Markov Decision Processes

DEPARTMENT OF COMPUTER SCIENCE
ST. FRANCIS XAVIER UNIVERSITY

CSCI-531 - Reinforcement Learning

Fall 2025

Beyond Multi-Armed Bandits

Bandits vs. Real-World Decisions

- **Bandits**: Each action is independent

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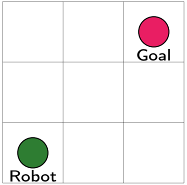
These are sequential decision processes with ripple effects through time

The Challenge of Sequential Decisions

Key Differences from Bandits

- **State matters**: Current situation affects future options



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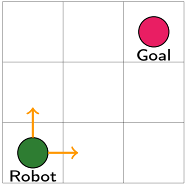

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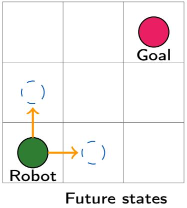

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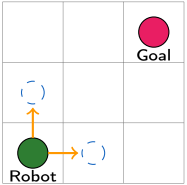

Future states

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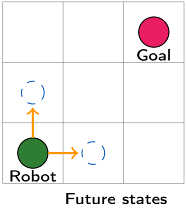

We need a mathematical framework for sequential decisions

What is a Markov Decision Process?

MDP: Mathematical Framework

A Markov Decision Process models sequential decision-making under uncertainty

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MDPs provide the foundation for virtually all modern RL algorithms

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MDP Tuple (S, A, T, R)

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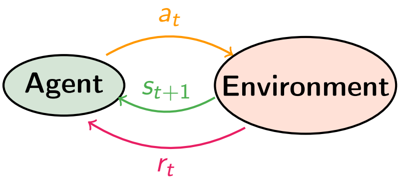
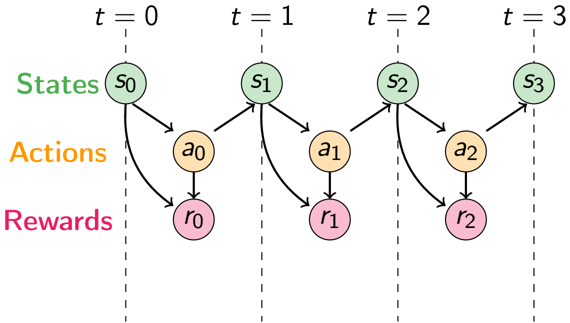


The Agent-Environment Interaction Loop



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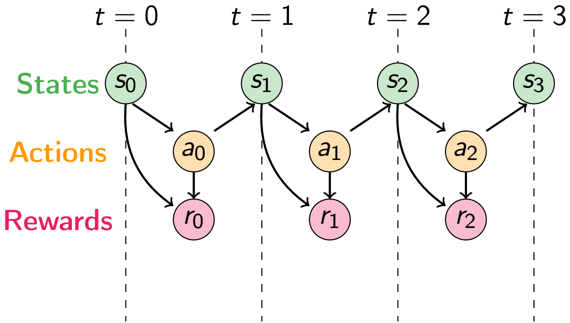

Trajectory Generation

This process generates a **trajectory** or **episode**:

$$s_0, a_0, r_0, s_1, a_1, r_1, s_2, a_2, r_2, \ldots$$

Transition Function: The World's Physics

Probabilistic Transitions

After taking action a_t in state s_t, next state s_{t+1} is determined by:

$$p(s'|s, a) = \text{Probability of moving to state } s' \text{ given state } s \text{ and action } a$$

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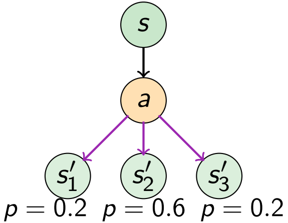

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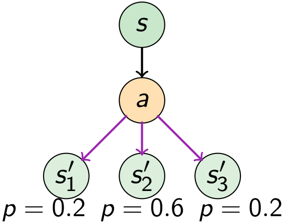

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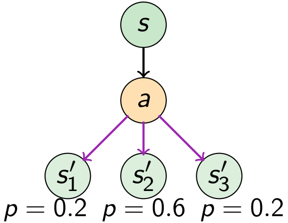

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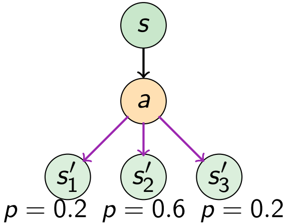

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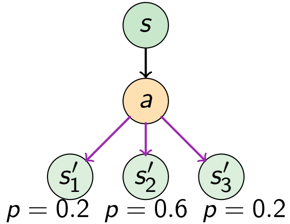

Note: $\sum_{s' \in S} p(s'|s, a) = 1$ for all $s \in S, a \in A$

The Markov Property

Markov Property Definition

The future depends only on the present, not on the past

Formally: All information needed to predict future states must be contained in the current state.

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Mathematical Expression

$$P(S_{t+1} = s' | S_t = s_t, A_t = a_t, S_{t-1} = s_{t-1}, \ldots, S_0 = s_0) = P(S_{t+1} = s' | S_t = s_t, A_t = a_t)$$

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Examples

- **Markovian**: Chess position (complete board state)
- **Non-Markovian**: "Take the third turn" (depends on path history)

Reward Function: The Learning Signal

Reward Function Purpose

$r(s, a)$ provides immediate feedback that guides the agent toward its goal

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- **Game playing**: $r = +1$ win, -1 loss, 0 otherwise

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Expected Return

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Expected Return

Return Definition

The **return** G_t is the cumulative reward from time t:

$$G_t = r_t + r_{t+1} + r_{t+2} + \cdots + r_T$$

The Problem with Infinite Horizons

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Solution: Discounted Return

Introduce **discount factor** $\gamma \in [0, 1]$:

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Discount Factor Interpretation

- $\gamma = 0$: Only immediate rewards matter (completely myopic)
- $\gamma = 1$: All future rewards equally important (completely farsighted)
- $\gamma = 0.9$: Future rewards matter, but less than immediate ones

Discount Factor Example

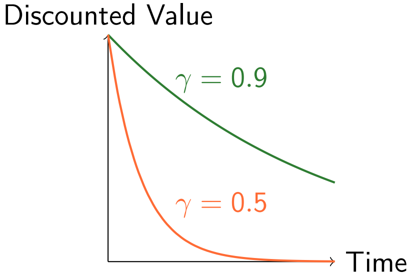
Scenario: Receive reward of 10 at each time step

With $\gamma = 0.5$:

$$\begin{aligned} G_0 &= 10 + 0.5 \times 10 + 0.5^2 \times 10 + \cdots \\ &= 10 + 5 + 2.5 + 1.25 + \cdots \\ &= \frac{10}{1 - 0.5} = 20 \end{aligned}$$

With $\gamma = 0.9$:

$$\begin{aligned} G_0 &= 10 + 9 + 8.1 + 7.29 + \cdots \\ &= \frac{10}{1 - 0.9} = 100 \end{aligned}$$



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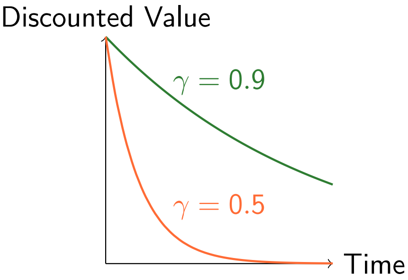

With $\gamma = 0.9$:

$$G_0 = 10 + 9 + 8.1 + 7.29 + \cdots$$
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Higher γ values future rewards more

Policies: Decision-Making Strategies

Policy Definition

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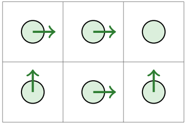

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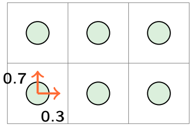

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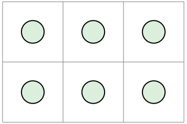

A policy completely specifies the agent's behavior

Value Functions: Evaluating Policies

State Value Function

The **value** of state s under policy π:

$$v_\pi(s) = \mathbb{E}_\pi[G_t | S_t = s] = \mathbb{E}_\pi\left[\sum_{k=0}^{\infty} \gamma^k r_{t+k} \middle| S_t = s\right]$$

"Expected return when starting in state s and following policy π"

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"Expected return when starting in state s and following policy π"

Action-Value Function (Q-Function)

The **value** of taking action a in state s under policy π:

$$q_\pi(s, a) = \mathbb{E}_\pi[G_t | S_t = s, A_t = a] = \mathbb{E}_\pi\left[\sum_{k=0}^{\infty} \gamma^k r_{t+k} \middle| S_t = s, A_t = a\right]$$

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Relationship: $v_\pi(s) = \sum_a \pi(a|s) q_\pi(s, a)$

Bellman Equation: The Key Recursive Relationship

Bellman Equation Derivation

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\end{aligned}$$

Bellman Equation: The Key Recursive Relationship

Bellman Equation Derivation

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Interpretation

- **Immediate reward**: $r(s, a)$
- **Future value**: $\gamma v_\pi(s')$ (discounted)
- **Weighted by probabilities**: Policy and transitions

Optimal Policies and Value Functions

Policy Comparison

Policy π is **better than** policy π' if:

$$v_\pi(s) \geq v_{\pi'}(s) \text{ for all states } s \in S$$

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Fundamental Theorem

There always exists at least one optimal policy that is better than or equal to all other policies.

Optimal Policies and Value Functions

Optimal Value Functions

Optimal state value function:

$$v^*(s) = \max_\pi v_\pi(s) \text{ for all } s \in S$$

Optimal action-value function:

$$q^*(s, a) = \max_\pi q_\pi(s, a) \text{ for all } s \in S, a \in A$$

Bellman Optimality Equations

Bellman Optimality Equation for v^*

$$
\begin{aligned}
v^*(s) &= \max_a q^*(s, a) \\
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Key Insight

Instead of averaging over policy probabilities, we take the **maximum** over all possible actions.

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Finding the Optimal Policy

Once we have v^*, the optimal policy is:

$$\pi^*(s) = \arg\max_a \sum_{s'} p(s'|s,a)[r(s,a) + \gamma v^*(s')]$$

Choose the action that achieves the maximum in the Bellman optimality equation

MDP Solution Methods

Dynamic Programming Methods

When we know the MDP model (S, A, T, R):

- **Policy Iteration**: Alternate between policy evaluation and improvement

MDP Solution Methods

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When we know the MDP model (S, A, T, R):

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Real-world applications often don't know transition probabilities:

- **Model-free RL**: Learn from experience without knowing T or R

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- **Q-Learning, SARSA**: Popular algorithms for this setting

MDP Applications in Modern AI

Computational Biology & Drug Discovery

- **State**: Molecular configuration, binding sites, chemical properties

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Large Language Model Training

- **State**: Model parameters, training data batch, loss landscape

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- **Challenge**: Extremely long horizons, uncertain outcomes

Key Skills: MDP Formulation

Problem Formulation Process

1. **Define State Space**: What information is crucial for decisions?

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Critical Questions

- Does your state representation satisfy the Markov property?
- Does your reward function capture what you actually want?
- Where might the MDP framework break down?

Current Research Challenges

Computational Challenges

- **Curse of Dimensionality**: State spaces grow exponentially

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- **Multi-Agent MDPs**: What happens when multiple agents interact?
- **Inverse RL**: Can we infer reward functions from behavior?
- **Safe RL**: How to ensure safety during learning?

Summary

What We've Learned

- **MDP Framework**: States, actions, transitions, rewards
- **Sequential Decision Making**: Actions have lasting consequences
- **Value Functions**: Evaluate policies and states
- **Optimal Solutions**: Bellman equations and dynamic programming

Next Steps

- Dynamic Programming algorithms (Policy/Value Iteration)
- Model-free reinforcement learning
- Temporal difference learning
- Deep reinforcement learning

From bandits to MDPs: The foundation is complete!