Function Approximations and Policy Gradients in Reinforcement Learning

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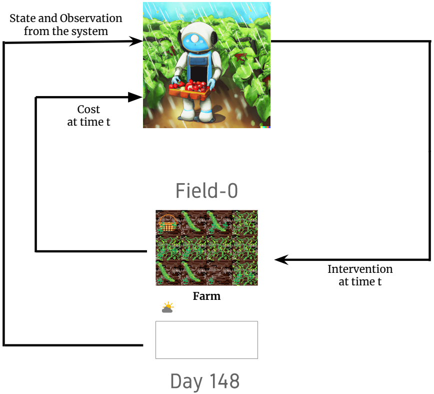
PART 1

Revisiting MDPs and RL Algorithms

RL: sequentially learning to take optimal decisions under uncertainty.



The goal of the agent is to compute a policy or strategy that maximises the reward accumulated over a time horizon.

Formalism of the Environment: Markov Decision Processes

A Markov Decision Process (MDP) is a tuple $\mathcal{M} \triangleq \langle \mathcal{S}, \mathcal{A}, \mathcal{P}, \mathcal{R}, \gamma \rangle$

- **State:** $s \in \mathcal{S} \subseteq \mathbb{R}^d$
- **Action/Intervention/Control:** $a \in \mathcal{A} \subseteq \mathbb{R}^d$
- **Transition function/dynamics:** $\mathcal{P}(.|s, a)$ induces a distribution over s_{t+1} for s_t, a_t (previously f)
- **Reward Function:** $\mathcal{R}(.|s, a)$ induces a distribution over $\mathbb{R}$ measuring goodness of an action a at state s (negative of cost function)

Formalism of the Agent: Policy and Value Function

- **Policy:** A deterministic or stochastic map $\pi(\cdot|s_t)$ from present state s_t to actions
- **How good or bas is your policy?** Value Function (Negative of cost of control)

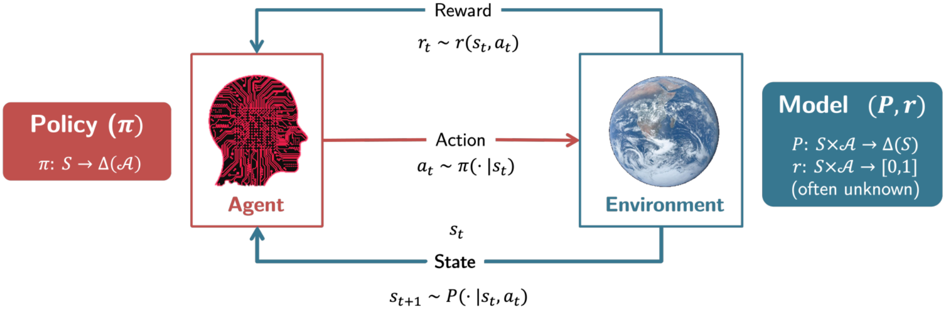
$$V_\pi(s_0) \triangleq \sum_{t=0}^{\infty} \gamma^t \mathcal{R}_t(s_t, \pi(s_t))$$

Or, action-value functions or Q values

$$Q_\pi(s_0, a_0) \triangleq \mathcal{R}(s_0, a_0) + \sum_{t=1}^{\infty} \gamma^t \mathcal{R}_t(s_t, \pi(s_t))$$

Goal: Find an optimal policy π^* maximising $V_\pi(s_0)$.

$$\textbf{Value:}\quad V^\pi(s) := \mathbb{E}_\pi\left[\sum_{t=0}^{\infty}\gamma^t r(s_t,a_t)\middle| s_0 = s\right] \Rightarrow \max_{\pi\in\Pi}\; V^\pi(s)$$



Courtesy: Niao He, RLSS 2023

A Generic Template of RL Algorithms: Generalised Policy Iteration

Algorithm Generalised Policy Iteration

```
Input: Initial Policy π_0
for episode k = 1, 2, ... do
    Observe an initial state s_0^k
    Rollouts: Collect trajectory data {r(s_h^k, a_h^k), s_{h+1}^k}_{h=0}^H and state s_{h+1}^k by playing policy π_k
    Policy Evaluation: Compute the value function of the policy V_{π_k}(s_0^k)
    Policy Optimisation: Use V_{π_k}(s_0^k) to compute a better policy π_{k+1}
end for
return policy π_K.
```

A Taxonomy of RL Algorithms

1. Level of interaction with the environment:
    - Online: Sequentially learn while collecting data by interacting with the environment
    - Offline: Use data collected in advance by some behavioural policy (e.g. Monte-Carlo methods)

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   - Value-based RL (Off-policy): Find optimal value function $V^*_{\mathcal{M}}$, use it to compute $\pi^\star$
   - Policy-based RL (On-policy): Evaluate π, improve π, and repeat

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3. Knowledge of the model:
   - Planning: $\mathcal{R}$ and $\mathcal{P}$ are known (dynamic programming)
   - Model-based/model-predictive/model-learning: estimate $\mathcal{R}$ and $\mathcal{P}$ from data yielded through interactions
   - Model-free: no knowledge of $\mathcal{R}$ and $\mathcal{P}$ is used– only transition data

Algorithm Iterative Policy Evaluation

Input: A policy π, steps K
Initialise: value function $V_0(s) = 0$ for all $s \in \mathcal{S}$
for steps $k = 1, 2, \dots, K$ **do**
  for states $s \in \mathcal{S}$ **do**
    Using collected dataset or by rolling out π, compute the Bellman update equation

$$V_k(s) \leftarrow \mathcal{T} V_{k-1}(s) = \mathcal{R}(s, \pi(s)) + \gamma \sum_{s' \in \mathcal{S}} \mathcal{P}(s'|s, \pi(s)) V_{k-1}(s') \tag{1}$$

  end for
end for
return estimated value function $V_\pi(s) \leftarrow V_K(s)$ for all s.

Greedy improvement: Bellman optimality equations

Value function

$$V^*_{\mathcal{M}}(s) = \max_a Q^*_{\mathcal{M}}(s,a)$$

Q-Value function

$$Q^*_{\mathcal{M}}(s,a) = \mathcal{T}^\star Q^*_{\mathcal{M}}(s,a) = \mathcal{R}(s,a) + \sum_{s' \in \mathcal{S}} \mathcal{P}(s'|s,a) V^*_{\mathcal{M}}(s)$$

Policy Improvement in MDPs with Discrete State-Actions → Q-value Iteration

Greedy improvement: Bellman optimality equations

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Algorithm Q-value iteration (Off-policy, Planning with full information)

1: **Input:** Steps K
2: **Initialise:** Q-value function $Q_0(s,a) = 0$ for all $s,a \in \mathcal{S} \times \mathcal{A}$
3: **for** episodes $k = 1, 2, \ldots, K$, and state-action pairs $(s,a) \in (\mathcal{S}, \mathcal{A})$ **do**
4: **Compute Q-table:** Evaluate the greedy policy using the Bellman update equation

$$Q_k(s, \pi(s)) \leftarrow \mathcal{R}(s, \pi(s)) + \gamma \sum_{s' \in \mathcal{S}} \mathcal{P}(s'|s, \pi(s)) \max_b Q_{k-1}(s', b) \tag{2}$$

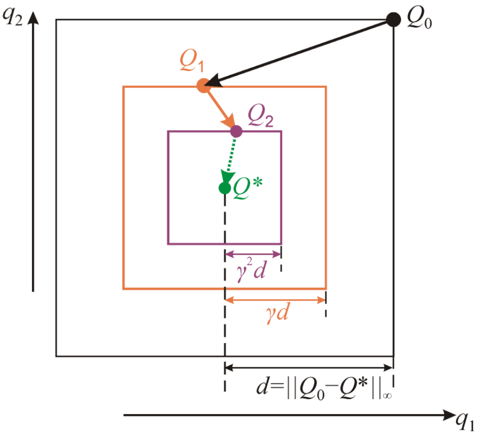
5: **end for**
6: **return** the **greedy policy** for all s

$$\pi_K(s) \in \arg\max_{a \in \mathcal{A}} Q_K(s,a) \tag{3}$$

Why Does Q-iteration Work?

Q-iteration is a fixed point contraction through stochastic approximation.

$$\|Q_k - Q^*_{\mathcal{M}}\|_\infty = \|\textcolor{red}{\mathcal{T}^\star} Q_{k-1} - Q^*_{\mathcal{M}}\|_\infty \leq \gamma \|Q_{k-1} - Q^*_{\mathcal{M}}\|_\infty$$



Alternative update of Equation (2)

$$Q_k(s) = (1-\alpha) Q_{k-1}(s) + \alpha \textcolor{red}{\mathcal{T}^\star} Q_{k-1}(s)$$

This works as
(1) Bellman operator is a contraction, and
(2) $\mu_k = (1-\alpha)\mu_{k-1} + \alpha \times$ new sample
is a consistent stochastic approximation of mean.

Limitations of GPIs in MDPs with Discrete State-Actions

Dynamic programming algorithms require an exact representation of value functions and policies.

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Thus, GPI with tabular MDPs suffer from:

- Discrete States
- No generlisation and only look-up tables
- Computationally expensive to handle large state-action spaces
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Approximate RL

Can we approximately learn good representations of transitions and rewards or directly the Q-value functions, and use them to find a good policy π?

Goal: Find a policy π and functional representation f such that the performance loss $\|V^*_{\mathcal{M}} - V^f_{\pi}\|$ is as small as possible

Four Key Challenges in RL

- *Planning in Large Spaces (Curse of Dimensionality)*
  – How to optimise the policy when the number of reachable states and decidable actions are big?
- *Succinct Representation of Information*
  – How to succinctly represent the available information regarding states, actions, dynamics and policies?
- *Exploration–Exploitation Trade-off (Effect of Incomplete Information)*
  – Should you try out new decisions which may prove to be beneficial or play as best as you can with your existing knowledge?
- *Planning under Incomplete Information (Exploration + Planning)*
  – How to estimate the effect of an action and how to predict the future state reached from a state through the action?

Four Key Challenges in RL and Solutions

- *Planning in Large Spaces (Curse of Dimensionality)*
  $\rightarrow$ Approximate RL
- *Succinct Representation of Information*
  $\rightarrow$ Abstractions (Frans) $+$ Approximate RL $++$
- *Exploration–Exploitation Trade-off (Effect of Incomplete Information)*
  $\rightarrow$ Bandits (Bert) $+$ Q-learning (Sean) $+$ Optimism (Friday)
- *Planning under Incomplete Information (Exploration $+$ Planning)*
  $\rightarrow$ Approximate RL $+$ Optimism (Friday)

PART 2

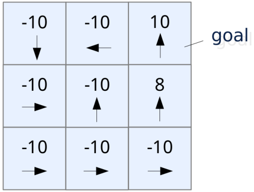
Function Approximations in RL
From Discrete to Continuous States: Dynamic Programming with Learning

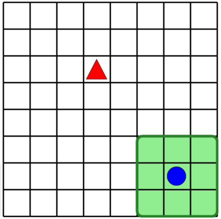
Q-table

-10 ↓	-10 ←	10 ↑	goal
-10 →	-10 ↑	8 ↑	
-10 →	-10 →	-10 →	

From Discrete to Continuous World: From Q-tables to Q-functions

Q-table





No generalisation across discretisations.

From Discrete to Continuous World: From Q-tables to Q-functions

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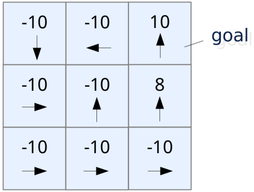

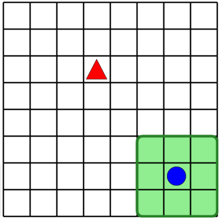

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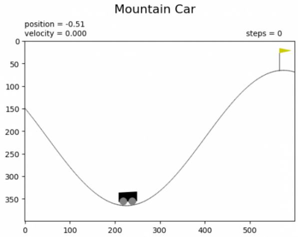
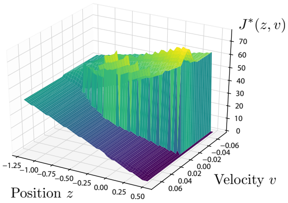
Q-function





Learn the Q-values as a function of (s, a).

Approximate RL

Problem

Exactly computing a Q-function across a continuous state-action space while looking into trajectories is not possible.

Question

Can we approximately learn good representations of transitions and rewards or directly the Q-value functions, and use them to find a good policy π?

Approximate RL: Planning with Learning (Step 1)

Problem

Exactly computing Q-function across continuous state-action space while using trajectories is not possible.

Question 1

Can we approximately learn generalisable and accurate representations of Q-value?

Solution:

Turn the Q-function computation into a learning problem.

$$Q_k(s,a) \leftarrow \mathcal{T}^\star Q_{k-1} = R(s,a) + \gamma \sum_{s' \in \mathcal{S}} \mathcal{P}(s'|s,\pi(s)) \max_b Q_{k-1}(s',b)$$

a. Write a parametric Bellman update:

$$\boxed{Q_\theta(s,a)} = R(s,a) + \gamma \sum_{s' \in \mathcal{S}} \mathcal{P}(s'|s,\pi(s)) \max_b \boxed{Q_\theta(s',b)}\,.$$

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b. Sample trajectories of $\{(s_i, a_i, r_i, s'_i)\}_{i=1}^n$, and solve the regression problem to learn $\theta^\star$:

$$\theta^\star = \arg\min_\theta \boxed{\sum_{i=1}^n \left(Q_\theta(s_i,a_i) - r_i - \gamma \max_b Q_\theta(s'_i,b)\right)^2}$$

Linear Models

$$Q^*_{\mathcal{M}} \in \left\{\theta^\top \phi(s,a), \theta \in \mathbb{R}^d\right\},$$

where $\phi : \mathcal{S} \times \mathcal{A} \to [0, M]$.

How to Choose a Function Approximation Space?

Linear Models

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Kernel Models

$$Q^*_{\mathcal{M}} \in \left\{\mathrm{GaussianProcess}(\mu_Q, \Sigma_V Q, \theta \in \mathbb{R}^d\right\}.$$

Neural Models

$$Q^*_{\mathcal{M}} \in \left\{f_\theta(s,a), \theta \in \mathbb{R}^d\right\}.$$

Approximate RL: Planning with Learning (Step 2)

$$\theta^\star = \arg\min_\theta \boxed{\sum_{i=1}^{n} \Big(Q_\theta(s_i, a_i) - r_i - \gamma \max_b Q_\theta(s'_i, b) \Big)^2}$$

Problem

Unlike in standard approximation schemes (e.g. supervised learning), we have only limited access to the target function, i.e. $Q^*_{\mathcal{M}}$.

Question 2

What would be a good way to generate data to directly learn optimal Q-value function?

Approximate RL: Planning with Learning (Step 2)

Problem

We have only limited access to the target function, i.e. $Q^*_{\mathcal{M}}$.

Question 2

What would be a good way to generate data to directly learn optimal Q-value function?

Solution:

GPI (e.g. Q-value iteration) tends to iteratively learn functions which are close to the optimal value function. Leverage the contraction to generate data.

$$\theta_{k+1} = \arg\min_{\theta} \sum_{i=1}^{n} \Big(Q_\theta(s_i, a_i) - r_i - \gamma \max_b Q_{\theta_k}(s_i', b) \Big)^2 \quad \text{for } k = 1, 2, \ldots$$

Question 3

How to use the learned Q-function $\hat{Q}_\pi$ to find a policy close to optimal $\pi^\star$?

Approximate RL: Planning with Learning (Step 3)

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How to use the learned Q-function $\hat{Q}_\pi$ to find a policy close to optimal $\pi^\star$?

Solution:

If $\hat{Q}_\pi$ is a good approximation of $Q^*_{\mathcal{M}}$, use it to compute the greedy policy.

$$\pi_K(s) = \arg\max_{a \in \mathcal{A}} \hat{Q}_{\theta_K}(s, a)$$

Why would it work?

An Approximate RL Algorithm: Fitted Q-iteration (FQI)

Three Components

1. Sample trajectories of $\{(s_i, a_i, r_i)\}_{i=1}^{n}$, and solve the regression problem with $r_i + \gamma \max_b Q_\theta(s'_i, b)$ as data and Q_θ as the parametric function to learn $\theta^\star$.

2. Use the $Q_{\theta_{k-1}}$ as the target function to generate data and apply regression iteratively.

3. If $\hat{Q}_{\theta_K}$ is a good approximation of $Q^*_{\mathcal{M}}$, use it to compute the greedy policy.

An Approximate RL Algorithm: Fitted Q-iteration (FQI)

Algorithm Fitted Q-Iteration (FQI)

Input: Steps K , initial state distribution ρ and initial policy π_0
Initialise: parameter of Q-value function θ_0
for episodes $k = 1, 2, \dots, K$ **do**
    Draw n samples $(s_i, a_i) \sim \rho\pi_0$.
    Draw n next states $s'_i \sim \mathcal{P}(\cdot|s_i, a_i)$ and rewards $r_i \sim \mathcal{R}(s_i, a_i)$
    Create a dataset $\mathcal{H}_k = \{(s_i, a_i), y_i\}$ such that $y_i \triangleq r_i + \gamma \max_b Q_{\theta_k}(s'_i, b)$
    Solve the regression problem

$$\theta_{k+1} = \arg\min_{\theta} \sum_{i=1}^{n} \left(Q_\theta(s_i, a_i) - r_i - \gamma \max_b Q_{\theta_k}(s'_i, b) \right)^2$$

end for
return the **greedy policy** for all s

$$\pi_K(s) \in \arg\max_{a \in \mathcal{A}} Q_{\theta_K}(s, a)$$

Why Does FQI Work?

Performance Loss to Learning Error: Contraction of Greedy Policy

$$\|V^*_{\mathcal{M}} - V_{\pi_K,\theta_K}\|_\infty \leq \frac{2\gamma}{1-\gamma}\|V^*_{\mathcal{M}} - V_{\theta_K}\|_\infty$$

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From Learning Error to Estimation and Approximation Errors (Lazaric et al., 2012)

$$\|V^*_{\mathcal{M}} - V_{n,\theta_K}\|_{\mathcal{P}\pi} \leq \left\|V^*_{\mathcal{M}} - \hat{V}_n\right\|_{\mathcal{P}\pi} + \left\|\hat{V}_n - V_{n,\theta_K}\right\|_{\mathcal{P}\pi}$$

- Estimation Error: Depends on the complexity of the function class and the coverage of samples collected
- Approximation Error: How good is the function class to approximate the optimal value function and generalise across state-action space.

Limitations of FQI

- FQI is an Offline RL algorithm.
- FQI loops over all possible actions to get next best action a_{t+1}:

$$\arg\max_{a \in \mathcal{A}} Q_\theta^k(s_t, a)$$

- FQI encounters instability (target depends on $Q_\theta^{k-1}(s_{t+1}, a)$).
- Collects data at every episode and forget them in the next one.

From FQI to DQN: Baby Steps to Deep RL

- DQN is an Online RL algorithm
- One forward pass to get all $Q_{\theta_k}(s_t, a)$
- Use a target network $Q_{\theta_{k-1}}(s_{t+1}, a)$ to ensure stability
- Uses replay buffer to reuse the data

Algorithm 1 Deep Q-learning with Experience Replay

Initialize replay memory $\mathcal{D}$ to capacity N
Initialize action-value function Q with random weights
for episode $= 1, M$ **do**
  Initialise sequence $s_1 = \{x_1\}$ and preprocessed sequenced $\phi_1 = \phi(s_1)$
  for $t = 1, T$ **do**
    With probability ϵ select a random action a_t
    otherwise select $a_t = \max_a Q^*(\phi(s_t), a; \theta)$
    Execute action a_t in emulator and observe reward r_t and image x_{t+1}
    Set $s_{t+1} = s_t, a_t, x_{t+1}$ and preprocess $\phi_{t+1} = \phi(s_{t+1})$
    Store transition $(\phi_t, a_t, r_t, \phi_{t+1})$ in $\mathcal{D}$
    Sample random minibatch of transitions $(\phi_j, a_j, r_j, \phi_{j+1})$ from $\mathcal{D}$
    Set $y_j = \begin{cases} r_j & \text{for terminal } \phi_{j+1} \\ r_j + \gamma \max_{a'} Q(\phi_{j+1}, a'; \theta) & \text{for non-terminal } \phi_{j+1} \end{cases}$
    Perform a gradient descent step on $(y_j - Q(\phi_j, a_j; \theta))^2$ according to equation $\boxed{3}$
  end for
end for

epsilon-greedy exploration

step in the environment

replay buffer and sampling

regression target

gradient step

Courtesy: Antoin Raffin, RLSS 2023

The Deadly Triad of RL

If we use FQI or DQN with experience replay, we face the deadly triads of RL.

1. **Function approximation:** Using a neural network or linear model to fit Q-values.
2. **Bootstrapping:** Using $\max_a Q_\theta(s, a)$ to construct the target data.
3. **Off-policy learning:** the replay holds data from a mixture of past policies.

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The Silver Lining or Myopia?

Empirically, we rarely see the deadly triad appearing destructively, while some explosions of Q-value that recover after an initial phase are common.

Do we need a better and new approach to approximate RL theory?

- Leverage Bellman operator's contraction to iteratively approximate $Q^*_{\mathcal{M}}$.
- Parametrise the Q-value functions and turn learning it into an iterative regression problem.

$$\theta_{k+1} = \arg\min_{\theta} \boxed{\sum_{i=1}^{n} \left(Q_\theta(s_i, a_i) - r_i - \gamma \max_b Q_{\theta_k}(s'_i, b) \right)^2} \quad \text{for } k = 1, 2, \ldots, K\,.$$

- Use a "good" data-generating policy to cover the state-action space and/or reuse the old collected data "smartly".
- Use greedy policy once a good approximation Q_{θ_K} is computed.

PART 3

Policy Gradient Algorithms
From Dynamic Programming to Parametric Policy Optimisation

Step 1: Policy Parametrisation. Represent the probability distribution over actions, i.e. a stochastic policy $\pi : \mathcal{S} \to \Delta_{\mathcal{A}}$, as a parametric family (π_θ).

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Discrete Actions

1. Direct Parametrisation:

$$\boxed{\pi_\theta(a|s) = \theta_{s,a}} \text{ such that } \sum_{s,a} \theta_{s,a} = 1 \text{ and } \theta_{s,a} \geq 0.$$

2. Log-linear Policy:

$$\pi_\theta(a|s) = \frac{\boxed{\exp(\theta^\top \phi(a,s))}}{\sum_{s,a} \exp(\theta^\top \phi(a,s))}.$$

3. Neural Softmax Policy:

$$\pi_\theta(a|s) = \frac{\boxed{\exp(f_\theta(a,s))}}{\sum_{s,a} \exp(f_\theta(a,s))}.$$

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Discrete Actions

1. Direct Parametrisation
2. Log-linear Policy
3. Neural Softmax Policy

$$\pi_\theta(a|s) = \frac{\exp(f_\theta(a,s))}{\sum_{s,a} \exp(f_\theta(a,s))}.$$

Continuous Actions

1. Gaussian:

$$\pi_\theta(a|s) = \frac{1}{\sqrt{2\pi\sigma_\theta^2(s)}} \exp\left(\frac{(a-\mu_\theta(s))^2}{2\sigma_\theta^2(s)}\right).$$

2. Beta (for Bounded Actions) [Chou et al., ICML 2017]:

$$\pi_\theta(a|s) = \mathrm{Beta}\left(\frac{a + A_{\max}}{2A_{\max}}; \alpha_\theta(s), \beta_\theta(s)\right).$$

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Step 2: Policy Optimisation. Find the parameter $\theta^\star$ that maximises the long-term expected reward

$$\theta^\star = \arg\max_\theta \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma \mathcal{R}(s_t, a_t) \mid s_0 \sim \rho, a_t \sim \pi_\theta(\cdot|s_t)\right]$$
$$= \arg\max_\theta \mathbb{E}_{s_0 \sim \rho}\left[V^{\pi_\theta}(s_0)\right]$$

Here, ρ is the initial state distribution.

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$$\begin{aligned}\theta^\star &= \arg\max_\theta \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma \mathcal{R}(s_t, a_t) \mid s_0 \sim \rho, a_t \sim \pi_\theta(\cdot|s_t)\right] \\ &= \arg\max_\theta \mathbb{E}_{s_0 \sim \rho}\left[V^{\pi_\theta}(s_0)\right]\end{aligned}$$

Here, ρ is the initial state distribution.

The Hill Ahead

$\mathbb{E}_{s_0 \sim \rho}\left[V^{\pi_\theta}(s_0)\right]$ is non-concave in θ.

Policy Gradient Algorithms

Apply gradient ascent on $J(\pi_\theta) = \mathbb{E}_{s_0 \sim \rho}\left[V^{\pi_\theta}(s_0)\right]$

$$\theta_{k+1} \leftarrow \theta_k + \eta_k \nabla_\theta J(\pi_\theta)\,.$$

Apply gradient ascent on $J(\pi_\theta) = \mathbb{E}_{s_0 \sim \rho}\left[V^{\pi_\theta}(s_0)\right]$

$$\theta_{k+1} \leftarrow \theta_k + \eta_k \nabla_\theta J(\pi_\theta)\,.$$

Issue

We cannot exactly compute the gradient of $J(\pi_\theta)$.

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$$\theta_{k+1} \leftarrow \theta_k + \eta_k \nabla_\theta J(\pi_\theta)\,.$$

Issue

We cannot exactly compute the gradient of $J(\pi_\theta)$.

Solution: Stochastic Approximation

Construct a stochastic estimate of $\nabla_\theta J(\pi_\theta)$ from data collected by playing π_{θ_k}.

Research Question

How to construct a "good" estimator of $\nabla_\theta J(\pi_\theta)$?

Theorem (Policy Gradient Theorem (Williams, 1992))

$$\nabla_\theta J(\pi_\theta) = \mathbb{E}_{\tau \sim \mathcal{P}_\theta}\left[Z(\tau)\sum_{t=0}^{\infty}\nabla_\theta \log \pi_\theta(a_t|s_t)\right]$$

The Policy Gradient Theorem

Theorem (Policy Gradient Theorem (Williams, 1992))

$$\nabla_\theta J(\pi_\theta) = \mathbb{E}_{\tau \sim \mathcal{P}_\theta} \left[Z(\tau) \sum_{t=0}^{\infty} \nabla_\theta \log \pi_\theta(a_t|s_t) \right]$$

- τ is a trajectory $\{s_1, a_1, \ldots, s_t, a_t, \ldots\}$ generated by the probability distribution induced by policy π_θ and transition function $\mathcal{P}$:

$$\mathcal{P}_\theta(\tau) = \rho(s_0) \prod_{t=0}^{\infty} \pi_\theta(a_t|s_t) \mathcal{P}(s_{t+1}|s_t, a_t)$$

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- $Z(\tau)$ is the return from the trajectory τ: $Z(\tau) \triangleq \sum_{t=0}^{\infty} \gamma^t r_t$.

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- τ is a trajectory $\{s_1, a_1, \ldots, s_t, a_t, \ldots\}$ generated by the probability distribution $\mathcal{P}_\theta(\tau)$ induced by policy π_θ and transition function $\mathcal{P}$.
- $Z(\tau)$ is the return from the trajectory τ: $Z(\tau) \triangleq \sum_{t=0}^{\infty} \gamma^t r_t$.
- The gradient $\nabla_\theta \log \pi_\theta(a_t|s_t) = \frac{\nabla_\theta \pi_\theta(a_t|s_t)}{\pi_\theta(a_t|s_t)}$ is called the score function and exists for differentiable parametric policies.

Example: Score Function of log-linear Policies

If $\pi_\theta(a|s) = \frac{\exp(\theta^\top \phi(a,s))}{\sum_{s,a} \exp(\theta^\top \phi(a,s))}$, then $\nabla_\theta \log \pi_\theta(a|s) = \phi(a,s) - \mathbb{E}_{a \sim \pi_\theta(\cdot|s)}[\phi(a,s)]$.

REINFORCE: The Monte-Carlo Estimator

Algorithm REINFORCE

Input: Learning rate η, episode number K
Initialise: Initial policy parameter θ_0
for episodes $k = 0, \ldots, K$ **do**
  Generate a trajectory τ_K from policy π_{θ_k}
  Estimate the gradient at $\theta = \theta_k$:

$$\nabla_\theta^{REINFORCE} J(\pi_\theta) \leftarrow \left(\sum_{t=0}^{\infty} \gamma_t r_t\right)\left(\sum_{t=0}^{\infty} \gamma_t \nabla_\theta \log \pi_\theta(a_t|s_t)\right)$$

  Apply policy gradient ascent

$$\theta_{k+1} \leftarrow \theta_k + \eta \nabla_\theta^{REINFORCE} J(\pi_\theta)\,|_{\theta=\theta_k}$$

end for

Algorithm REINFORCE

Input: Learning rate η, episode number K
Initialise: Initial policy parameter θ_0
for episodes $k = 0, \dots, K$ **do**
    Generate a trajectory τ_K from policy π_{θ_k}
    Estimate the gradient at $\theta = \theta_k$:

$$\nabla_\theta^{REINFORCE} J(\pi_\theta) \leftarrow \left(\sum_{t=0}^{\infty} \gamma_t r_t\right) \left(\sum_{t=0}^{\infty} \gamma_t \nabla_\theta \log \pi_\theta(a_t|s_t)\right)$$

    Apply policy gradient ascent

$$\theta_{k+1} \leftarrow \theta_k + \eta \nabla_\theta^{REINFORCE} J(\pi_\theta) \mid_{\theta=\theta_k}$$

end for

- A single *infinite-length* trajectory is enough to create an unbiased estimate without learning transition $\mathcal{P}$.
- Estimator has high variance due to correlation of $Z(\tau)$ and $\{\pi_\theta(a_t|s_t)\}_t$.

How to leverage the Markovianity in estimation?

Q-value Function version of Policy Gradient Theorem

$$\nabla_\theta J(\pi_\theta) = \mathbb{E}_{\tau\sim\mathcal{P}_\theta}\left[\left(\sum_{t=0}^{\infty}\gamma^s r_i\right)\sum_{t=0}^{\infty}\nabla_\theta \log \pi_\theta(a_t|s_t)\right] = \mathbb{E}_{\tau\sim\mathcal{P}_\theta}\left[\sum_{t=0}^{\infty}\left(\sum_{i=t}^{\infty}\gamma^i r_i\right)\nabla_\theta \log \pi_\theta(a_t|s_t)\right]$$

$$= \mathbb{E}_{\tau\sim\mathcal{P}_\theta}\left[\sum_{t=0}^{\infty}\gamma^t Q_{\pi_\theta}(s_t, a_t)\,\nabla_\theta \log \pi_\theta(a_t|s_t)\right]$$

How to decrease variance of the estimator?

Baseline Function version of Policy Gradient Theorem

$$\begin{aligned}\nabla_\theta J(\pi_\theta) &= \mathbb{E}_{\tau\sim\mathcal{P}_\theta}\left[\sum_{t=0}^{\infty} \gamma^t Q_{\pi_\theta}(s_t,a_t)\,\nabla_\theta \log \pi_\theta(a_t|s_t)\right]\\ &= \mathbb{E}_{\tau\sim\mathcal{P}_\theta}\left[\sum_{t=0}^{\infty} \gamma^t \left(Q_{\pi_\theta}(s_t,a_t) - b(s_t)\right) \nabla_\theta \log \pi_\theta(a_t|s_t)\right]\end{aligned}$$

if the baseline function satisfies $\mathbb{E}_{a\sim\pi_\theta}[b(s)\nabla_\theta \log \pi_\theta(a|s)] = 0$.

REINFORCE: The Q-function and Advantage Function based Estimators

How to decrease variance of the estimator?

Baseline Function version of Policy Gradient Theorem

$$\nabla_\theta J(\pi_\theta) = \mathbb{E}_{\tau \sim \mathcal{P}_\theta}\left[\sum_{t=0}^{\infty} \gamma^t \left(Q_{\pi_\theta}(s_t, a_t) - b(s_t) \right) \nabla_\theta \log \pi_\theta(a_t|s_t)\right] \quad (4)$$

if the baseline function satisfies $\mathbb{E}_{a \sim \pi_\theta}[b(s)\nabla_\theta \log \pi_\theta(a|s)] = 0$.

A good choice of $b(s)$ is $V_{\pi_\theta}(s)$.

Advantage Function version of Policy Gradient Theorem

$$\begin{aligned}\nabla_\theta J(\pi_\theta) &= \mathbb{E}_{\tau \sim \mathcal{P}_\theta}\left[\sum_{t=0}^{\infty} \gamma^t \left(Q_{\pi_\theta}(s_t, a_t) - V_{\pi_\theta}(s_t) \right) \nabla_\theta \log \pi_\theta(a_t|s_t)\right] \\ &= \mathbb{E}_{\tau \sim \mathcal{P}_\theta}\left[\sum_{t=0}^{\infty} \gamma^t A_{\pi_\theta}(s_t, a_t) \nabla_\theta \log \pi_\theta(a_t|s_t)\right]\end{aligned}$$

Algorithm Natural Policy Gradient (NPG)

1: **Input:** Learning rate η, episode number K
2: **Initialise:** Initial policy parameter θ_0
3: **for** episodes $k = 0, \ldots, K$ **do**
4: Generate a trajectory τ_K from policy π_{θ_k}
5: Estimate the gradient at $\theta = \theta_k$
6: Estimate the covariance Σ_{θ_k} at $\theta = \theta_k$
7: Apply covariance/curvature-calibrated policy gradient ascent

$$\theta_{k+1} \leftarrow \theta_k + \eta \left(\Sigma_{\theta_k}\right)^{\dagger} \hat{\nabla}_\theta J(\pi_\theta) \;|_{\theta=\theta_k}$$

8: **end for**

Here, $\Sigma_{\theta_k} = \mathbb{E}_{\tau \sim \mathcal{P}_{\theta_k}} \left[\nabla_\theta \log \pi_\theta(a|s) \left(\nabla_\theta \log \pi_\theta(a|s)\right)^\top \right]$

We can reinterpret the NPG as a proximal gradient ascent step:

$$\theta_{k+1} = \arg\max_{\theta} J(\pi_\theta) \quad \text{s.t.} \quad \mathrm{KL}\left(\mathcal{P}_{\theta_k} || \mathcal{P}_\theta\right) \leq \epsilon .$$

where we do a second order approximation of KL: $\frac{1}{2}(\theta - \theta_k)^\top \Sigma_{\theta_k} (\theta - \theta_k) \leq \epsilon$.

Different Proximal Estimators and Optimisers: PPO, TRPO,...

We can reinterpret the NPG as a proximal gradient ascent step:

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where we do a second order approximation of KL: $\boxed{\frac{1}{2}(\theta - \theta_k)^\top \Sigma_{\theta_k}(\theta - \theta_k) \leq \epsilon}$.

Success of this approach motivates development of different proximal policy gradient algorithms.

TRPO (Schulman et al., 2015)

$$\max_{\theta} \mathbb{E}_{\tau \sim \mathcal{P}_{\theta_k}}\left[\frac{\pi_\theta(a|s)}{\pi_{\theta_k}(a|s)} A_{\pi_\theta}(s,a)\right] \quad \text{s.t.} \quad \mathbb{E}_{s \sim \mathcal{P}_{\theta_k}}\left[\mathrm{KL}\left(\pi_\theta(\cdot|s) || \pi_{\theta_k}(\cdot|s)\right)\right] \leq \epsilon\,.$$

PPO (Schulman et al., 2017)

$$\max_{\theta} \mathbb{E}_{\tau \sim \mathcal{P}_{\theta_k}}\left[\min\left\{\frac{\pi_\theta(a|s)}{\pi_{\theta_k}(a|s)} A_{\pi_\theta}(s,a), \mathrm{clip}\left(\frac{\pi_\theta(a|s)}{\pi_{\theta_k}(a|s)}; 1+\delta, 1-\delta\right) A_{\pi_\theta}(s,a)\right\}\right]\,.$$

When Does Policy Gradient Work?: Convergence Analysis

Optimisation Perspective

When $J(\pi_\theta)$ is a "concave-like" function, the stochastic gradient ascent would work.

$$J(\pi_{\theta^\star}) - J(\pi_\theta) = \mathcal{O}\left(\|\nabla_\theta J(\pi_\theta)\|\right) .$$

[1] 1. Lin Xiao. On the convergence rates of policy gradient methods. JMLR, 2022.
2. Alekh Agarwal, Sham M. Kakade, Jason D. Lee, and Gaurav Mahajan. On the theory of policy gradient methods: Optimality, approximation, and distribution shift. JMLR, 2021.
3. Alekh Agarwal, Sham M Kakade, Jason D Lee, and Gaurav Mahajan. Optimality and approximation with policy gradient methods in markov decision processes. COLT, 2020.

When Does Policy Gradient Work?: Convergence Analysis

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$$J(\pi_{\theta^\star}) - J(\pi_\theta) = \mathcal{O}\left(\|\nabla_\theta J(\pi_\theta)\|\right) .$$

Statistical Perspective

If we have data with enough "coverage" of the state-action space and we have an unbiased estimator, we can apply the policy gradient theorems almost surely.

$$\|\nabla_\theta J(\pi_\theta) - \widehat{\nabla}_\theta J(\pi_\theta)\| \leq \epsilon(\#samples, \delta) \quad \text{with probability } 1-\delta.$$

For details, check some interesting works below.[1]

[1] 1. Lin Xiao. On the convergence rates of policy gradient methods. JMLR, 2022.
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Challenges in Policy-based RL Algorithm Design

1. Hard to choose the good stepsize
   - Use clipping, hyperparameter tuning
2. High sample complexity if we cannot use the samples collected from previous policies
   - Use importance sampling, replay buffer
3. The stochastic gradient estimators suffer high variance
   - Use baseline functions with actor-critic methods

PART 4

What's ahead?
Actor-Critic Algorithms, Exploration–Exploitation Trade-offs, and ....

Value-based RL (Critics)

Approach: Learn the optimal Value or Q-value function

Algorithms: Value/Q-value Iteration, Q-learning, Fitted Q-iteration, DQN

Pros: Low variance, good convergence guarantees

Cons: Scales badly with dimensions

Actors vs. Critics: Value-based RL vs. Policy-based RL

Value-based RL (Critics)

Approach: Learn the optimal Value or Q-value function

Algorithms: Value/Q-value Iteration, Q-learning, Fitted Q-iteration, DQN

Pros: Low variance, good convergence guarantees

Cons: Scales badly with dimensions

Policy-based RL (Actors)

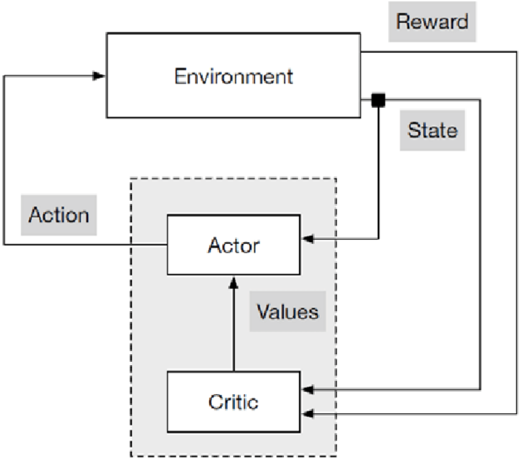
Approach: Learn the optimal (parametrised) policy directly

Algorithms: Policy Iteration, REINFORCE, NPG, TRPO, PPO

Pros: Scales for large state-action spaces

Cons: High variance and sample complexity

Actor-Critic Algorithms



What We Have not Covered?

- What are the theoretical guarantees of RL algorithms? How to derive them?
  $\rightarrow$ Convergence analysis
  $\rightarrow$ Regret upper bounds
  $\rightarrow$ Stability analysis
  $\rightarrow$ Sample-complexity bounds

- How to understand generalisation ability of the learned function approximators and corresponding RL policies?
  $\rightarrow$ Learning theory and generalisation errors meet RL

- How to explore either while collecting data for RL training or while running the RL algorithm itself?
  $\rightarrow$ Exploration–exploitation trade-offs

- How to be robust and safe while learning and execution?
  $\rightarrow$ Robust MDPs and Safe RL

Thanks to our collaborators, teachers, and the audience!

Questions?

References I