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

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About Me



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Tutorial Material

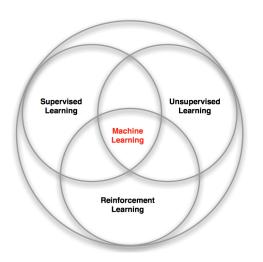


 $\verb|https://terranovafr.github.io/teaching/2024-EASSS-Course|\\$

Overview

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

Paradigms of Machine Learning



 $Image\ Source:\ https://medium.com/dataseries/reinforcement-learning-mimics-human-learning-bc701d6ccc08$

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

Reinforcement Learning

- **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 ↔
 maximize cumulative expected reward

Example:

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

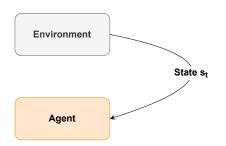
RL Elements - Environment & Agent

Environment

Agent

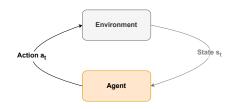
Interaction starts at timestep t

RL Elements - State



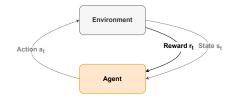
- Input for the agent
- Represents the context where the agent is located
- Agent must learn which elements of the state are relevant
- May not have full visibility of the environment

RL Elements - Action



- 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



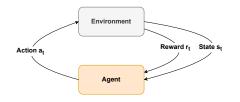
- Evaluation of the action taken in the previous state \leftrightarrow r_t | a_t, s_t
- Represents a prize or penalty for the action
- Guides the agent in adjusting its behavior for similar future states

RL Elements - Next State



- Resulting outcome of the action taken in the previous state ↔
 s_{t+1} | a_t, s_t
- ullet 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 → action → reward, next state
- Sequential decision-making inspired by how humans learn

RL Elements - Simplistic Formulation

• The agent policy maps a state to an action:

Action =
$$\pi(State)$$
 where π is the policy

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

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

where ${\cal E}$ represents the environment's dynamics

• The overall loop can be summarized as:

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

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 $T \to \infty$

• 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

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: (S, A, P, R, γ)

 \mathcal{S} : State space

 \mathcal{A} : Action space

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

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

 γ : Discount factor

Model-based Methods

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

- **Know** \mathcal{R} : Determines the quality of a_t 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

Model-Free Methods

Indirectly approximate environment by approximating the policy:

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

Return

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}, \ldots : Rewards received at each time step
 - γ : Discount factor, $0 \le \gamma \le 1$



Discounting rewards

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

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

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

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

• 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

Model-Free Methods

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

Policy-based methods

- **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:

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

Value-based methods

- **Objective:** Approximate a function that provides the quality (value) of each action in a given state
- 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:

$$\pi(s) = \arg\max_{a} Q(s, a)$$

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

Actor-critic methods

- 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

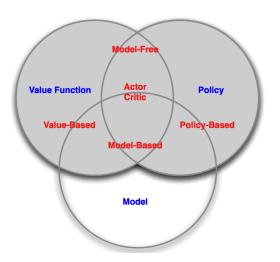


Image Source: Odonkor, Philip & Lewis, Kemper. (2018). Control of Shared Energy Storage Assets Within Building Clusters Using Reinforcement Learning. 10.1115/DETC2018-86094.

Algorithms for Learning

- **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

Optimality

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:

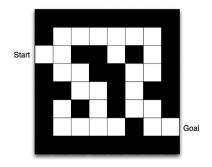
$$\pi^*(a|s) = P(a|s)$$

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

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



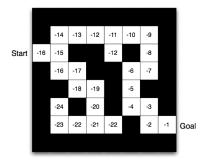
Grid World



Slide credit: D. Silver

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

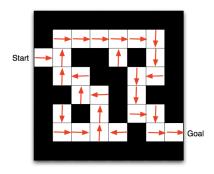
Grid World



Slide credit: D. Silver

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

Grid World



Slide credit: D. Silver

- Optimal policy function $\pi^*(a|s)$
- The optimal policy is deterministic
- Actions that maximize expected return in each state

Tabular RL

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	te 1 V ^π (S1)	
State 2	$V^{\pi}(S2)$	
State M	$V^{\pi}(SM)$	

	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 value function

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

Limitations of Tabular RL

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

RL Elements - Discrete vs Continuous

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

Function Approximation

Parameterized Models:

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

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

ullet Here, heta represents the parameters of the function to be optimized for the return maximization

Function Approximators

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

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

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

 $\theta \in \Theta$, parameter space

Function Approximators

$$\begin{array}{ll} \pi_{\theta}: & \mathcal{S} \times \theta \rightarrow \mathcal{A} \\ V_{\theta}^{\pi}: & \mathcal{S} \times \theta \rightarrow \mathbb{R} \\ Q_{\theta}^{\pi}: & \mathcal{S} \times \theta \rightarrow \mathbb{R}^{|\mathcal{A}|} \\ & \theta \in \Theta \text{, parameter space} \end{array}$$

Function Approximators

• 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: Efficients algorithms for iterative optimization
- Deep RL relies on deep learning, using neural networks (NN) as function approximators

Deep Learning

- **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

Neural Networks as Function Approximators

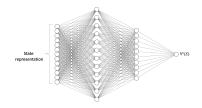
General Update Rule:

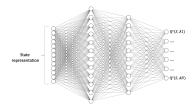
$$\theta \leftarrow \theta - \alpha \nabla_{\theta} J(\theta)$$

where

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

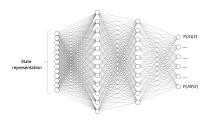
Deep Reinforcement Learning





NN approximating the value function

 $\ensuremath{\mathsf{NN}}$ approximating the action-value function



NN approximating the policy function.

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

Established DRL Algorithms

- Value-Based
 - Deep Q-Network (DQN)
 - . . .
- Policy-Based
 - Proximal Policy Optimization (PPO)
 - Trust Region Policy Optimization (TRPO)
 - ...
- Actor-Critic
 - Advantage Actor Critic (A2C)
 - ...

Deep Q-Network (DQN)

• 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
- 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
- **3** Randomly sample a mini-batch of k transitions (s_i, a_i, r_i, s'_i) from the replay buffer

DQN Algorithm (Part 2)

Ompute target Q-values using the Bellman equation:

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

Ompute the loss over the mini-batch:

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

Update the Q-network by minimizing the loss:

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

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 $Q_{\theta}(s,a)$
- Initialize an empty replay buffer
- Collect experience (s, a, r, s') from the environment using the Q-network and store it in the replay buffer
- **3** Randomly sample a mini-batch of k transitions (s_i, a_i, r_i, s_i') from the replay buffer

DQN Algorithm (Part 2)

3 Compute target Q-values using the target network $Q_{ heta^-}$:

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

Ompute the loss over the mini-batch:

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

Update the Q-network by minimizing the loss:

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

- Periodically update the target network weights to match the online network weights
- Pepeat from step 3 until convergence



ϵ -greedy Strategy

- 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:

$$a_t = egin{cases} ext{random action} & ext{with probability } \epsilon \ ext{arg max}_a \ Q_{ heta}(s_t, a) & ext{with probability } 1 - \epsilon \end{cases}$$

ϵ Decay in ϵ -Greedy Strategy

- Purpose of Epsilon Decay:
 - Start with high exploration to gather diverse experiences
 - Gradually shift towards exploitation to refine the policy
- Epsilon Linear Decay Function:

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

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

DQN Algorithm (Part 1)

- **1** Initialize Q-network $Q_{\theta}(s, a)$ with random weights θ
- $oldsymbol{Q}$ Initialize target network $Q_{ heta^-}(s,a)$ with the same weights as $Q_{ heta}(s,a)$
- Initialize an empty replay buffer
- Collect experience (s, a, r, s') from the environment
 - ullet with probability ϵ , select a random action
 - otherwise, select the action that maximizes $Q_{\theta}(s, a)$
- **3** 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^-} :

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

Ompute the loss over the mini-batch:

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

Update the Q-network by minimizing the loss:

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

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



DQN Improvements

- 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):

$$L(heta) = \mathbb{E}_t \left[\mathsf{clip} \left(rac{\pi_{ heta}(a_t | s_t)}{\pi_{ heta_{\mathsf{old}}}(a_t | s_t)}, 1 - \epsilon, 1 + \epsilon
ight) \hat{A}_t
ight]$$

- 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
- **②** Compute the advantage $\hat{A}(s,a)$ for each time step
- Update the policy network by maximizing the PPO objective (simplified):

$$L(heta) = \mathbb{E}_t \left[\mathsf{clip} \left(rac{\pi_{ heta}(a_t|s_t)}{\pi_{ heta_{\mathsf{old}}}(a_t|s_t)}, 1 - \epsilon, 1 + \epsilon
ight) \hat{A}_t
ight]$$

Repeat steps 2 to 4 until convergence

Recap

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

Best Practices for RL Experiments

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

Best Practices for RL Experiments

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

Best Practices for RL Experiments

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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 Learning to predict by the methods of temporal differences

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See you soon at the lab session!

Installation Toolkit

• Installation Toolkit:

- Conda Environment: Anaconda or Miniconda
- IDE: Install an Integrated Development Environment (IDE) like PyCharm or VSCode for coding
- Requirements File: Download the environment.yml file from https://terranovafr.github.io/teaching/2024-EASSS-Course.
 - Use the command: conda env create -f environment.yml to install the necessary libraries