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/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

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Reinforcement Learning (RL)

From *Wikipedia*:

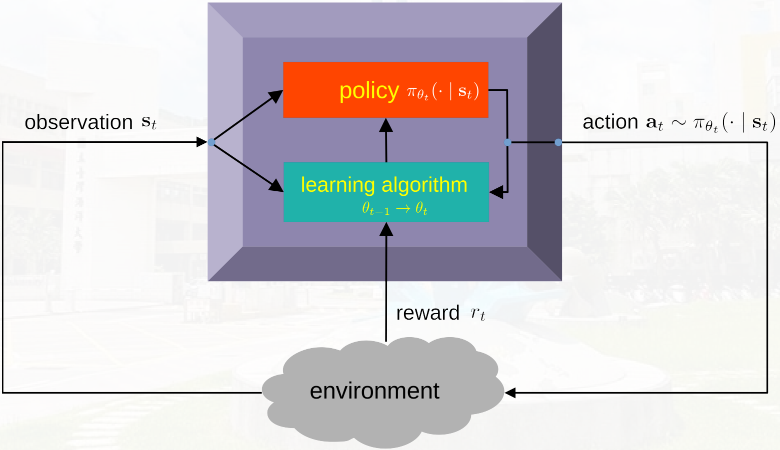
- *Reinforcement learning (RL) is an interdisciplinary area of machine learning and optimal control concerned with how an intelligent agent should take actions in a dynamic environment in order to maximize a reward signal.*
- *Reinforcement learning is one of the three basic machine learning paradigms, 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 ($\mathbf{s}_t \to \mathbf{s}_{t+1}$).
  - the agent receives the **reward** $r(\mathbf{s}_t, \mathbf{a}_t)$.
- Goal of the agent: learn a policy $\pi_{\boldsymbol{\theta}}(\mathbf{a}_t, \mathbf{s}_t)$.
  - A distribution over the actions given the current state $\mathbf{s}_t$ and the parameter $\boldsymbol{\theta}$.
    - $\boldsymbol{\theta}$: can be regarded as a machine learning model.

RL Setting


policy $\pi_{\theta_t}(\cdot \mid \mathbf{s}_t)$
learning algorithm
$\theta_{t-1} \to \theta_t$
observation $\mathbf{s}_t$
action $\mathbf{a}_t \sim \pi_{\theta_t}(\cdot \mid \mathbf{s}_t)$
reward r_t
environment

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: $\pi_{\boldsymbol{\theta}}(\mathbf{s}_t, \mathbf{a}_t)$
- 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: $\tau = (\mathbf{s}_0, \mathbf{a}_0, \mathbf{s}_1, \mathbf{a}_1, \ldots, \mathbf{s}_T, \mathbf{a}_T)$
- Probability of a trajectory:

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

- 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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- Each long trajectory could happen with extremely low probability.

Markov Decision Process (MDP) (3/3)

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

Outline

The Log-derivative Trick

Log-derivative Trick

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

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

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

Estimate of the gradient

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

- Sampling the trajectories and rewards to have its estimate.

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- Let's unpack the gradient of $\log p_{\boldsymbol{\theta}}(\tau)$:

Estimate of the gradient

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

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

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

Update after T steps

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

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

  Since we have the gradient

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

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

Update after a sequence of N trajectories

- Given trajectories $\tau^{(1)}, \tau^{(2)}, \ldots, \tau^{(N)}$, each consists of T_i steps.

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

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update rule: (η: the step-size)

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

or a time-step-averaged alternative:

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

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

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

Online single-episode update: (η: the step-size)

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

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

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

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

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

Discussions