

# Markov Decision Process, Optimal Solutions, Monte Carlo Methods

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unless otherwise stated

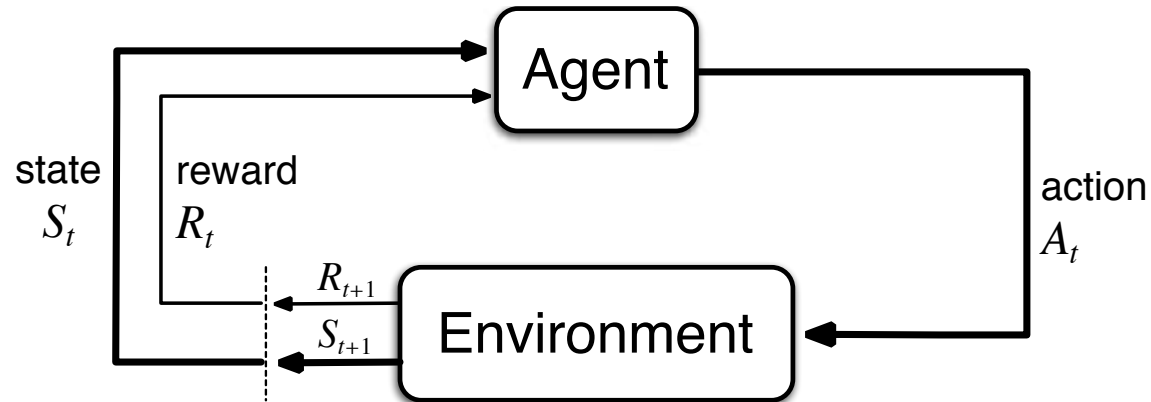


Figure 3.1 of "Reinforcement Learning: An Introduction, Second Edition".

A Markov decision process (MDP) is a quadruple  $(\mathcal{S}, \mathcal{A}, p, \gamma)$ , where:

- $\mathcal{S}$  is a set of states,
- $\mathcal{A}$  is a set of actions,
- $p(S_{t+1} = s', R_{t+1} = r | S_t = s, A_t = a)$  is a probability that action  $a \in \mathcal{A}$  will lead from state  $s \in \mathcal{S}$  to  $s' \in \mathcal{S}$ , producing a reward  $r \in \mathbb{R}$ ,
- $\gamma \in [0, 1]$  is a *discount factor*.

Let a *return*  $G_t$  be  $G_t \stackrel{\text{def}}{=} \sum_{k=0}^{\infty} \gamma^k R_{t+1+k}$ . The goal is to optimize  $\mathbb{E}[G_0]$ .

# Multi-armed Bandits as MDP

To formulate  $n$ -armed bandits problem as MDP, we do not need states. Therefore, we could formulate it as:

- one-element set of states,  $\mathcal{S} = \{S\}$ ;
- an action for every arm,  $\mathcal{A} = \{a_1, a_2, \dots, a_n\}$ ;
- assuming every arm produces rewards with a distribution of  $\mathcal{N}(\mu_i, \sigma_i^2)$ , the MDP dynamics function  $p$  is defined as

$$p(S, r | S, a_i) = \mathcal{N}(r | \mu_i, \sigma_i^2).$$

One possibility to introduce states in multi-armed bandits problem is to have separate reward distribution for every state. Such generalization is usually called *Contextualized Bandits* problem. Assuming that state transitions are independent on rewards and given by a distribution  $next(s)$ , the MDP dynamics function for contextualized bandits problem is given by

$$p(s', r | s, a_i) = \mathcal{N}(r | \mu_{i,s}, \sigma_{i,s}^2) \cdot next(s' | s).$$

# (State-)Value and Action-Value Functions

A *policy*  $\pi$  computes a distribution of actions in a given state, i.e.,  $\pi(a|s)$  corresponds to a probability of performing an action  $a$  in state  $s$ .

To evaluate a quality of a policy, we define *value function*  $v_\pi(s)$ , or *state-value function*, as

$$v_\pi(s) \stackrel{\text{def}}{=} \mathbb{E}_\pi [G_t | S_t = s] = \mathbb{E}_\pi \left[ \sum_{k=0}^{\infty} \gamma^k R_{t+k+1} \mid S_t = s \right].$$

An *action-value function* for a policy  $\pi$  is defined analogously as

$$q_\pi(s, a) \stackrel{\text{def}}{=} \mathbb{E}_\pi [G_t | S_t = s, A_t = a] = \mathbb{E}_\pi \left[ \sum_{k=0}^{\infty} \gamma^k R_{t+k+1} \mid S_t = s, A_t = a \right].$$

Evidently,

$$\begin{aligned} v_\pi(s) &= \mathbb{E}_\pi [q_\pi(s, a)], \\ q_\pi(s, a) &= \mathbb{E}_\pi [R_{t+1} + \gamma v_\pi(S_{t+1}) | S_t = s, A_t = a]. \end{aligned}$$

Optimal state-value function is defined as

$$v_*(s) \stackrel{\text{def}}{=} \max_{\pi} v_{\pi}(s),$$

analogously

$$q_*(s, a) \stackrel{\text{def}}{=} \max_{\pi} q_{\pi}(s, a).$$

Any policy  $\pi_*$  with  $v_{\pi_*} = v_*$  is called an *optimal policy*. Such policy can be defined as

$$\pi_*(s) \stackrel{\text{def}}{=} \arg \max_a q_*(s, a) = \arg \max_a \mathbb{E}[R_{t+1} + \gamma v_*(S_{t+1}) | S_t = s, A_t = a].$$

## Existence

Under some mild assumptions, there always exists a unique optimal state-value function, unique optimal action-value function, and (not necessarily unique) optimal policy. The mild assumptions are that either termination is guaranteed from all reachable states, or  $\gamma < 1$ .

Dynamic programming is an approach devised by Richard Bellman in 1950s.

To apply it to MDP, we now consider finite-horizon problems (i.e., with episodes of bounded length) with finite number of states  $\mathcal{S}$  and actions  $\mathcal{A}$ , and known MDP dynamics  $p$ .

The following recursion (which must hold for an optimal value function in a MDP, because future decisions does not depend on the current one) is usually called the *Bellman equation*:

$$\begin{aligned} v_*(s) &= \max_a \mathbb{E} [R_{t+1} + \gamma v_*(S_{t+1}) | S_t = s, A_t = a] \\ &= \max_a \sum_{s', r} p(s', r | s, a) [r + \gamma v_*(s')]. \end{aligned}$$

It can be also shown that if a value function satisfies the Bellman equation, it is already optimal.

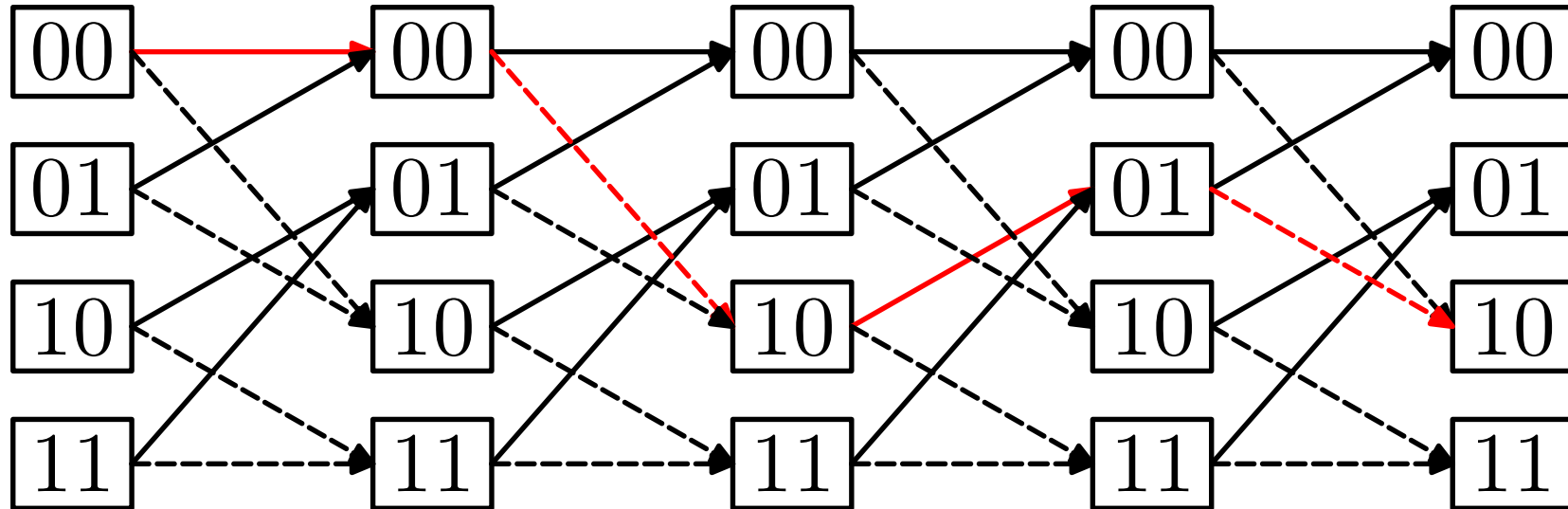
To turn the Bellman equation into an algorithm, we change the equal signs to assignments:

$$v_0(s) \leftarrow 0$$
$$v_{k+1}(s) \leftarrow \max_a \mathbb{E} [R_{t+1} + \gamma v_k(S_{t+1}) | S_t = s, A_t = a].$$

It is easy to show that if the problem consists of episodes of length at most  $T$  steps, the optimal value function is reached after  $T$  iteration of the above assignment (we can show by induction that  $v_k(s)$  is the maximum return reachable from state  $s$  in  $k$  steps).

# Relations to Graph Algorithms

Searching for optimal value functions of deterministic problems is in fact search for the shortest path in a suitable graph.



[https://upload.wikimedia.org/wikipedia/commons/a/a0/Convolutional\\_code\\_trellis\\_diagram.svg](https://upload.wikimedia.org/wikipedia/commons/a/a0/Convolutional_code_trellis_diagram.svg)



$$v_{k+1}(s) \leftarrow \max_a \mathbb{E} [R_{t+1} + \gamma v_k(S_{t+1}) | S_t = s, A_t = a].$$

Bellman-Ford-Moore algorithm:

```
# input: graph `g`, initial vertex `s`
for v in g.vertices: d[v] = 0 if v == s else +∞

for i in range(len(g.vertices) - 1):
    for e in g.edges:
        if d[e.source] + e.length < d[e.target]:
            d[e.target] = d[e.source] + e.length
```

# Bellman Backup Operator

Our goal is now to handle also infinite horizon tasks, using discount factor of  $\gamma < 1$ .

For any value function  $v \in \mathbb{R}^{|\mathcal{S}|}$  we define *Bellman backup operator*  $B : \mathbb{R}^{|\mathcal{S}|} \rightarrow \mathbb{R}^{|\mathcal{S}|}$  as

$$Bv(s) \stackrel{\text{def}}{=} \max_a \mathbb{E} [R_{t+1} + \gamma v(S_{t+1}) | S_t = s, A_t = a].$$

It is not difficult to show that Bellman backup operator is a *contraction*:

$$\max_s |Bv_1(s) - Bv_2(s)| \leq \gamma \max_s |v_1(s) - v_2(s)|.$$

Considering a normed vector space  $\mathbb{R}^{|\mathcal{S}|}$  with sup-norm  $\|\cdot\|_\infty$ , from Banach fixed-point theorem it follows there exist a *unique value function*  $v_*$  such that

$$Bv_* = v_*.$$

Such unique  $v_*$  is the *optimal value function*, because it satisfies the Bellman equation.

Furthermore, iterative application of  $B$  on arbitrary  $v$  converges to  $v_*$ , because

$$\|Bv - v_*\|_\infty = \|Bv - Bv_*\|_\infty \leq \gamma \|v - v_*\|,$$

and therefore  $B^n v \rightarrow v_*$ .

# Value Iteration Algorithm

We can turn the iterative application of Bellman backup operator into an algorithm.

$$Bv(s) \stackrel{\text{def}}{=} \max_a \mathbb{E} [R_{t+1} + \gamma v(S_{t+1}) | S_t = s, A_t = a]$$

## Value Iteration, for estimating $\pi \approx \pi_*$

Algorithm parameter: a small threshold  $\theta > 0$  determining accuracy of estimation  
Initialize  $V(s)$ , for all  $s \in \mathcal{S}$ , arbitrarily except that  $V(\text{terminal}) = 0$

Loop:

```
|  $\Delta \leftarrow 0$   
| Loop for each  $s \in \mathcal{S}$ :  
|    $v \leftarrow V(s)$   
|    $V(s) \leftarrow \max_a \sum_{s',r} p(s', r | s, a) [r + \gamma V(s')]$   
|    $\Delta \leftarrow \max(\Delta, |v - V(s)|)$   
until  $\Delta < \theta$ 
```

Output a deterministic policy,  $\pi \approx \pi_*$ , such that  
$$\pi(s) = \arg \max_a \sum_{s',r} p(s', r | s, a) [r + \gamma V(s')]$$

*Modification of Algorithm 4.4 of "Reinforcement Learning: An Introduction, Second Edition".*

# Value Iteration Algorithm

Although we have described the so-called *synchronous* implementation requiring two arrays for  $v$  and  $Bv$ , usual implementations are *asynchronous* and modify the value function in place (if a fixed ordering is used, usually such value iteration is called *Gauss-Seidel*).

Even with such asynchronous update value iteration can be proven to converge, and usually performs better in practise.

# Bellman Backup Operator as a Contraction

To show that Bellman backup operator is a contraction, we proceed as follows:

$$\begin{aligned}
 \|Bv_1 - Bv_2\|_\infty &= \left\| \max_a \mathbb{E} [R_{t+1} + \gamma v_1(S_{t+1})] - \max_a \mathbb{E} [R_{t+1} + \gamma v_2(S_{t+1})] \right\|_\infty \\
 &\leq \max_a \left( \left\| \mathbb{E} [R_{t+1} + \gamma v_1(S_{t+1})] - \mathbb{E} [R_{t+1} + \gamma v_2(S_{t+1})] \right\|_\infty \right) \\
 &= \max_a \left( \left\| \sum_{s',r} p(s',r|s,a) \gamma (v_1(s') - v_2(s')) \right\|_\infty \right) \\
 &= \gamma \max_a \left( \left\| \sum_{s',r} p(s'|s,a) (v_1(s') - v_2(s')) \right\|_\infty \right) \\
 &\leq \gamma \|v_1 - v_2\|_\infty,
 \end{aligned}$$

where the second line follows from  $|\max_x f(x) - \max_x g(x)| \leq \max_x |f(x) - g(x)|$  and the last line from the fact that from any given  $s$  and  $a$ , the  $\sum_{s'} p(s'|s,a)$  sums to 1.

# Speed of Convergence

Assuming maximum reward is  $R_{\max}$ , we have that

$$v_*(s) \leq \sum_{t=0}^{\infty} \gamma^t R_{\max} = \frac{R_{\max}}{1 - \gamma}.$$

Starting with  $v(s) \leftarrow 0$ , we have

$$\|B^k v - v_*\|_{\infty} \leq \gamma^k \|v - v_*\|_{\infty} = \gamma^k \frac{R_{\max}}{1 - \gamma}.$$

Compare to finite horizon case, where  $B^T v = v_*$ .

# Policy Iteration Algorithm

We now propose another approach of computing optimal policy. The approach, called *policy iteration*, consists of repeatedly performing *policy evaluation* and *policy improvement*.

## Policy Evaluation

Given a policy  $\pi$ , policy evaluation computes  $v_\pi$ .

Recall that

$$\begin{aligned} v_\pi(s) &\stackrel{\text{def}}{=} \mathbb{E}_\pi [G_t | S_t = s] \\ &= \mathbb{E}_\pi [R_{t+1} + \gamma v_\pi(S_{t+1}) | S_t = s] \\ &= \sum_a \pi(a|s) \sum_{s',r} p(s', r | s, a) [r + \gamma v_\pi(s')]. \end{aligned}$$

If the dynamics of the MDP  $p$  is known, the above is a system of linear equations, and therefore,  $v_\pi$  can be computed exactly.



The equation

$$v_{\pi}(s) = \sum_a \pi(a|s) \sum_{s',r} p(s', r|s, a) [r + \gamma v_{\pi}(s')]$$

is called *Bellman equation for  $v_{\pi}$*  and analogously to Bellman optimality equation, it can be proven that

- under the same assumptions as before ( $\gamma < 1$  or termination),  $v_{\pi}$  exists and is unique;
- $v_{\pi}$  is a fixed point of the Bellman equation

$$v_{k+1}(s) = \sum_a \pi(a|s) \sum_{s',r} p(s', r|s, a) [r + \gamma v_k(s')];$$

- iterative application of the Bellman equation to any  $v$  converges to  $v_{\pi}$ .

## Iterative Policy Evaluation, for estimating $V \approx v_\pi$

Input  $\pi$ , the policy to be evaluated

Algorithm parameter: a small threshold  $\theta > 0$  determining accuracy of estimation

Initialize  $V(s)$ , for all  $s \in \mathcal{S}$ , arbitrarily except that  $V(\text{terminal}) = 0$

Loop:

$\Delta \leftarrow 0$

Loop for each  $s \in \mathcal{S}$ :

$v \leftarrow V(s)$

$V(s) \leftarrow \sum_a \pi(a|s) \sum_{s',r} p(s', r | s, a) [r + \gamma V(s')]$

$\Delta \leftarrow \max(\Delta, |v - V(s)|)$

until  $\Delta < \theta$

*Modification of Algorithm 4.1 of "Reinforcement Learning: An Introduction, Second Edition".*

# Policy Improvement

Given  $\pi$  and computed  $v_\pi$ , we would like to *improve* the policy. A straightforward way to do so is to define a policy using a *greedy* action

$$\begin{aligned}\pi'(s) &\stackrel{\text{def}}{=} \arg \max_a q_\pi(s, a) \\ &= \arg \max_a \sum_{s', r} p(s', r | s, a) [r + \gamma v_\pi(s')].\end{aligned}$$

For such  $\pi'$ , we can easily show that

$$q_\pi(s, \pi'(s)) \geq v_\pi(s).$$

# Policy Improvement Theorem

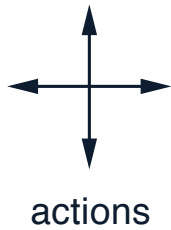
Let  $\pi$  and  $\pi'$  be any pair of deterministic policies, such that  $q_\pi(s, \pi'(s)) \geq v_\pi(s)$ .

Then for all states  $s$ ,  $v_{\pi'}(s) \geq v_\pi(s)$ .

The proof is straightforward, we repeatedly expand  $q_\pi$  and use the assumption of the policy improvement theorem:

$$\begin{aligned}
 v_\pi(s) &\leq q_\pi(s, \pi'(s)) \\
 &= \mathbb{E}[R_{t+1} + \gamma v_\pi(S_{t+1}) | S_t = s, A_t = \pi'(s)] \\
 &= \mathbb{E}_{\pi'}[R_{t+1} + \gamma v_\pi(S_{t+1}) | S_t = s] \\
 &\leq \mathbb{E}_{\pi'}[R_{t+1} + \gamma q_\pi(S_{t+1}, \pi'(S_{t+1})) | S_t = s] \\
 &= \mathbb{E}_{\pi'}[R_{t+1} + \gamma \mathbb{E}[R_{t+2} + \gamma v_\pi(S_{t+2}) | S_{t+1}, A_{t+1} = \pi'(S_{t+1})] | S_t = s] \\
 &= \mathbb{E}_{\pi'}[R_{t+1} + \gamma R_{t+2} + \gamma^2 v_\pi(S_{t+2}) | S_t = s] \\
 &\dots \\
 &\leq \mathbb{E}_{\pi'}[R_{t+1} + \gamma R_{t+2} + \gamma^2 R_{t+3} + \dots | S_t = s] = v_{\pi'}(s)
 \end{aligned}$$

# Policy Improvement Example



	1	2	3
4	5	6	7
8	9	10	11
12	13	14	

$R_t = -1$   
on all transitions

Example 4.1 of "Reinforcement Learning: An Introduction, Second Edition".

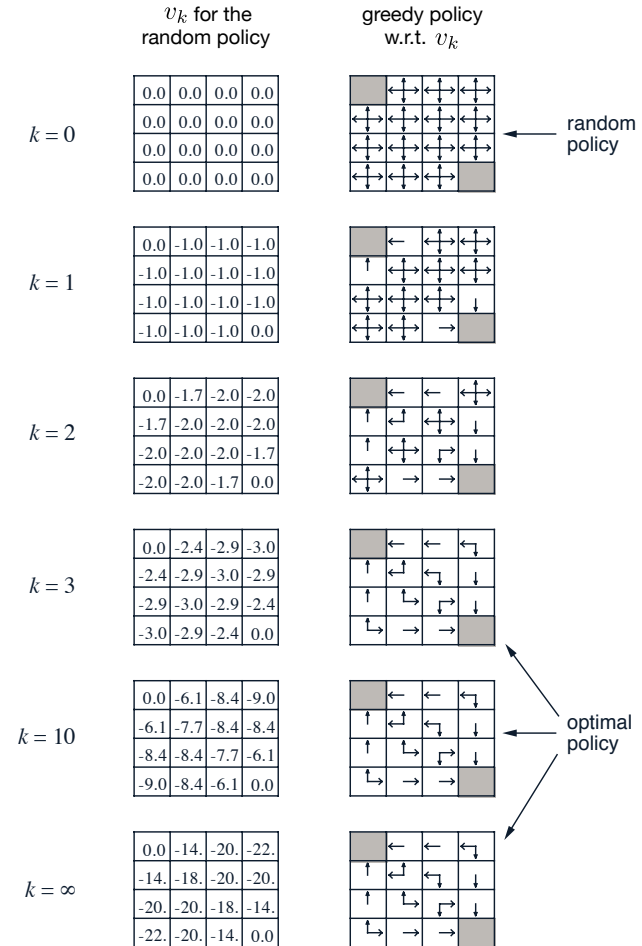


Figure 4.1 of "Reinforcement Learning: An Introduction, Second Edition".

# Policy Iteration Algorithm

Policy iteration consists of repeatedly performing policy evaluation and policy improvement:

$$\pi_0 \xrightarrow{E} v_{\pi_0} \xrightarrow{I} \pi_1 \xrightarrow{E} v_{\pi_1} \xrightarrow{I} \pi_2 \xrightarrow{E} v_{\pi_2} \xrightarrow{I} \dots \xrightarrow{I} \pi_* \xrightarrow{E} v_{\pi_*}.$$

The result is a sequence of monotonically improving policies  $\pi_i$ . Note that when  $\pi' = \pi$ , also  $v_{\pi'} = v_{\pi}$ , which means Bellman optimality equation is fulfilled and both  $v_{\pi}$  and  $\pi$  are optimal.

Considering that there is only a finite number of policies, the optimal policy and optimal value function can be computed in finite time (contrary to value iteration, where the convergence is only asymptotic).

Note that when evaluating policy  $\pi_{k+1}$ , we usually start with  $v_{\pi_k}$ , which is assumed to be a good approximation to  $v_{\pi_{k+1}}$ .

Policy Iteration (using iterative policy evaluation) for estimating  $\pi \approx \pi_*$

1. Initialization

$V(s) \in \mathbb{R}$  and  $\pi(s) \in \mathcal{A}(s)$  arbitrarily for all  $s \in \mathcal{S}$

2. Policy Evaluation

Loop:

$\Delta \leftarrow 0$

Loop for each  $s \in \mathcal{S}$ :

$v \leftarrow V(s)$

$V(s) \leftarrow \sum_{s',r} p(s',r|s,\pi(s)) [r + \gamma V(s')]$

$\Delta \leftarrow \max(\Delta, |v - V(s)|)$

until  $\Delta < \theta$  (a small positive number determining the accuracy of estimation)

3. Policy Improvement

*policy-stable*  $\leftarrow$  *true*

For each  $s \in \mathcal{S}$ :

*old-action*  $\leftarrow \pi(s)$

$\pi(s) \leftarrow \operatorname{argmax}_a \sum_{s',r} p(s',r|s,a) [r + \gamma V(s')]$

If *old-action*  $\neq \pi(s)$ , then *policy-stable*  $\leftarrow$  *false*

If *policy-stable*, then stop and return  $V \approx v_*$  and  $\pi \approx \pi_*$ ; else go to 2

Algorithm 4.3 of "Reinforcement Learning: An Introduction, Second Edition".

Note that value iteration is in fact a policy iteration, where policy evaluation is performed only for one step:

$$\pi'(s) = \arg \max_a \sum_{s',r} p(s', r | s, a) [r + \gamma v(s')] \quad (\textit{policy improvement})$$

$$v'(s) = \sum_a \pi'(a|s) \sum_{s',r} p(s', r | s, a) [r + \gamma v(s')] \quad (\textit{one step of policy evaluation})$$

Substituting the former into the latter, we get

$$v'(s) = \max_a \sum_{s',r} p(s', r | s, a) [r + \gamma v(s)] = Bv(s).$$



# Generalized Policy Iteration

Therefore, it seems that to achieve convergence, it is not necessary to perform policy evaluation exactly.

*Generalized Policy Evaluation* is a general idea of interleaving policy evaluation and policy improvement at various granularity.

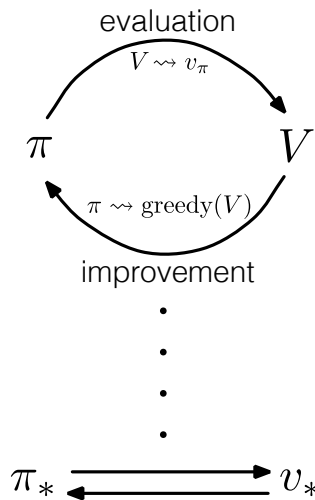


Figure in Section 4.6 of "Reinforcement Learning: An Introduction, Second Edition".

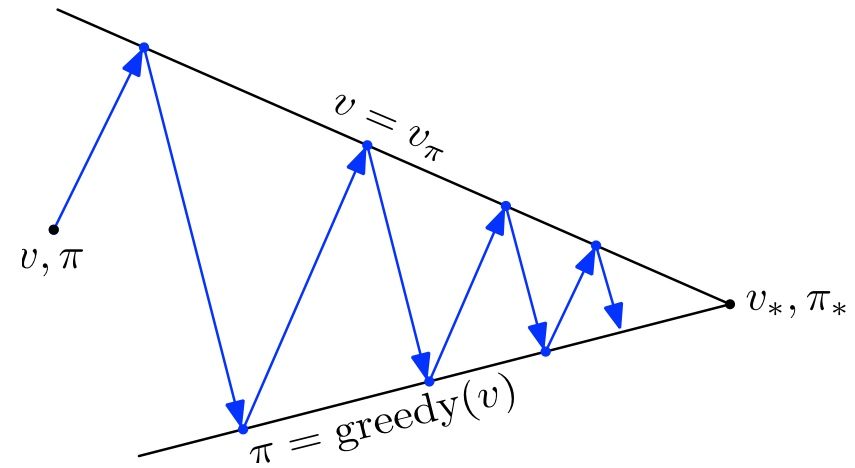


Figure in Section 4.6 of "Reinforcement Learning: An Introduction, Second Edition".

If both processes stabilize, we know we have obtained optimal policy.

We now present the first algorithm for computing optimal policies without assuming a knowledge of the environment dynamics.

However, we still assume there are finitely many states  $\mathcal{S}$  and we will store estimates for each of them.

Monte Carlo methods are based on estimating returns from complete episodes. Furthermore, if the model (of the environment) is not known, we need to estimate returns for the action-value function  $q$  instead of  $v$ .

We can formulate Monte Carlo methods in the generalized policy improvement framework.

Keeping estimated returns for the action-value function, we perform policy evaluation by sampling one episode according to current policy. We then update the action-value function by averaging over the observed returns, including the sampled episode.

To guarantee convergence, we need to visit each state infinitely many times. One of the simplest way to achieve that is to assume *exploring starts*, where we randomly select the first state and first action, each pair with nonzero probability.

Furthermore, if a state-action pair appears multiple times in one episode, the sampled returns are not independent. The literature distinguishes two cases:

- *first visit*: only the first occurrence of a state-action pair in an episode is considered
- *every visit*: all occurrences of a state-action pair are considered.

Even though first-visit is easier to analyze, it can be proven that for both approaches, policy evaluation converges. Contrary to the Reinforcement Learning: An Introduction book, which presents first-visit algorithms, we use every-visit.

## Monte Carlo ES (Exploring Starts), for estimating $\pi \approx \pi_*$

Initialize:

$\pi(s) \in \mathcal{A}(s)$  (arbitrarily), for all  $s \in \mathcal{S}$

$Q(s, a) \in \mathbb{R}$  (arbitrarily), for all  $s \in \mathcal{S}, a \in \mathcal{A}(s)$

$Returns(s, a) \leftarrow$  empty list, for all  $s \in \mathcal{S}, a \in \mathcal{A}(s)$

Loop forever (for each episode):

Choose  $S_0 \in \mathcal{S}, A_0 \in \mathcal{A}(S_0)$  randomly such that all pairs have probability  $> 0$

Generate an episode from  $S_0, A_0$ , following  $\pi$ :  $S_0, A_0, R_1, \dots, S_{T-1}, A_{T-1}, R_T$

$G \leftarrow 0$

Loop for each step of episode,  $t = T-1, T-2, \dots, 0$ :

$G \leftarrow \gamma G + R_{t+1}$

Append  $G$  to  $Returns(S_t, A_t)$

$Q(S_t, A_t) \leftarrow \text{average}(Returns(S_t, A_t))$

$\pi(S_t) \leftarrow \text{argmax}_a Q(S_t, a)$

*Modification (no first-visit) of algorithm 5.3 of "Reinforcement Learning: An Introduction, Second Edition".*

A policy is called  $\varepsilon$ -soft, if

$$\pi(a|s) \geq \frac{\varepsilon}{|\mathcal{A}(s)|}.$$

For  $\varepsilon$ -soft policy, Monte Carlo policy evaluation also converges, without the need of exploring starts.

We call a policy  $\varepsilon$ -greedy, if one action has maximum probability of  $1 - \varepsilon + \frac{\varepsilon}{|\mathcal{A}(s)|}$ .

The policy improvement theorem can be proved also for the class of  $\varepsilon$ -soft policies, and using  $\varepsilon$ -greedy policy in policy improvement step, policy iteration has the same convergence properties. (We can embed the  $\varepsilon$ -soft behaviour “inside” the environment and prove equivalence.)

## On-policy every-visit Monte Carlo for $\varepsilon$ -soft Policies

Algorithm parameter: small  $\varepsilon > 0$

Initialize  $Q(s, a) \in \mathbb{R}$  arbitrarily (usually to 0), for all  $s \in \mathcal{S}, a \in \mathcal{A}$

Initialize  $C(s, a) \in \mathbb{Z}$  to 0, for all  $s \in \mathcal{S}, a \in \mathcal{A}$

Repeat forever (for each episode):

- Generate an episode  $S_0, A_0, R_1, \dots, S_{T-1}, A_{T-1}, R_T$ , by generating actions as follows:
  - With probability  $\varepsilon$ , generate a random uniform action
  - Otherwise, set  $A_t \stackrel{\text{def}}{=} \arg \max_a Q(S_t, a)$
- $G \leftarrow 0$
- For each  $t = T - 1, T - 2, \dots, 0$ :
  - $G \leftarrow \gamma G + R_{T+1}$
  - $C(S_t, A_t) \leftarrow C(S_t, A_t) + 1$
  - $Q(S_t, A_t) \leftarrow Q(S_t, A_t) + \frac{1}{C(S_t, A_t)} (G - Q(S_t, A_t))$