535514: Reinforcement Learning
Lecture 5 — Regularized MDPs and Policy Optimization

Ping-Chun Hsieh

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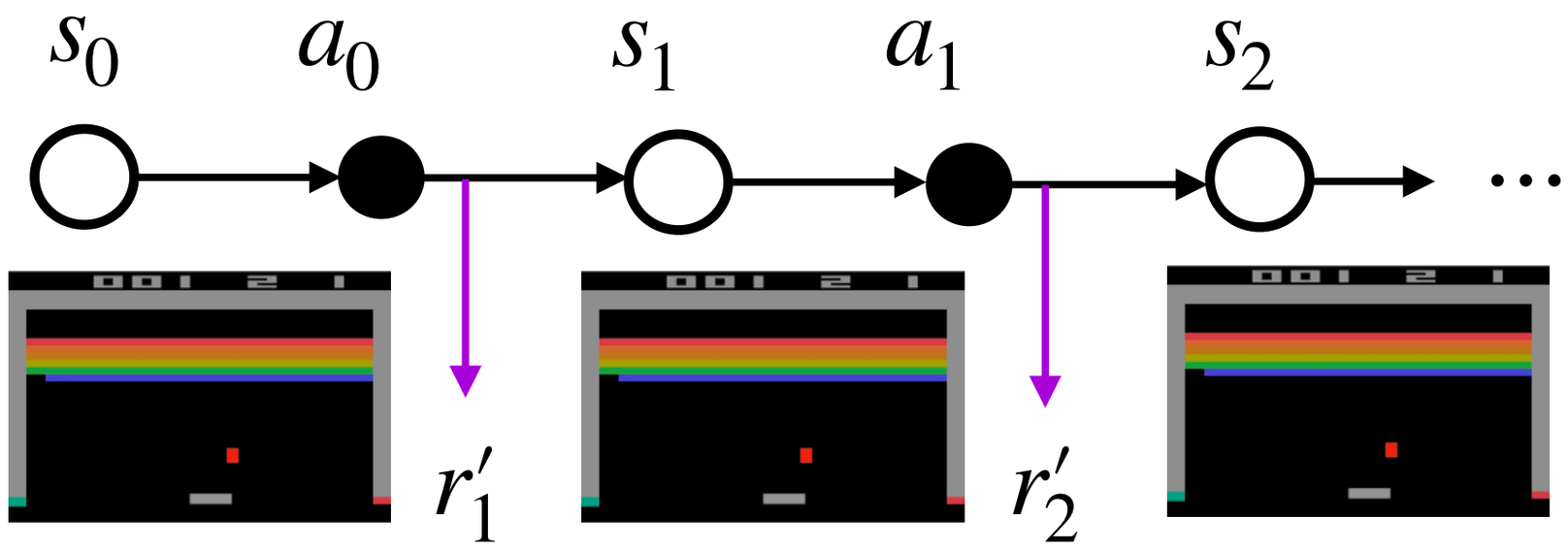
Review: *Regularized MDPs*

Regularized MDP = Standard MDP + Regularized rewards!



- A regularized MDP can be specified by $(\mathcal{S}, \mathcal{A}, P, R, \Omega, \gamma)$
  - $\Omega(\cdot)$: A function that maps an *action distribution* to a *real number*

Value Functions of *Regularized MDPs*

	Unregularized MDP	Regularized MDP
Return	$G_t := r_{t+1} + \gamma r_{t+2} + \gamma^2 r_{t+3} + \cdots$	$G_t := r_{t+1} + \gamma\big(r_{t+2} + \Omega(\pi(\,\cdot\,\vert s_{t+1})\big) + \gamma^2\big(r_{t+3} + \Omega(\pi\cdot\vert s_{t+2})\big) + \cdots$
Value function	$V^\pi(s) := \mathbb{E}[G_t \vert s_t = s; \pi]$	$V^\pi_\Omega(s) :=$
Q function	$Q^\pi(s,a) := \mathbb{E}[G_t \vert s_t = s, a_t = a; \pi]$	$Q^\pi_\Omega(s,a) :=$
Bellman expectation equations	$V^\pi(s) = \sum_{a\in\mathcal{A}} \pi(a\vert s) Q^\pi(s,a)$ $Q^\pi(s,a) = R_{s,a} + \gamma \sum_{s'\in\mathcal{S}} P^a_{ss'} V^\pi(s')$	

Next Question: *How to find* V^{π}_{Ω}*?*

Regularized Bellman Expectation Operator

- Regularized Bellman Expectation Operator

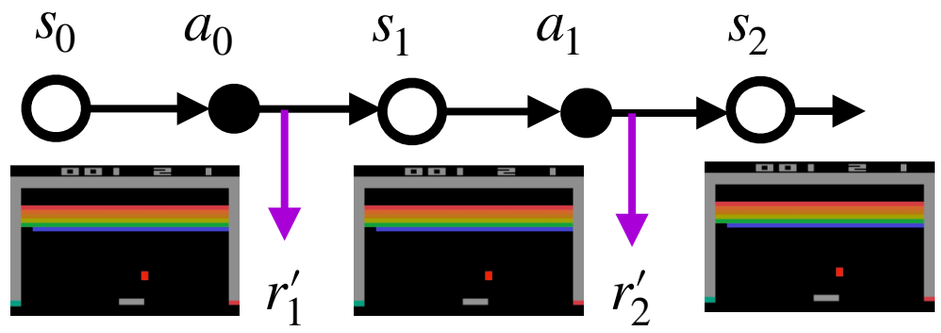
$$[T_\Omega^\pi V](s) := [T^\pi V](s) + \underbrace{\Omega(\pi(\,\cdot\,|\,s))}_{\text{regularization term}}$$
$$= \underbrace{R_s^\pi + \Omega(\pi(\,\cdot\,|\,s))}_{\text{regularized immediate reward}} + \gamma P_{ss'}^\pi V$$

- Question: Is T_Ω^π a contraction? *Yes! (in L_∞-norm)*
- Therefore, under T_Ω^π, there is a unique fixed point, which is the regularized value function V_Ω^π
- To find V_Ω^π, we can use the (regularized) IPE method

Geist et al., "A Theory of Regularized Markov Decision Processes," ICML 2019

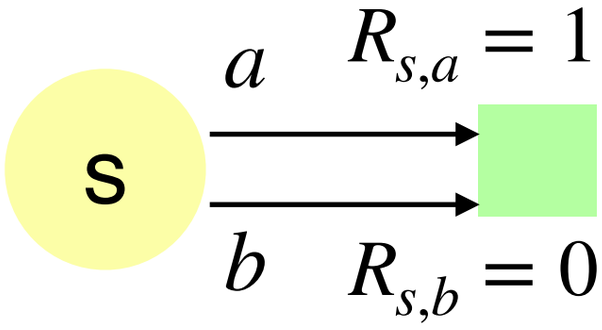
Next Question: *How to define “optimality” for regularized MDPs?*

Optimal Value Functions of *Regularized MDPs*



	Unregularized MDP	Regularized MDP
Optimal value functions	$V^*(s) := \max_{\pi \in \Pi} V^\pi(s)$	$V^*_\Omega(s) :=$
Optimal Q functions	$Q^*(s,a) := \max_{\pi \in \Pi} Q^\pi(s,a)$	$Q^*_\Omega(s,a) :=$

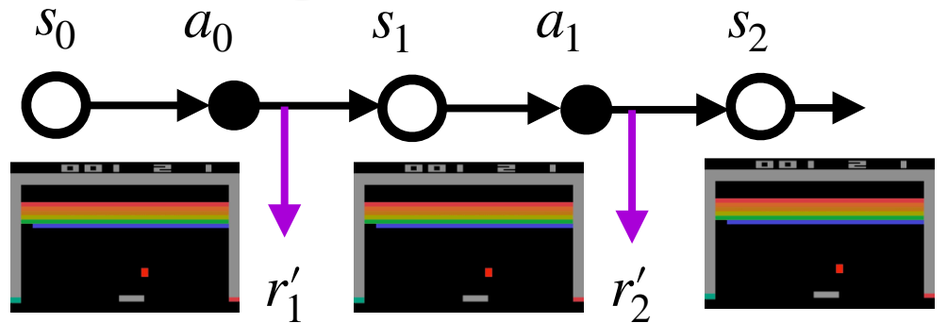
Example: A Simple One-State Regularized MDP



Suppose we choose entropy regularizer
$\Omega(\pi(\cdot|s)) \equiv H(\pi(\cdot|s))$

- **Question 1**: $V^*_\Omega(s)$ = ? $Q^*_\Omega(s,a)$ = ? $Q^*_\Omega(s,b)$ = ?
- **Question 2**: Which policy π can achieve $V^*_\Omega(s)$, i.e., $V^\pi_\Omega(s) = V^*_\Omega(s)$?

Bellman Optimality Equations of *Regularized MDPs*



	Unregularized MDP	Regularized MDP
Bellman optimality equations	$V^*(s) = \max_{a \in \mathcal{A}} R_s^a + \gamma P_s^a V^*$ $= \max_{\pi \in \Pi} R_s^\pi + \gamma P_s^\pi V^*$ $Q^*(s,a) = R_s^a + \gamma E_{s' \sim P(\cdot\|s,a)}[V^*(s')]$	$V_\Omega^*(s) = \max_{\pi \in \Pi} R_s^\pi + \gamma P_s^\pi V_\Omega^*$ $Q_\Omega^*(s,a) = R_s^a + \gamma E_{s' \sim P(\cdot\|s,a)}[V_\Omega^*(s')]$

- Next Question: How to obtain $V_\Omega^*(s)$ and $Q_\Omega^*(s,a)$?

(See HW1 problem for more details)

Next Topic: Policy Optimization

Policy Optimization Framework:

- Consider a parametric policy class: $\{\pi_\theta | \theta \in \Theta \subset \mathbb{R}^d\}$
- View RL as an optimization problem: $\max_\theta V^{\pi_\theta}(\mu) := \mathbb{E}_{s_0 \sim \mu}[V^{\pi_\theta}(s_0)]$

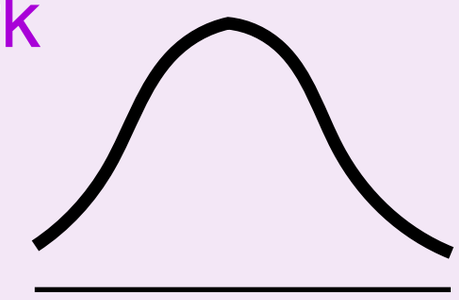
Example:

1. Parametrize the policy by a neural network

s

$\pi_\theta(\cdot)$

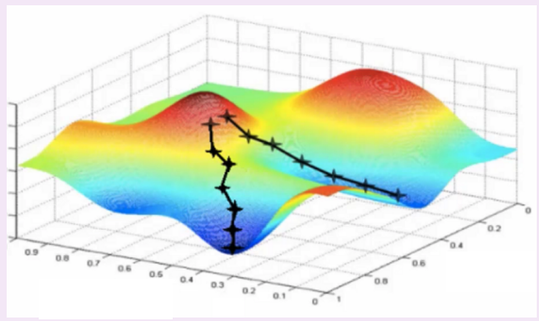
Neural network



A deterministic action or an action distribution

2. Update π_θ iteratively, e.g., by gradient ascent (GA)

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



- Question: Why using $V^\pi(\mu)$ as the objective (instead of each individual $V^\pi(s)$)?

3 Challenges in Policy Optimization

(C1) How to parametrize the policy?

(C2) How to solve the optimization problem in a model-free manner?

1. Policy gradient (PG)
2. Model-free prediction (aka model-free policy evaluation)

(C3) Any theoretical guarantee of PG?

Typical Examples of Parametric Policies

Discrete action space

- Softmax policies: $\pi_\theta(a \mid s) = \dfrac{\exp(\theta_{s,a})}{\sum_{a' \in \mathcal{A}} \exp(\theta_{s,a'})}$
- Linear softmax policies: $\pi_\theta(a \mid s) = \dfrac{\exp(\theta^T \phi_{s,a})}{\sum_{a' \in \mathcal{A}} \exp(\theta^T \phi_{s,a'})}$
- Neural softmax policies: $\pi_\theta(a \mid s) = \dfrac{\exp(f_\theta(s,a))}{\sum_{a' \in \mathcal{A}} \exp(f_\theta(s,a'))}$

Continuous action space

- Gaussian policies: $a \sim \mathcal{N}(f_\theta(s), \sigma^2)$

Questions: Are these parametric policies general enough?

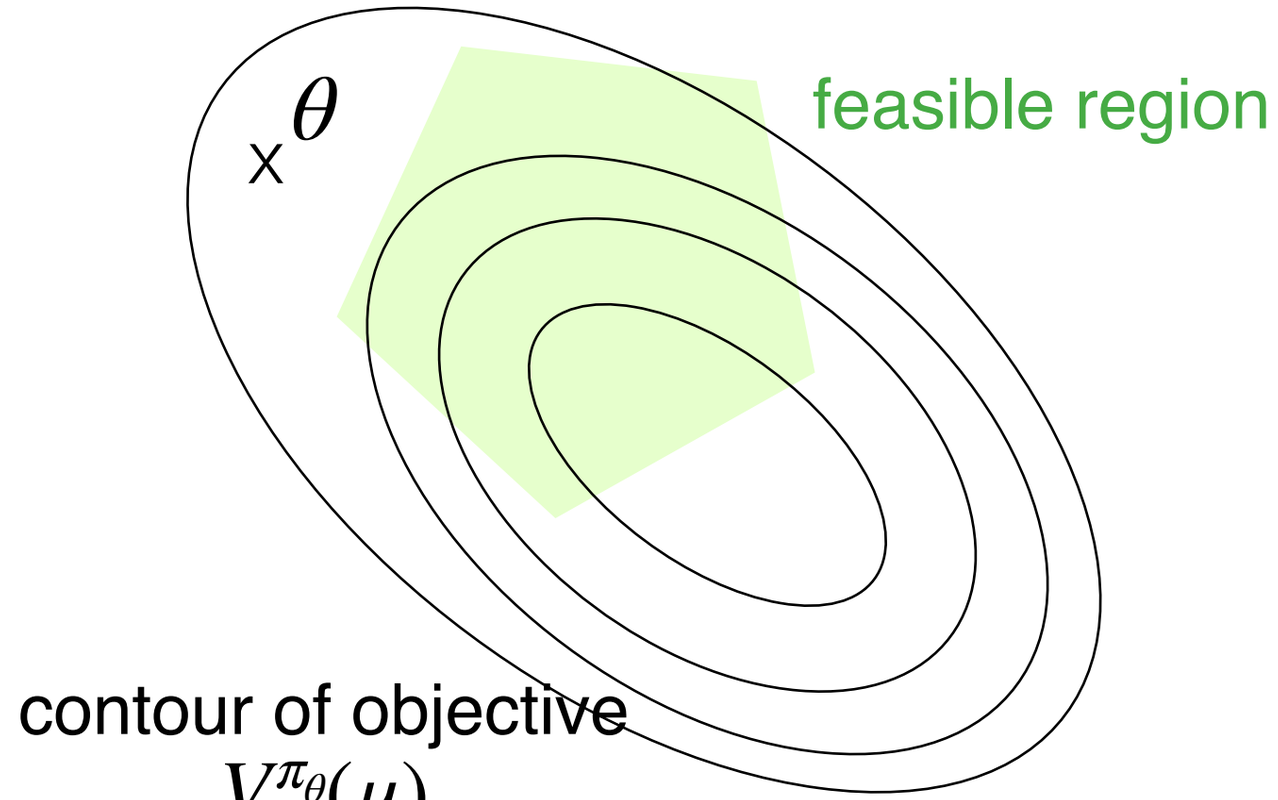
(We will come back to this momentarily)

How About Direct Tabular Parametrization?

- Question: Can we do direct parametrization, i.e., $\pi_\theta(a \mid s) = \theta_{s,a}$?
- Possible, but now we face constrained policy optimization

$$\max_{\theta \in \Theta} V^{\pi_\theta}(\mu)$$

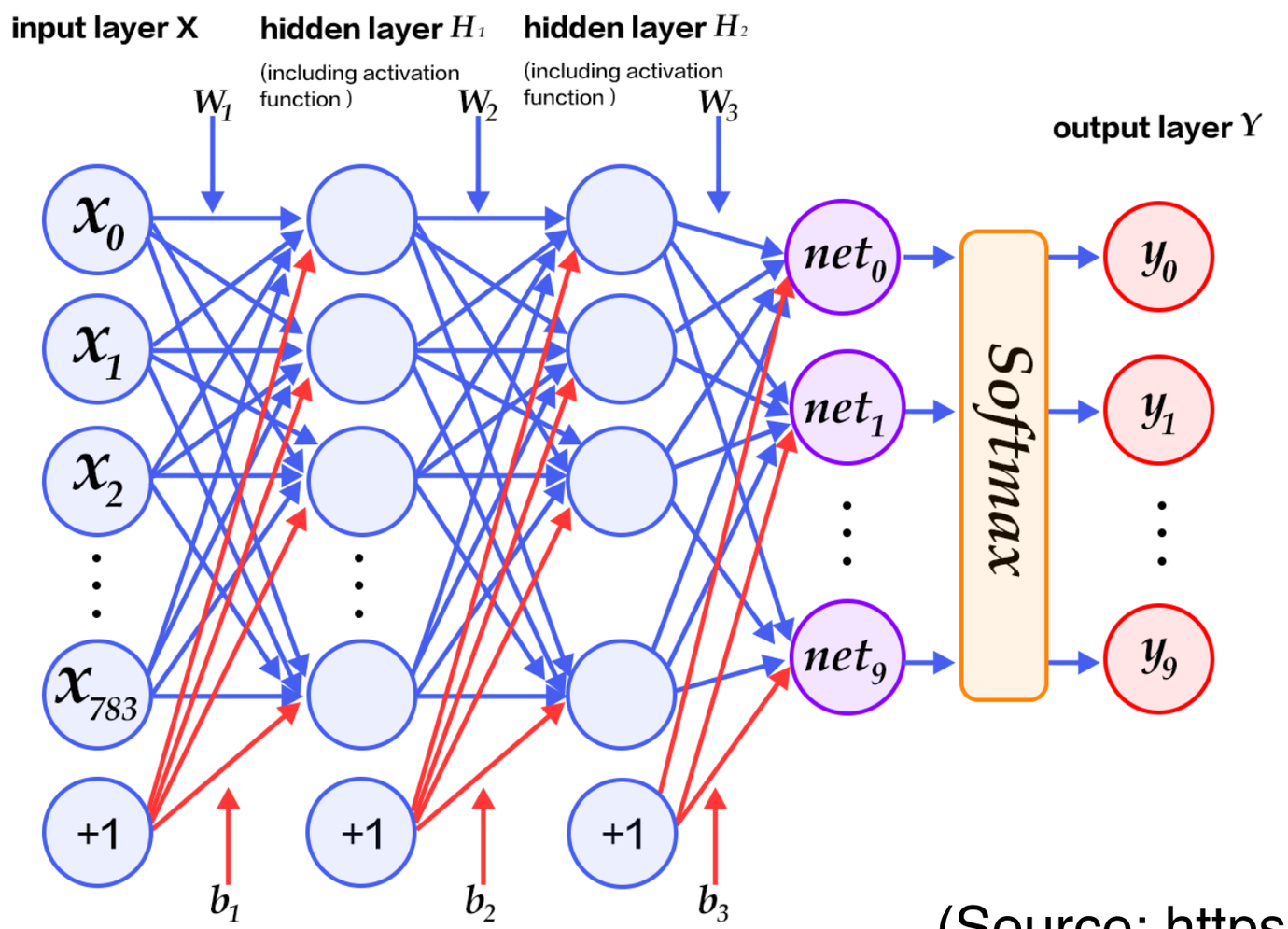
subject to $\sum_a \theta_{s,a} = 1, \forall s$



- In this case, *projection* is needed to ensure a valid probability distribution (often computationally heavy)

Neural Softmax Policies

- Neural softmax policies: $$\pi_\theta(a \mid s) = \frac{\exp(f_\theta(s, a))}{\sum_{a' \in \mathcal{A}} \exp(f_\theta(s, a'))}$$
  - θ denotes all the weights and biases of a neural net



(Source: https://files.ifi.uzh.ch/ddis/)

Policy Gradient (PG)

Historical Accounts on PG

Policy Gradient Methods for Reinforcement Learning with Function Approximation

Richard S. Sutton, David McAllester, Satinder Singh, Yishay Mansour
AT&T Labs – Research, 180 Park Avenue, Florham Park, NJ 07932

Abstract

Function approximation is essential to reinforcement learning, but the standard approach of approximating a value function and determining a policy from it has so far proven theoretically intractable. In this paper we explore an alternative approach in which the policy is explicitly represented by its own function approximator, independent of the value function, and is updated according to the gradient of expected reward with respect to the policy parameters. Williams's REINFORCE method and actor–critic methods are examples of this approach. Our main new result is to show that the gradient can be written in a form suitable for estimation from experience aided by an approximate action-value or advantage function. Using this result, we prove for the first time that a version of policy iteration with arbitrary differentiable function approximation is convergent to a locally optimal policy.

Richard Sutton
(U of Alberta & DeepMind)

Satinder Singh
(UMich & DeepMind)

A seminal paper on PG in NIPS 1999

Review: Some Useful Notations

- Question: To apply GA, what do we need?
- Policy gradient! $\nabla_\theta V^{\pi_\theta}(\mu)$ (μ: distribution of initial state)

Some useful notations

- 1. Sample return $G(\tau)$ along a trajectory $\tau = (s_0, a_0, r_1, \cdots)$

$$G(\tau) := \sum_{t=0}^{\infty} \gamma^t \cdot r_{t+1}(\tau)$$

- 2. Value function written in $R(\tau)$

$$V^{\pi_\theta}(\mu) = \mathbb{E}_{\tau \sim P_\mu^{\pi_\theta}}[G(\tau)] = \sum_{\tau} G(\tau) P_\mu^{\pi_\theta}(\tau)$$

Review: Some Useful Notations (Cont.)

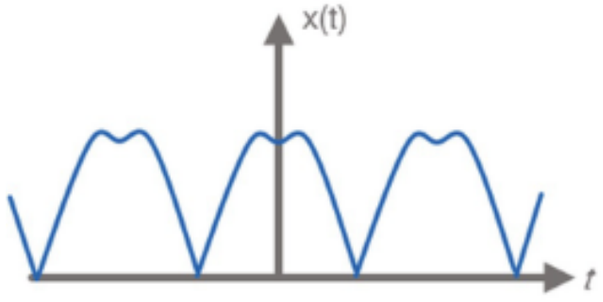
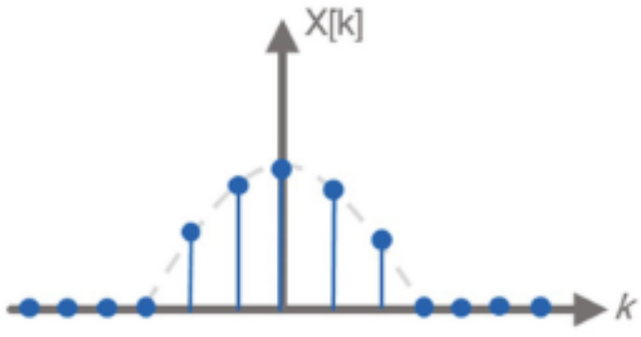
- 3. Discounted state visitation distribution (aka “occupancy measure”)

$$d^{\pi}_{s_0}(s) := (1-\gamma)\sum_{t=0}^{\infty}\gamma^t P(s_t = s \,|\, s_0, \pi)$$

$$d^{\pi}_{\mu}(s) := \mathbb{E}_{s_0\sim\mu}\left[d^{\pi}_{s_0}(s)\right]$$

- Question: What’s the purpose of $(1-\gamma)$ in the above?

State Visitation Distribution: An Analogy

	Time domain		Frequency domain
Fourier Series		≡	

	Time domain		Distribution domain
RL Objective Function	$\mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^t r_t \middle\| s_0 \sim \mu; \pi_\theta\right]$	=	$\mathbb{E}_{s\sim d_\mu^{\pi_\theta}, a\sim\pi(\cdot\|s)}\left[R(s,a)\right]$

(We will use this form several times in the sequel)

The Policy Gradient: Inherent Difficulty

- Issue: Computing $\nabla_\theta V^{\pi_\theta}(\mu)$ might seem highly non-trivial…
- Recall: $V^{\pi_\theta}(\mu) = \mathbb{E}_{\tau \sim P_\mu^{\pi_\theta}}[G(\tau)] = \sum_\tau G(\tau) P_\mu^{\pi_\theta}(\tau)$

- $V^{\pi_\theta}(\mu)$ is affected by θ in two ways:

1. θ determines $\pi_\theta(\cdot \mid s)$
2. The actions taken by π_θ affect the state visitation accordingly

Expressions of The Policy Gradient

- **Expressions of Policy Gradient (aka Policy Gradient Theorem)**:

(P1) Total reward: $\nabla_\theta V^{\pi_\theta}(\mu) = \mathbb{E}_{\tau \sim P_\mu^{\pi_\theta}}\left[G(\tau) \sum_{t=0}^{\infty} \nabla_\theta \log \pi_\theta(a_t \mid s_t)\right]$

(P2) REINFORCE: $\nabla_\theta V^{\pi_\theta}(\mu) = \mathbb{E}_{\tau \sim P_\mu^{\pi_\theta}}\left[\sum_{t=0}^{\infty} \gamma^t Q^{\pi_\theta}(s_t, a_t) \nabla_\theta \log \pi_\theta(a_t \mid s_t)\right]$

(P3) Q-value and discounted state visitation:

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

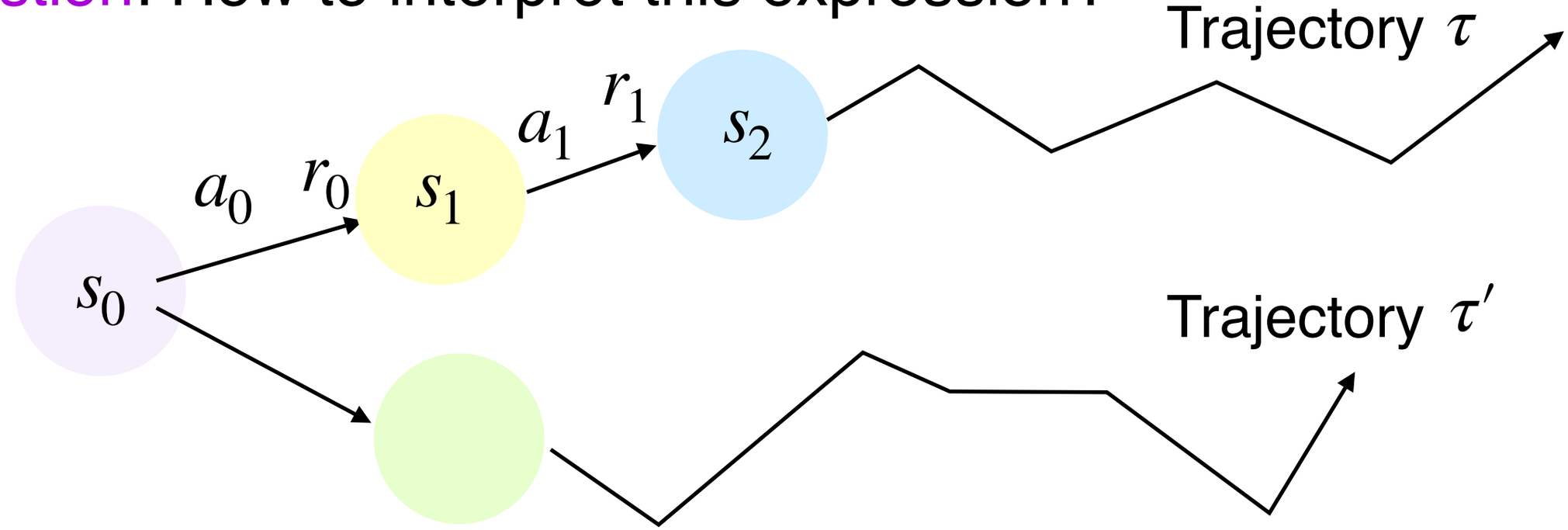
- Question: Why do we care about various expressions?
- Each expression gives us an RL algorithm!

[AJK, Chapter 11]

(P1) Total Reward Policy Gradient

- Want to show: $\nabla_\theta V^{\pi_\theta}(\mu) = \mathbb{E}_{\tau \sim P_\mu^{\pi_\theta}}\left[G(\tau) \sum_{t=0}^{\infty} \nabla_\theta \log \pi_\theta(a_t \mid s_t) \right]$

- Question: How to interpret this expression?



1. $G(\tau) > 0$:

2. $G(\tau) < 0$:

- Question: Can you find out any potential issue?

(P1) Total Reward Policy Gradient (Cont.)

- Want to show: $\nabla_\theta V^{\pi_\theta}(\mu) = \mathbb{E}_{\tau \sim P_\mu^{\pi_\theta}}\left[G(\tau) \sum_{t=0}^{\infty} \nabla_\theta \log \pi_\theta(a_t \mid s_t) \right]$
- Recall: $V^{\pi_\theta}(\mu) = \mathbb{E}_{\tau \sim P_\mu^{\pi_\theta}}[G(\tau)] = \sum_\tau G(\tau) P_\mu^{\pi_\theta}(\tau)$

$$
\begin{aligned}
\nabla_\theta V^{\pi_\theta}(\mu) &= \sum_\tau G(\tau) \nabla_\theta P_\mu^{\pi_\theta}(\tau) \\
&= \sum_\tau G(\tau) \left(P_\mu^{\pi_\theta}(\tau) \cdot \nabla_\theta \log P_\mu^{\pi_\theta}(\tau) \right) \\
&= \sum_\tau G(\tau) \left(P_\mu^{\pi_\theta}(\tau) \cdot \nabla_\theta \log(\mu(s_0)\pi_\theta(a_0 \mid s_0) P(s_1 \mid s_0, a_0)\pi_\theta(a_1 \mid s_1) \cdots) \right) \\
&= \sum_\tau G(\tau) \left(P_\mu^{\pi_\theta}(\tau) \cdot \sum_{t=0}^{\infty} \nabla_\theta \log \pi(a_t \mid s_t) \right) \\
&= \mathbb{E}_{\tau \sim P_\mu^{\pi_\theta}}\left[G(\tau) \sum_{t=0}^{\infty} \nabla_\theta \log \pi_\theta(a_t \mid s_t) \right]
\end{aligned}
$$

(Not a rigorous proof)

Technical Subtlety in the Proof of (P1):

- For τ of infinite length, $\nabla_\theta P_\mu^{\pi_\theta}(\tau)$ needs to be handled more carefully
- Idea: Consider "truncated trajectories" and take the limit

1. Without loss of generality, assume $R(s,a) \in [0,1]$

   Define $\tau^{(k)}$ to be the truncated version of τ up to step k

   Define $V_k^{\pi_\theta}(\mu) = \sum_{\tau^{(k)}} G(\tau^{(k)}) P_\mu^{\pi_\theta}(\tau^{(k)})$

2. Then, $\lim_{k\to\infty} V_k^{\pi_\theta}(\mu) = V^{\pi_\theta}(\mu)$ (by Monotone convergence theorem)

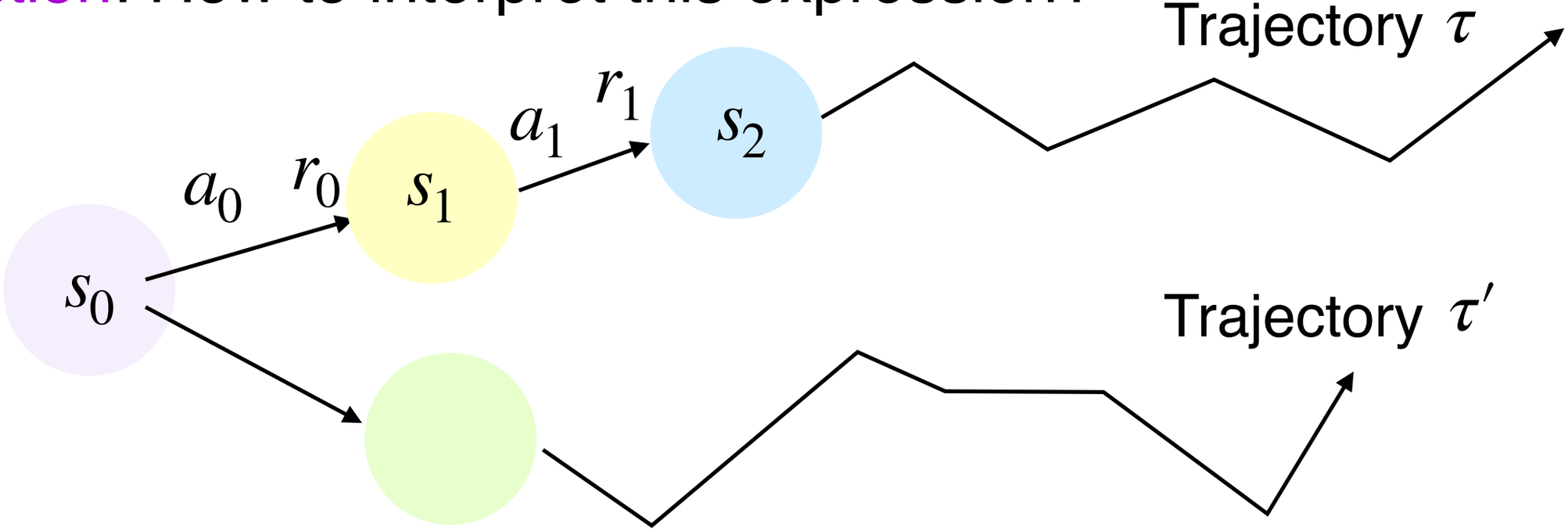
3. Next, we need to verify that $\lim_{k\to\infty} \nabla_\theta V_k^{\pi_\theta}(\mu) = \nabla_\theta V^{\pi_\theta}(\mu)$ by showing "uniform convergence" of $\nabla_\theta V_k^{\pi_\theta}(\mu)$ [Rudin 1976, Thm 7.17]

(Note that it is not always valid to interchange ∇ and $\lim$)

(P2) REINFORCE Policy Gradient

- Want to show: $\nabla_\theta V^{\pi_\theta}(\mu) = \mathbb{E}_{\tau \sim P_\mu^{\pi_\theta}}\left[\sum_{t=0}^{\infty} \gamma^t Q^{\pi_\theta}(s_t, a_t) \nabla_\theta \log \pi_\theta(a_t \mid s_t)\right]$

- Question: How to interpret this expression?



1. $Q(s, a) > 0$:

2. $Q(s, a) < 0$:

- Question: Can you find out any potential issue?

(P2) REINFORCE Policy Gradient

- Want to show: $\nabla_\theta V^{\pi_\theta}(\mu) = \mathbb{E}_{\tau \sim P_\mu^{\pi_\theta}}\left[\sum_{t=0}^{\infty} \gamma^t Q^{\pi_\theta}(s_t, a_t) \nabla_\theta \log \pi_\theta(a_t \mid s_t) \right]$
- Idea: prove by induction
- Recall: $V^{\pi_\theta}(s_0) = \sum_{a_0 \in \mathcal{A}} \pi_\theta(a_0 \mid s_0) Q^{\pi_\theta}(s_0, a_0)$

$$\nabla_\theta V^{\pi_\theta}(s_0) = \sum_{a_0} \nabla_\theta \left(\pi_\theta(a_0 \mid s_0) Q^{\pi_\theta}(s_0, a_0) \right)$$

$$= \underbrace{\sum_{a_0} \nabla_\theta \left(\pi_\theta(a_0 \mid s_0) \right) Q^{\pi_\theta}(s_0, a_0)}_{(1)} + \underbrace{\sum_{a_0} \pi_\theta(a_0 \mid s_0) \nabla \left(Q^{\pi_\theta}(s_0, a_0) \right)}_{(2)}$$

$$(1) = \sum_{a_0} \pi_\theta(a_0 \mid s_0) \cdot \nabla_\theta \left(\log \pi_\theta(a_0 \mid s_0) \right) \cdot Q^{\pi_\theta}(s_0, a_0)$$

$$= \mathbb{E}_{\tau \sim P_{s_0}^{\pi_\theta}}\left[\nabla_\theta \left(\log \pi_\theta(a_0 \mid s_0) \right) \cdot Q^{\pi_\theta}(s_0, a_0) \right]$$

(P2) REINFORCE Policy Gradient (Cont.)

$$
\begin{aligned}
(2) &= \sum_{a_0} \pi_\theta(a_0 \mid s_0)\, \nabla \Big(Q^{\pi_\theta}(s_0, a_0) \Big) \\
&= \sum_{a_0} \pi_\theta(a_0 \mid s_0)\, \nabla_\theta \Big(r(s_0, a_0) + \gamma \sum_{s_1} P(s_1 \mid s_0, a_0) \cdot V^{\pi_\theta}(s_1) \Big) \\
&= \sum_{a_0} \pi_\theta(a_0 \mid s_0) \Big(\gamma \sum_{s_1} P(s_1 \mid s_0, a_0) \cdot \nabla_\theta V^{\pi_\theta}(s_1) \Big) \\
&= \mathbb{E}_{\tau \sim P^{\pi_\theta}_{s_0}} \Big[\gamma \nabla_\theta V^{\pi_\theta}(s_1) \Big]
\end{aligned}
$$

By combining (1) and (2):

$$
\nabla_\theta V^{\pi_\theta}(s_0) = \mathbb{E}_{\tau \sim P^{\pi_\theta}_{s_0}} \Big[\nabla_\theta \big(\log \pi_\theta(a_0 \mid s_0) \big) \cdot Q^{\pi_\theta}(s_0, a_0) \Big] + \mathbb{E}_{\tau \sim P^{\pi_\theta}_{s_0}} \Big[\gamma \nabla_\theta V^{\pi_\theta}(s_1) \Big]
$$

This is a recursion!

(P2) REINFORCE Policy Gradient (Cont.)

Given the recursion:

$$\nabla_\theta V^{\pi_\theta}(s_0) = \mathbb{E}_{\tau \sim P_{s_0}^{\pi_\theta}}\Big[\nabla_\theta\big(\log \pi_\theta(a_0 \,|\, s_0)\big) \cdot Q^{\pi_\theta}(s_0, a_0)\Big] + \mathbb{E}_{\tau \sim P_{s_0}^{\pi_\theta}}\Big[\gamma \nabla_\theta V^{\pi_\theta}(s_1)\Big]$$

- We can verify that:

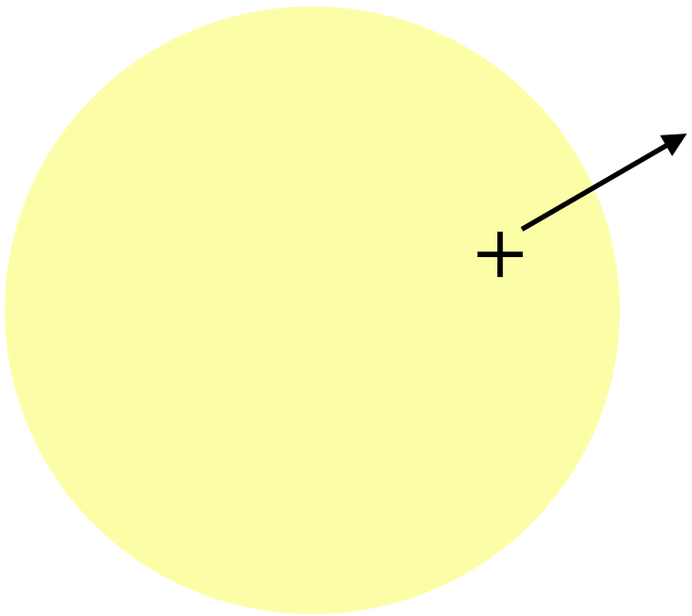
$$\nabla_\theta V^{\pi_\theta}(\mu) = \mathbb{E}_{\tau \sim P_\mu^{\pi_\theta}}\Big[\sum_{t=0}^{\infty} \gamma^t Q^{\pi_\theta}(s_t, a_t)\, \nabla_\theta \log \pi_\theta(a_t \,|\, s_t)\Big]$$

(P3) Q-Value and Discounted State Visitation

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

- Question: How to interpret this expression?

Sample space of (s, a)



1. $Q(s,a) > 0$:

2. $Q(s,a) < 0$:

- Question: Why is this expression useful?

(P3) Q-Value and Discounted State Visitation (Cont.)

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

- Proof idea: Use the following lemma and (P2)

- **Lemma (From Trajectories to Visitation)**:

  For any function $f(s,a) : \mathcal{S}\times\mathcal{A}\to\mathbb{R}$, we have

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

- Proof: Expand RHS and recollect terms to get LHS (HW1)