# Mathematics for Machine Learning

Continuous Optimization
 Introduction to the Policy Gradient Trick

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#### 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/r̃grosse/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)

Policy Gradient

ML Math - Continuous Optimization
Markov Decision Process (MDP)

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2 Policy Gradient

### Reinforcement Learning (RL)

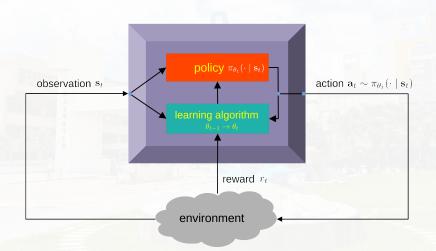
#### From Wikipedia:

- 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 s<sub>t</sub>.
  - the agent then takes an action  $\mathbf{a}_t$  which can affect the state  $(\mathbf{s}_t \to \mathbf{s}_{t+1})$ .
  - 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  $\boldsymbol{\theta}$ .
    - $\theta$ : 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.
  - **s**<sub>t</sub> can be observed directly.



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

- Trajectory or rollout:  $\tau = (s_0, a_0, s_1, a_1, \dots, s_T, a_T)$
- Probability of a trajectory:

$$p(\tau) = p(s_0) \pi_{\theta}(a_0 | s_0) p(s_1 | s_0, a_0) \pi_{\theta}(a_1 | s_1) p(s_2 | s_1, a_1)$$

$$\cdots p(s_T | s_{T-1}, a_{T-1}) \pi_{\theta}(a_T | s_T).$$

- 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.

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- $\star$  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

$$\begin{split} \frac{\partial}{\partial \boldsymbol{\theta}} \, \mathbb{E}_{p_{\boldsymbol{\theta}}(\tau)}[\, r(\tau)\,] &= \frac{\partial}{\partial \boldsymbol{\theta}} \sum_{\tau} r(\tau) \, p_{\boldsymbol{\theta}}(\tau) = \sum_{\tau} r(\tau) \, \frac{\partial p_{\boldsymbol{\theta}}(\tau)}{\partial \boldsymbol{\theta}} \\ &= \sum_{\tau} r(\tau) \, p_{\boldsymbol{\theta}}(\tau) \, \frac{\partial}{\partial \boldsymbol{\theta}} \log p_{\boldsymbol{\theta}}(\tau) \\ &= \mathbb{E}_{p_{\boldsymbol{\theta}}(\tau)} \Big[\, r(\tau) \, \frac{\partial}{\partial \boldsymbol{\theta}} \log p_{\boldsymbol{\theta}}(\tau) \, \Big]. \end{split}$$

### Estimate of the gradient

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

Sampling the trajectories and rewards to have its estimate.

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### Estimate of the gradient

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

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

#### REINFORCE: vanilla Monte-Carlo estimator

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

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

Since we have the gradient

$$\mathbb{E}_{\tau}\Big[\mathit{r}(\tau)\sum_{t=0}^{T}\nabla_{\theta}\log\pi_{\theta}(\mathbf{a}_{t}\mid\mathbf{s}_{t})\Big].$$

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

$$\theta_{t+1} \leftarrow \theta_t + \eta r(\tau) \nabla_{\theta} \log \pi_{\theta}(\mathbf{a}_t \mid \mathbf{s}_t)$$
 for  $t = 0, 1, ..., T$ .

# 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

$$\mathbb{E}\big[P_t \nabla_{\boldsymbol{\theta}} \log \pi_{\boldsymbol{\theta}}(\mathbf{a}_t \mid \mathbf{s}_t)\big] = 0, \quad \text{since}$$

$$\begin{split} \mathbb{E}_{\mathbf{a}_t \sim \pi_{\boldsymbol{\theta}}(\cdot \mid \mathbf{s}_t)} \big[ \nabla_{\boldsymbol{\theta}} \log \pi_{\boldsymbol{\theta}}(\mathbf{a}_t \mid \mathbf{s}_t) \big] &= \sum_{\mathbf{a}} \pi_{\boldsymbol{\theta}}(\mathbf{a} \mid \mathbf{s}_t) \nabla_{\boldsymbol{\theta}} \log \pi_{\boldsymbol{\theta}}(\mathbf{a}_t \mid \mathbf{s}_t) \big] \\ &= `\nabla_{\boldsymbol{\theta}} \sum \pi_{\boldsymbol{\theta}}(\mathbf{a} \mid \mathbf{s}_t) = 0. \end{split}$$

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

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

# **Discussions**