

# Mathematics for Machine Learning

## — Continuous Optimization

### Introduction to the Policy Gradient Trick

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Fall 2025

## Credits for the resource

- The slides are based on the textbooks and reference lectures:
  - *Marc Peter Deisenroth, A. Aldo Faisal, and Cheng Soon Ong: Mathematics for Machine Learning. Cambridge University Press. 2020.*
  - *Roger Grosse's Course Lectures on Neural Networks and Deep Learning*  
([https://www.cs.toronto.edu/~rgrosse/courses/csc421\\_2019/](https://www.cs.toronto.edu/~rgrosse/courses/csc421_2019/)).
- We could partially refer to the monograph:  
*Francesco Orabona: A Modern Introduction to Online Learning.*  
<https://arxiv.org/abs/1912.13213>

# Outline

- 1 Markov Decision Process (MDP)
- 2 Policy Gradient

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# Reinforcement Learning (RL)

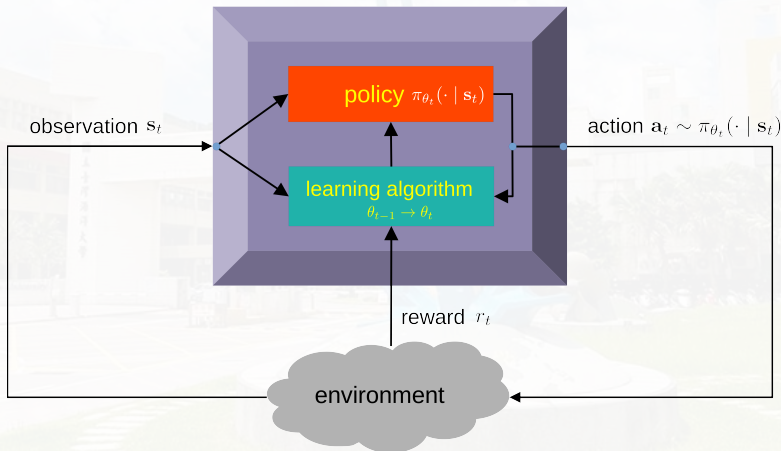
From *Wikipedia*:

- *Reinforcement learning (RL) is an interdisciplinary area of machine learning and optimal control concerned with how an intelligent agent should **take actions** in a **dynamic environment** in order to **maximize a reward signal**.*
- *Reinforcement learning is one of the three basic machine learning paradigms, alongside supervised learning and unsupervised learning.*
- Example of RL environments: [link].

# RL Setting

- Each **agent** interacts with an **environment** (static or dynamic).
- In each time step  $t$ ,
  - the agent receives feedback or observations from the environment about the **state**  $\mathbf{s}_t$ .
  - the agent then takes an action  $\mathbf{a}_t$  which can affect the state ( $\mathbf{s}_t \rightarrow \mathbf{s}_{t+1}$ ).
  - the agent receives the **reward**  $r(\mathbf{s}_t, \mathbf{a}_t)$ .
- Goal of the agent: learn a policy  $\pi_{\theta}(\mathbf{a}_t, \mathbf{s}_t)$ .
  - A distribution over the actions given the current state  $\mathbf{s}_t$  and the parameter  $\theta$ .
    - $\theta$ : can be regarded as a machine learning model.

# RL Setting



# Markov Decision Process (MDP) (1/3)

- Markov decision process (MDP): an RL environment setting.
- Assumption: all information is encapsulated in the current state  $\mathbf{s}_t$ ; transitions are independent of past states.

## MDP components

- initial state distribution  $p(\mathbf{s}_0)$ .
  - policy:  $\pi_{\theta}(\mathbf{s}_t, \mathbf{a}_t)$
  - transition prob.:  $p(\mathbf{s}_{t+1} \mid \mathbf{s}_t, \mathbf{a}_t)$ .
  - reward function:  $r(\mathbf{s}_t, \mathbf{a}_t)$ .
- 
- We consider **fully observable** environment.
    - $\mathbf{s}_t$  can be observed **directly**.



# Markov Decision Process (MDP) (2/3)

- **Trajectory** or **rollout**:  $\tau = (\mathbf{s}_0, \mathbf{a}_0, \mathbf{s}_1, \mathbf{a}_1, \dots, \mathbf{s}_T, \mathbf{a}_T)$
- Probability of a trajectory:

$$p(\tau) = p(\mathbf{s}_0) \pi_{\theta}(\mathbf{a}_0 \mid \mathbf{s}_0) p(\mathbf{s}_1 \mid \mathbf{s}_0, \mathbf{a}_0) \pi_{\theta}(\mathbf{a}_1 \mid \mathbf{s}_1) p(\mathbf{s}_2 \mid \mathbf{s}_1, \mathbf{a}_1) \cdots p(\mathbf{s}_T \mid \mathbf{s}_{T-1}, \mathbf{a}_{T-1}) \pi_{\theta}(\mathbf{a}_T \mid \mathbf{s}_T).$$

- Return for a trajectory:  $r(\tau) = \sum_{t=0}^T r(\mathbf{s}_t, \mathbf{a}_t)$ .
- **Goal**: Maximize  $R := \mathbb{E}_{p(\tau)}[r(\tau)]$ .
- The expectation is over the environment's dynamics and the policy, but we only have control over the **policy**.

# Markov Decision Process (MDP) (3/3)

- ★ What's the issue when we compute  $p(\tau)$  and  $R$ ?

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- ★ What's the issue when we compute  $p(\tau)$  and  $R$ ?
- Each long trajectory could happen with extremely low probability.
- Problematic to derive  $\frac{dR}{d\theta}$ .

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# The Log-derivative Trick

## Log-derivative Trick

$$\frac{\partial}{\partial \theta} \log p(\tau) = \frac{1}{p(\tau)} \frac{\partial}{\partial \theta} p(\tau).$$

- Hence, the gradient of the expected return turns out to be

$$\begin{aligned} \frac{\partial}{\partial \theta} \mathbb{E}_{p_{\theta}(\tau)}[r(\tau)] &= \frac{\partial}{\partial \theta} \sum_{\tau} r(\tau) p_{\theta}(\tau) = \sum_{\tau} r(\tau) \frac{\partial p_{\theta}(\tau)}{\partial \theta} \\ &= \sum_{\tau} r(\tau) p_{\theta}(\tau) \frac{\partial}{\partial \theta} \log p_{\theta}(\tau) \\ &= \mathbb{E}_{p_{\theta}(\tau)} \left[ r(\tau) \frac{\partial}{\partial \theta} \log p_{\theta}(\tau) \right]. \end{aligned}$$

# Estimate of the gradient

$$\frac{\partial}{\partial \theta} \mathbb{E}_{p_{\theta}(\tau)}[r(\tau)] = \mathbb{E}_{p_{\theta}(\tau)} \left[ r(\tau) \frac{\partial}{\partial \theta} \log p_{\theta}(\tau) \right].$$

- Sampling the trajectories and rewards to have its estimate.

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- Sampling the trajectories and rewards to have its estimate.
- Let's unpack the gradient of  $\log p_{\theta}(\tau)$ :

$$\begin{aligned} \frac{\partial}{\partial \theta} \log p_{\theta}(\tau) &= \frac{\partial}{\partial \theta} \log \left[ p(\mathbf{s}_0) \prod_{t=0}^T \pi_{\theta}(\mathbf{a}_t \mid \mathbf{s}_t) \prod_{t=1}^T p(\mathbf{s}_t \mid \mathbf{s}_{t-1}, \mathbf{a}_{t-1}) \right] \\ &= \frac{\partial}{\partial \theta} \log \left( \prod_{t=0}^T \pi_{\theta}(\mathbf{a}_t \mid \mathbf{s}_t) \right) \\ &= \sum_{t=0}^T \frac{\partial}{\partial \theta} \log(\pi_{\theta}(\mathbf{a}_t \mid \mathbf{s}_t)). \end{aligned}$$

# Update after $T$ steps

- Let a trajectory be  $\tau = (\mathbf{s}_0, \mathbf{a}_0, \dots, \mathbf{s}_T, \mathbf{a}_T)$  and define the episode return

$$r(\tau) = \sum_{k=0}^T r(\mathbf{s}_k, \mathbf{a}_k).$$

Since we have the gradient

$$\nabla_{\theta} \mathbb{E}_{p_{\theta}(\tau)}[r(\tau)] = \mathbb{E}_{p_{\theta}(\tau)} \left[ r(\tau) \sum_{t=0}^T \nabla_{\theta} \log \pi_{\theta}(\mathbf{a}_t | \mathbf{s}_t) \right].$$

- Issue:**

- How to perform the expectation  $\mathbb{E}_{p_{\theta}(\tau)}[\cdot]$ ?

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$$\nabla_{\theta} \mathbb{E}_{p_{\theta}(\tau)}[r(\tau)] \approx \frac{1}{N} \sum_{i=1}^N r(\tau^{(i)}) \sum_{t=0}^{T_i} \nabla_{\theta} \log \pi_{\theta}(\mathbf{a}_t^{(i)} \mid \mathbf{s}_t^{(i)}).$$

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**update rule:** ( $\eta$ : the step-size)

$$\theta' \leftarrow \theta + \eta \frac{1}{N} \sum_{i=1}^N r(\tau^{(i)}) \sum_{t=0}^{T_i} \nabla_{\theta} \log \pi_{\theta}(\mathbf{a}_t^{(i)} \mid \mathbf{s}_t^{(i)}).$$

or equivalently,

$$\theta' \leftarrow \theta + \eta \frac{1}{\sum_i^N T_i + 1} \sum_{i=1}^N \sum_{t=0}^{T_i} r(\tau^{(i)}) \nabla_{\theta} \log \pi_{\theta}(\mathbf{a}_t^{(i)} \mid \mathbf{s}_t^{(i)}).$$

# An online iterative update approach

Given a trajectory  $\tau = (\mathbf{s}_0, \mathbf{a}_0, \dots, \mathbf{s}_T, \mathbf{a}_T)$  and define the episode return

$$r(\tau) = \sum_{k=0}^T r(\mathbf{s}_k, \mathbf{a}_k).$$

Since the gradient is

$$\nabla_{\theta} \mathbb{E}_{p_{\theta}(\tau)}[r(\tau)] = \mathbb{E}_{p_{\theta}(\tau)} \left[ r(\tau) \sum_{t=0}^T \nabla_{\theta} \log \pi_{\theta}(\mathbf{a}_t | \mathbf{s}_t) \right],$$

**Online single-episode update:** ( $\eta$ : the step-size)

$$\theta_{t+1} \leftarrow \theta_t + \eta r(\tau) \underbrace{\nabla_{\theta} \log \pi_{\theta}(\mathbf{a}_t | \mathbf{s}_t)}_{\text{accumulated with } t} \quad \text{for } t = 0, 1, \dots, T.$$

# Credit only future rewards (still unbiased)

Split the total return at time  $t$  into past and future parts:

$$r(\tau) = \underbrace{\sum_{k=0}^{t-1} r(\mathbf{s}_k, \mathbf{a}_k)}_{P_t} + \underbrace{\sum_{k=t}^T r(\mathbf{s}_k, \mathbf{a}_k)}_{F_t =: r_t(\tau)}.$$

Then  $\mathbb{E}[P_t \nabla_{\theta} \log \pi_{\theta}(\mathbf{a}_t | \mathbf{s}_t)] = 0$ , since

$$\begin{aligned} \mathbb{E}_{\mathbf{a}_t \sim \pi_{\theta}(\cdot | \mathbf{s}_t)}[\nabla_{\theta} \log \pi_{\theta}(\mathbf{a}_t | \mathbf{s}_t)] &= \sum_{\mathbf{a}} \pi_{\theta}(\mathbf{a} | \mathbf{s}_t) \nabla_{\theta} \log \pi_{\theta}(\mathbf{a}_t | \mathbf{s}_t) \\ &= \nabla_{\theta} \sum_{\mathbf{a}} \pi_{\theta}(\mathbf{a} | \mathbf{s}_t) = 0. \end{aligned}$$

Hence we may drop  $P_t$  to have the gradient without bias.

**Update rule:**  $\theta_{t+1} \leftarrow \theta_t + \alpha r_t(\tau) \nabla_{\theta} \log \pi_{\theta}(\mathbf{a}_t | \mathbf{s}_t), \quad t = 0, 1, \dots, T.$

# Discussions