

Deep Reinforcement Learning: Foundations and Practical Environment Setup for Real-World Applications

Franco Terranova

Université de Lorraine, CNRS, Inria, LORIA

franco.terranova@inria.fr

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About Me



Name: Franco Terranova

PhD Student @ Université de Lorraine / INRIA / CNRS / LORIA

Current Project: Deep Reinforcement Learning for Cyber-Attack Paths Prediction

Previous Project: Deep Reinforcement Learning for a Self-driving Telescope

Website: <https://terranovafr.github.io>





<https://terranovalfr.github.io/teaching/2024-EASSS-Course>

Overview

- 1 Markov Decision Process
- 2 Model-Based vs Model-Free Methods
- 3 Learning Methods
- 4 Tabular vs Deep Reinforcement Learning
- 5 Deep Q-Network and Proximal Policy Optimization
- 6 Best Practices for RL Experiments

Paradigms of Machine Learning

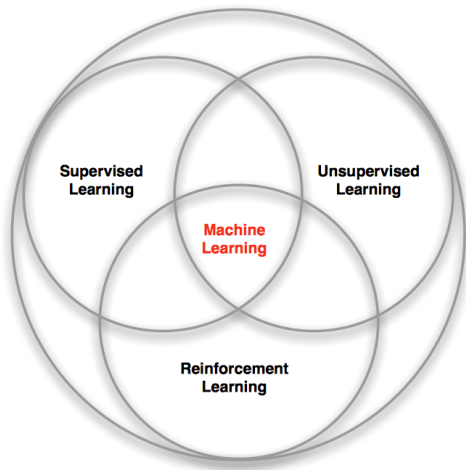


Image Source: <https://medium.com/dataserries/reinforcement-learning-mimics-human-learning-bc701d6ccc08>

Supervised Learning

- **Definition:** Learning from labeled data
- **Label:** The known output or correct answer for a given input
- **Data:** (x, y) — input and label
- **Goal:** Learn a function to map $x \rightarrow y$
- **Applications:** Classification, Regression, etc.

Example:

- Email spam detection: Emails with text labeled as "spam" or "not spam"
- Cat/Dog Image Classification: Images of cats and dogs labeled by type

Unsupervised Learning

- **Definition:** Finding patterns in unlabeled data
- **Data:** x — input data with no labels
- **Goal:** Discover hidden structures or patterns in the data
- **Applications:** Clustering, Dimensionality Reduction, etc.

Example:

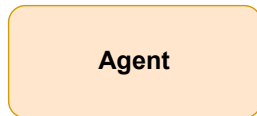
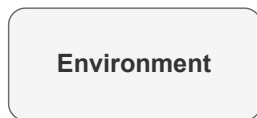
- Customer segmentation in marketing: Grouping customers based on purchasing behavior
- Anomaly detection: Identifying unusual patterns in data, such as fraud detection in financial transactions

- **Definition:** Learning by interacting through trial and error with an **environment** that provides a **reward signal** (distinct from labels)
- **Goal:** Learn the optimal decision-making strategy in its context \leftrightarrow maximize cumulative expected reward

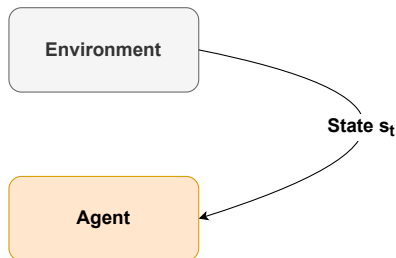
Example:

- Game Playing: Agents learn strategies for games like Chess
- Drone Navigation: Agent navigating towards a destination by avoiding obstacles

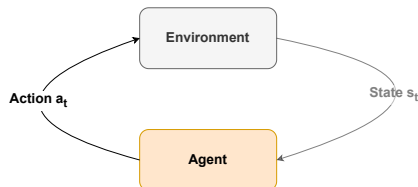
RL Elements - Environment & Agent



Interaction starts at timestep t

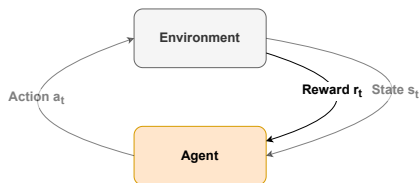


- Input for the agent
- Represents the context where the agent is located
- Agent must learn which elements of the state are relevant
- May not have full visibility of the environment



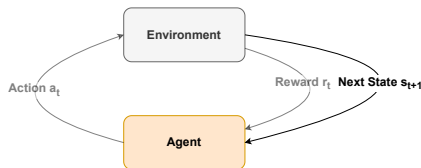
- Output for the agent
- Action produced conditional on the state provided as input $\leftrightarrow a_t|s_t$
- Represents the modification the agent wants to make to the environment state

RL Elements - Reward



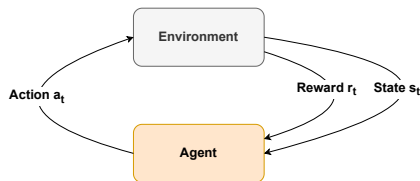
- Evaluation of the action taken in the previous state $\leftrightarrow r_t \mid a_t, s_t$
- Represents a prize or penalty for the action
- Guides the agent in adjusting its behavior for similar future states

RL Elements - Next State



- Resulting outcome of the action taken in the previous state $\leftrightarrow s_{t+1} \mid a_t, s_t$
- Advances the timestep to $t + 1$
- Enables the sequential decision-making

RL Elements - Trial and error



- Agent learns through a loop of trial and error: state \rightarrow action \rightarrow reward, next state
- Sequential decision-making inspired by how humans learn

- The agent policy maps a state to an action:

$$\text{Action} = \pi(\text{State}) \quad \text{where } \pi \text{ is the policy}$$

- The environment maps an action and state to the next state and reward:

$$\text{Next State, Reward} = \mathcal{E}(\text{State}, \text{Action})$$

where \mathcal{E} represents the environment's dynamics

- The overall loop can be summarized as:

$$\text{State}_{t+1}, \text{Reward}_t = \mathcal{E}(\text{State}_t, \pi(\text{State}_t))$$

What Makes RL Different?

- **No Supervisor:** Driven by reward signals, not explicit labeled data
- **Sequential Decision Making:** Optimization of long-term rewards through a series of actions over time
- **Delayed Feedback:** Feedback may be delayed, potentially sacrificing short-term rewards for long-term gains
- **Exploration vs. Exploitation:** Choosing between trying new actions or using known strategies

RL Definitions: Episodes, Trajectory, and Iterations

- **Episode:** A complete sequence of steps from the initial state to a terminal state or goal, after which the process restarts
- **Trajectory τ :** A sequence of states, actions, and rewards from the start to the end of an episode

$$\tau = (s_0, a_0, r_0, s_1, a_1, r_1, \dots, s_T, a_T, r_T)$$

Finite Episode: Episode length $T < \infty$

Infinite Episode: Episode length $T \rightarrow \infty$

- **Cutoff or Goal:** The condition or point at which an episode ends

Steps for RL Formulation

- Identify the State (s):
 - Determine what information defines the current situation of the agent
- Define the Actions (a):
 - Specify the possible decisions or moves the agent can take from each state
- Specify the Reward (r):
 - Decide how to quantify the feedback for each action in a given state
- Design the Environment Interaction:
 - Define state transitions and reward assignments based on actions
 - Specify episode structure, including length and termination criteria

Example - Breakout (Atari Game)

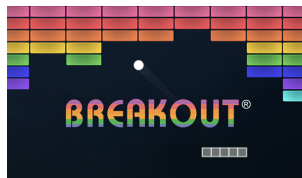


Image from <https://www.coolmathgames.com/fr/0-atari-breakout>

- **State Space:**

- Raw pixel values from the game screen, 2D array of pixels

- **Action Space:**

- Discrete actions: moving the paddle left, right, or no action

- **Reward Function:**

- Positive reward for destroying bricks
- Negative reward for losing the ball

- **Episode:**

- Starts with the paddle at the bottom and the ball in motion
- Ends when the ball falls below the paddle or all bricks are destroyed

Example - AlphaGo (Go Game)

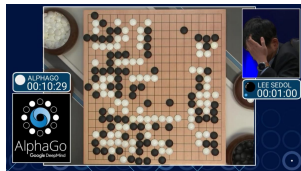


Image from Engadget

- **State Space:**
 - Board configurations, including the positions of black and white stones
- **Action Space:**
 - Placing a stone at any empty intersection on the board
- **Reward Function:**
 - Positive reward for winning the game
 - Negative reward for losing
- **Episode:**
 - Begins with an empty board
 - Ends when a winner is determined

Markov Decision Process (MDP) Formulation

MDP: $(\mathcal{S}, \mathcal{A}, \mathcal{P}, \mathcal{R}, \gamma)$

\mathcal{S} : State space

\mathcal{A} : Action space

\mathcal{P} : $\mathcal{S} \times \mathcal{A} \rightarrow \mathcal{S}$, State transition function

\mathcal{R} : $\mathcal{S} \times \mathcal{A} \rightarrow \mathbb{R}$, Reward function

γ : Discount factor

One approach to finding optimal behavior in an environment involves approximating \mathcal{P} and \mathcal{R} :

- **Know \mathcal{R} :** Determines the quality of each action in s_t for each t
- **Know \mathcal{P} :** Predicts s_{t+1} based on a_t in s_t . Allows recalculation of \mathcal{P} and \mathcal{R} based on s_{t+1} and a_{t+1}
- **Challenges:** This approach can be impractical for real-world problems

Indirectly approximate environment by approximating the policy:

- **Policy Approximation:** Learn a policy $\pi(s) \rightarrow a$, which maps states s to actions a
- **Objective:** Optimize the policy to maximize the cumulative expected reward (or return) over time

Return (G_t): The total accumulated reward an agent expects to receive starting from time step t

- **Definition:**

$$G_t = r_{t+1} + \gamma r_{t+2} + \gamma^2 r_{t+3} + \dots = \sum_{k=0}^{\infty} \gamma^k r_{t+k+1}$$

- **Finite Episode:** The sum is limited to a fixed number of steps, T , rather than extending to infinity
- **Components:**
 - r_{t+1}, r_{t+2}, \dots : Rewards received at each time step
 - γ : Discount factor, $0 \leq \gamma \leq 1$

Role of Discount Factor (γ):

- **Trade-off Decision:** Determines the trade-off between immediate rewards and future rewards
- $\gamma = 0$: Focuses only on immediate reward

$$G_t = r_{t+1}$$

- $\gamma = 1$: Values future rewards as much as immediate rewards

$$G_t = r_{t+1} + r_{t+2} + r_{t+3} + \dots = \sum_{k=0}^{\infty} r_{t+k+1}$$

- **Practical Use:** strictly between 0 and 1

Summary

- RL is a ML paradigm involving a loop of trial and error
- The reward signal guides the learning process
- Environment modeled as MDP
- Model-free methods preferred for real-world problems
- Maximization of $\mathbb{E}_{\pi}[G_t]$ properly setting γ

We do not approximate \mathcal{P} and \mathcal{R} , we approximate them indirectly:

- **Policy-Based:** The policy $\pi(a|s)$
- **Value-Based:** Value functions $V(s)$ or $Q(s, a)$
- **Actor-Critic:** Both policy $\pi(a|s)$ and value functions

- **Objective:** Directly learn a policy $\pi(a|s)$ representing the agent
- The policy (π) outputs the probability of taking action a in state s

$$\pi(a|s) = P(a_t = a | s_t = s)$$

- **Optimization Problem:** Train the policy to maximize the cumulative expected reward:

$$J(\pi) = \mathbb{E}_{\pi}[G_t]$$

- **Objective:** Approximate a function that provides the quality (value) of states or actions
- **Potential Options:**
 - **State Value Function ($V(s)$):** Estimates the expected return starting from state s and following a particular policy π :

$$V(s) = \mathbb{E}_{\pi}[G_t | s_t = s]$$

- **Action Value Function ($Q(s, a)$):** Estimates the expected return of taking action a in state s and following a particular policy π :

$$Q(s, a) = \mathbb{E}_{\pi}[G_t | s_t = s, a_t = a]$$

Interconnection of π , V , and Q

- **From Q to π :** Optimal policy can be derived directly by selecting actions with the highest Q -value:

$$\pi(s) = \arg \max_a Q(s, a)$$

- However, we have no direct mapping from V to π
- Same from π to V or Q

- **Objective:** Combine policy-based and value-based methods to improve learning
- **Components:**
 - **Actor:** Learns the policy $\pi(a|s)$ to select actions
 - **Critic:** Estimates the value function $V(s)$ to evaluate the quality of the states
- Leveraging the value estimate to inform the policy updates

RL Intersections

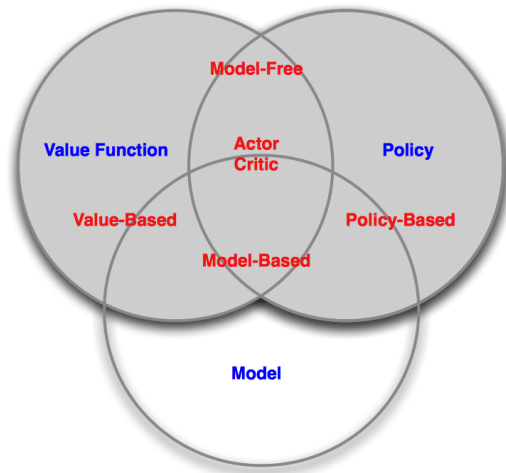


Image Source: Odonkor, Philip & Lewis, Kemper. (2018). Control of Shared Energy Storage Assets Within Building Clusters Using Reinforcement Learning. 10.1115/DETC2018-86094.

- **Objective:** Find functions that maximize $\mathbb{E}_\pi[G_t]$ using iterative optimization methods
- **Value-Based Methods:**
 - Update Formula: Bellman Equation
- **Policy-Based Methods:**
 - Update Formula: Policy Gradient Theorem, ...
- **Actor-Critic Methods:**
 - Combination of update formulas to reach the approximation of actor and critic

Derive Optimal Policy in RL Problems:

- From Policy-Based / Actor-Critic Methods: directly derive the optimal policy (π^*)
- From Value-Based Methods:
 - Approximate the optimal action-value function (Q^*)
 - Derive the optimal policy (π^*) from this function:

$$\pi^*(a|s) = \arg \max_a Q^*(s, a)$$

How to choose?

Choosing the right RL method:

• Policy-Based / Actor-Critic Methods:

- Converge to probabilistic (stochastic) policies
- Reason: Optimize a policy $\pi(a|s)$, that inherently approximate a probability distribution:

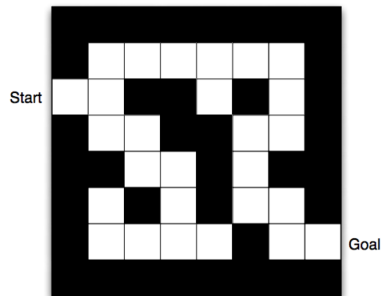
$$\pi^*(a|s) = P(a|s)$$

• Value-Based Methods:

- Converge to deterministic policies
- Reason: Derive the policy by selecting the unique maximum action in each state:

$$\pi^*(a|s) = \arg \max_a Q^*(s, a)$$

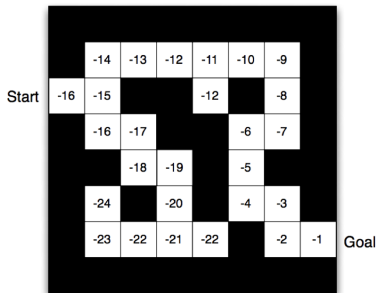
Grid World



- State: (x,y) position
- Action: up, down, left, right
- Rewards: -1 per time-step
- Episode termination: Reach goal

Slide credit: D. Silver

Grid World



- Optimal value function $V_{\pi}^*(s)$
- Expected return in each state

Slide credit: D. Silver

Tabular RL Overview:

- **Definition:** Uses tables (arrays) to represent and approximate policies and value functions
- **Tabular Representation:**
 - Value Function Table
 - Action-Value Function Table
 - Policy Function Table

Tabular RL

	Value
State 1	$V^\pi(S1)$
State 2	$V^\pi(S2)$
....	
State M	$V^\pi(SM)$

Tabular representation of the value function

	Action 1	Action 2	Action N
State 1	$Q^\pi(S1, A1)$	$Q^\pi(S1, A2)$		$Q^\pi(S1, AN)$
State 2	$Q^\pi(S2, A1)$	$Q^\pi(S2, A2)$		$Q^\pi(S2, AN)$
....				
State M	$Q^\pi(SM, A1)$	$Q^\pi(SM, A2)$		$Q^\pi(SM, AN)$

Tabular representation of the action-value function

	Action 1	Action 2	Action N
State 1	$P(A1 S1)$	$P(A2 S1)$		$P(AN S1)$
State 2	$P(A1 S2)$	$P(A2 S2)$		$P(AN S2)$
....				
State M	$P(A1 SM)$	$P(A2 SM)$		$P(AN SM)$

Tabular representation of the policy

Challenges and Limitations:

- **Scalability:**

- **Optimization:** Slow convergence and inefficient learning in large environments
- **Memory:** Tables become impractical with large state or action spaces due to memory constraints

- **Generalization:**

- No ability to generalize across unseen states or actions

- **Continuous Spaces:**

- Inapplicable for environments with continuous state and action spaces

Discrete vs Continuous Spaces:

- **Discrete:**

- **Definition:** Finite/countable states/actions
- **Example:** Board games

- **Continuous:**

- **Definition:** Infinite states/actions
- **Example:** Robot arm angles
- **Note:** Requires specialized algorithms

- **Mixed:**

- **Definition:** Both discrete and continuous elements
- **Example:** Video games with levels and player control
- **Note:** May need hybrid approaches

- **Parameterized Models:**

- Represent the policy $\pi(a|s)$, action-value function $Q(s, a)$, or value function $V(s)$ using a parameterized function:

$$\pi_{\theta}(a|s) \quad Q_{\theta}(s, a) \quad V_{\theta}(s)$$

- Here, θ represents the parameters of the function to be optimized for the return maximization

Function Approximators

$$\pi_{\theta} : \mathcal{S} \times \theta \rightarrow \mathcal{A}$$

$$V_{\theta}^{\pi} : \mathcal{S} \times \theta \rightarrow \mathbb{R}$$

$$Q_{\theta}^{\pi} : \mathcal{S} \times \mathcal{A} \times \theta \rightarrow \mathbb{R}$$

$\theta \in \Theta$, parameter space

Function Approximators

$$\pi_{\theta} : \mathcal{S} \times \theta \rightarrow \mathcal{A}$$

$$V_{\theta}^{\pi} : \mathcal{S} \times \theta \rightarrow \mathbb{R}$$

$$Q_{\theta}^{\pi} : \mathcal{S} \times \theta \rightarrow \mathbb{R}^{|\mathcal{A}|}$$

$\theta \in \Theta$, parameter space

- **Advantages:**

- **Generalization:** Handle large or continuous state and action spaces by generalizing across similar states and actions
 - **Efficiency:** Reduce memory usage compared to tabular methods
 - **Optimization:** Efficient algorithms for iterative optimization
- **Deep RL** relies on deep learning, using neural networks (NN) as function approximators

- **Definition:** A subset of machine learning involving NNs with multiple layers
- **Architecture:** Composed of input, hidden, and output layers
- **Universal Function Approximator:** NNs are capable of approximating any continuous function to a desired level of accuracy, given enough neurons and layers
- Uses **backpropagation** to adjust weights, with **gradients** computed to minimize error through optimization algorithms

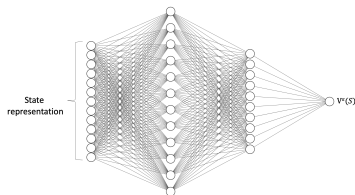
General Update Rule:

$$\theta \leftarrow \theta - \alpha \nabla_{\theta} J(\theta)$$

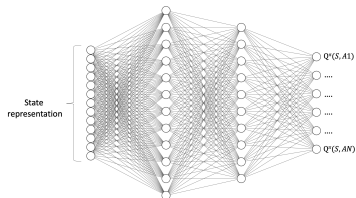
where

- θ denotes the model parameters
- α is the learning rate
- $\nabla_{\theta} J(\theta)$ represents the gradient of the loss function $J(\theta)$
- Iterative update formulas will be used to define the loss function for updating the function parameters θ

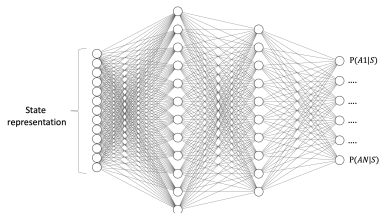
Deep Reinforcement Learning



NN approximating the value function



NN approximating the action-value function



NN approximating the policy function.

Images generated with <https://alexlenail.me/NN-SVG/>

- **Value-Based**

- Deep Q-Network (DQN)
- ...

- **Policy-Based**

- Proximal Policy Optimization (PPO)
- Trust Region Policy Optimization (TRPO)
- ...

- **Actor-Critic**

- Advantage Actor Critic (A2C)
- ...

- **What is DQN?**

- Combines Q-learning with deep NNs
- Approximates the Q-value function

$$Q(s, a; \theta) \approx Q^*(s, a)$$

- Uses an experience replay to store and reuse experiences
- Widely used version incorporates additional strategies to improve learning

DQN Algorithm (Part 1)

- 1 Initialize Q-network $Q_\theta(s, a)$ with random weights θ
- 2 Initialize an empty replay buffer
- 3 Collect experience (s, a, r, s') from the environment using the Q-network and store it in the replay buffer
- 4 Randomly sample a mini-batch of k transitions (s_i, a_i, r_i, s'_i) from the replay buffer

DQN Algorithm (Part 2)

- 5 Compute target Q-values using the Bellman equation:

$$y_i = r_i + \gamma \max_{a'} Q_{\theta}(s'_i, a')$$

- 6 Compute the loss over the mini-batch:

$$L(\theta) = \frac{1}{2k} \sum_{i=1}^k (y_i - Q_{\theta}(s_i, a_i))^2$$

- 7 Update the Q-network by minimizing the loss:

$$\theta \leftarrow \theta - \eta \nabla_{\theta} L(\theta)$$

- 8 Repeat from step 3 until convergence

Target Network

- **Concept:** A target network is a separate Q-network $Q_{\theta^-}(s, a)$ that provides stable Q-value estimates for the Bellman equation
- **Purpose:** Avoid instability in learning due to rapidly changing Q-values
- Periodically update the target network weights to match the online network weights $Q_{\theta}(s, a)$

DQN Algorithm (Part 1)

- 1 Initialize Q-network $Q_{\theta}(s, a)$ with random weights θ
- 2 **Initialize target network $Q_{\theta-}(s, a)$ with the same weights as $Q_{\theta}(s, a)$**
- 3 Initialize an empty replay buffer
- 4 Collect experience (s, a, r, s') from the environment using the Q-network and store it in the replay buffer
- 5 Randomly sample a mini-batch of k transitions (s_i, a_i, r_i, s'_i) from the replay buffer

DQN Algorithm (Part 2)

- 5 **Compute target Q-values using the target network $Q_{\theta-}$:**

$$y_i = r_i + \gamma \max_{a'} Q_{\theta-}(s'_i, a')$$

- 6 Compute the loss over the mini-batch:

$$L(\theta) = \frac{1}{2k} \sum_{i=1}^k (y_i - Q_{\theta}(s_i, a_i))^2$$

- 7 Update the Q-network by minimizing the loss:

$$\theta \leftarrow \theta - \eta \nabla_{\theta} L(\theta)$$

- 8 **Periodically update the target network weights to match the online network weights**
- 9 Repeat from step 3 until convergence

- **Concept:** Balances exploration and exploitation in action selection
- **Strategy:**
 - With probability ϵ , select a random action (exploration)
 - With probability $1 - \epsilon$, select the action that maximizes the Q-value (exploitation)
- **Equation:**

$$a_t = \begin{cases} \text{random action} & \text{with probability } \epsilon \\ \arg \max_a Q_\theta(s_t, a) & \text{with probability } 1 - \epsilon \end{cases}$$

- **Purpose of Epsilon Decay:**

- Start with high exploration to gather diverse experiences
- Gradually shift towards exploitation to refine the policy

- **Epsilon Linear Decay Function:**

$$\epsilon_t = \max(\epsilon_{\min}, \epsilon_0 \cdot \text{decay_rate}^t)$$

- ϵ_t : Epsilon value at time t
- ϵ_0 : Initial epsilon value
- decay_rate : Rate at which epsilon decreases
- ϵ_{\min} : Minimum value epsilon can decay to

DQN Algorithm (Part 1)

- ① Initialize Q-network $Q_\theta(s, a)$ with random weights θ
- ② Initialize target network $Q_{\theta^-}(s, a)$ with the same weights as $Q_\theta(s, a)$
- ③ Initialize an empty replay buffer
- ④ Collect experience (s, a, r, s') from the environment
 - **with probability ϵ , select a random action**
 - **otherwise, select the action that maximizes $Q_\theta(s, a)$**
- ⑤ Randomly sample a mini-batch of k transitions (s_i, a_i, r_i, s'_i) from the replay buffer

DQN Algorithm (Part 2)

- 5 Compute target Q-values using the target network Q_{θ^-} :

$$y_i = r_i + \gamma \max_{a'} Q_{\theta^-}(s'_i, a')$$

- 6 Compute the loss over the mini-batch:

$$L(\theta) = \frac{1}{2k} \sum_{i=1}^k (y_i - Q_{\theta}(s_i, a_i))^2$$

- 7 Update the Q-network by minimizing the loss:

$$\theta \leftarrow \theta - \eta \nabla_{\theta} L(\theta)$$

- 8 Periodically update the target network weights to match the online network weights
- 9 Repeat from step 3 until convergence

- **Dueling DQN:** Improve value estimation
- **Double DQN:** Reduces overestimation bias
- **Prioritized Replay:** Changes sampling strategy
- **Noisy DQN:** Noisy networks instead of ϵ -greedy
- **Distributional DQN:** From expected Q-value to distribution

Proximal Policy Optimization (PPO)

- **What is PPO?**

- An optimization algorithm aimed to approximate a policy function

$$\pi_{\theta}(a|s) \approx \text{Optimal Policy Distribution}$$

- Optimizes the policy using a clipped surrogate objective (here simplified):

$$L(\theta) = \mathbb{E}_t \left[\text{clip} \left(\frac{\pi_{\theta}(a_t|s_t)}{\pi_{\theta_{\text{old}}}(a_t|s_t)}, 1 - \epsilon, 1 + \epsilon \right) \hat{A}_t \right]$$

- Uses clipping to ensure stable and reliable updates by preventing large policy changes
 - Uses the advantage of the action \hat{A}_t for the update

PPO Algorithm

- 1 Initialize the policy network π_θ with random weights
- 2 Collect data by interacting with the environment using the current policy
- 3 Compute the advantage $\hat{A}(s, a)$ for each time step
- 4 Update the policy network by maximizing the PPO objective (simplified):

$$L(\theta) = \mathbb{E}_t \left[\text{clip} \left(\frac{\pi_\theta(a_t|s_t)}{\pi_{\theta_{\text{old}}}(a_t|s_t)}, 1 - \epsilon, 1 + \epsilon \right) \hat{A}_t \right]$$

- 5 Repeat steps 2 to 4 until convergence

- **Model-Free Methods:**

- Do not require a model of the environment
- Suited for real-world complexities

- **Classes of Methods:**

- Value-Based (e.g., DQN), Policy-Based (e.g., PPO), and Actor-Critic

- **Tabular RL Limitations:**

- Struggle with large or continuous state/action spaces

- **Deep NNs:**

- Address scalability issues by approximating functions in complex environments

Extra

Reporting and Analysis

- Plot reward versus steps/episodes to visualize learning progress and convergence
- Use relevant metrics, such as reward or domain-specific measures, for evaluation
- Document experimental settings and results for reproducibility and future reference

Generalization and Robustness

- Assess how well the policy generalizes to new or unseen environments
- Evaluate the algorithm's robustness to different conditions or noise

Comparison

- Compare multiple RL algorithms to identify the most effective approach
- Explore hyper-parameters or use hyperparameter optimization techniques
- Conduct multiple runs with different random seeds to ensure result robustness and reproducibility
- Report confidence intervals (CIs) to improve reliability with few runs

Others

- Consider normalization of the observation space and reward signal
- Consider the sample efficiency of algorithms
- Consider the NN size or function approximator used
- Determine which environment parameters affect learning and how

Partially Observable Markov Decision Process

POMDP: (S, A, T, R, Ω, O)

S : State space (hidden states)

A : Action space

Ω : Observation space

O : $S \times \Omega \rightarrow [0, 1]$, Observation function

P : $S \times A \rightarrow S$, State transition function

R : $S \times A \rightarrow \mathbb{R}$, Reward function

Challenges and Algorithms for POMDPs

- More suited for modeling realistic scenarios
- Some information may not be available at deployment phase
- **Challenges:**
 - Incomplete or noisy information
 - Hidden states complicate decision-making
- Need DRL to converge also in front of partial observability

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See you soon at the lab session!

- **Installation Toolkit:**

- **Conda Environment:** Anaconda, Miniconda, or pip
- **IDE:** Install an Integrated Development Environment (IDE) like PyCharm or VSCode for coding
- **Requirements File:** Download the `environment.yml` or `requirements.txt` file from the code in <https://terranoafr.github.io/teaching/2024-EASSS-Course>.
 - Use the command: `conda env create -f environment.yml` or `pip install -r requirements.txt` to install the necessary libraries