Reinforcement learning

Master CPS, Year 2 Semester 1

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Part III

Exact reinforcement learning

Part III in plan

- Reinforcement learning problem
- Optimal solution
- Exact dynamic programming
- **Exact reinforcement learning**
- Approximation techniques
- Approximate dynamic programming
- Approximate reinforcement learning

Algorithm landscape

By model usage:

- Model-based: f, ρ known a priori
- Model-free: f, ρ unknown (reinforcement learning)

By interaction level:

- Offline: algorithm runs in advance
- Online: algorithm runs with the system

Exact vs. approximate:

- Exact: x, u small number of discrete values
- Approximate: x, u continuous (or many discrete values)

RL on the machine learning spectrum

Supervised learning — Reinforcement learning — Unsupervised learning

← more informative feedback — less informative feedback

- Supervised: for each training sample, **correct output** known
- Unsupervised: only input samples, **no outputs**; find patterns in the data
- Reinforcement: correct actions not available, **only rewards**

But note: RL finds **dynamical optimal control**!

Contents part III

1. Monte Carlo, MC
2. Exploration
3. Temporal differences, TD
4. Accelerating TD methods
5. Recap

Reminder: Policy iteration

Policy iteration with Q-functions

initialize policy h_0 arbitrarily
repeat at each iteration ℓ
1: policy evaluation: find Q^{h_ℓ}
2: policy improvement:
find $h_{\ell+1}(x) = \arg\max_u Q^{h_\ell}(x, u)$
until convergence to h^*

Note: In RL, we generally use **Q-functions** so policy improvement does not require a model

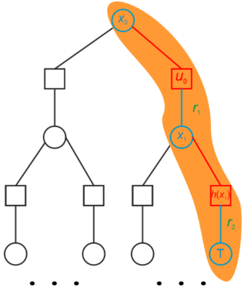
Policy evaluation

To find Q^h:

- So far: model-based methods
- Reinforcement learning: **model not available**
- Learn Q^h from offline data or via **online interaction with the system**

"Monte-Carlo" policy evaluation

Recall: $Q^h(x_0, u_0) = \sum_{k=0}^{\infty} \gamma^k r_{k+1}$

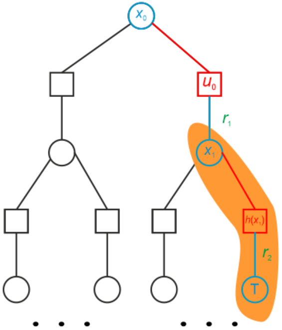


- Trajectory from (x_0, u_0) to x_K (**terminal**) using $u_1 = h(x_1)$, $u_2 = h(x_2)$, etc.

$\Rightarrow$ $Q^h(x_0, u_0)$ = return along trajectory:

$$Q^h(x_0, u_0) = \sum_{j=0}^{K-1} \gamma^j r_{j+1}$$

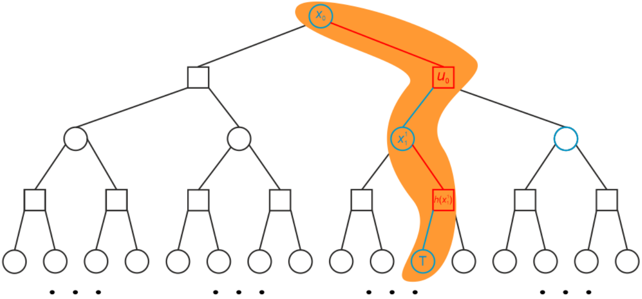
"Monte-Carlo" policy evaluation (cont'd)



- Moreover, at each step k:

$$Q^h(x_k, u_k) = \sum_{j=k}^{K-1} \gamma^{j-k} r_{j+1}$$

Monte-Carlo policy evaluation: Stochastic case



- N trajectories (differing due to stochastic transitions)
- Estimated Q value = **mean** of the returns, e.g.

$$Q^h(x_0, u_0) = \frac{1}{N} \sum_{i=1}^{N} \sum_{j=0}^{K_i - 1} \gamma^j r_{i,j+1}$$

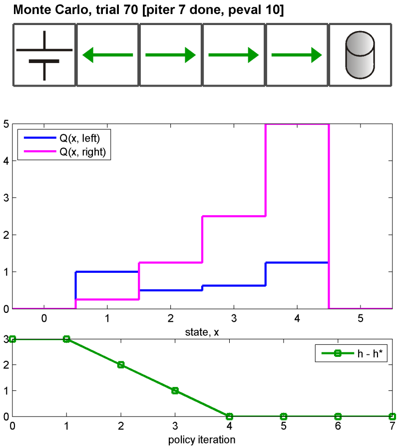
Monte-Carlo policy iteration

Monte-Carlo policy iteration

for each iteration ℓ **do**
  perform N trajectories applying h_ℓ
  reset to 0 accumulator $A(x, u)$, counter $C(x, u)$
  for each step k of each trajectory i **do**
    $A(x_k, u_k) \leftarrow A(x_k, u_k) + \sum_{j=k}^{K_i - 1} \gamma^{j-k} r_{i,j+1}$ (return)
    $C(x_k, u_k) \leftarrow C(x_k, u_k) + 1$
  end for
  $Q^{h_\ell}(x, u) \leftarrow A(x, u) / C(x, u)$
  $h_{\ell+1}(x) \leftarrow \arg\max_u Q^{h_\ell}(x, u)$
end for

Note: must guarantee that **terminal state is reached**!

Cleaning robot: Monte Carlo, demo



The need for exploration

In the MC estimate:

$$Q^h(x, u) \leftarrow A(x, u)/\mathbf{C(x, u)}$$

how to ensure $C(x, u) > 0$ – **information** about each (x, u)?

1. Initial states x_0 representative
2. Actions:
   u_0 representative, sometimes different from $h(x_0)$
   and additionally, possibly:
   u_k representative, sometimes different from $h(x_k)$

Exploration-exploitation dilemma

- **Exploration** is necessary:
  actions different from the current policy
- **Exploitation** of current knowledge is necessary:
  current policy must be applied for good performance

The exploration-exploitation dilemma
– essential in all RL algorithms

(not only in MC)

ε-greedy strategy

- Simple solution to the exploration-exploitation dilemma: **ε-greedy**

$$u_k = \begin{cases} h(x_k) = \arg\max_u Q(x_k, u) & \text{with probability } (1-\varepsilon_k) \\ \text{a uniformly random action} & \text{w.p. } \varepsilon_k \end{cases}$$

- **Exploration probability** $\varepsilon_k \in (0, 1)$
  usually decreased over time
- Main disadvantage: when exploring, actions are fully random, leading to poor performance

Softmax strategy

- Action selection:

$$u_k = u \text{ w.p. } \frac{e^{Q(x_k,u)/\tau_k}}{\sum_{u'} e^{Q(x_k,u')/\tau_k}}$$

  where $\tau_k > 0$ is the **exploration temperature**
- Taking $\tau \to 0$, greedy selection recovered; $\tau \to \infty$ gives uniform random
- Compared to ε-greedy, better actions are more likely to be applied even when exploring

Bandit-based exploration

At single state, exploration modeled as **multi-armed bandit**:

- Action j = arm with reward distribution ρ_j, expectation μ_j
- Best arm (optimal action) has expected value μ^*
- At step k, we pull arm (try action) j_k, getting $r_k \sim \rho_{j_k}$
- **Objective:** After n pulls, small regret: $\sum_{k=1}^{n} \mu^* - \mu_{j_k}$

UCB algorithm

Often-used algorithm: after n steps, pick arm with largest **upper confidence bound**:

$$b(j) = \widehat{\mu}_j + \sqrt{c\frac{\log n}{n_j}}$$

where:

- $\widehat{\mu}_j$ = mean of rewards observed for arm j so far
- n_j = how many times arm j was pulled
- c tunable constant, e.g. $3/2$

These are only a few simple methods, many others exist, e.g. Bayesian exploration, intrinsic rewards, optimistic initialization etc.

Monte-Carlo with incremental updates

Consider the return sample from step k onwards:

$$R_k = \sum_{j=k}^{K-1} \gamma^{j-k} r_{j+1}$$

Instead of averaging such samples to get Q, perform **incremental updates**:

$$Q(x_k, u_k) \leftarrow Q(x_k, u_k) + \alpha_k [R_k - Q(x_k, u_k)]$$

where α_k is a step size, or **learning rate**

Discussion

- Incremental MC motivated by time-varying problems (recent samples have larger weights), but works in time-invariant MDPs as well
- No longer need to store accumulators A and counters C, just directly the Q-values
- If α satisfies "stochastic-approximation" conditions:
  1. decreases to 0, $\sum_{k=0}^{\infty} \alpha_k^2 = \text{finite}$
  2. but not too quickly, $\sum_{k=0}^{\infty} \alpha_k \to \infty$

  method converges: lim when # of samples $\to \infty$ = Q-value

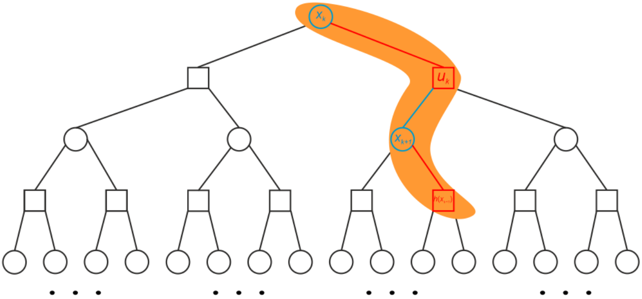
From Monte-Carlo to temporal differences

To avoid waiting until trajectory finishes, recall Bellman equation:

$$Q^h(x, u) = \mathrm{E}_{x'} \left\{ \tilde{\rho}(x, u, x') + \gamma Q^h(x', h(x')) \right\}$$

and use the return estimate:

$$\hat{R}_k = r_{k+1} + \gamma Q(x_{k+1}, h(x_{k+1}))$$



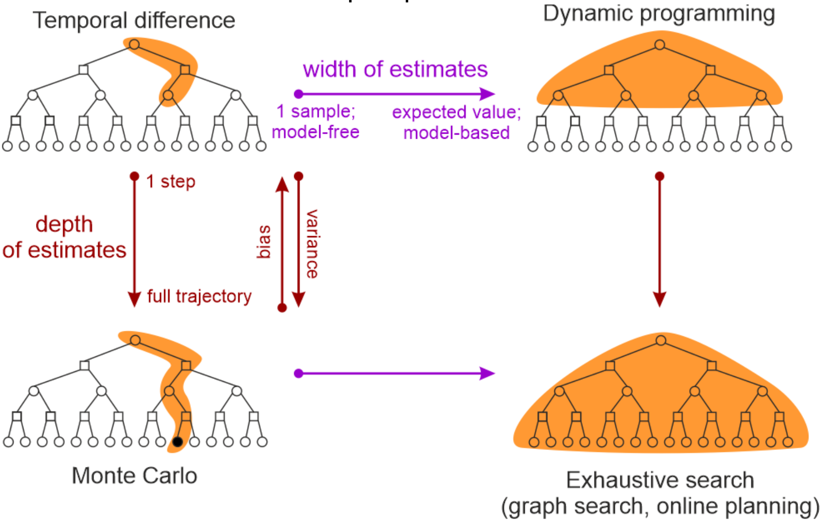
Temporal differences (TD)

Otherwise, update remains the same, but let us make the return estimate explicit:

$$
\begin{aligned}
Q(x_k, u_k) &\leftarrow Q(x_k, u_k) + \alpha_k[\hat{R}_k - Q(x_k, u_k)] \\
&= Q(x_k, u_k) + \alpha_k[r_{k+1} + \gamma Q(x_{k+1}, h(x_{k+1})) - Q(x_k, u_k)]
\end{aligned}
$$

- $[\dots]$ is the **temporal difference** between two estimates of $Q(x_k, u_k)$, using information at subsequent time steps
- Model-free, data-based updates (like MC): r_{k+1}, x_{k+1} e.g. observed while interacting online
- Updates estimate $Q(x_k, u_k)$ using another estimate, $Q(x_{k+1}, h(x_{k+1}))$: **bootstrapping**
- Dynamic programming also bootstraps, but using a model

TD vs. MC vs. DP: Unified perspective



TD for policy evaluation

TD for policy evaluation

for each trajectory **do**
  initialize x_0, choose the initial action u_0
  repeat at each step k
    apply u_k, measure x_{k+1}, receive r_{k+1}
    choose the **next** action $u_{k+1} \sim h(x_{k+1})$
    $$Q(x_k, u_k) \leftarrow Q(x_k, u_k) + \alpha_k \cdot \\ [r_{k+1} + \gamma Q(x_{k+1}, u_{k+1}) - Q(x_k, u_k)]$$
  until trajectory finished
end for

Note: we replaced $h(x_{k+1})$ by u_{k+1}, chosen according to h

Exploration-exploitation

choose the next action $u_{k+1} \sim h(x_{k+1})$

- Information about $(x, u) \neq (x, h(x))$ necessary
  $\Rightarrow$ **exploration**
- h must be followed
  $\Rightarrow$ **exploitation**

- E.g. ε-greedy:

$$u_{k+1} = \begin{cases} h(x_{k+1}) & \text{w.p. } (1 - \varepsilon_{k+1}) \\ \text{unif. random} & \text{w.p. } \varepsilon_{k+1} \end{cases}$$

Recall: MC

MC policy iteration

for each iteration ℓ **do**
  perform N trajectories applying h_ℓ
  reset to 0 accumulator $A(x, u)$, counter $C(x, u)$
  for each step k of each trajectory i **do**
    $A(x_k, u_k) \leftarrow A(x_k, u_k) + \sum_{j=k}^{K_i-1} \gamma^{j-k} r_{i,j+1}$ (return)
    $C(x_k, u_k) \leftarrow C(x_k, u_k) + 1$
  end for
  $Q^{h_\ell}(x, u) \leftarrow A(x, u)/C(x, u)$
  $h_{\ell+1}(x) \leftarrow \arg\max_u Q^{h_\ell}(x, u)$
end for

Optimistic policy improvement

- Policy unchanged for N trajectories

$\Rightarrow$ Algorithm learns slowly

- Policy improvement after each trajectory

  = **optimistic**

- We will also use ε-greedy exploration

Optimistic MC

Optimistic MC

initialize to 0 accumulator $A(x, u)$, counter $C(x, u)$
for each trajectory **do**
execute trajectory, e.g., applying ε-greedy:

$$u_k = \begin{cases} \arg\max_u Q(x_k, u) & \text{w.p. } (1 - \varepsilon_k) \\ \text{unif. random} & \text{w.p. } \varepsilon_k \end{cases}$$

for each step k **do**
$A(x_k, u_k) \leftarrow A(x_k, u_k) + \sum_{j=k}^{K-1} \gamma^{j-k} r_{j+1}$
$C(x_k, u_k) \leftarrow C(x_k, u_k) + 1$
end for
$Q(x, u) \leftarrow A(x, u)/C(x, u)$
end for

- h implicit, greedy in Q
- update of $Q \Rightarrow$ implicit improvement of h

Optimism in TD

- Earlier TD algorithm: fixed h
- What is the fastest we can improve h in TD?
  After each transition.

$\Rightarrow$ interpretation: policy iteration
optimistic at the transition level

- h implicit, greedy in Q
  (updating $Q \Rightarrow$ implicit improvement of h)

SARSA

SARSA with ε-greedy

for each trajectory **do**

initialize x_0

$$u_0 = \begin{cases} \arg\max_u Q(x_0, u) & \text{w.p. } (1 - \varepsilon_0) \\ \text{unif. random} & \text{w.p. } \varepsilon_0 \end{cases}$$

repeat at each step k

apply u_k, measure x_{k+1}, receive r_{k+1}

$$u_{k+1} = \begin{cases} \arg\max_u Q(x_{k+1}, u) & \text{w.p. } (1 - \varepsilon_{k+1}) \\ \text{unif. random} & \text{w.p. } \varepsilon_{k+1} \end{cases}$$

$$Q(x_k, u_k) \leftarrow Q(x_k, u_k) + \alpha_k \cdot \\ [r_{k+1} + \gamma Q(x_{k+1}, u_{k+1}) - Q(x_k, u_k)]$$

until trajectory finished

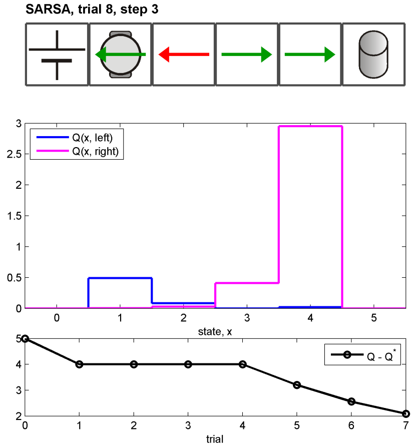
end for

Origin of name "SARSA"

$(x_k, u_k, r_{k+1}, x_{k+1}, u_{k+1}) =$
(**S**tate, **A**ction, **R**eward, **S**tate, **A**ction) = **SARSA**

Cleaning robot: SARSA, demo

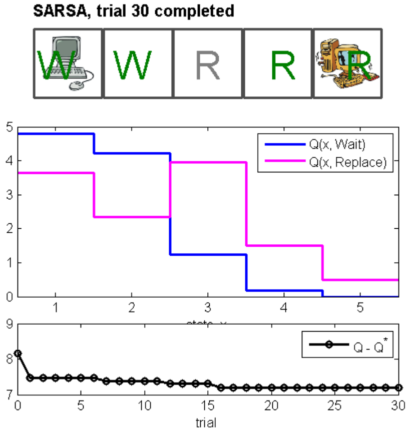
Parameters: $\alpha = 0.2$, $\varepsilon = 0.3$ (constant)
$x_0 = 2$ or 3 (random)



Machine replacement: SARSA, demo

Parameters: $\alpha = 0.1$, $\varepsilon = 0.3$ (constant), 20 steps per trajectory

$x_0 = 1$



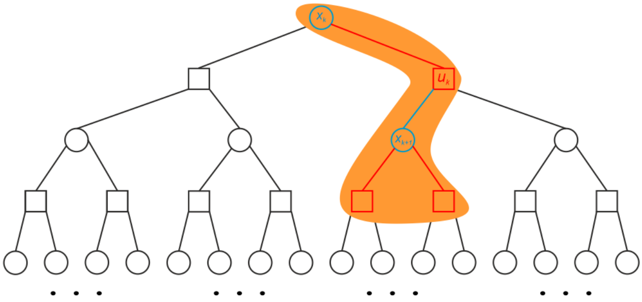
Bootstrapping estimate of Q^*

Bellman optimality equation:

$$Q^*(x,u) = \mathrm{E}_{x'}\left\{\tilde{\rho}(x,u,x') + \gamma \max_{u'} Q^*(x',u')\right\}$$

leads to estimate:

$$\hat{Q}_k = r_{k+1} + \gamma \max_{u'} Q(x_{k+1}, u')$$



TD update for Q^*

$$
\begin{aligned}
Q(x_k, u_k) \leftarrow & Q(x_k, u_k) + \alpha_k [\hat{Q}_k - Q(x_k, u_k)] \\
& [r_{k+1} + \gamma \max_{u'} Q(x_{k+1}, u') - Q(x_k, u_k)]
\end{aligned}
$$

Q-learning

Q-learning with ε-greedy

for each trajectory **do**
  initialize x_0
  repeat at each step k

$$u_k = \begin{cases} \arg\max_u Q(x_k, u) & \text{w.p. } (1 - \varepsilon_k) \\ \text{unif. random} & \text{w.p. } \varepsilon_k \end{cases}$$

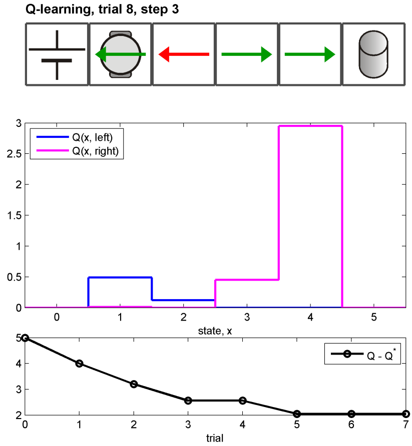
  apply u_k, measure x_{k+1}, receive r_{k+1}

$$Q(x_k, u_k) \leftarrow Q(x_k, u_k) + \alpha_k \cdot \left[r_{k+1} + \gamma \max_{u'} Q(x_{k+1}, u') - Q(x_k, u_k)\right]$$

  until trajectory finished
end for

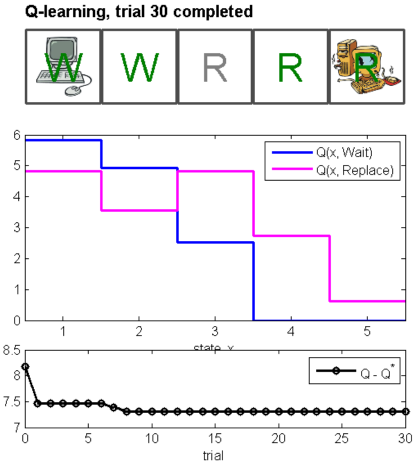
Cleaning robot: Q-learning, demo

Parameters – same as SARSA: $\alpha = 0.2$, $\varepsilon = 0.3$ (constant)
$x_0 = 2$ or 3 (random)



Machine replacement: Q-learning, demo

Parameters: $\alpha = 0.1$, $\varepsilon = 0.3$ (constant), 20 steps per trajectory
$x_0 = 1$



1. Monte Carlo, MC

2. Exploration

3. Temporal differences, TD
   - Introduction
   - SARSA
   - Q-learning
   - Discussion

4. Accelerating TD methods

5. Recap

Convergence

Conditions for convergence to Q^*:

1. All pairs (x, u) continue to be updated: ensured by **exploration**, e.g. ε-greedy
2. Stochastic-approximation conditions: learning rate decreases to zero, $\sum_{k=0}^{\infty} \alpha_k^2 =$ finite, but not too quickly: $\sum_{k=0}^{\infty} \alpha_k \to \infty$

Additionally, for SARSA:

3. The policy must become greedy at infinity e.g. $\lim_{k\to\infty} \varepsilon_k = 0$

On-policy / off-policy

SARSA: **on-policy**

- Always estimates the Q-function of the current policy

Q-learning: **off-policy**

- Independently of the current policy,
  always estimates the optimal Q-function

TD: Discussion

Advantages

- Simple to understand and implement
- Low complexity $\Rightarrow$ fast execution

SARSA vs. Q-learning

- SARSA less complex than Q-learning
  (no max in the Q-function update)

Learning rate and exploration sequences α_k, ε_k
significantly influence performance

Main disadvantage

- Large amount of data required

1. Monte Carlo, MC
2. Exploration
3. Temporal differences, TD
4. Accelerating TD methods
   - Motivation
   - Experience replay
   - n-step returns
5. Recap

The need to accelerate TD

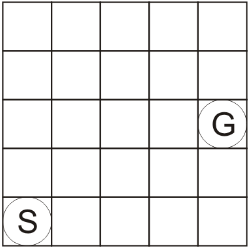
Main disadvantage: TD learns slowly – **requires a lot of data**

In practice, data costs:

- time
- profit (low performance due to exploration)
- system wear

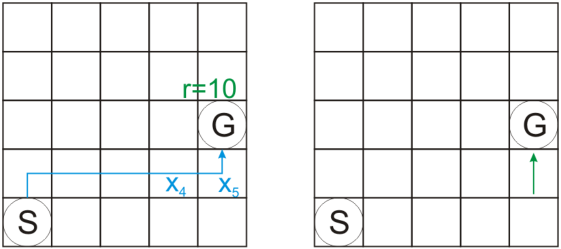
Accelerating RL = **efficient use of data**

Example: 2D navigation



- Navigation in a discrete 2D world from **S**tart to **G**oal
- Reward $= 10$ only upon reaching G (terminal state)

Example: TD



- We choose SARSA, $\alpha = 1$; initialize $Q = 0$
- Updates along trajectory on the left:

$$\ldots$$
$$Q(x_4, u_4) = 0 + \gamma \cdot Q(x_5, u_5) = 0$$
$$Q(x_5, u_5) = 10 + \gamma \cdot 0 = 10$$

- A new transition from x_4 to x_5 needed to propagate the information to x_4!

Accelerating TD: 2 ideas

1. Store and **replay experience**
2. Use **n-step returns**

1. Monte Carlo, MC
2. Exploration
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   - n-step returns
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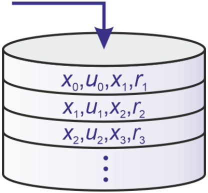
Experience replay (ER)

- Store each transition $(x_k, u_k, x_{k+1}, r_{k+1})$ (and for SARSA, also u_{k+1}) in a database



- At each step, **replay** m transitions from database (in addition to normal updates)

Q-learning with ER

Q-learning with ER

for each trajectory **do**
  initialize x_0
  repeat at each step k
    apply u_k, measure x_{k+1}, receive r_{k+1}
    $Q(x_k, u_k) \leftarrow Q(x_k, u_k) + \alpha_k \cdot$
    $$[r_{k+1} + \gamma \max_{u'} Q(x_{k+1}, u') - Q(x_k, u_k)]$$
    add $(x_k, u_k, x_{k+1}, r_{k+1})$ to the database
    ReplayExperience
  until trajectory ends
end for

ReplayExperience procedure

ReplayExperience

loop m times

fetch a transition (x, u, x', r) from the database

$$Q(x,u) \leftarrow Q(x,u) + \alpha \cdot \left[r + \gamma \max_{u'} Q(x', u') - Q(x,u)\right]$$

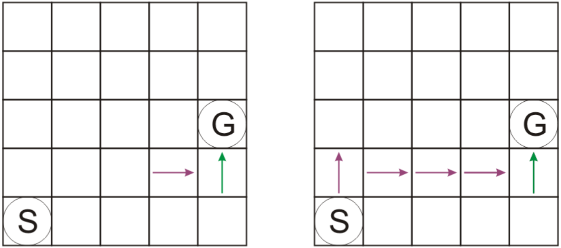
end loop

Replay direction

Order of replaying transitions:

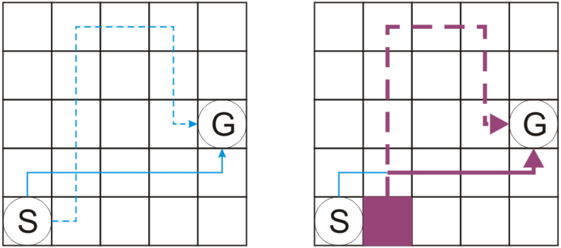
1. Forward
2. Backward
3. Arbitrary

Example: Influence of replay direction



- Green: normal updates, purple: experience replay
- Left: forward replay; right: backward replay
- **Backward replay** preferable in exact RL

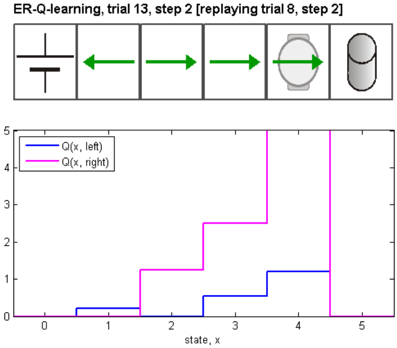
Example: Aggregating information



- Experience replay **aggregates information** from multiple trajectories
- The indicated cell benefits from information along both trajectories

Cleaning robot: Q-learning with ER, demo

Parameters: $\alpha = 0.2$, $\varepsilon = 0.3$, $m = 5$, backward direction
$x_0 = 2$ or 3 (random)



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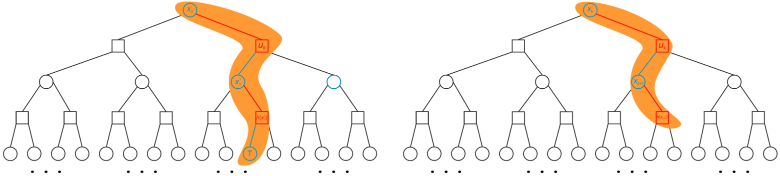
   - Motivation
   - Experience replay
   - n-step returns
5. Recap

Recall: MC and TD return estimates

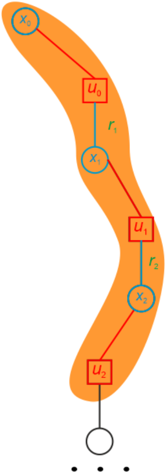


$$R_k = \sum_{j=k}^{K-1} \gamma^{j-k} r_{j+1}$$

$$\hat{R}_k = r_{k+1} + \gamma Q(x_{k+1}, h(x_{k+1}))$$

Is there something in-between?

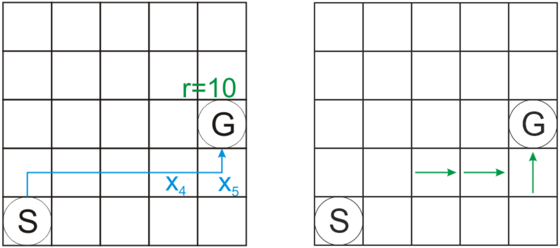
Middle ground: n-step return



SARSA (on-policy):

$$\begin{aligned}\hat{R}_k =& r_{k+1} + \gamma r_{k+2} + \ldots + \gamma^{n-1} r_{k+n} \\ &+ \gamma^n Q(x_{k+n}, u_{k+n})\end{aligned}$$

Example: Effect of n-step return

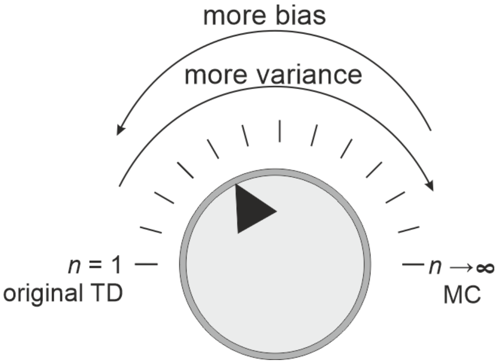


For $n = 3$:

$$Q(x_5, u_5) = 10 + 0 \quad \text{(terminal)}$$
$$Q(x_4, u_4) = 0 + \gamma 10 + 0 \quad \text{(terminal)}$$
$$Q(x_3, u_3) = 0 + \gamma 0 + \gamma^2 10 + 0 \quad \text{(terminal)}$$
$$Q(x_2, u_2) = 0 + \gamma 0 + \gamma^2 0 + \gamma^3 0 \quad \text{(bootstrap)}$$
$$\dots$$

TD versus MC

- $n = 1$ recovers TD, $n \to \infty$ recovers MC
- Intermediate values mix TD and MC, leading to a tunable bias-variance tradeoff



1. Monte Carlo, MC
2. Exploration
3. Temporal differences, TD
4. Accelerating TD methods
5. Recap

Recap: Methods in Part III

Monte-Carlo methods, MC:

- MC policy iteration
- MC with incremental updates

Exploration-exploitation dilemma:

- ε-greedy widely used
- Many other solutions exist, like UCB

Temporal differences, TD:

- TD for policy evaluation
- Optimistic policy improvements
- SARSA
- Q-learning

Accelerating TD:

- Experience replay
- n-step returns

Key terms in this part

- Monte-Carlo methods
- exploration-exploitation dilemma
- ϵ-greedy, softmax, bandits
- optimistic policy improvement
- learning rate
- bootstrapping
- temporal differences
- SARSA
- Q-learning
- experience replay
- n-step returns

Exercises

1. Does the exponential schedule $\alpha_k = \alpha^k$, with $\alpha \in (0,1)$ a constant, satisfy the stochastic approximation conditions?
2. Is Q-learning guaranteed to converge when $\varepsilon_k = \varepsilon$, a constant in $(0,1)$? What about SARSA? How about when you use an exponential decrease $\varepsilon_k = \varepsilon^k$?
3. Would a Monte-Carlo algorithm that improves the policy after every transition (like TD) make sense?
4. Would Q-learning (without n-step returns as they are nontrivial in the off-policy case) propagate information faster than SARSA for the gridworld trajectory example?

Exercises (cont'd)

5. Assuming that we have access to a model **only for the purposes of policy improvement**, provide V-function alternates for all algorithms in this part. Do this in the same order as for Q-functions:
   - Monte Carlo estimates, averaging-based and incremental
   - Bootstrapping estimates and updates
   - Policy evaluation, SARSA, and Q-learning

   Don't forget to draw trees and highlights, it will help you visualize things.