \cdot \gamma \cdot \left( \sum_{a'} \left( \nabla_{\theta} \pi_{\theta}(a'|s') q_{\pi_{\theta}}(s',a') \right) + \pi_{\theta}(a'|s') \sum_{s''} P(s''|s',a') \gamma \cdot \nabla_{\theta} V_{\pi_{\theta}}(s'') \right) \\ &= \sum_{x \in S} \sum_{k=0}^{\infty} \mathbb{P}(s_{0} \to x, k, \pi_{\theta}) \gamma^{k} \sum_{a} \nabla_{\theta} \pi_{\theta}(a|x) q_{\pi_{\theta}}(x,a) \\ &= \sum_{s} p^{\pi_{\theta}}(s) \sum_{a} \nabla_{\theta} \pi_{\theta}(a|s) q_{\pi_{\theta}}(s,a) \end{split}$$

We derived the policy gradient theorem for the episodic setting. Now we suppose our task is no longer episodic. Again, let us assume that the initial state is fixed  $s_0$ . In this case, we define

$$V(\theta) = \lim_{h \to \infty} \frac{1}{h} \sum_{t=1}^{h} \mathbb{E}_{\pi_{\theta}}[R_t] = \lim_{t \to \infty} \mathbb{E}_{s, a \sim \pi_{\theta}}[R_t] = \sum_{s} \mu(s) \sum_{a} \pi_{\theta}(a|s) \sum_{s', r} P(s', r|s, a) r.$$

where  $\mu(s) := \lim_{t \to \infty} \mathbb{P}(s_t = s | a_{0:t} \sim \pi_{\theta})$ . We call  $\mu(s)$  the steady-state distribution i.e. we say that as time progresses, the probability of being in a state s converges. We assume that this distribution is independent of the initial state, which is called an ergodicity assumption. In particular, if we execute actions by sampling from the policy  $\pi_{\theta}$ , then we remain in this distribution:

$$\sum_{s} \mu(s) \sum_{a} \pi_{\theta}(a \mid s) p(s' \mid s, a) = \mu(s')$$

for all  $s' \in \mathcal{S}$ .

In the continuing case, we define

$$G_t := R_{t+1} - V(\theta) + R_{t+2} - V(\theta) + \cdots$$

and using this, we define,  $V_{\pi_{\theta}}(s) := \mathbb{E}_{\pi_{\theta}}[G_t|s_t = s], \ q_{\pi_{\theta}}(s, a) = \mathbb{E}_{\pi_{\theta}}[G_t|s_t = s, a_t = a].$ 

We prove the following theorem, which is analogous to the episodic setting:

**Theorem 8.** (Policy Gradient Theorem (continuous case)) Suppose, our task is continuous. Furthermore, suppose our start state is  $s_0$  for all trajectories. Then,

$$\nabla_{\theta} V(\theta) \propto \sum_{s} \mu(s) \sum_{a} q_{\pi_{\theta}}(s, a) \nabla_{\theta} \pi_{\theta}(a|s).$$

Proof.

$$\nabla_{\theta} V_{\pi_{\theta}}(s) = \nabla \left[ \sum_{a} \pi_{\theta}(a|s) q_{\pi_{\theta}}(s, a) \right]$$

$$= \sum_{a} \left[ \nabla_{\theta} \pi_{\theta}(a|s) q_{\pi_{\theta}}(s, a) + \pi_{\theta}(a|s) \nabla_{\theta} q_{\pi_{\theta}}(s, a) \right]$$

$$= \sum_{a} \left[ \nabla_{\theta} \pi_{\theta}(a|s) q_{\pi_{\theta}}(s, a) + \pi_{\theta}(a|s) \nabla_{\theta} \sum_{s', r} P(s', r|s, a) (r - V(\theta) + V_{\pi_{\theta}}(s')) \right]$$

$$= \sum_{a} \left[ \nabla_{\theta} \pi_{\theta}(a|s) q_{\pi_{\theta}}(s, a) + \pi_{\theta}(a|s) \left[ -\nabla_{\theta} V(\theta) + \sum_{s'} P(s'|s, a) \nabla_{\theta} V_{\pi_{\theta}}(s') \right] \right]$$

$$\nabla_{\theta} V(\theta) = \sum_{a} \left[ \nabla_{\theta} \pi_{\theta}(a|s) q_{\pi_{\theta}}(s, a) + \pi_{\theta}(a|s) \sum_{s'} P(s'|s, a) \nabla_{\theta} V_{\pi_{\theta}}(s') \right] - \nabla_{\theta} V_{\pi_{\theta}}(s)$$

Now, the left hand side is independent of s, so we can do a weighted sum over s (weighted by

 $\mu(s)$ :

$$\sum_{s} \mu(s) \nabla_{\theta} V(\theta) = \sum_{s} \mu(s) \left( \sum_{a} \left[ \nabla_{\theta} \pi_{\theta}(a|s) q_{\pi_{\theta}}(s, a) + \pi_{\theta}(a|s) \sum_{s'} P(s'|s, a) \nabla_{\theta} V_{\pi_{\theta}}(s') \right] - \nabla_{\theta} V_{\pi_{\theta}}(s) \right)$$

$$\nabla_{\theta} V(\theta) = \sum_{s} \mu(s) \sum_{a} \nabla_{\theta} \pi_{\theta}(a|s) q_{\pi_{\theta}}(s, a) +$$

$$\sum_{s} \mu(s) \sum_{a} \pi_{\theta}(a|s) \sum_{s'} P(s'|s, a) \nabla_{\theta} V_{\pi_{\theta}}(s') - \sum_{s} \mu(s) \nabla_{\theta} V_{\pi_{\theta}}(s)$$

$$= \sum_{s} \mu(s) \sum_{a} \nabla_{\theta} \pi_{\theta}(a|s) q_{\pi_{\theta}}(s, a) +$$

$$\sum_{s'} \sum_{s} \mu(s) \sum_{a} \pi_{\theta}(a|s) P(s'|s, a) \nabla_{\theta} V_{\pi_{\theta}}(s') - \sum_{s} \mu(s) \nabla_{\theta} V_{\pi_{\theta}}(s)$$

$$= \sum_{s} \mu(s) \sum_{a} \nabla_{\theta} \pi_{\theta}(a|s) q_{\pi_{\theta}}(s, a) + \sum_{s'} \mu(s') \nabla_{\theta} V_{\pi_{\theta}}(s') - \sum_{s} \mu(s) \nabla_{\theta} V_{\pi_{\theta}}(s)$$

$$= \sum_{s} \mu(s) \sum_{a} \pi_{\theta}(a|s) \nabla_{\theta} \pi_{\theta}(a|s)$$

$$= \sum_{s} \mu(s) \sum_{a} \pi_{\theta}(a|s) \nabla_{\theta} \pi_{\theta}(a|s)$$

$$= \sum_{s} \mu(s) \sum_{a} \pi_{\theta}(s, a) \nabla_{\theta} \pi_{\theta}(a|s)$$

where in the second last line we used the fact that  $\mu(s') = \sum_s \mu(s) \sum_a \pi_{\theta}(a|s) P(s'|s,a)$ .

This is a very interesting and powerful result - the fact that the same theory holds for both episodic and non-episodic tasks after the simple, understandable redefinition of  $G_t$ . In fact, the new way of seeing  $G_t$  is similar to the introduction of baselines in methods like REINFORCE.

#### 2.3 REINFORCE

Using our derivation, we have our first policy gradient algorithm. So far, we have:

$$\nabla_{\theta} V(\theta) = \mathbb{E}_{\tau \sim P_{\theta}(\tau)} \left[ \left( \sum_{t=0}^{T} \nabla_{\theta} \log \pi_{\theta}(a_{t}|s_{t}) \right) \left( \sum_{t'=0}^{T} r(s_{t'}, a_{t'}) \right) \right].$$

REINFORCE is an on-policy algorithm that approximates this by sampling multiple trajectories rolled out by policy  $\pi_{\theta}$  and then letting:

$$\nabla_{\theta} V(\theta) \approx \frac{1}{m} \sum_{i=1}^{m} \left( \sum_{t=0}^{T} \nabla_{\theta} \log \pi_{\theta}(a_{i,t}|s_{i,t}) \right) \left( \sum_{t'=0}^{T} r(s_{i,t'}, a_{i,t'}) \right)$$

Intuitive interpretation: One way to interpret this update rule is to note that we are maximizing the log-likelihood of each trajectory sampled - except we are weighing them by their

returns. In other words, if a trajectory yields higher returns, we are increasing the log-likelihood of that with a larger weight than one that yields lower returns.

#### Problems with REINFORCE:

- 1. Since this is an on-policy method, we require sampling multiple trajectories for each update to the policy.
- 2. The algorithm has high variance since the trajectory samples are often quite noisy (especially in most real-world environments). More precisely,  $\sum_{t'=1}^{T} r(s_{i,t'}, a_{i,t'})$  has high variance. As such, REINFORCE is a quite slow algorithm in most cases.

We will next introduce a couple of algorithms that are aimed towards solving these issues.

#### 2.4 REINFORCE using causality

The update rule we derived so far is

$$\nabla_{\theta} V(\theta) \approx \frac{1}{m} \sum_{i=1}^{m} \left( \sum_{t=0}^{T} \nabla_{\theta} \log \pi_{\theta}(a_{i,t}|s_{i,t}) \right) \left( \sum_{t'=0}^{T} r(s_{i,t'}, a_{i,t'}) \right).$$

Recall the intuition we provided in the previous section: we are maximizing log probability of each action weighted by the "goodness" of the action i.e. the returns achieved by executing the action. Now, notice that the action at time t cannot affect the rewards at time t' < t. In other words, when we maximize the log-likelihood of taking a particular action  $a_{i,t}$  from a state  $s_{i,t}$ , should we really weigh it by the reward attained from the entire trajectory? Intuitively, it makes more sense to weigh it by the rewards attained from that time t onward in the trajectory i since only the rewards attained after executing  $a_{i,t}$  gives us a signal for how good the action is. With this in mind, we have the following modification:

$$\nabla_{\theta} V(\theta) \approx \frac{1}{m} \sum_{i=1}^{m} \left( \sum_{t=0}^{T} \nabla_{\theta} \log \pi_{\theta}(a_{i,t}|s_{i,t}) \right) \left( \sum_{t'=t}^{T} r(s_{i,t'}, a_{i,t'}) \right).$$

The term  $\sum_{t'=t}^{T} r(s_{i,t'}, a_{i,t'})$  is called reward-to-go. In other words, we are using the "reward to go" from time t.

```
Algorithm: REINFORCE (with causality)
  1: Initialize policy parameters \theta
  2: for iteration = 1, 2, \ldots do
            Collect a set of trajectories \{\tau^i\} by running the policy \pi_{\theta}(a_t|s_t)
            for each trajectory \tau^i do
  4:
                 for each timestep t in \tau^i do Compute return: G_t^i = \sum_{t'=t}^T r(s_{t'}^i, a_{t'}^i)
  5:
  6:
                  end for
  7:
            end for
  8:
            Update the policy parameters:
  9:
                  \nabla_{\theta} V(\theta) \approx \sum_{i} \sum_{t} \nabla_{\theta} \log \pi_{\theta}(a_{t}^{i} | s_{t}^{i}) G_{t}^{i}
\theta \leftarrow \theta + \alpha \nabla_{\theta} V(\theta)
10: end for
```

Intuitive interpretation: we are updating the policy parameters by taking a step in the direction of  $\nabla_{\theta}V(\theta) \approx \sum_{i} \sum_{t} (\nabla_{\theta} \log \pi_{\theta}) G_{t}^{i}$ . Focus on the term  $\sum_{i} \sum_{t} (\nabla_{\theta} \log \pi_{\theta})$ . A step in this direction is essentially maximizing the probability of  $A = a \mid s$  under  $\pi_{\theta}$ , which is what maximum likelihood estimation does! Since this is scaled by  $G_{t}^{i}$ , it takes a step in a direction that is closed aligned with high  $G_{t}^{i}$  actions i.e., actions that we expect to give higher returns.

Here is a more formal derivation of this causality idea:

So far, in the derivation of the policy gradient, we assumed we wanted to maximize  $\mathbb{E}_{\pi_{\theta}}[R(\tau)]$ . What if we instead choose to maximize the reward at one time-step,  $r_t$ , only? Following the same steps of derivation, we would arrive at

$$\nabla_{\theta} \mathbb{E}_{\pi_{\theta}}[r_t] = \mathbb{E}_{\pi_{\theta}} \left[ \sum_{t'=0}^{t} \nabla_{\theta} \log \pi_{\theta}(a_{t'} \mid s_{t'}) r_t \right].$$

Now, we can take the sum of rewards over time  $t' = 0, \dots, T$  to get

$$\nabla_{\theta} \mathbb{E}_{\pi_{\theta}}[r_t] = \mathbb{E}_{\pi_{\theta}} \left[ \sum_{t=0}^{T} r_t \sum_{t'=0}^{t} \nabla_{\theta} \log \pi_{\theta}(a_{t'} \mid s_{t'}) \right]$$
$$= \mathbb{E}_{\pi_{\theta}} \left[ \sum_{t=0}^{T} \nabla_{\theta} \log \pi_{\theta}(a_t \mid s_t) \sum_{t'=t}^{T} r_{t'} \right].$$

#### 2.5 REINFORCE with baseline

To further reduce variance, we introduce a baseline:

$$\nabla_{\theta} V(\theta) \approx \frac{1}{m} \sum_{i=1}^{m} \left( \sum_{t=0}^{T} \nabla_{\theta} \log \pi_{\theta}(a_{i,t}|s_{i,t}) \right) \left( \sum_{t'=0}^{T} r(s_{i,t'}, a_{i,t'}) - b(s_{i,t'}) \right).$$

where b is any arbitrary function as long as it does not depend on  $a_t$ .

Intuitive explanation: in REINFORCE, we sample trajectories and maximize the log probability of actions based on how good they were. Subtracting an appropriate baseline (we will discuss what are appropriate baselines soon) is equivalent to asking "Are the returns from this action better than expected?" We choose a baseline that gives us a sense of  $V_{\pi_{\theta}}(s_{i,t'})$  because that is the expected returns from the state.

What baseline should we choose? We usually choose baselines that are either constant or depends only on  $s_{i,t'}$  but not on  $a_{i,a'}$ .

- 1. We usually select  $b(s) = \mathbb{E}_{\tau \sim \pi_{\theta}}[r(\tau) \mid s_0 = s]$ .
- 2. We could also use a learned state value function parametrized by  $\phi$ ,

$$v_{\phi}(s_t) =: b(s_t).$$

Note that either choice gives is an unbiased modification of the original update rule derived from the policy gradient theorem:

**Proposition 9.** Subtracting the baseline b (that does not depend on action) is unbiased in expectation i.e.,

$$\nabla_{\theta} V(\theta) = \mathbb{E}_{s \sim p^{\pi_{\theta}}, a \sim \pi_{\theta}(\cdot | s)} \left[ \left( \nabla_{\theta} \log \pi_{\theta}(a | s) \right) \left( Q_{\pi_{\theta}}(s, a) - b(s) \right) \right]$$

where  $\nabla_{\theta}V(\theta)$  is computed as in the policy gradient theorem (theorem 7).

Proof. We show

$$\mathbb{E}_{\tau \sim P_{\theta}(\tau)} \left[ \left( \sum_{t=0}^{T} (\nabla_{\theta} \log \pi_{\theta}(a_{t}|s_{t})) V^{\pi_{\theta}}(s_{t}) \right) \right] = 0.$$

$$\mathbb{E}_{\tau \sim P_{\theta}(\tau)} \left[ \left( \sum_{t=0}^{T} (\nabla_{\theta} \log \pi_{\theta}(a_{t}|s_{t})) V^{\pi_{\theta}}(s_{t}) \right) \right]$$

$$= \sum_{t=0}^{T} \mathbb{E}_{\tau \sim P_{\theta}(\tau)} \left[ (\nabla_{\theta} \log \pi_{\theta}(a_{t}|s_{t})) V^{\pi_{\theta}}(s_{t}) \right]$$

$$= \sum_{t=0}^{T} \sum_{s_{t}} \mathbb{P}(s_{0} \to s_{t}, t, \pi_{\theta}) \sum_{a_{t}} \pi_{\theta}(a_{t} \mid s_{t}) (\nabla_{\theta} \log \pi_{\theta}(a_{t}|s_{t})) V^{\pi_{\theta}}(s_{t})$$

$$= \sum_{t=0}^{T} \sum_{s_{t}} \mathbb{P}(s_{0} \to s_{t}, t, \pi_{\theta}) V^{\pi_{\theta}}(s_{t}) \sum_{a_{t}} \pi_{\theta}(a_{t} \mid s_{t}) (\nabla_{\theta} \log \pi_{\theta}(a_{t}|s_{t}))$$

$$= \sum_{t=0}^{T} \sum_{s_{t}} \mathbb{P}(s_{0} \to s_{t}, t, \pi_{\theta}) V^{\pi_{\theta}}(s_{t}) \sum_{a_{t}} \nabla_{\theta} \pi_{\theta}(a_{t} \mid s_{t})$$

$$= \sum_{t=0}^{T} \sum_{s_{t}} \mathbb{P}(s_{0} \to s_{t}, t, \pi_{\theta}) V^{\pi_{\theta}}(s_{t}) \nabla_{\theta} \left( \sum_{a_{t}} \pi_{\theta}(a_{t} \mid s_{t}) \right)$$

$$= \sum_{t=0}^{T} \sum_{s_{t}} \mathbb{P}(s_{0} \to s_{t}, t, \pi_{\theta}) V^{\pi_{\theta}}(s_{t}) \nabla_{\theta} (1)$$

$$= \sum_{t=0}^{T} \sum_{s_{t}} \mathbb{P}(s_{0} \to s_{t}, t, \pi_{\theta}) V^{\pi_{\theta}}(s_{t}) \cdot 0$$

$$= 0.$$

We can actually find the baseline that reduces the variance the most in a principled manner:

**Proposition 10.**  $b = \frac{\mathbb{E}[g(\tau)^2 r(\tau)]}{\mathbb{E}[g(\tau)^2]}$  minimizes the variance:

$$\operatorname{Var} := \mathbb{E}_{\tau \sim P_{\theta}(\tau)} \left[ (\nabla_{\theta} \log P_{\theta}(\tau)(r(\tau) - b))^{2} \right] - \mathbb{E}_{\tau \sim P_{\theta}(\tau)} \left[ \nabla_{\theta} \log P_{\theta}(\tau)(r(\tau) - b) \right]^{2}.$$

Here  $g(\tau)$  is the gradient  $\nabla_{\theta} \log P_{\theta}(\tau)$ .

*Proof.* Take the derivative with respect to the baseline b and, after a little bit of algebra, you get the desired expression.

In other words, the optimal baseline is the expected reward but weighted by the magnitude of our gradients. In practice, we end up just using the expected reward as the baseline.

```
Algorithm: REINFORCE with baseline
  1: Initialize policy parameters \theta
  2: for iteration = 1, 2, \ldots do
                Collect a set of trajectories \{\tau^i\}_{i=1}^N by running the policy \pi_{\theta}(a_t|s_t)
  3:
                for each trajectory \tau^i do
                       \begin{array}{l} \textbf{for each timestep } t \text{ in } \tau^i \textbf{ do} \\ \text{Compute return: } G_t^i = \sum_{t'=t}^T r(s_{t'}^i, a_{t'}^i) \end{array}
  5:
  6:
                       end for
  7:
                end for
  8:
               Compute b = \frac{1}{N} \sum_{i=1}^{N} r(\tau^{i})

Update the policy parameters:

\nabla_{\theta} V(\theta) \approx \sum_{i} \sum_{t} \nabla_{\theta} \log \pi_{\theta}(a_{t}^{i} | s_{t}^{i}) (G_{t}^{i} - b)

\theta \leftarrow \theta + \alpha \nabla_{\theta} V(\theta)
  9:
 10:
11: end for
```

```
REINFORCE with Baseline using learned value-function baseline
```

**Input:** a differentiable policy parameterization  $\pi(a \mid s, \theta)$ 

**Input:** a differentiable state-value function parameterization  $\hat{v}(s, \mathbf{w})$ 

Algorithm parameters: step sizes  $\alpha^{\theta} > 0$ ,  $\alpha^{\mathbf{w}} > 0$ 

Initialize policy parameter  $\theta \in \mathbb{R}^{d'}$  and state-value weights  $\mathbf{w} \in \mathbb{R}^{d}$  (e.g., to 0)

Loop forever (for each episode):

- Generate an episode  $S_0, A_0, R_1, \ldots, S_{T-1}, A_{T-1}, R_T$ , following  $\pi(\cdot \mid \cdot, \boldsymbol{\theta})$
- Loop for each step of the episode t = 0, 1, ..., T 1:

$$-G \leftarrow \sum_{k=t+1}^{T} \gamma^{k-t-1} R_k$$

$$-\delta \leftarrow G - \hat{v}(S_t, \mathbf{w})$$

$$-\mathbf{w} \leftarrow \mathbf{w} + \alpha^{\mathbf{w}} \delta \nabla \hat{v}(S_t, \mathbf{w})$$

$$-\theta \leftarrow \theta + \alpha^{\theta} \gamma^t \delta \nabla \ln \pi (A_t \mid S_t, \theta)$$
(G<sub>t</sub>)

#### 2.6 On-Policy Actor-Critic Methods

Let us consider the baseline  $b(s_{i,t'}) = V_{\pi_{\theta}}(s_{i,t'})$  i.e. the true state-value function under policy  $\pi_{\theta}$ . We will see how to get this value function soon. We also replace the reward to go with the state-action value function for taking  $a_{i,t'}$  from  $s_{i,t'}$  (as seen in the sampled trajectory) i.e.  $Q_{\pi_{\theta}}(s_{i,t'})$ . Then, note that the factor multiplying the gradient of the log of our policy becomes  $Q_{\pi_{\theta}}(s_{i,t'}) - V_{\pi_{\theta}}(s_{i,t'}) = r(s_{i,t'}) + \gamma \cdot \mathbb{E}_{s_{t'+1} \sim P(\cdot|s_{i,t'},a_{i,t'})}[V_{\pi_{\theta}}(s_{t'+1})] = A^{\pi_{\theta}}(s_{i,t'},a_{i,t'})$ . This is the main idea in this section.

Actor-Critic methods replace the reward to go  $\sum_{t'=t}^{T} r(s_{i,t'}, a_{i,t'})$  with  $r(s_{i,t}, a_{i,t}) + \gamma V_{\phi}^{\pi_{\theta}}(s_{i,t+1})$ .

As for the baseline, we use  $V_{\theta}(s_{i,t})$ . Then, we can replace  $\sum_{t'=t}^{T} r(s_{i,t'}, a_{i,t'})$  in REINFORCE with the advantage function  $A^{\pi_{\theta}}(s_{i,t'}, a_{i,t'}) \approx r(s_{i,t}, a_{i,t}) + \gamma V_{\phi}^{\pi_{\theta}}(s_{i,t+1}) - V_{\phi}^{\pi_{\theta}}(s_{i,t})$ . Note that here we removed the expectation over the next state  $s_{i,t+1}$  with just a single sample estimate from the trajectory i. This can be a poor estimate. In general, the better the estimate of the advantage, the lower the variance.

Actor-critic methods use a learned value function  $V_{\phi}^{\pi_{\theta}}(s_t)$ . This is trained using supervised regression. Suppose that our training set (using the rollouts by policy  $\pi_{\theta}$ ) is of the form  $\{(s_{i,t}, \sum_{t'=t}^T r(s_{i,t'}, a_{i,t'}))\}$ . Then, we train via minimizing

$$\frac{1}{2} \sum_{i} \sum_{t} \left\| V_{\phi}^{\pi_{\theta}}(s_{i,t}) - \left( \sum_{t'=t}^{T} r(s_{i,t'}, a_{i,t'}) \right) \right\|^{2}.$$

Alternatively, we can also train this by using a boostrapped estimate of the target:

$$\frac{1}{2} \sum_{i} \sum_{t} \left| \left| V_{\phi}^{\pi_{\theta}}(s_{i,t}) - \left( r(s_{i,t}, a_{i,t}) + V_{\phi}^{\pi_{\theta}}(s_{i,t+1}) \right) \right| \right|^{2}.$$

## One-step Actor-Critic (episodic), for estimating $\pi_{\theta} \approx \pi_*$

**Input:** a differentiable policy parameterization  $\pi(a \mid s, \theta)$ 

**Input:** a differentiable state-value function parameterization  $\hat{v}(s, \mathbf{w})$ 

Parameters: step sizes  $\alpha^{\theta} > 0$ ,  $\alpha^{\mathbf{w}} > 0$ Initialize policy parameter  $\boldsymbol{\theta} \in \mathbb{R}^{d'}$  and state-value weights  $\mathbf{w} \in \mathbb{R}^{d}$  (e.g., to  $\mathbf{0}$ )

Loop forever (for each episode):

- Initialize S (first state of episode)
- $I \leftarrow 1$
- Loop while S is not terminal (for each time step):
  - $-A \sim \pi(\cdot \mid S, \boldsymbol{\theta})$
  - Take action A, observe S', R
  - $-\delta \leftarrow R + \gamma \hat{v}(S', \mathbf{w}) \hat{v}(S, \mathbf{w})$

(if S' is terminal, then  $\hat{v}(S', \mathbf{w}) \doteq 0$ )

- $-\mathbf{w} \leftarrow \mathbf{w} + \alpha^{\mathbf{w}} \delta \nabla \hat{v}(S, \mathbf{w})$
- $-\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \alpha^{\theta} I \delta \nabla \ln \pi (A \mid S, \boldsymbol{\theta})$
- $-I \leftarrow \gamma I$
- $-S \leftarrow S'$

#### 2.7 Making inroads to off-policy policy gradient

Suppose, we collected trajectories using policy  $\pi_{\theta}$  and we know the returns from these trajectories. Can we use them to make updates to a different policy  $\pi_{\theta'}$ ?

Given policy  $\pi_{\theta'}$ , we want to maximize  $V(\theta') = \mathbb{E}_{\tau \sim p_{\theta'}(\tau)}[r(\tau)]$ . Using importance-sampling, we can write:

$$V(\theta) = \mathbb{E}_{\tau \sim p_{\theta}} \left[ \frac{p_{\theta'}(\tau)}{p_{\theta}(\tau)} r(\tau) \right]$$
$$\nabla_{\theta} V(\theta) = \mathbb{E}_{\tau \sim p_{\theta}} \left[ \frac{p_{\theta'}(\tau)}{p_{\theta}(\tau)} \nabla_{\theta'} \log(p_{\theta'}(\tau)) r(\tau) \right]$$

Then, using the full expression for the probability of any trajectory, we get

$$\nabla_{\theta} V(\theta) = \mathbb{E}_{\tau \sim p_{\theta}} \left[ \prod_{t=1}^{T} \frac{\pi_{\theta'}(a_{t} \mid s_{t})}{\pi_{\theta}(a_{t} \mid s_{t})} \left( \sum_{t=1}^{T} \nabla_{\theta'} \log \pi_{\theta'}(a_{t} \mid s_{t}) \right) r(\tau) \right]$$

$$= \mathbb{E}_{\tau \sim p_{\theta}} \left[ \prod_{t=1}^{T} \frac{\pi_{\theta'}(a_{t} \mid s_{t})}{\pi_{\theta}(a_{t} \mid s_{t})} \left( \sum_{t=1}^{T} \nabla_{\theta'} \log \pi_{\theta'}(a_{t} \mid s_{t}) \right) \left( \sum_{t=1}^{T} r(s_{t}, a_{t}) \right) \right]$$

Rewrite this:

$$\nabla_{\theta} V(\theta) = \mathbb{E}_{\tau \sim p_{\theta}} \left[ \left( \sum_{t=1}^{T} \nabla_{\theta'} \log \pi_{\theta'}(a_{t} \mid s_{t}) \right) \left( \prod_{t'=1}^{t} \frac{\pi_{\theta'}(a_{t'} \mid s_{t'})}{\pi_{\theta}(a_{t'} \mid s_{t'})} \right) \left( \sum_{t'=t}^{T} r(s_{t'}, a_{t'}) \left( \prod_{t''=t}^{t'} \frac{\pi_{\theta'}(a_{t''} \mid s_{t''})}{\pi_{\theta}(a_{t''} \mid s_{t''})} \right) \right) \right]$$

And then we get, using causality:

$$\nabla_{\theta} V(\theta) = \mathbb{E}_{\tau \sim p_{\theta}} \left[ \left( \sum_{t=1}^{T} \nabla_{\theta'} \log \pi_{\theta'}(a_t \mid s_t) \right) \left( \prod_{t'=1}^{t} \frac{\pi_{\theta'}(a_{t'} \mid s_{t'})}{\pi_{\theta}(a_{t'} \mid s_{t'})} \right) \left( \sum_{t'=t}^{T} r(s_{t'}, a_{t'}) \right) \right]$$

## 2.8 Off-Policy Actor-Critic (OffPAC)

This section is not really new - we just use importance sampling. The derivation will assume continuous state and action spaces. We want to estimate the policy gradient off-policy from trajectories sampled from a distinct behaviour policy  $\beta(a|s) \neq \pi_{\theta}(a|s)$ . In this setting, the performance objective is the value function of the target policy,  $\pi_{\theta}$ , averaged over the state distribution of the behaviour policy  $\beta(a|s)$ :

$$J_{\beta}(\pi_{\theta}) = \int_{\mathcal{S}} p^{\beta}(s) V^{\pi_{\theta}}(s) = \int_{\mathcal{S}} \int_{\mathcal{A}} p^{\beta}(s) \pi_{\theta}(a|s) Q^{\pi_{\theta}}(s,a) dads.$$

The policy gradient becomes (after approximating by dropping  $\nabla_{\theta} Q^{\pi_{\theta}}(s, a)$ ):

$$\nabla_{\theta} J_{\beta}(\pi_{\theta}) = \mathbb{E}_{s \sim p^{\beta}, a \sim \beta} \left[ \frac{\pi_{\theta}(a|s)}{\beta(a|s)} \nabla_{\theta} \log \pi_{\theta}(a|s) Q^{\pi_{\theta}}(s, a) \right].$$

OffPAC (Off-Policy Actor Critic) algorithm uses the behavior policy  $\beta(a|s)$  to generate trajectories. A critic estimates  $V^{\phi}(s) \approx V^{\pi_{\theta}}(s)$  off-policy by gradient temporal-difference learning. Instead of the unknown  $Q^{\pi_{\theta}}(s,a)$ , the temporal-difference error  $\delta_t = r_{t+1} + \gamma V^{\phi}(s_{t+1}) - V^{\phi}(s_t)$  is used.

#### 2.9 Performance Difference Lemma

We want to prove a few results that are building blocks for trust regional policy optimisation.

Firstly, note that the probability of sampling any particular trajectory  $\tau = (s_0, a_0, r_0, s_1, a_1, ...)$  is  $P_{\theta}(\tau) = \prod_{i=0}^{\infty} \pi_{\theta}(a_i|s_i) P(s_{i+1}|s_i, a_i)$ . The probability of sampling a particular trajectory  $\tau$  such that  $s_t = s$  is  $P_{\theta}(s_t = s) = \sum_{a_0} \sum_{s_1} ... \sum_{s_{t-1}} \sum_{a_{t-1}} \left( \prod_{i=1}^{T-2} \pi_{\theta}(a_i|s_i) P(s_{i+1}|s_i, a_i) \right) \pi_{\theta}(a_{t-1}|s_{t-1}) P(s_t = s \mid s_{t-1}, a_{t-1})$ .

Let the distribution over all states induced by  $\pi_{\theta}$  be:

$$d^{\pi_{\theta}}(s) := (1 - \gamma) \sum_{t=0}^{\infty} \gamma^{t} P_{\theta}(s_{t} = s).$$

The factor  $(1 - \gamma)$  is a normalization constant and this distribution simply discounts states visited later in time.

Lemma 11. 
$$\mathbb{E}_{\tau \sim P_{\theta}}\left[\sum_{t=0}^{\infty} \gamma^t f(s_t, a_t)\right] = \frac{1}{1-\gamma} \mathbb{E}_{s \sim d^{\pi_{\theta}}}\left[\mathbb{E}_{a \sim \pi_{\theta}(\cdot \mid s)}\left[f(s, a)\right]\right]$$

Proof.

$$\mathbb{E}_{\tau \sim P_{\theta}} \left[ \sum_{t=0}^{\infty} \gamma^{t} f(s_{t}, a_{t}) \right]$$

$$\begin{split} &= \sum_{\tau} P_{\theta}(\tau) \sum_{t=0}^{\infty} \gamma^{t} f(s_{t}, a_{t}) \\ &= \sum_{\tau} \prod_{i=0}^{\infty} \pi_{\theta}(a_{i}|s_{i}) P(s_{i+1}|s_{i}, a_{i}) \sum_{t=0}^{\infty} \gamma^{t} f(s_{t}, a_{t}) \\ &= \sum_{a_{0}} \sum_{s_{1}} \sum_{a_{1}} \cdots \prod_{i=0}^{\infty} \pi(a_{i}|s_{i}) P(s_{i+1}|s_{i}, a_{i}) \sum_{t=0}^{\infty} \gamma^{t} f(s_{t}, a_{t}) \\ &= \sum_{a_{0}} \sum_{s_{1}} \sum_{a_{1}} \cdots \prod_{i=0}^{\infty} \pi(a_{i}|s_{i}) P(s_{i+1}|s_{i}, a_{i}) \sum_{t=0}^{\infty} \gamma^{t} f(s_{t}, a_{t}) \\ &= \sum_{a_{0}} \gamma^{t} \sum_{a_{0}} \sum_{s_{1}} \sum_{a_{1}} \cdots \sum_{s_{t}} \sum_{a_{t}} \sum_{s_{t+1}} \prod_{i=0}^{t} \pi_{\theta}(a_{i}|s_{i}) P(s_{i+1}|s_{i}, a_{i}) f(s_{t}, a_{t}) \\ &= \sum_{t=0}^{\infty} \gamma^{t} \sum_{s_{t+1}} (\cdots) f(s_{t}, a_{t}) \\ &= \sum_{t=0}^{\infty} \gamma^{t} \sum_{s_{t}} \sum_{a_{t}} \left( \sum_{a_{0}} \cdots \sum_{s_{t-1}} \sum_{a_{t-1}} \prod_{i=0}^{t-1} \pi_{\theta}(a_{i}|s_{i}) P(s_{i+1}|s_{i}, a_{i}) \right) \pi_{\theta}(a_{t}|s_{t}) f(s_{t}, a_{t}) \\ &= \sum_{t=0}^{\infty} \gamma^{t} \sum_{s_{1}} \sum_{a_{t}} P_{\theta}(s_{t}) \pi_{\theta}(a_{t}|s_{t}) f(s_{t}, a_{t}) \\ &= \sum_{t=0}^{\infty} \gamma^{t} \sum_{s_{1}} \sum_{a_{1}} P_{\theta}(s_{t}) \pi_{\theta}(a_{t}|s_{t}) f(s_{t}, a_{t}) \\ &= \frac{1}{1-\gamma} (1-\gamma) \sum_{t=0}^{\infty} \gamma^{t} \sum_{s_{t}} P_{\theta}(s_{t}) \mathbb{E}_{a \sim \pi_{\theta}} \left[ f(s_{t}, a) \right] \\ &= \frac{1}{1-\gamma} \mathbb{E}_{s \sim d^{\pi_{\theta}}} \left[ \mathbb{E}_{a \sim \pi_{\theta}} \left[ f(s_{t}, a) \right] \right] \end{split}$$

**Theorem 12.** (Performance Difference Lemma)

$$V_{\pi}(s_0) - V_{\pi'}(s_0) = \frac{1}{1 - \gamma} \mathbb{E}_{s \sim d^{\pi}} \left[ \mathbb{E}_{a \sim \pi(s)} \left[ A^{\pi'}(s, a) \right] \right]$$

where the advantage function is  $A^{\pi}(s, a) := q^{\pi}(s, a) - V^{\pi}(s)$ .

Proof.

$$\begin{split} &V_{\pi}(s_{0}) - V_{\pi'}(s_{0}) \\ &= \mathbb{E}_{\tau \sim P^{\pi}} \left[ \sum_{t=0}^{\infty} \gamma^{t} R(s_{t}, a_{t}) \right] + \mathbb{E}_{\tau \sim P^{\pi}} \left[ \sum_{t=0}^{\infty} \gamma^{t+1} V_{\pi'}(s_{t+1}) \right] - \mathbb{E}_{\tau \sim P^{\pi}} \left[ \sum_{t=0}^{\infty} \gamma^{t+1} V_{\pi'}(s_{t+1}) \right] - V_{\pi'}(s_{0}) \\ &= \mathbb{E}_{\tau \sim P^{\pi}} \left[ \sum_{t=0}^{\infty} \gamma^{t} (R(s_{t}, a_{t}) + \gamma V_{\pi'}(s_{t+1})) - \sum_{t=0}^{\infty} \gamma^{t+1} V_{\pi'}(s_{t+1}) - V_{\pi'}(s_{0}) \right] \end{split}$$

Now, we expand the first term:

$$\mathbb{E}_{\tau \sim P^{\pi}} \left[ \sum_{t=0}^{\infty} \gamma^{t} \left( R(s_{t}, a_{t}) + \gamma V_{\pi'}(s_{t+1}) \right) \right]$$

$$= \sum_{t=0}^{\infty} \gamma^{t} \mathbb{E}_{\tau \sim P^{\pi}} \left[ R(s_{t}, a_{t}) + \gamma V^{\pi'}(s_{t+1}) \right]$$

$$= \sum_{t=0}^{\infty} \gamma^{t} \mathbb{E}_{s_{t} \sim P^{\pi}} \left[ \mathbb{E}_{a_{t} \sim P^{\pi}} \left[ \mathbb{E}_{s_{t+1} \sim P^{\pi}} \left[ R(s, a) + \gamma V^{\pi'}(s_{t+1}) \mid s = s_{t}, a = a_{t} \right] \mid s = s_{t} \right] \right]$$

$$= \sum_{t=0}^{\infty} \gamma^{t} \mathbb{E}_{s_{t}, a_{t} \sim P^{\pi}} \left[ R(s, a) + \gamma \sum_{s_{t+1}} P(s_{t+1} \mid s_{t}, a_{t}) V^{\pi'}(s_{t+1}) \mid s = s_{t}, a = a_{t} \right]$$

$$= \sum_{t=0}^{\infty} \gamma^{t} \mathbb{E}_{\tau \sim P^{\pi}} \left[ Q^{\pi'}(s, a) \mid s = s_{t}, a = a_{t} \right]$$

$$= \mathbb{E}_{\tau \sim P^{\pi}} \left[ \sum_{t=0}^{\infty} \gamma^{t} Q^{\pi'}(s_{t}, a_{t}) \right]$$

Therefore, we get

$$V^{\pi}(s_0) - V^{\pi'}(s_0) = \mathbb{E}_{\tau \sim P^{\pi}} \left[ \sum_{t=0}^{\infty} \gamma^t \left( Q^{\pi'}(s_t, a_t) - V^{\pi'}(s_t) \right) \right]$$
$$= \mathbb{E}_{\tau \sim P^{\pi}} \left[ \sum_{t=0}^{\infty} \gamma^t A^{\pi'}(s_t, a_t) \right]$$
$$= \frac{1}{1 - \gamma} \mathbb{E}_{s \sim d^{\pi}} \left[ \mathbb{E}_{a \sim \pi} \left[ A^{\pi'}(s, a) \right] \right]$$

Sometimes, as in [2], this lemma has the following equivalent expression:

**Proposition 13.** (Performance Difference Lemma (2)) Given two policies  $\pi$  and  $\pi'$ ,

$$V(\pi') - V(\pi) = \mathbb{E}_{\tau \sim \pi'} \left[ \sum_{t=0}^{\infty} \gamma^t A_{\pi}(s_t, a_t) \right].$$

Proof. We write:

$$A_{\pi}(s, a) = \mathbb{E}_{s' \in P(s'|s, a)} \left[ r(s, a) + \gamma V_{\pi}(s') - V_{\pi}(s) \right].$$

Then.

$$\begin{split} \mathbb{E}_{\pi'} \left[ \sum_{t=0}^{\infty} \gamma^t A_{\pi}(s_t, a_t) \right] &= \mathbb{E}_{\pi'} \left[ \sum_{t=0}^{\infty} \gamma^t \left( r(s_t, a_t) + \gamma V_{\pi}(s_{t+1}) - V_{\pi}(s_t) \right) \right] \\ &= \mathbb{E}_{\pi'} \left[ -V_{\pi}(s_0) + \sum_{t=0}^{\infty} \gamma^t \left( r(s_t, a_t) \right) \right] \\ &= -\mathbb{E}_{s_0 \sim \rho_0} [V_{\pi}(s_0)] + \mathbb{E}_{\pi'} [\sum_{t=0}^{\infty} \gamma^t r_t] \\ &= -V(\pi) + V(\pi'). \end{split}$$

## 2.10 Covariant/natural policy gradient

So far, our update rules were aimed towards computing

$$\theta \leftarrow \theta + \alpha \nabla_{\theta} V(\theta)$$

to update the policy  $\pi_{\theta}(a \mid s)$ . However, controlling the learning rate to maximize  $V(\theta)$  is non-trivial. Some parameters of your policy ultimately end up affecting  $V(\theta)$  more than others and choosing one constant  $\alpha$  that controls the learning rate for all the parameters is difficult. We would want to have higher learning rates for parameters that do not change the policy very much and smaller learning rates for those that do.

Now, notice that using a first-order Taylor expansion, we can write:

$$\arg \max_{\theta'} V(\theta') \approx \arg \max_{\theta'} V(\theta) + (\theta' - \theta)^T \nabla_{\theta} V(\theta).$$

So, we aim to solve  $\arg \max_{\theta'} (\theta' - \theta)^T \nabla_{\theta} V(\theta)$  such that  $||\theta' - \theta|| \leq \epsilon$  (so that the Taylor approximation is valid). We can reframe this problem in the policy space: we aim to solve  $\arg \max_{\theta'} (\theta' - \theta)^T \nabla_{\theta} V(\theta)$  such that  $D(\pi_{\theta'} || \pi_{\theta}) \leq \epsilon$  where D is a divergence-measure [3].

We can choose D to be the KL-divergence. In this case, we can approximate (using the second-order Taylor approximation)  $D_{KL}(\pi_{\theta'} \mid\mid \pi_{\theta}) \approx (\theta' - \theta)^T F(\theta' - \theta)$  where F is the Fisher information matrix, i.e.  $F = \mathbb{E}_{\pi_{\theta}}[(\nabla_{\theta} \log \pi_{\theta}(a \mid s))(\nabla_{\theta} \log \pi_{\theta}(a \mid s))^T]$ . Then, the problem becomes:  $\arg \max_{\theta'} (\theta' - \theta)^T \nabla_{\theta} V(\theta)$  such that  $||\theta' - \theta||_F^2 \leq \epsilon$ . Then, the update rule becomes

$$\theta \leftarrow \theta + \alpha F^{-1} \nabla_{\theta} V(\theta)$$

## 2.11 Trust Region Policy Optimization (TRPO)

In this section, we discuss the building blocks of TRPO.

Let 
$$V(\pi) = \mathbb{E}_{\pi}[\sum_{t=0}^{\infty} \gamma^{t} r_{t}]$$
. Recall:  $Q_{\pi}(s_{t}, a_{t}) = \mathbb{E}_{\pi}[\sum_{l=0}^{\infty} \gamma^{l} r_{t+l} \mid s_{t}, a_{t}], V_{\pi}(s_{t}) = \mathbb{E}_{\pi}[\sum_{l=0}^{\infty} \gamma^{l} r_{t+l} \mid s_{t}]$  and  $A_{\pi}(s, a) = Q_{\pi}(s, a) - V_{\pi}(s)$  where  $a_{t} \sim \pi(a_{t} \mid s_{t})$ .

Recall the improper discounted state distribution  $p^{\pi}(s) = \sum_{k=0}^{\infty} \gamma^{k} \mathbb{P}(s_0 \to s, k, \pi)$ . Using this, we can write the performance difference lemma as:

$$V(\pi') - V(\pi) = \sum_{t=0}^{\infty} \sum_{s} P(s_t = s \mid \pi') \sum_{a} \pi'(a \mid s) \gamma^t A_{\pi}(s, a)$$
$$= \sum_{s} \sum_{t=0}^{\infty} \gamma^t P(s_t = s \mid \pi') \sum_{a} \pi'(a \mid s) A_{\pi}(s, a)$$
$$= \sum_{s} p^{\pi'}(s) \sum_{a} \pi'(a \mid s) A_{\pi}(s, a)$$

Note:  $V(\pi') - V(\pi) \ge 0$  if, at every state s, we have that  $\sum_a \pi'(a \mid s) A_{\pi}(s, a) \ge 0$ .

Now, the first building block of TRPO is the local approximation of this as

$$L_{\pi}(\pi') = V(\pi) + \sum_{s} p^{\pi}(s) \sum_{a} \pi'(a \mid s) A_{\pi}(s, a)$$

where we have replaced  $p^{\pi'}$  with  $p^{\pi'}$ . Note that when our policy  $\pi_{\theta}(a \mid s)$  is differentiable, then, for the parameters  $\theta_0$ , we have that  $L_{\pi_{\theta_0}}(\pi_{\theta_0}) = V(\pi_{\theta_0})$  and  $\nabla_{\theta}L_{\pi_{\theta_0}}(\pi_{\theta})|_{\theta=\theta_0} = \nabla_{\theta}V(\pi_{\theta})|_{\theta=\theta_0}$ . Therefore, if the update  $\pi_{\theta_0} \to \pi'$  is small enough such that  $L_{\pi_{\theta_0}}(\pi_{\theta_0})$  improves, then we see an improvement in the value V as well. However, controlling the learning rate that ensures this is difficult. TRPO aims to solve this issue.

The guiding principal comes from the following theorem [2]:

**Theorem 14.** Let  $\alpha = D_{\text{TV}}^{\text{max}}(\pi_{\text{old}}, \pi_{\text{new}}) = \max_{s} D_{\text{TV}}(\pi_{\text{old}}(\cdot \mid s) || \pi_{\text{new}}(\cdot \mid s))$ . Then,

$$V(\pi_{\text{new}}) \ge L_{\pi_{\text{old}}}(\pi_{\text{new}}) - \frac{4\epsilon\gamma}{(1-\gamma)^2}\alpha^2$$

where  $\epsilon = \max_{s,a} |A_{\pi}(s,a)|$ .

The main building blocks are the following two definitions and lemma:

**Definition 8.** ( $\alpha$ -coupled policy pair). We call  $(\pi, \pi')$  an  $\alpha$ -coupled policy pair if the joint distribution  $(a, a') \mid s$  is such that  $\mathbb{P}(a \neq a' \mid s) \leq \alpha$  for all s.

We also define

$$\bar{A}(s) = \mathbb{E}_{a \sim \pi'(\cdot|s)} \left[ A_{\pi}(s, a) \right].$$

Then, we have the following lemma:

**Lemma 15.** Let  $(\pi, \pi')$  be an  $\alpha$ -coupled policy pair. Then, for all states s,

$$|\bar{A}(s)| \leq 2\alpha \max_{s,a} |A_{\pi}(s,a)|.$$

Proof.

$$\bar{A}(s) = \mathbb{E}_{a' \sim \pi'} [A_{\pi}(s, a')]$$

$$= \mathbb{E}_{(a, a') \sim (\pi, \pi')} [A_{\pi}(s, a') - A_{\pi}(s, a)]$$

as  $\mathbb{E}_{a \sim \pi}[A_{\pi}(s, a)] = 0$ . Then, continuing:

$$\bar{A}(s) = \mathbb{E}_{(a,a') \sim (\pi,\pi')}[A_{\pi}(s,a') - A_{\pi}(s,a)]$$

$$= \sum_{a'} \pi'(a' \mid s) \sum_{a \neq a'} \pi(a \mid s)(A_{\pi}(s,a') - A_{\pi}(s,a))$$

$$|\bar{A}(s)| = |\sum_{a'} \pi'(a' \mid s) \sum_{a \neq a'} \pi(a \mid s)(A_{\pi}(s,a') - A_{\pi}(s,a))|$$

$$\leq |\sum_{a'} \pi'(a' \mid s) \sum_{a \neq a'} \pi(a \mid s)(A_{\pi}(s,a'))| + |\sum_{a'} \pi'(a' \mid s) \sum_{a \neq a'} \pi(a \mid s)(A_{\pi}(s,a))|$$

$$\leq |\sum_{a'} \pi'(a' \mid s) \sum_{a \neq a'} \pi(a \mid s)(\max_{s,a} A_{\pi}(s,a))| + |\sum_{a'} \pi'(a' \mid s) \sum_{a \neq a'} \pi(a \mid s)(\max_{s,a} A_{\pi}(s,a))|$$

$$= |\max_{s,a} A_{\pi}(s,a)| 2 \sum_{a'} \pi'(a' \mid s) \sum_{a \neq a'} \pi(a \mid s)|$$

$$= 2\alpha |\max_{s,a} A_{\pi}(s,a)|$$

$$\leq 2\alpha \max_{s,a} |A_{\pi}(s,a)|$$

**Lemma 16.** Let  $(\pi, \pi')$  be an  $\alpha$ -coupled policy pair. Then,

$$|\mathbb{E}_{s_t \sim \pi'} \left[ \bar{A}(s_t) \right] - \mathbb{E}_{s_t \sim \pi} \left[ \bar{A}(s_t) \right] | \le 2\alpha \max_s |\bar{A}(s)| \le 4\alpha (1 - (1 - \alpha)^t) \max_s |A_{\pi}(s, a)|.$$

*Proof.* Let  $n_t$  be the number of time steps such that  $a_i \neq a_i'$  for i < t and  $a_i \sim \pi, a_i' \sim \pi'$ . This denotes the number of times  $\pi$  and  $\pi'$  take different actions before time step t. Then,

$$\mathbb{E}_{s_t \sim \pi'} \left[ \bar{A}(s_t) \right] = P(n_t = 0) \mathbb{E}_{s_t \sim \pi' \mid n_t = 0} \left[ \bar{A}(s_t) \right] + P(n_t > 0) \mathbb{E}_{s_t \sim \pi' \mid n_t > 0} \left[ \bar{A}(s_t) \right].$$

Similarly,

$$\mathbb{E}_{s_{t} \sim \pi} \left[ \bar{A}(s_{t}) \right] = P(n_{t} = 0) \mathbb{E}_{s_{t} \sim \pi \mid n_{t} = 0} \left[ \bar{A}(s_{t}) \right] + P(n_{t} > 0) \mathbb{E}_{s_{t} \sim \pi \mid n_{t} > 0} \left[ \bar{A}(s_{t}) \right].$$

Now,

$$\mathbb{E}_{s_t \sim \pi' \mid n_t = 0} \left[ \bar{A}(s_t) \right] = \mathbb{E}_{s_t \sim \pi \mid n_t = 0} \left[ \bar{A}(s_t) \right]$$

since  $n_t = 0 \implies \pi$  and  $\pi'$  executed the same actions on all time steps less than t. Then,

$$\begin{split} & \mathbb{E}_{s_t \sim \pi'} \left[ \bar{A}(s_t) \right] - \mathbb{E}_{s_t \sim \pi} \left[ \bar{A}(s_t) \right] \\ &= P(n_t > 0) \left( \mathbb{E}_{s_t \sim \pi' \mid n_t > 0} \left[ \bar{A}(s_t) \right] - \mathbb{E}_{s_t \sim \pi \mid n_t > 0} \left[ \bar{A}(s_t) \right] \right). \end{split}$$

Now, since  $\pi$  and  $\pi'$  are  $\alpha$ -coupled, then,  $\mathbb{P}(a=a'\mid s)\geq 1-\alpha$ , so  $P(n_t=0)\geq (1-\alpha)^t$  and

$$P(n_t > 0) < 1 - (1 - \alpha)^t$$
.

On the other hand, using triangle inequality,

$$\left| \mathbb{E}_{s_t \sim \pi' \mid n_t > 0} \left[ \bar{A}(s_t) \right] - \mathbb{E}_{s_t \sim \pi \mid n_t > 0} \left[ \bar{A}(s_t) \right] \right| \tag{2}$$

$$\leq |\mathbb{E}_{s_t \sim \pi'|n_t > 0} \left[ \bar{A}(s_t) \right] | + |\mathbb{E}_{s_t \sim \pi|n_t > 0} \left[ \bar{A}(s_t) \right] | \tag{3}$$

$$\leq 2 \max_{s} |\bar{A}(s)| \tag{4}$$

$$\leq 4\alpha \max_{s,a} |A_{\pi}(s,a)| \tag{5}$$

(6)

Then,

$$\begin{split} & \left| \mathbb{E}_{s_t \sim \pi'} \left[ \bar{A}(s_t) \right] - \mathbb{E}_{s_t \sim \pi} \left[ \bar{A}(s_t) \right] \right| \\ &= \left| P(n_t > 0) \left( \mathbb{E}_{s_t \sim \pi' \mid n_t > 0} \left[ \bar{A}(s_t) \right] - \mathbb{E}_{s_t \sim \pi \mid n_t > 0} \left[ \bar{A}(s_t) \right] \right) \right| \\ &\leq 4\alpha (1 - (1 - \alpha)^t) \max_{s, a} \left| A_{\pi}(s, a) \right|. \end{split}$$

Now we prove theorem 14:

*Proof.* Denote  $\pi = \pi_{\text{old}}$  and  $\pi' = \pi_{\text{new}}$ . Let  $\epsilon = \max_{s,a} |A_{\pi}(s,a)|$ . Then, using performance difference lemma and the definition of  $\bar{A}(s)$ :

$$V(\pi') - V(\pi) = \mathbb{E}_{\tau \sim \pi'} \left[ \sum_{t=0}^{\infty} \gamma^t A_{\pi}(s_t, a_t) \right]$$
$$= \mathbb{E}_{\tau \sim \pi'} \left[ \sum_{t=0}^{\infty} \gamma^t \bar{A}(s_t) \right]$$

On the other hand,

$$L_{\pi}(\pi') = V(\pi) + \mathbb{E}_{s \sim p^{\pi}, a \sim \pi'}[A_{\pi}(s, a)]$$
$$= V(\pi) + \mathbb{E}_{\tau \sim \pi} \left[ \sum_{t=0}^{\infty} \gamma^{t} \bar{A}(s_{t}) \right].$$

Combining:

$$|V(\pi') - L_{\pi}(\pi')| \leq \sum_{t=0}^{\infty} \gamma^{t} \left| \mathbb{E}_{\tau \sim \pi'} [\bar{A}(s_{t})] - \mathbb{E}_{\tau \sim \pi} [\bar{A}(s_{t})] \right|$$

$$\sum_{t=0}^{\infty} \gamma^{t} 4\epsilon \alpha (1 - (1 - \alpha)^{t})$$

$$= 4\epsilon \alpha \left( \frac{1}{1 - \gamma} - \frac{1}{1 - \gamma(1 - \alpha)} \right)$$

$$= \frac{4\alpha^{2} \gamma \epsilon}{(1 - \gamma)(1 - \gamma(1 - \alpha))}$$

$$= \frac{4\alpha^{2} \gamma \epsilon}{(1 - \gamma)(1 - \gamma(1 - \alpha))}$$

$$\leq \frac{4\alpha^{2} \gamma \epsilon}{(1 - \gamma)^{2}}.$$

Now, if we have two policies  $\pi$  and  $\pi'$  such that  $\max_s D_{\mathrm{TV}}(\pi(\cdot \mid s) | |\pi'(\cdot \mid s)) \leq \alpha$ , then we can define an  $\alpha$ -coupled policy with the appropriate marginals by Theorem 23. Therefore, take  $\alpha = \max_s D_{\mathrm{TV}}(\pi(\cdot \mid s) | |\pi'(\cdot \mid s))$ , plug this into  $\frac{4\alpha^2 \gamma \epsilon}{(1-\gamma)^2}$  to conclude.

From theorem 14, by noting that  $D_{\text{TV}}(p||q)^2 \leq D_{\text{KL}}(p||q)$ , we get that

$$V(\pi') \ge L_{\pi}(\pi') - \frac{4\epsilon\gamma}{(1-\gamma)^2} D_{\mathrm{KL}}^{\mathrm{max}}(\pi, \pi').$$

Using this, we can find a preliminary algorithm:

Algorithm: Policy iteration guaranteeing non-decreasing expected return V

- 1: **Initialize** policy  $\pi_0$
- 2: **for**  $i = 0, 1, 2, \ldots$  until convergence **do**
- 3: Compute all advantage values  $A_{\pi_i}(s, a)$
- 4: Solve the constrained optimization problem:

$$\pi_{i+1} = \arg \max_{\pi} \left[ L_{\pi_i}(\pi) - CD_{\text{KL}}^{\text{max}}(\pi_i, \pi) \right]$$
 where  $C = \frac{4\epsilon\gamma}{(1-\gamma)^2}$  and  $L_{\pi_i}(\pi) = V(\pi_i) + \sum_s p^{\pi_i}(s) \sum_a \pi(a|s) A_{\pi_i}(s, a)$ 

5: end for

This algorithm has guaranteed monotonic improvement. We can now use it to derive TRPO. Let  $V(\theta) := V(\pi_{\theta})$ ,  $L_{\theta}(\theta') := L_{\pi_{\theta}}(\pi_{\theta'})$ , and  $D_{\text{KL}}(\theta \parallel \theta') := D_{\text{KL}}(\pi_{\theta} \parallel \pi_{\theta'})$ . We saw that:

$$V(\theta) \ge L_{\theta_{\text{old}}}(\theta) - CD_{\text{KL}}^{\text{max}}(\theta_{\text{old}}, \theta)$$

with equality at  $\theta = \theta_{\text{old}}$ . Thus, we can improve  $V(\theta)$  by solving the following optimization problem:

$$\max_{\theta} L_{\theta_{\text{old}}}(\theta) - CD_{\text{KL}}^{\text{max}}(\theta_{\text{old}}, \theta)$$

However, choosing the step size here is tricky - if we use  $C = \frac{4\epsilon\gamma}{(1-\gamma)^2}$ , then the step sizes become small. Instead, we solve the following with a trust region constraint:

$$\max_{\theta} L_{\theta_{\text{old}}}(\theta) \tag{7}$$

subject to 
$$D_{\text{KL}}^{\text{max}}(\theta_{\text{old}}, \theta) \le \delta$$
 (8)

In practice, we use the average KL divergence:  $\bar{D}_{\mathrm{KL}}^{p^{\theta_{\mathrm{old}}}}(\theta_{\mathrm{old}}, \theta) = \mathbb{E}_{s \sim p^{\theta_{\mathrm{old}}}}[D_{\mathrm{KL}}(\pi_{\theta_{\mathrm{old}}}(\cdot \mid s) || \pi_{\theta}(\cdot \mid s))]$ 

Lastly, we show how to estimate the objective and constraint functions using Monte Carlo simulation. We replace the objective  $\sum_s p^{\theta_{\text{old}}}(s) \sum_a \pi_{\theta}(a \mid s) A_{\theta_{\text{old}}}(s,a)$  with  $\frac{1}{1-\gamma} \mathbb{E}_{s \sim \theta_{\text{old}}, a \sim \pi_{\theta}(\cdot \mid s)} [A_{\theta_{\text{old}}}(s,a)]]$ . Lastly, we use importance sampling. Altogether, we have:

$$\max_{\theta} \mathbb{E}_{s \sim p^{\theta_{\text{old}}}, a \sim \pi_{\theta_{\text{old}}}} \left[ \frac{\pi_{\theta}(a \mid s)}{\pi_{\theta_{\text{old}}}(a \mid s)} A_{\theta_{\text{old}}}(s, a) \right]$$
(9)

subject to 
$$\mathbb{E}_{s \sim p^{\theta_{\text{old}}}} \left[ D_{\text{KL}} \left( \pi_{\theta_{\text{old}}} (\cdot \mid s) \parallel \pi_{\theta} (\cdot \mid s) \right) \right] \leq \delta$$
 (10)

The alternative version is the optimize the following:

$$\max_{\theta} \mathbb{E}_{s \sim p^{\theta_{\text{old}}}, a \sim \pi_{\theta_{\text{old}}}} \left[ \frac{\pi_{\theta}(a \mid s)}{\pi_{\theta_{\text{old}}}(a \mid s)} A_{\theta_{\text{old}}}(s, a) - \beta \cdot D_{\text{KL}} \left( \pi_{\theta_{\text{old}}}(\cdot \mid s) \parallel \pi_{\theta}(\cdot \mid s) \right) \right]$$
(11)

The second version comes from the first via the method of Lagrange multipliers so these are two equivalent formulations. However, comparing these two versions, tuning  $\delta$  (in the first version) is generally easier than tuning  $\beta$  in the second version. Also, for the second version in practice, TRPO uses the *maximum* over KL divergences conditioned on each state instead of the mean. In other words, optimize:

$$\max_{\theta} \mathbb{E}_{s \sim p^{\theta_{\text{old}}}, a \sim \pi_{\theta_{\text{old}}}} \left[ \frac{\pi_{\theta}(a \mid s)}{\pi_{\theta_{\text{old}}}(a \mid s)} A_{\theta_{\text{old}}}(s, a) \right] - \beta \cdot \max_{s} \left[ D_{\text{KL}} \left( \pi_{\theta_{\text{old}}}(\cdot \mid s) \parallel \pi_{\theta}(\cdot \mid s) \right) \right]$$
(13)

TRPO solves this optimization problem by making a linear approximation to the objective  $L_{\pi_{\theta_{\text{old}}}}(\pi_{\theta})$ , a quadratic approximation to the constraint and then using a conjugate gradient algorithm.

Then, the problem becomes:

$$\max_{\theta} \quad g \cdot (\theta - \theta_{\text{old}}) - \frac{\beta}{2} (\theta - \theta_{\text{old}})^T F(\theta - \theta_{\text{old}})$$

where 
$$g = \frac{\partial}{\partial \theta} L_{\pi_{\theta_{\text{old}}}}(\pi_{\theta}) \Big|_{\theta = \theta_{\text{old}}}$$
 and  $F = \frac{\partial^2}{\partial \theta^2} \text{KL}_{\pi_{\theta_{\text{old}}}}(\pi_{\theta}) \Big|_{\theta = \theta_{\text{old}}}$ .

This problem can be solved efficiently using the conjugate gradient algorithm.

## 2.12 Proximal Policy Optimization (PPO)

(This section is written independently of the previous section on trust regional policy optimization so that it is self-complete, which means there are some repetitions here)

There are two major issues with vanilla policy gradient methods. Firstly, it is difficult to optimize in the sense that it is difficult to find the right step size to use in gradient descent. The input data distribution is non-stationary - you sample trajectories using a learned policy, then you use those samples to update your policy, then you use this updated policy to sample new trajectories. However, if, at any point in time, you use a set of bad samples and therefore, your optimisation step is wrong, this could lead to performance collapse - with the bad samples,

you take a "wrong step" to get a poor policy, with which you sample new trajectories which are also poor which you then use to optimise again. The second issue is that the algorithm is sample inefficient - with any particular set of sampled trajectories, we carry out one step of gradient descent and then throw those samples out. For future optimisation steps, we sample new trajectories. Although we have made some modifications to the basic vanilla PG algorithm like we found the actor-critic methods, they are still insufficient in completely curbing these issues.

We now derive the building blocks of Trust Region Policy Optimisation (TRPO): We already saw the performance difference lemme:

$$V_{\pi'} - V_{\pi} = \frac{1}{1 - \gamma} \mathbb{E}_{s \sim d^{\pi'}} \left[ \mathbb{E}_{a \sim \pi'} \left[ A^{\pi}(s, a) \right] \right]$$

Now, suppose, our current policy is  $\pi$ . In our next step, we essentially want to maximize the difference between  $V_{\pi'} - V_{\pi}$ . Therefore,

$$\arg \max_{\pi'} V_{\pi'} - V_{\pi} = \arg \max_{\pi'} \frac{1}{1 - \gamma} \mathbb{E}_{s \sim d^{\pi'}} \left[ \mathbb{E}_{a \sim \pi'} \left[ A^{\pi}(s, a) \right] \right]$$

$$= \arg \max_{\pi'} \frac{1}{1 - \gamma} \mathbb{E}_{s \sim d^{\pi'}} \left[ \mathbb{E}_{a \sim \pi} \left[ \frac{\pi'(a|s)}{\pi(a|s)} A^{\pi}(s, a) \right] \right]$$

$$\approx \arg \max_{\pi'} \frac{1}{1 - \gamma} \mathbb{E}_{s \sim d^{\pi}} \left[ \mathbb{E}_{a \sim \pi} \left[ \frac{\pi'(a|s)}{\pi(a|s)} A^{\pi}(s, a) \right] \right]$$

$$=: \arg \max_{\pi'} \mathcal{L}_{\pi}(\pi')$$

where, in the second last line, we made the approximation  $d^{\pi'} \approx d^{\pi}$ . This approximation only holds true if

$$||V_{\pi'} - V_{\pi} - \mathcal{L}_{\pi}(\pi')|| \le C\sqrt{\mathbb{E}_{s_t \sim \pi} \left[D_{KL}(\pi(\cdot|s_t)||\pi'(\cdot|s_t))\right]}$$

With this, TRPO maximises  $\mathcal{L}_{\pi}(\pi')$  subject to  $\mathbb{E}_{s \sim \pi}[D_{KL}(\pi(\cdot|s)||\pi'(\cdot|s))] \leq \delta$ . Note that, in actual implementation, we use a learned approximation for the advantage function.

Also note that we get monotonic improvement since the KL divergence is zero when  $\pi' = \pi$  whereas  $\mathcal{L}_{\pi}(\pi) = 0$  too, therefore, the performance of  $\pi'$  is at least as good as  $\pi$ .

PPO [4] slightly modifies this - instead of placing a harsh constraint in the optimization process (which requires conjugate gradient descent otherwise), instead PPO brings in 2 variants. The first is to maximize  $\mathbb{E}_{s_t \sim d^{\pi}, a_t \sim \pi} \left[ \frac{\pi'(a_t|s_t)}{\pi(a_t|s_t)} A^{\pi}(s_t, a_t) - \beta \cdot D_{KL}(\pi'(\cdot|s_t)||\pi(\cdot|s_t)) \right]$ . If the KL-divergence is too high, we adaptively increase  $\beta$  and if it is small, then we decrease  $\beta$ . The other

variant is as follows - define  $r_t(\theta) := \frac{\pi_{\theta'}(a_t|s_t)}{\pi_{\theta}(a_t|s_t)}$ . Then, maximize

$$\mathbb{E}_{\tau \sim \pi_{\theta}} \left[ \sum_{t=0}^{T-1} \left[ \min(r_t(\theta) A^{\pi_{\theta}}(s_t, a_t), \operatorname{clip}(r_t(\theta), 1 - \epsilon, 1 + \epsilon) A^{\pi_{\theta}}(s_t, a_t)) \right] \right]$$

The second variant is more commonly used. In practical implementations, we often add an entropy bonus (similar to SAC) to encourage exploration and prevent collapsing to a local optimal.

Intuition: let's see what this algorithm really does. Consider the vanilla algorithm that maximizes  $\mathbb{E}_{\tau \sim \pi_{\theta}} \left[ \sum_{t} r_{t}(\theta) A^{\pi_{\theta}}(s_{t}, a_{t}) \right]$ . If we take the gradient of this with respect to  $\theta'$ , then, we get  $\mathbb{E}_{\tau \sim \pi_{\theta}} \left[ \sum_{t} r_{t}(\theta) \nabla_{\theta'} (\log \pi_{\theta'}(a_{t} \mid s_{t})) A^{\pi_{\theta}}(s_{t}, a_{t}) \right]$ . Now, if  $A^{\pi_{\theta}}(s_{t}, a_{t})$  is positive, this means we take a gradient step in the direction given by  $\nabla_{\theta'} (\log \pi_{\theta'}(a_{t} \mid s_{t}))$ . If this step is too large, then we will have left the "trust region" in TRPO where  $\pi_{\theta'}$  is close to  $\pi_{\theta}$ . If we compute the gradient of the PPO objective, we can see that when  $A^{\pi_{\theta}}(s_{t}, a_{t})$  and whenever  $r_{t}(\theta) > 1 + \epsilon$ , the gradient becomes zero i.e. whenver we have left the trust region, we do not update policy anymore suggesting that we need new data and cannot use our old data from previous policy anymore.

In both variants, the algorithm uses an advantage estimator  $\hat{A}^{\pi}(s_t, a_t)$ . PPO uses Generalized Advantage Estimator (GAE) which we discuss now.

First, we define N-step advantage estimators:

$$\hat{A}_{t}^{(1)} = r_{t} + \gamma V(s_{t+1}) - V(s_{t})$$

$$\hat{A}_{t}^{(2)} = r_{t} + \gamma r_{t+1} + \gamma V(s_{t+2}) - V(s_{t})$$

$$\hat{A}_{t}^{(\infty)} = r_{t} + \gamma r_{t+1} + \gamma^{2} r_{t+2} + \dots - V(s_{t}).$$

If we define

$$\delta_t^V = r_t + \gamma V(s_{t+1}) - V(s_t),$$

then, these become:

$$\hat{A}_{t}^{(1)} = \delta_{t}^{V},$$

$$\hat{A}_{t}^{(2)} = \delta_{t}^{V} + \gamma \delta_{t+1}^{V},$$

$$\hat{A}_{t}^{(k)} = \sum_{l=1}^{k-1} \gamma^{l} \delta_{t+l}^{V}.$$

Thus, generally,

$$\hat{A}_{t}^{(k)} = \sum_{l=0}^{k-1} \gamma^{l} r_{t+l} + \gamma^{k} V(s_{t+k}) - V(s_{t}).$$

GAE is an exponentially-weighted average of k-step estimators:

$$\begin{split} \hat{A}_t^{GAE(\gamma,\lambda)} &= (1-\lambda) \left( \hat{A}_t^{(1)} + \lambda \hat{A}_t^{(2)} + \lambda^2 \hat{A}_t^{(3)} + \ldots \right) \\ &= (1-\lambda) \left( \delta_t^V + \lambda (\delta_t^V + \gamma \delta_{t+1}^V + \gamma^2 \delta_{t+2}^V) + \ldots \right) \\ &= (1-\lambda) \left( \delta_t^V (1+\lambda+\lambda^2+\ldots) + \gamma \delta_{t+1}^V (\lambda+\lambda^2+\ldots) + \ldots \right) \\ &= (1-\lambda) \left( \delta_t^V \frac{1}{1-\lambda} + \gamma \delta_{t+1}^V \frac{\lambda}{1-\lambda} + \gamma^2 \delta_{t+2}^V \frac{\lambda^2}{1-\lambda} + \ldots \right) \\ &= \sum_{l=0}^{\infty} (\gamma \lambda)^l \delta_{t+l}^V. \end{split}$$

PPO uses a truncated version of a GAE:

$$\hat{A}_t = \sum_{l=0}^{T-t-1} (\gamma \lambda)^l \delta_{t+l}^V$$

```
Algorithm: PPO (Actor-Critic Style)

1: for iteration = 1, 2, ... do
2: for actor = 1, 2, ..., N do
3: Run policy \pi_{\theta_{\text{old}}} in environment for T timesteps
4: Compute advantage estimates \hat{A}_1, \ldots, \hat{A}_T
5: end for
6: Optimize surrogate objective L with respect to \theta, using K epochs and minibatch size M \leq NT
7: \theta_{\text{old}} \leftarrow \theta
8: end for
```

```
Algorithm: PPO with GAE
  1: Initialize parameters \phi, environment state s
  2: for iteration k = 1, 2, \dots do
                \phi_{\text{old}} \leftarrow \phi
                (\tau, s) = \text{rollout}(s, \pi_{\phi_{\text{old}}})
  4:
               (s_1, a_1, r_1, \dots, s_T) = \tau
               v_t = V_\phi(s_t) for t = 1:T
               (A_{1:T}, y_{1:T}) = GAE(r_{1:T}, v_{1:T}, \gamma, \lambda)
  7:
               for m = 1: M do
\rho_t = \frac{\pi_{\phi}(a_t|s_t)}{\pi_{\phi_{\text{old}}}(a_t|s_t)} \text{ for } t = 1: T
\tilde{\rho}_t = \text{clip}(\rho_t) \text{ for } t = 1: T
10:
                      \mathcal{L}(\phi) = \frac{1}{T} \sum_{t=1}^{T} \left[ \lambda_{TD} (V_{\phi}(s_t) - y_t)^2 - \lambda_{PG} \min(\rho_t A_t, \tilde{\rho}_t A_t) - \lambda_{\text{ent}} \mathbb{H}(\pi_{\phi}(\cdot|s_t)) \right]
\phi \leftarrow \phi - \eta \nabla_{\phi} \mathcal{L}(\phi)
11:
12:
                end for
13:
14: end for
```

## 2.13 Soft Actor-Critic (SAC)

Soft Actor-Critic [5] is an off-policy actor-critic algorithm that aims to learn a policy that maximizes rewards while also acting as stochastically as possible. In other words, if there are two actions that both achieve the same maximum rewards, our goal would be to assign nearly equal probability mass to both of them. This falls under a general framework called maximum entropy reinforcement learning where the goal is to maximize (assume a finite horizon task with discount factor  $\gamma = 0$ ):

$$J(\theta) = \sum_{t=0}^{T} \mathbb{E}_{s_t \sim p^{\pi_{\theta}}, a_t \sim \pi_{\theta}} \left[ r(s_t, a_t) + \alpha H(\pi(\cdot \mid s_t)) \right]$$
 (15)

where H(p) is the entropy of the distribution p.

There are many benefits to learning such policies. Firstly, sometimes we would want our agents to learn multiple strategies for solving a task. Imagine building an agent that plays chess - it would be a problem if the agent acts deterministically (or close to deterministically) because then its opponent could very well predict its moves. Secondly, a highly stochastic policy would also end up doing more exploration allowing us to potentially uncover even more optimal strategies as training progresses, instead of collapsing to suboptimal ones.

First, we define the modified Bellman backup operator that gets us the soft Q-value corresponding to  $J(\theta)$  as in equation 15:

**Definition 9.** (Bellman backup for soft Q-value). The soft Q-value of a fixed policy  $\pi$  can be computed by repeatedly applying the modified Bellman backup operator:

$$\tau^{\pi} Q_{\pi}(s_t, a_t) := r(s_t, a_t) + \gamma \mathbb{E}_{s_{t+1} \sim p(\cdot | s_t, a_t)} [V(s_{t+1})]$$

where

$$V(s_t) = \mathbb{E}_{a_t \sim \pi} \left[ Q_{\pi}(s_t, a_t) - \log \pi(a_t \mid s_t) \right].$$

The fact that this converges comes from the following result:

**Lemma 17.** For any mapping  $Q_{\pi}^0: \mathcal{S} \times \mathcal{A} \to \mathbb{R}$  with  $|\mathcal{A}| < \infty$  and  $Q_{\pi}^{k+1} = \tau^{\pi} Q_{\pi}^{k}$ . Then, the sequence  $Q_{\pi}^{k}$  converges to the soft Q-value of  $\pi$  as  $k \to \infty$ .

Proof. Define  $r_{\pi}(s_t, a_t) = r(s_t, a_t) + \mathbb{E}_{s_{t+1} \sim P(\cdot | s_t, a_t)} [H(\pi(\cdot | s_{t+1}))]$ . Then,  $Q_{\pi}(s_t, a_t) \leftarrow r_{\pi}(s_t, a_t) + \gamma \mathbb{E}_{s_{t+1} \sim P, a_{t+1} \sim \pi} [Q(s_{t+1}, a_{t+1})]$  is the update rule. Given  $|\mathcal{A}| < \infty$ , the entropy augment reward  $r_{\pi}$  is bounded. Using this, we can show the convergence as required following similar steps as for classical policy evaluation.

Given this evaluation, we can then do policy improvement as follows:

$$\pi_{\text{new}} = \arg\min_{\pi' \in \Pi} D_{\text{KL}} \left( \pi'(\cdot \mid s_t) \mid\mid \frac{\exp(Q_{\pi_{\text{old}}}(s_t, \cdot))}{Z^{\pi_{\text{old}}}(s_t)} \right)$$

where  $Z^{\pi_{\text{old}}}$  is the partition function that normalizes the distribution. We can prove that this results in an improved policy as follows:

**Lemma 18.** Let  $\pi_{\text{old}} \in \Pi$  and let  $\pi_{\text{new}}$  be the resulting policy from the soft-policy improvement step. Then,  $Q^{\pi_{\text{new}}}(s_t, a_t) \geq Q^{\pi_{\text{old}}}(s_t, a_t)$  for all  $(s_t, a_t) \in \mathcal{S} \times \mathcal{A}$  with  $|\mathcal{A}| < \infty$ .

*Proof.* Given  $\pi_{\text{old}}$  with corresponding  $Q^{\pi_{\text{old}}}$  and  $V^{\pi_{\text{old}}}$ , we can define

$$\pi_{\text{new}}(\cdot \mid s_t) = \arg\min_{\pi' \in \Pi} D_{\text{KL}}(\pi'(\cdot \mid s_t) \mid\mid \exp(Q^{\pi_{\text{old}}}(s_t, \cdot) - \log Z^{\pi_{\text{old}}}(s_t)))$$
$$=: \arg\min_{\pi' \in \Pi} J_{\pi_{\text{old}}}(\pi'(\cdot \mid s_t)).$$

Now,  $J_{\pi_{\text{old}}}(\pi_{\text{new}}(\cdot|s_t)) \leq J_{\pi_{\text{old}}}(\pi_{\text{old}}(\cdot|s_t))$  since we could choose  $\pi_{\text{new}} = \pi_{\text{old}}$  in our minimization process. Therefore, expanding this line, we get:

$$\mathbb{E}_{a_t \sim \pi_{\text{new}}} [\log \pi_{\text{new}}(a_t \mid s_t) - Q^{\pi_{\text{old}}}(s_t, a_t) + \log Z^{\pi_{\text{old}}}(s_t)]$$

$$\leq \mathbb{E}_{a_t \sim \pi_{\text{old}}} [\log \pi_{\text{old}}(a_t \mid s_t) - Q^{\pi_{\text{old}}}(s_t, a_t) + \log Z^{\pi_{\text{old}}}(s_t)]$$

Since  $Z^{\pi_{\text{old}}}$  is independent of  $a_t$ , this reduces to

$$\mathbb{E}_{a_t \sim \pi_{\text{new}}}[Q^{\pi_{\text{old}}}(s_t, a_t) - \log \pi_{\text{new}}(a_t \mid s_t)] \ge V^{\pi_{\text{old}}}(s_t).$$

Then,

$$Q^{\pi_{\text{old}}}(s_{t}, a_{t}) = r(s_{t}, a_{t}) + \gamma \mathbb{E}_{s_{t+1} \sim P} \left[ V^{\pi_{\text{old}}}(s_{t+1}) \right]$$

$$\leq r(s_{t}, a_{t}) + \gamma \mathbb{E}_{s_{t+1} \sim P} \left[ \mathbb{E}_{a_{t+1} \sim \pi_{\text{new}}} \left[ Q^{\pi_{\text{old}}}(s_{t+1}, a_{t+1}) - \log \pi_{\text{new}}(a_{t+1} \mid s_{t+1}) \right] \right].$$
...
$$\leq Q^{\pi_{\text{new}}}(s_{t}, a_{t})$$

where the expansion uses  $\mathbb{E}_{a_t \sim \pi_{\text{new}}}[Q^{\pi_{\text{old}}}(s_t, a_t) - \log \pi_{\text{new}}(a_t \mid s_t)] \geq V^{\pi_{\text{old}}}(s_t)$ . The convergence follows from the previous lemma.

The soft-policy iteration algorithm essentially works like policy iteration except we alternate between soft policy evaluation and soft policy improvement as described above. This algorithm will, in fact, converge to the optimal policy as proven in the following theorem:

**Theorem 19.** The soft policy iteration algorithm over  $\pi \in \Pi$  converges to a policy  $\pi^*$  such that  $Q^{\pi^*}(s_t, a_t) \geq Q^{\pi}(s_t, a_t)$  for all  $\pi \in \Pi$  and  $(s_t, a_t) \in \mathcal{S} \times \mathcal{A}$ , assuming  $|\mathcal{A}| < \infty$ .

*Proof.* We know by the previous lemma that  $Q^{\pi_i}$  is monotonically increasing. However,  $Q^{\pi}$  is bounded above since the reward and entropy (given  $|\mathcal{A}| < \infty$ ) are bounded above. Therefore, the policy iteration will converge to some  $\pi^*$ . Now, we claim that this policy is optimal. Since  $\pi^*$  is the policy at convergence, we have that  $J_{\pi^*}(\pi^*(\cdot|s_t)) < J_{\pi^*}(\pi(\cdot|s_t))$  for all  $\pi \in \Pi$  such that  $\pi \neq \pi^*$ . From this, we can easily show that  $Q^{\pi^*}(s_t, a_t) > Q^{\pi}(s_t, a_t)$  for all  $s_t$  and  $s_t$ .

The catch, however, is that performing the exact optimization in each of these steps may not be tractable. We now describe the practical algorithm we get from SAC.

In SAC, we parametrize three function:  $V_{\psi}(s_t)$  (to estimate the soft state-value function),  $Q_{\phi}(s_t, a_t)$  (to estimate the soft state-action value function) and  $\pi_{\theta}(a_t|s_t)$ . Although technically we do not need to have separate function approximators for V and Q, doing this improves training stability. In practice,  $V_{\psi}(s_t)$  and  $Q_{\phi}(s_t, a_t)$  could be neural networks where as the policy could be Gaussian with mean and covariance given by neural networks.

The soft value function is trained to minimize the following loss:

$$J_V(\psi) = \mathbb{E}_{s_t \sim \mathcal{D}} \left[ \frac{1}{2} \left( V_{\psi}(s_t) - \mathbb{E}_{a_t \sim \pi_{\theta}(\cdot|s_t)} \left[ Q_{\phi}(s_t, a_t) - \log \pi_{\theta}(a_t|s_t) \right] \right)^2 \right].$$

Here  $\mathcal{D}$  is the replay buffer. The gradient is computed as the following unbiased estimator:

$$\nabla_{\psi} J_V(\psi) = \nabla_{\psi} V_{\psi}(s_t) (V_{\psi}(s_t) - Q_{\phi}(s_t, a_t) + \log \pi_{\theta}(a_t|s_t))$$

where the actions are sampled  $a_t \sim \pi_{\theta}(\cdot|s_t)$ .

The soft Q-function is trained to minimize the soft Bellman residual:

$$J_Q(\phi) = \mathbb{E}_{s_t, a_t \sim \mathcal{D}} \left[ \frac{1}{2} \left( Q_{\phi}(s_t, a_t) - \hat{Q}(s_t, a_t) \right)^2 \right]$$

where  $\hat{Q}(s_t, a_t) = r(s_t, a_t) + \gamma \mathbb{E}_{s_{t+1} \sim p} \left[ V_{\bar{\psi}}(s_{t+1}) \right]$ . Here  $V_{\bar{\psi}}$  is our target network where  $\bar{\psi}$  is an exponentially moving average of the value network weights. The gradient of this is computed as the estimator:

$$\nabla_{\phi}(J_O(\phi)) = \nabla_{\phi}Q_{\phi}(s_t, a_t)(Q_{\phi}(s_t, a_t) - r(s_t, a_t) - \gamma V_{\bar{\phi}}(s_{t+1})).$$

Finally, we can find the policy by minimizing the expected KL-divergence:

$$J_{\pi}(\phi) = \mathbb{E}_{s_t \sim \mathcal{D}} \left[ D_{\mathrm{KL}} \left( \pi_{\phi}(\cdot \mid s_t) \mid\mid \frac{\exp\left(Q_{\theta}(s_t, \cdot)\right)}{Z_{\theta}(s_t)} \right) \right].$$

To minimize this, we use the reparametrization trick: let  $a_t = f_{\phi}(\epsilon_t; s_t)$  where  $\epsilon_t$  is an input noise vector sampled from a fixed distribution (say, normal). Then,

$$J_{\pi}(\phi) = \mathbb{E}_{\mathbf{s}_{t} \sim \mathcal{D}, \boldsymbol{\epsilon}_{t} \sim \mathcal{N}} \left[ \log \pi_{\phi} \left( f_{\phi}(\boldsymbol{\epsilon}_{t}; \mathbf{s}_{t}) \mid \mathbf{s}_{t} \right) - Q_{\theta} \left( \mathbf{s}_{t}, f_{\phi}(\boldsymbol{\epsilon}_{t}; \mathbf{s}_{t}) \right) \right].$$

Here we ignored the partition function since it does not depend on  $\phi$ .

Then,

$$\hat{\nabla}_{\phi} J_{\pi}(\phi) = \nabla_{\phi} \log \pi_{\phi}(\mathbf{a}_t \mid \mathbf{s}_t) + (\nabla_{\mathbf{a}_t} \log \pi_{\phi}(\mathbf{a}_t \mid \mathbf{s}_t) - \nabla_{\mathbf{a}_t} Q_{\theta}(\mathbf{s}_t, \mathbf{a}_t)) \nabla_{\phi} f_{\phi}(\boldsymbol{\epsilon}_t; \mathbf{s}_t),$$

```
Algorithm 1: Soft Actor-Critic
  1: Initialize parameter vectors \psi, \bar{\psi}, \theta, \phi
  2: for each iteration do
             for each environment step do
                   a_t \sim \pi_\phi(a_t \mid s_t)
  4:
                  s_{t+1} \sim p(s_{t+1} \mid s_t, a_t)
                  \mathcal{D} \leftarrow \mathcal{D} \cup \{(s_t, a_t, r(s_t, a_t), s_{t+1})\}
  6:
             end for
            for each gradient step do
  8:
                  \psi \leftarrow \psi - \lambda_V \hat{\nabla}_{\psi} J_V(\psi)
  9:
                  for i \in \{1, 2\} do
10:
                        \theta_i \leftarrow \theta_i - \lambda_Q \hat{\nabla}_{\theta_i} J_Q(\theta_i)
12:
                  \phi \leftarrow \phi - \lambda_{\pi} \hat{\nabla}_{\phi} J_{\pi}(\phi)
13:
                   \bar{\psi} \leftarrow \tau \psi + (1 - \tau)\bar{\psi}
14:
             end for
15:
16: end for
```

### 2.14 Deterministic Policy Gradient Methods (DPG)

**Notation:** We denote  $r_t^{\gamma} = \sum_{k=t}^{\infty} \gamma^{k-t} r(s_k, a_k)$ . Then,  $V^{\pi}(s) = \mathbb{E}[r_1^{\gamma} | S_1 = s; \pi]$  and  $Q^{\pi}(s, a) = \mathbb{E}[r_1^{\gamma} | S_1 = s, A_1 = a; \pi]$ . The density at state s' after transitioning for t timesteps from state s is  $p(s \to s', t, \pi)$ . The improper, discounted state distribution is  $p^{\pi}(s') := \int_{\mathcal{S}} \sum_{t=1}^{\infty} \gamma^{t-1} p_1(s) p(s \to s', t, \pi) ds$ .

Suppose,  $\mathcal{A} = \mathbb{R}^m$  and  $\mathcal{S} = \mathbb{R}^d$ .

**Goal:** Learn a policy which maximizes  $J(\pi) := \mathbb{E}[r_1^{\gamma}|\pi]$ . With our notation, this becomes:

$$J(\pi_{\theta}) = \int_{\mathcal{S}} p^{\pi}(s) \int_{\mathcal{A}} \pi_{\theta}(s, a) r(s, a) dads = \mathbb{E}_{s \sim p^{\pi}, a \sim \pi_{\theta}} [r(s, a)].$$

Intuition behind the deterministic policy gradient theorem:

Most model-free RL algorithms use policy evaluation and policy improvement together. Evaluation approximates  $Q^{\pi}(s,a)$  and then improvement updates the policy, most often through  $\pi^{k+1}(s) = \arg \max_a Q^{\pi^k}(s,a)$ . However, in continuous action spaces, this is difficult since the  $\arg \max_a \text{ requires a global maximisation at each step and our action space is very large (because it is continuous). Instead, the idea is to move the policy in the direction of the gradient of <math>Q^{\pi^k}$  (instead of maximizing it altogether). Then

$$\theta^{k+1} = \theta^k + \alpha \mathbb{E}_{s \sim p^{\theta_k}} [\nabla_{\theta} Q^{\pi^{\theta^k}}(s, \pi^{\theta^k}(s))].$$

By chain rule this becomes

$$\theta^{k+1} = \theta^k + \alpha \mathbb{E}_{s \sim p^{\theta_k}} [\nabla_{\theta} \pi^{\theta}(s) \nabla_a Q^{\pi^{\theta^k}}(s, a)|_{a = \pi^{\theta}(s)}].$$

**Notation:** To distinguish between stochastic and deterministic policy, we will use  $\mu_{\theta}(s)$  as our deterministic policy.

More formally, our performance objective is

$$J(\mu_{\theta}) = \int_{\mathcal{S}} p^{\mu_{\theta}}(s) r(s, \mu_{\theta}(s)) ds = \mathbb{E}_{s \sim p^{\mu_{\theta}}} \left[ r(s, \mu_{\theta}(s)) \right]$$

Then.

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

$$\tag{16}$$

On-policy algorithm: We have a critic that estimates the action-value function while the actor updates the policy by ascending the gradient of the action-value function (using equation 16). The critic,  $Q^w(s, a)$  approximates  $Q^{\mu}(s, a)$ . The update rules are:

$$\delta_{t} = r_{t} + \gamma Q^{w}(s_{t+1}, a_{t+1}) - Q^{w}(s_{t}, a_{t})$$

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

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

**Off-policy algorithm:** Suppose we have trajectories generated by behavior policy  $\pi(s, a)$ . The new objective becomes:

$$J_{\pi}(\mu_{\theta}) = \int_{\mathcal{S}} p^{\pi}(s) V^{\mu}(s) ds = \int_{\mathcal{S}} p^{\pi}(s) Q^{\mu}(s, \mu_{\theta}(s)) ds$$

and the update rule becomes

$$\nabla_{\theta} J_{\pi}(\mu(\theta)) \approx \int_{\mathcal{S}} p^{\pi}(s) \nabla_{\theta} \mu_{\theta}(a|s) Q^{\mu}(s,a) ds = \mathbb{E}_{s \sim p^{\pi}} \left[ \nabla_{\theta} \mu_{\theta}(s) \nabla_{a} Q^{\mu}(s,a) |_{a = \mu_{\theta}(s)} \right].$$

Now we can develop an actor-critic algorithm similar to the on-policy case:our critic is  $Q^w(s,a)$ :

$$\delta_t = r_t + \gamma Q^w(s_{t+1}, \mu_{\theta}(s_{t+1})) - Q^w(s_t, a_t)$$

$$w_{t+1} = w_t + \alpha_w \delta_t \nabla_w Q^w(s_t, a_t)$$

$$\theta_{t+1} = \theta_t + \alpha_\theta \nabla_\theta \mu_{\theta}(s_t) \nabla_a Q^w(s_t, a_t)|_{a = \mu_{\theta}(s)}$$

## References

- [1] R. S. Sutton and A. G. Barto, *Reinforcement Learning: An Introduction*, 2nd ed. The MIT Press, 2018.
- [2] J. Schulman, S. Levine, P. Moritz, M. I. Jordan, and P. Abbeel, "Trust region policy optimization," 2017. [Online]. Available: https://arxiv.org/abs/1502.05477
- [3] J. Peters and S. Schaal, "Natural actor-critic," Neurocomput., vol. 71, no. 7–9, p. 1180–1190, Mar. 2008. [Online]. Available: https://doi.org/10.1016/j.neucom.2007.11.026
- [4] J. Schulman, F. Wolski, P. Dhariwal, A. Radford, and O. Klimov, "Proximal policy optimization algorithms," 2017. [Online]. Available: https://arxiv.org/abs/1707.06347
- [5] T. Haarnoja, A. Zhou, P. Abbeel, and S. Levine, "Soft actor-critic: Off-policy maximum entropy deep reinforcement learning with a stochastic actor," 2018. [Online]. Available: https://arxiv.org/abs/1801.01290
- [6] D. A. Levin and Y. Peres, Markov Chains and Mixing Times, 2nd ed. American Mathematical Society, 2009.
- [7] D. Silver, G. Lever, N. M. O. Heess, T. Degris, D. Wierstra, and M. A. Riedmiller, "Deterministic policy gradient algorithms," in *International Conference on Machine Learning*, 2014. [Online]. Available: https://api.semanticscholar.org/CorpusID:13928442
- [8] L. Weng, "A (long) peek into reinforcement learning," lilianweng.github.io, 2018. [Online]. Available: https://lilianweng.github.io/posts/2018-02-19-rl-overview/

## A Probability

#### A.1 Total Variation Distance

This section is reading notes from [6].

#### A.1.1 Defintions and Properties

Total variation distance is a metric for measuring the distance between two distributions.

**Definition 10.** (Total Variation Distance). The total variation distance between two probability distributions  $\mu$  and  $\nu$  on  $\mathcal{X}$  is defined by

$$||\mu - \nu||_{\text{TV}} = \max_{A \subseteq \mathcal{X}} |\mu(A) - \nu(A)|.$$

We have the equivalent formulation:

**Proposition 20.** For  $\mu$  and  $\nu$  distributions on  $\mathcal{X}$ , we have:

$$||\mu - \nu||_{\text{TV}} = \frac{1}{2} \sum_{x \in \mathcal{X}} |\mu(x) - \nu(x)||$$

*Proof.* Let  $B = \{x : \mu(x) \ge \nu(x)\}$  and let  $A \subset \mathcal{X}$  be any event. Then,

$$\mu(A) - \nu(A) \le \mu(A \cap B) - \nu(A \cap B)$$
  
$$\le \mu(B) - \nu(B).$$

Similarly,

$$\nu(A) - \mu(A) \le \nu(B^C) - \mu(B^C).$$

Note that  $\mu(B) - \nu(B) = \nu(B^C) - \mu(B^C)$  since probabilities sum to 1.

$$\mu(B) - \nu(B) + \nu(B^C) - \mu(B^C) = \sum_{x \in B} |\mu(x) - \nu(x)| + \sum_{x \in B^C} |\nu(x) - \mu(x)| = \sum_x |\mu(x) - \nu(x)|.$$

Now, consider A as in the definition of the TV distance - this A is either B or  $B^C$  i.e.  $|\mu(A) - \nu(A)|$  is maximize when either A = B or  $A = B^C$ . Then,

$$||\mu - \nu||_{\text{TV}} = \frac{1}{2} (\mu(B) - \nu(B) + \nu(B^C) - \mu(B^C)) = \frac{1}{2} \sum_{x} |\mu(x) - \nu(x)|.$$

Corollary 21. We also have that (using the proof above)

$$||\mu - \nu||_{\text{TV}} = \sum_{x \in \mathcal{X}, \mu(x) \ge \nu(x)} \mu(x) - \nu(x).$$

Corollary 22. Total variation distance satisfies the triangle inequality:

$$||\mu - \nu||_{\text{TV}} \le ||\mu - \eta||_{\text{TV}} + ||\eta - \nu||_{\text{TV}}$$

#### A.1.2 Coupling

A coupling of two probability distributions is a way of defining a joint distribution over two random variables such that their marginals match the original distributions. More formally:

**Definition 11.** (Coupling). A coupling of two probability distributions  $\mu$  and  $\nu$  is a pair of random variables (X,Y) defined on a single probability space such that the marginal distribution of X is  $\mu$  and the marginal distribution Y is  $\nu$ . So, the coupling (X,Y) satisfies  $\mathbb{P}(X=x) = \mu(x)$  and  $\mathbb{P}(Y=y) = \nu(y)$ .

Example: Consider  $\mu$  and  $\nu$  both be Bernoulli random variables with parameter 0.5. One way to couple  $\mu$  and  $\nu$  is to define the joint distribution (X,Y) such that  $\mathbb{P}(X=x,Y=y)=\frac{1}{4}$  for all x,y. Another way is to define X to be the independent Bernoulli variable and let Y=X.

Given a coupling (X,Y) with joint distribution  $\pi(X,Y) = P(X=x,Y=y)$ , by the law of total probability  $\sum_x \pi(X=x,Y=y) = \nu(y)$  (and the same for the marginal of X). Conversely, if we have a probability distribution  $\pi$  on  $\mathcal{X} \times \mathcal{X}$  such that  $\sum_y \pi(x,y) = \mu(x)$  and  $\sum_x \pi(x,y) = \nu(y)$ , we can find a pair of random variables (X,Y) that have  $\pi$  as their joint distribution, and so (X,Y) is a coupling of  $\mu$  and  $\nu$ .

**Proposition 23.** Let p and q be two probability distributions on  $\mathcal{X}$ . Then,

$$||p-q||_{\mathrm{TV}} = \inf\{\mathbb{P}(X \neq Y) \mid (X,Y) \text{ is a coupling of } p \text{ and } q\}.$$

In fact, there is a coupling where this infimum is achieved which we call the optimal coupling.

*Proof.* For any coupling of p and q and any event  $A \subset \mathcal{X}$ , we have that:

$$\begin{aligned} p(A) - q(A) &= \mathbb{P}(X \in A) - \mathbb{P}(Y \in A) \\ &\leq \mathbb{P}(X \in A, Y \not\in A) \\ &\leq \mathbb{P}(X \neq Y). \end{aligned}$$

where the second inequality comes from noting:

$$\mathbb{P}\{X\in A\} - \mathbb{P}\{Y\in A\} = \mathbb{P}\{X\in A, Y\in A\} + \mathbb{P}\{X\in A, Y\notin A\} - \mathbb{P}\{X\in A, Y\in A\} - \mathbb{P}\{X\notin A, Y\in A\}.$$

As such,

$$||p-q||_{\text{TV}} \leq \inf\{\mathbb{P}(X \neq Y) \mid (X,Y) \text{ is a coupling of } p \text{ and } q\}.$$

Now, we construct a coupling for which this is an equality.

Let  $m = \sum_{x \in \mathcal{X}} \min(p(x), q(x))$ . Then,

$$m = \sum_{x \in \mathcal{X}, p(x) \le q(x)} p(x) + \sum_{x \in \mathcal{X}, p(x) > q(x)} q(x)$$
$$= 1 - \sum_{x \in \mathcal{X}, p(x) > q(x)} (p(x) - q(x))$$
$$= 1 - ||p - q||_{\text{TV}}$$

where the second inequality comes from adding and subtracting  $\sum_{x \in \mathcal{X}, p(x) > q(x)} p(x)$ .

So

$$m = 1 - ||p - q||_{\text{TV}}.$$

Now, flip a coin with probability of heads equal to  $m = 1 - ||p - q||_{TV}$ .

- 1. If we get heads, then define Z as follows: sample x from the probability distribution  $\psi(x) = \frac{\min(p(x), q(x))}{m}$  and set X = Y = Z.
- 2. If we get tails, then choose X from the probability distribution

$$\varphi_1(x) = \begin{cases} \frac{p(x) - q(x)}{\|p - q\|_{\text{TV}}} & \text{if } p(x) > q(x), \\ 0 & \text{otherwise,} \end{cases}$$

and choose Y independently from the distribution:

$$\varphi_2(y) = \begin{cases} \frac{p(y) - q(y)}{\|\mu - \nu\|_{\text{TV}}} & \text{if } p(y) > q(y), \\ 0 & \text{otherwise.} \end{cases}$$

(Note: when the coin gives us tails,  $X \neq Y$  as  $\varphi_1$  and  $\varphi_2$  are positive on disjoint subsets of  $\mathcal{X}$ )

Then,

$$m\psi + (1-m)\varphi_1 = p$$
  
$$m\psi + (1-m)\varphi_2 = q$$

so we get the appropriate marginals. Also, X = Y if and only if the coin toss gives us heads which happens with probability m, so  $P(X \neq Y) = m = ||p - q||_{TV}$ .