

Monte Carlo Methods



DEPARTMENT OF COMPUTER SCIENCE
ST. FRANCIS XAVIER UNIVERSITY

CSCI-531 - Reinforcement Learning

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From Model-Based to Model-Free Learning

Dynamic Programming Limitations

- ▶ Requires **complete knowledge** of the environment

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- ▶ No need for transition probabilities

Real-World Motivation

Think About...

How would you learn to play a new video game?

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Key Insight

Most real problems are more like the video game scenario!

The Monte Carlo Approach

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$$\text{Value} = \text{Expected Return}$$

If we can collect many returns from a state, we can **average** them to estimate the true value!

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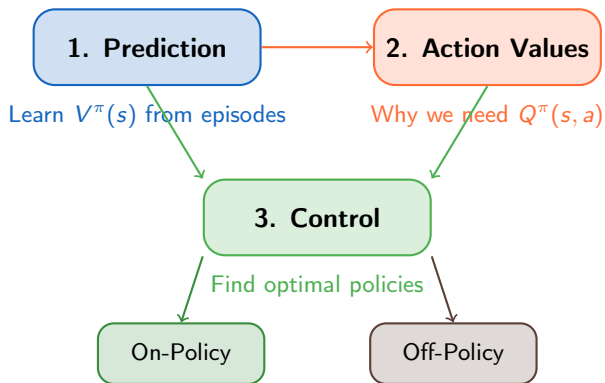
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Important Note

Model still needed for interaction, but not for learning!

Learning Roadmap: Our Journey Through Monte Carlo

Where We're Going



Monte Carlo Prediction: The Basic Idea

The Process

1. Follow policy π to generate **episodes**

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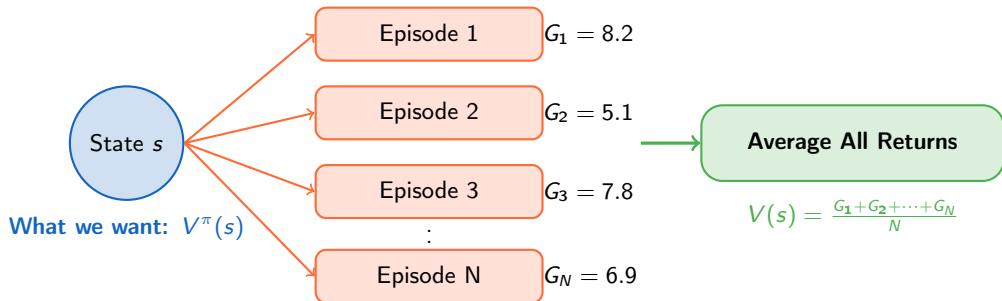
Mathematical Foundation

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

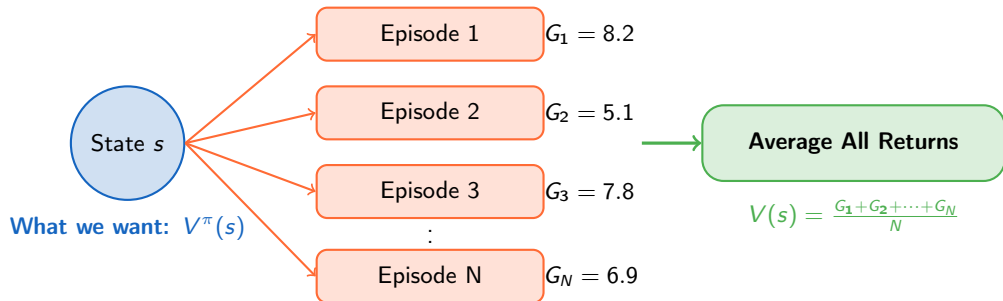
$$V(s) \approx \frac{1}{N} \sum_{i=1}^N G_i$$

where G_i are returns from N visits to state s .

Episode Collection: The Visual Process



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Key Insight

More episodes \Rightarrow Better estimate of true value!

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Convergence Guarantee

As $N \rightarrow \infty$, $V(s) \rightarrow v_{\pi}(s)$ by the **Law of Large Numbers**

Concrete Example: Blackjack

Consider playing Blackjack with a simple policy:

- ▶ Hit if hand value < 17
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Sample Episodes from State "Hand = 16"

Episode	Outcome	Return
1	Bust	-1
2	Win	+1
3	Bust	-1
4	Bust	-1
5	Lose	-1

Concrete Example: Blackjack

Worked Example and Value Estimate

Worked episodes (hand = 16), assume $\gamma = 1$:

- ▶ Episode 1: Bust $\rightarrow R = -1 \Rightarrow G = -1$
- ▶ Episode 2: Win $\rightarrow R = +1 \Rightarrow G = +1$
- ▶ Episode 3: Bust $\rightarrow R = -1 \Rightarrow G = -1$
- ▶ Episode 4: Bust $\rightarrow R = -1 \Rightarrow G = -1$
- ▶ Episode 5: Lose $\rightarrow R = -1 \Rightarrow G = -1$

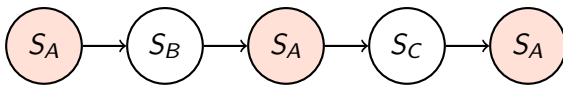
Averaging these returns:

$$V(\text{Hand} = 16) \approx \frac{-1 + 1 + (-1) + (-1) + (-1)}{5} = -0.6.$$

First-Visit vs Every-Visit Monte Carlo

A Key Decision

If we visit the same state multiple times in an episode, should we count all visits or just the first one?



State S_A visited 3 times

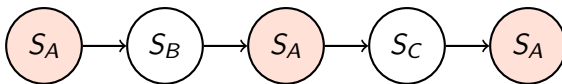
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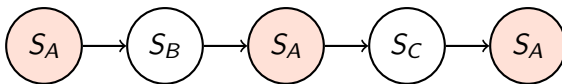
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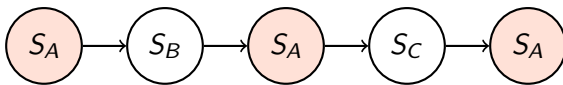
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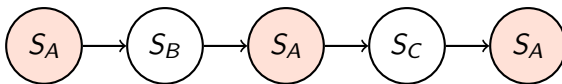
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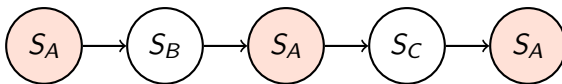
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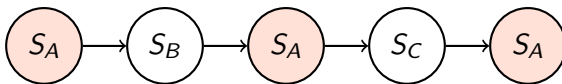
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- ▶ More data per episode



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First-Visit vs Every-Visit — Small numeric example

Episode

Consider the episode (with $\gamma = 1$):

$$S_A \xrightarrow{2} S_B \xrightarrow{1} S_A \xrightarrow{3} S_C \xrightarrow{0}$$

- ▶ First-Visit for S_A : use return from its first occurrence: $G_0 = 2 + 1 + 3 + 0 = 6$.
- ▶ Every-Visit for S_A : include returns from each visit: first visit $G_0 = 6$, second visit (at time 2) $G_2 = 3 + 0 = 3$.

Discussion: First-Visit yields one sample per episode (independent), Every-Visit yields multiple correlated samples but more data per episode.

Why Does This Choice Matter?

Different Perspectives

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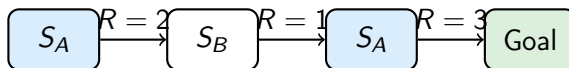
Practical Guidelines

- ▶ **Use First-Visit** for theoretical guarantees and textbook implementations
- ▶ **Use Every-Visit** for faster learning and limited computational budget

Interactive Example: Computing Returns

Activity

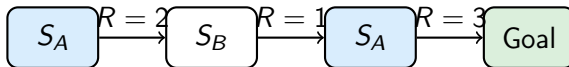
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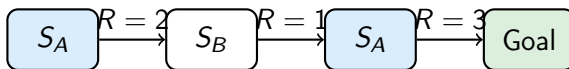
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- From first visit to S_A : $G_0 = 2 + 0.9 \times 1 + 0.9^2 \times 3 = 4.33$

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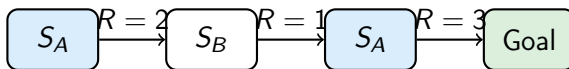
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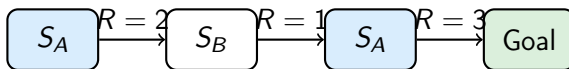
Value Estimates

- ▶ First-Visit MC: $V(S_A) = 4.33$

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Value Estimates

- ▶ First-Visit MC: $V(S_A) = 4.33$
- ▶ Every-Visit MC: $V(S_A) = \frac{4.33+3}{2} = 3.67$

Monte Carlo Prediction Algorithm

Algorithm First-Visit Monte Carlo Prediction

```

1: Input: Policy  $\pi$ , number of episodes  $N$ 
2: Initialize:  $V(s) \in \mathbb{R}$  arbitrarily,  $\forall s \in S$ ;  $Returns(s) \leftarrow$  empty list,  $\forall s \in S$ 
3: for  $episode = 1$  to  $N$  do
4:   Generate episode using  $\pi$ :  $S_0, A_0, R_1, S_1, A_1, R_2, \dots, S_{T-1}, A_{T-1}, R_T$ 
5:    $G \leftarrow 0$ 
6:   for  $t = T - 1, T - 2, \dots, 0$  do
7:      $G \leftarrow \gamma G + R_{t+1}$ 
8:     if  $S_t \notin \{S_0, S_1, \dots, S_{t-1}\}$  then
9:       Append  $G$  to  $Returns(S_t)$ 
10:       $V(S_t) \leftarrow \text{average}(Returns(S_t))$ 
11:    end if
12:  end for
13: end for

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Common Mistakes and Pitfalls

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Why do we go backwards through the episode?

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Why do we go backwards through the episode?

- ▶ Returns are calculated from **future rewards**
- ▶ Working backwards ensures we have all future rewards available
- ▶ More efficient than recalculating from scratch each time

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Pitfall #2: Insufficient Episodes

How many episodes do we need?

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How many episodes do we need?

- ▶ Depends on state space size and variance
- ▶ Start with **1000+ episodes** for simple problems
- ▶ Monitor convergence of value estimates

From Prediction to Control: What's Missing?

What We've Learned So Far

- ▶ We can estimate **state values** $V^\pi(s)$ using episodes

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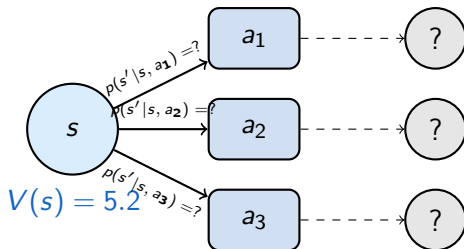
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- ▶ **But we don't know** $p(s'|s, a)$ in model-free settings!
- ▶ We need a different approach...

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Discussion Question

If we have perfect state values $V^*(s)$, can we immediately determine the optimal policy without knowing the model?

Which action is best?



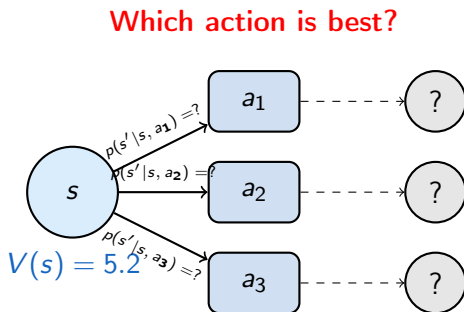
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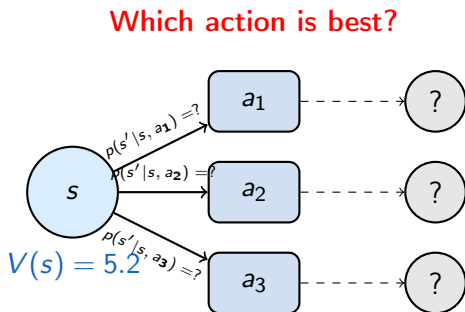
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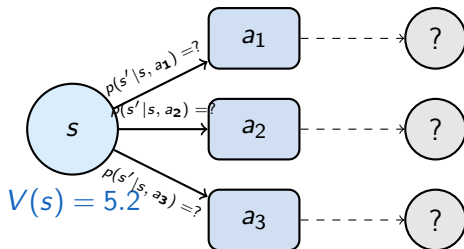
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- ▶ **Requires** transition probabilities $p(s'|s, a)$
- ▶ Not available in model-free settings!

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The Fundamental Problem: State Values Aren't Enough

Imagine This Scenario

You're playing a game and reach this state:

You have **perfect knowledge** that being here is worth $+5.2$ points on average

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Available Actions

► **Action A**: Move left

The Fundamental Problem: State Values Aren't Enough

Imagine This Scenario

You're playing a game and reach this state:

You have **perfect knowledge** that being here is worth +5.2 points on average

The Question

What should you do next?

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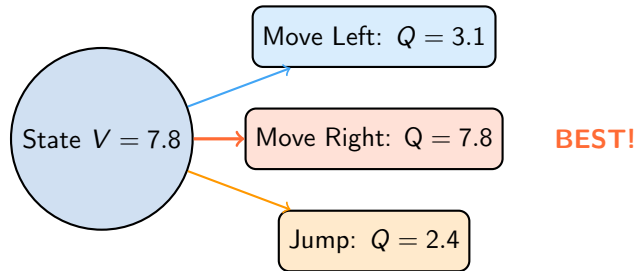
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The Problem

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- ▶ State value doesn't tell you!

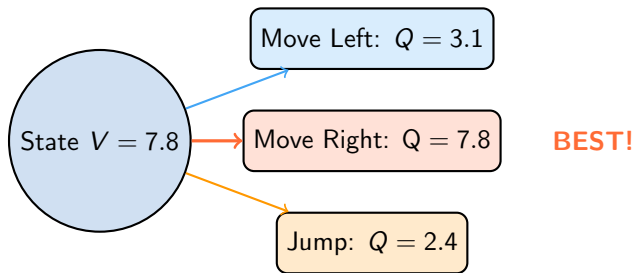
Action Values: The Missing Piece

What We Really Need



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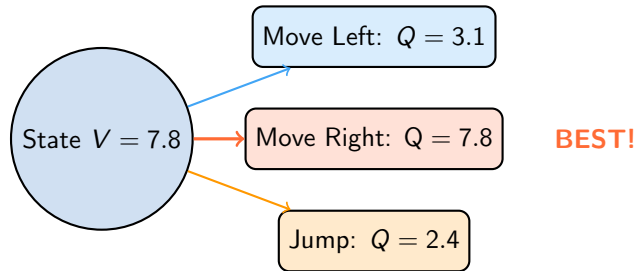


Now We Can Decide!

- **Move Right** has highest Q-value (7.8)

Action Values: The Missing Piece

What We Really Need



Now We Can Decide!

- ▶ **Move Right** has highest Q-value (7.8)
- ▶ **Simple policy**: $\pi(s) = \arg \max_a Q(s, a)$

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The Key Insight

Action values give us direct decision-making power!

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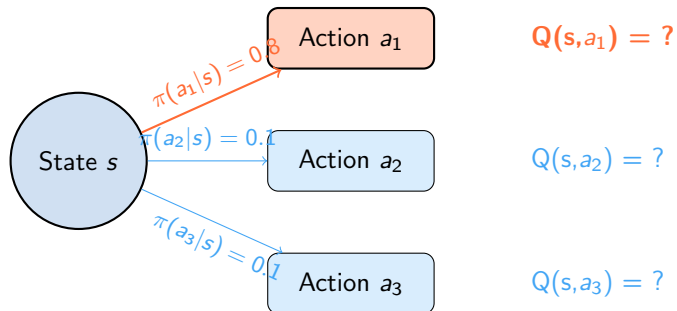
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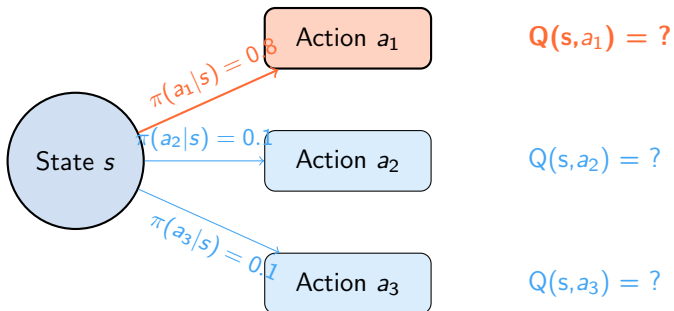
New Challenge

Exploration Problem: All actions must be visited to get good estimates!

The Exploration Problem



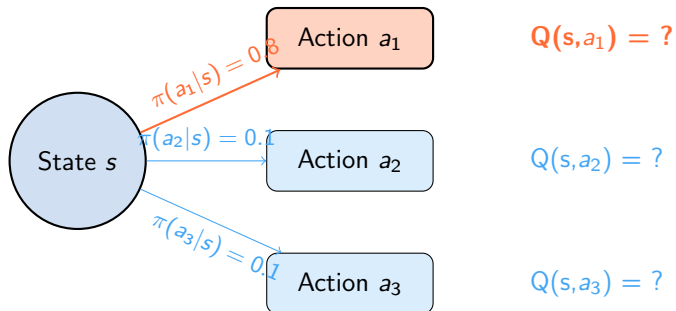
The Exploration Problem



The Dilemma

- **Greedy action** gets lots of data \rightarrow good estimate

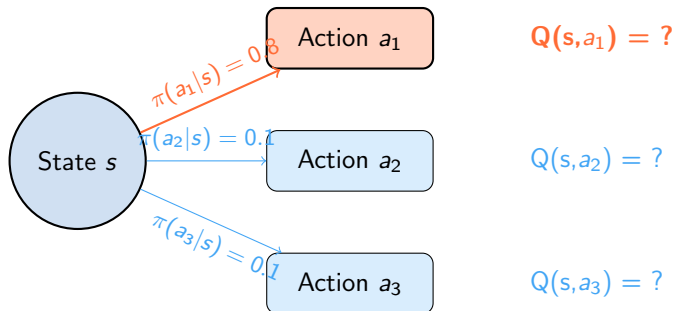
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- ▶ **Greedy action** gets lots of data → good estimate
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The Exploration Problem



The Dilemma

- ▶ **Greedy action** gets lots of data → good estimate
- ▶ **Other actions** get little data → poor estimates
- ▶ How do we know if unexplored actions are actually better?

Solutions to the Exploration Problem

Option 1: Exploring Starts

- ▶ Every episode starts with random state-action pair

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- ▶ Example: **ϵ -greedy policies**

On-Policy Monte Carlo Control

The Approach

- ▶ Learn the value of the **same policy** we're following

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$$\pi(a|s) = \begin{cases} 1 - \epsilon + \frac{\epsilon}{|A|} & \text{if } a = \arg \max_a Q(s, a) \\ \frac{\epsilon}{|A|} & \text{otherwise} \end{cases}$$

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Key Properties

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Key Properties

- ▶ **Soft policy:** All actions have non-zero probability
- ▶ **Improvement guarantee:** Any ϵ -greedy policy w.r.t. Q_π is better than π

ϵ -Greedy Policy Example

Interactive Example

State s has 3 actions with $\epsilon = 0.2$:

$$Q(s, a_1) = 5, Q(s, a_2) = 3, Q(s, a_3) = 1$$

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What happens as we learn and Q values change?

Algorithm On-Policy First-Visit MC Control

```

1: Initialize:  $Q(s, a) \in \mathbb{R}$  arbitrarily,  $\forall s \in S, a \in A$ 
2: Initialize:  $\pi \leftarrow$  arbitrary  $\epsilon$ -soft policy;  $Returns(s, a) \leftarrow$  empty list,  $\forall s \in S, a \in A$ 
3: for each episode do
4:   Generate episode using  $\pi$ :  $S_0, A_0, R_1, \dots, S_{T-1}, A_{T-1}, R_T$ 
5:    $G \leftarrow 0$ 
6:   for  $t = T - 1, T - 2, \dots, 0$  do
7:      $G \leftarrow \gamma G + R_{t+1}$ 
8:     if  $(S_t, A_t) \notin \{(S_0, A_0), \dots, (S_{t-1}, A_{t-1})\}$  then
9:       Append  $G$  to  $Returns(S_t, A_t)$ 
10:       $Q(S_t, A_t) \leftarrow \text{average}(Returns(S_t, A_t))$ 
11:       $A^* \leftarrow \arg \max_a Q(S_t, a)$ 
12:      for all  $a \in A$  do
13:        
$$\pi(a|S_t) \leftarrow \begin{cases} 1 - \epsilon + \frac{\epsilon}{|A|} & \text{if } a = A^* \\ \frac{\epsilon}{|A|} & \text{otherwise} \end{cases}$$

14:      end for

```

Concrete Example Part 1: Q-Value Update

Current Situation

State: Hand = 16, Actions: Hit or Stand

Action	Current Q-value	Returns History
Hit	$Q(16, \text{Hit}) = 0.2$	[0.1, 0.3]
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- ▶ $Q(16, \text{Hit}) = \frac{0.1+0.3+0.7}{3} = 0.37$
- ▶ **Result:** Hit improved from 0.2 to 0.37, Stand stays 0.5

Concrete Example Part 2: Policy Update

Current Q-Values

Action	Q-value
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Policy Update with $\epsilon = 0.1$:

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Off-Policy Monte Carlo: Motivation

Limitation of On-Policy Methods

What's the best policy on-policy MC can find?

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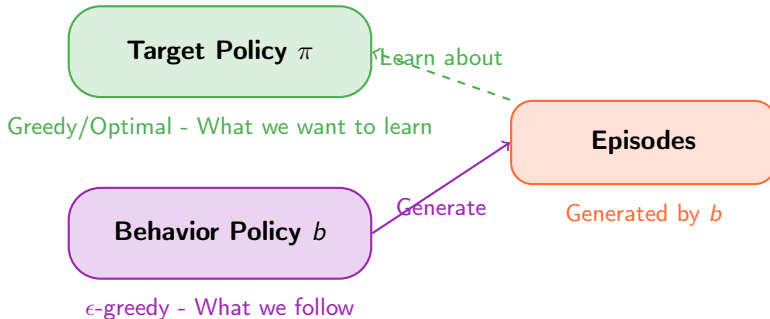
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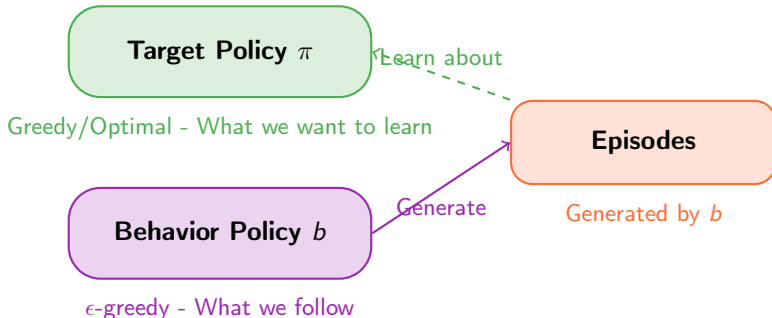
Off-Policy Solution

- ▶ Use two policies:
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 - ▶ Behavior Policy b : The policy we follow for exploration
- ▶ Learn about π using data generated by b

Off-Policy Concept Visualization



Off-Policy Concept Visualization



Coverage Assumption

$\pi(a|s) > 0 \Rightarrow b(a|s) > 0$ for all s, a

Why is this assumption crucial?

Simple Analogy: YouTube Gaming Videos

Imagine You Want to Know...

How good are speedrunners at this game?

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- ▶ Casual player videos are **over-represented** for safe moves

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The Solution: Weight the Gameplay

- ▶ Casual player videos are **over-represented** for safe moves
- ▶ Weight risky moves by $\frac{0.80}{0.20} = 4.0$
- ▶ This "up-weights" the rare risky gameplay we want to learn about

From Gaming to Reinforcement Learning

The Connection

YouTube Gaming	RL Off-Policy
Casual players	Behavior policy b
Speedrunners	Target policy π
Strategy choices	Episode actions
Game scores	Episode returns
Weight = 0.80/0.20	Weight = $\pi(a s)/b(a s)$

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Key Insight

When gameplay comes from the "wrong" player type, we reweight it to match the strategy we want to learn!

Importance Sampling Intuition

The Problem

We have episodes from policy b , but want to learn about policy π . How do we account for the difference?

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- ▶ Suppose b takes action a_1 with probability 0.8
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The Solution: Importance Sampling

Weight each episode by the ratio of its probability under π vs b

Importance Sampling Mathematics

Importance Sampling Ratio

$$\begin{aligned}\rho_{t:T-1} &= \frac{\text{Prob of trajectory under } \pi}{\text{Prob of trajectory under } b} \\ &= \frac{\prod_{k=t}^{T-1} \pi(A_k|S_k)p(S_{k+1}|S_k, A_k)}{\prod_{k=t}^{T-1} b(A_k|S_k)p(S_{k+1}|S_k, A_k)} \\ &= \prod_{k=t}^{T-1} \frac{\pi(A_k|S_k)}{b(A_k|S_k)}\end{aligned}$$

Importance Sampling Mathematics

Importance Sampling Ratio

$$\begin{aligned}
 \rho_{t:T-1} &= \frac{\text{Prob of trajectory under } \pi}{\text{Prob of trajectory under } b} \\
 &= \frac{\prod_{k=t}^{T-1} \pi(A_k|S_k)p(S_{k+1}|S_k, A_k)}{\prod_{k=t}^{T-1} b(A_k|S_k)p(S_{k+1}|S_k, A_k)} \\
 &= \prod_{k=t}^{T-1} \frac{\pi(A_k|S_k)}{b(A_k|S_k)}
 \end{aligned}$$

Key Insight

Transition probabilities cancel out. Only depends on policies.

Importance Sampling: Numerical Example

Episode Trajectory

Episode: $S_0 \xrightarrow{A_0} S_1 \xrightarrow{A_1} S_2$

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- At S_0 : $\pi(A_0|S_0) = 0.1$, $b(A_0|S_0) = 0.3$

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$$\begin{aligned}\rho &= \frac{\pi(A_0|S_0)}{b(A_0|S_0)} \times \frac{\pi(A_1|S_1)}{b(A_1|S_1)} \\ &= \frac{0.1}{0.3} \times \frac{0.8}{0.4} = \frac{1}{3} \times 2 = \frac{2}{3}\end{aligned}$$

Algorithm Off-Policy Monte Carlo Prediction

- 1: **Initialize:** $Q(s, a) \in \mathbb{R}$ arbitrarily, $\forall s \in S, a \in A$
 - 2: **Initialize:** $C(s, a) \leftarrow 0$, $\forall s \in S, a \in A$
 - 3: **for** each episode **do**
 - 4: $b \leftarrow$ any policy with coverage of π
 - 5: Generate episode using b : $S_0, A_0, R_1, \dots, S_{T-1}, A_{T-1}, R_T$
 - 6: $G \leftarrow 0$, $W \leftarrow 1$
 - 7: **for** $t = T - 1, T - 2, \dots, 0$ and $W \neq 0$ **do**
 - 8: $G \leftarrow \gamma G + R_{t+1}$
 - 9: $C(S_t, A_t) \leftarrow C(S_t, A_t) + W$
 - 10: $Q(S_t, A_t) \leftarrow Q(S_t, A_t) + \frac{W}{C(S_t, A_t)} [G - Q(S_t, A_t)]$
 - 11: $W \leftarrow W \cdot \frac{\pi(A_t|S_t)}{b(A_t|S_t)}$
 - 12: **end for**
 - 13: **end for**
-

Weighted Importance Sampling: Key Features

Implementation Details

- ▶ Uses **incremental implementation** with weighted average

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- ▶ **Robustness**: Handles impossible trajectories gracefully
- ▶ **Convergence**: Weighted averaging often has better properties

Algorithm Off-Policy Monte Carlo Control

```

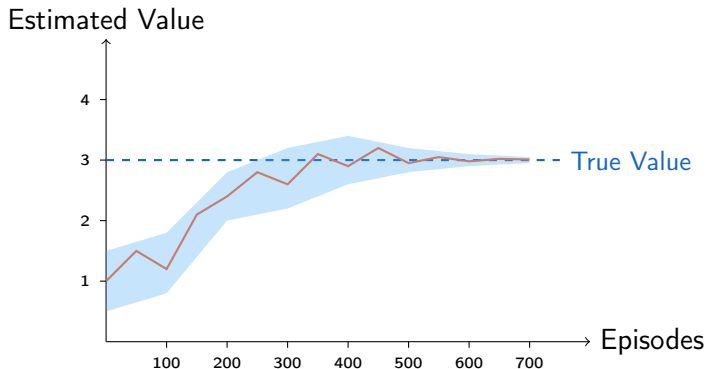
1: Initialize:  $\pi(s) \leftarrow \arg \max_a Q(s, a)$  (greedy policy)
2: for each episode do
3:    $b \leftarrow$  any policy with coverage of  $\pi$ 
4:   Generate episode using  $b$ :  $S_0, A_0, R_1, \dots, S_{T-1}, A_{T-1}, R_T$ 
5:    $G \leftarrow 0, W \leftarrow 1$ 
6:   for  $t = T - 1, T - 2, \dots, 0$  and  $W \neq 0$  do
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10:     $\pi(S_t) \leftarrow \arg \max_a Q(S_t, a)$ 
11:    if  $A_t \neq \pi(S_t)$  then
12:      break (exit inner loop)
13:    end if
14:     $W \leftarrow W \cdot \frac{1}{b(A_t|S_t)}$ 
15:  end for

```

Learning Progress: How Monte Carlo Converges

What Does Learning Look Like?

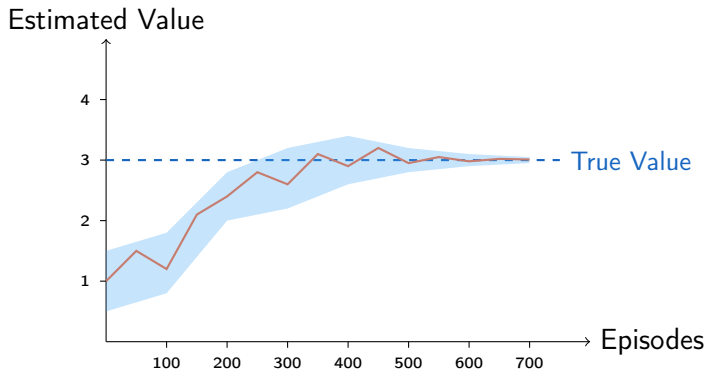
Let's visualize how our value estimates improve over time



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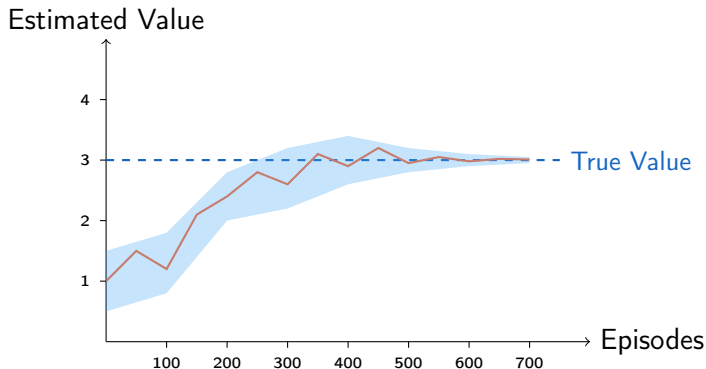


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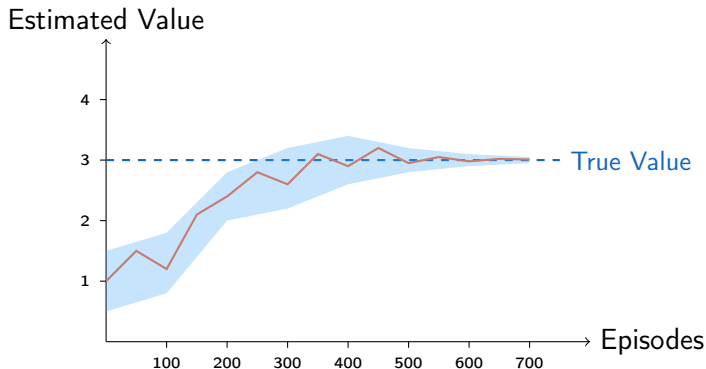


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Key Observations

Practical Learning Considerations

What Affects Convergence Speed?

Faster Convergence:

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Faster Convergence:

- ▶ Low variance returns

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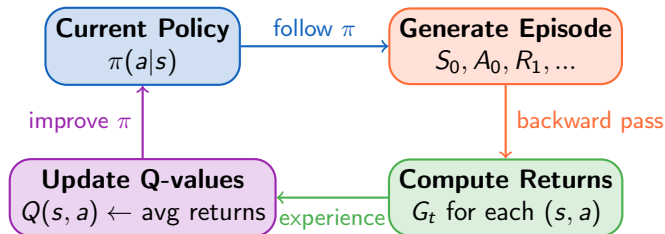
Slower Convergence:

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- ▶ Stochastic environments

Monte Carlo Control: The Complete Loop

The Big Picture

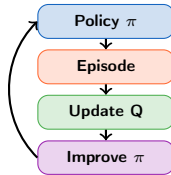
How do all the pieces fit together?



Repeat until convergence

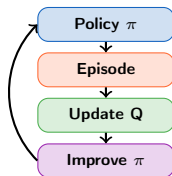
On-Policy vs Off-Policy Control Flow

On-Policy Monte Carlo



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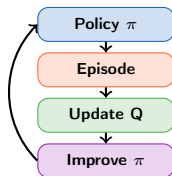
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- ▶ Same policy for **acting** and **learning**

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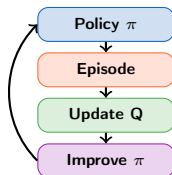
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- ▶ Same policy for **acting** and **learning**
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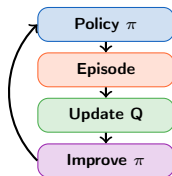
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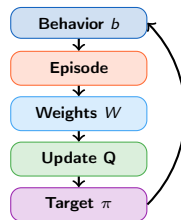
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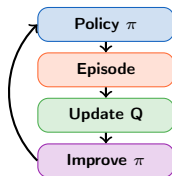
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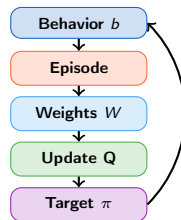
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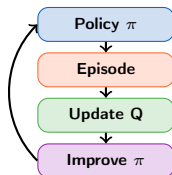
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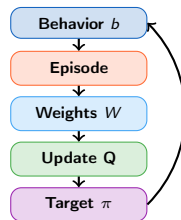
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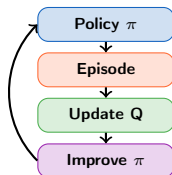
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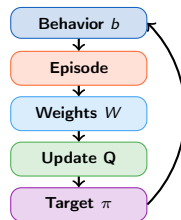
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- ▶ More complex (importance sampling)
- ▶ Better exploration potential

On-Policy vs Off-Policy: Trade-offs

On-Policy

Advantages:

- ▶ Simpler to understand
- ▶ Lower variance
- ▶ Faster convergence
- ▶ Easier to implement

Disadvantages:

- ▶ Limited to ϵ -soft policies
- ▶ Cannot learn deterministic optimal policy

Off-Policy

Advantages:

- ▶ Can learn optimal deterministic policy
- ▶ More general and powerful
- ▶ Can reuse data from any policy

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Discussion

When would you choose each approach?

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- ▶ Consider computational budget

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What should you consider when implementing Monte Carlo methods?

Common Issues

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- ▶ Slow convergence for large state spaces
- ▶ Need sufficient exploration

Key Takeaways

What We've Learned

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- ▶ What if episodes are very long or infinite?
- ▶ Next: **Temporal Difference Learning** - combine MC and DP benefits