UNIVERSITY OF TECHNOLOGY
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Deep Reinforcement Learning

Dynamic Programming

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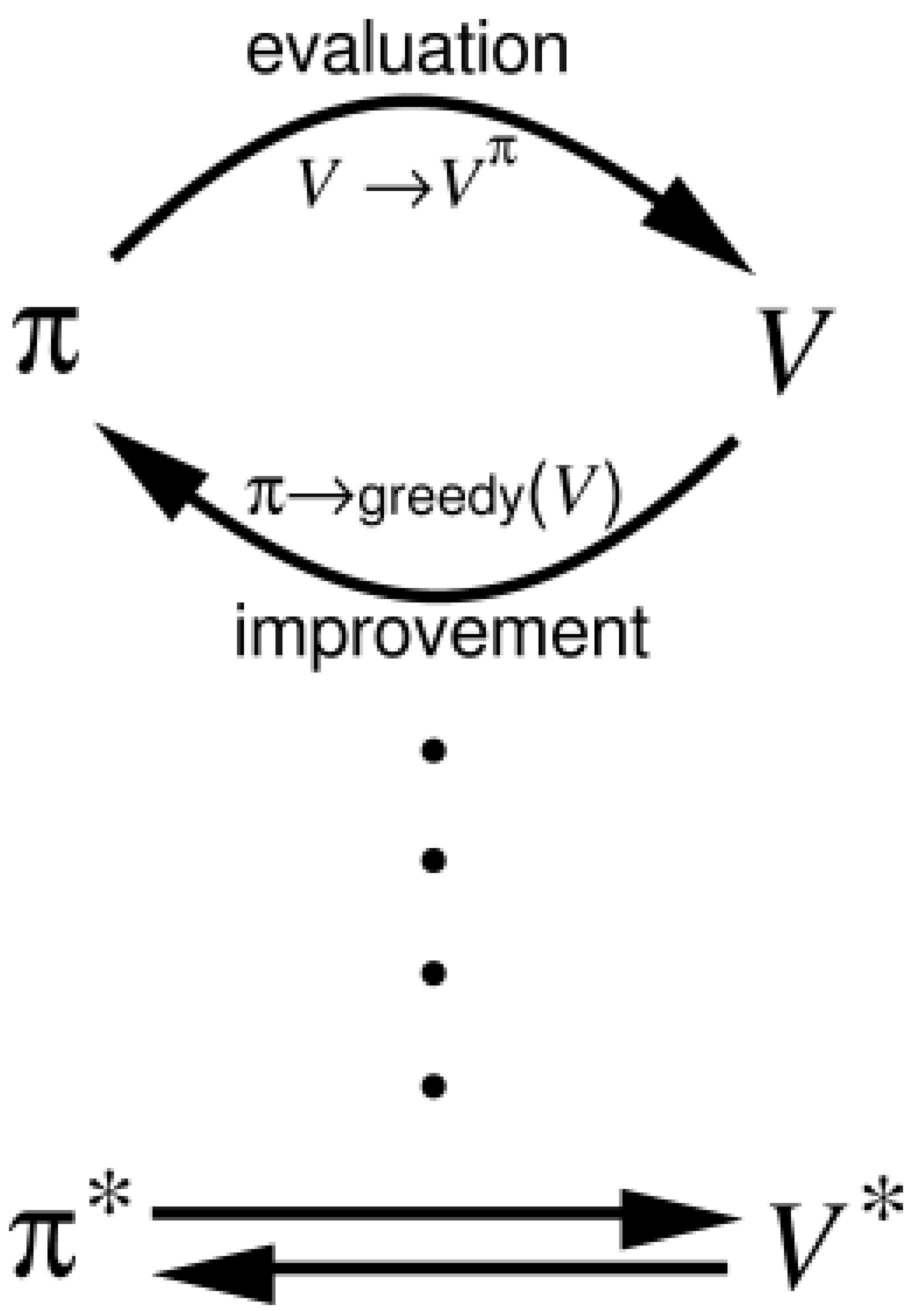
https://tu-chemnitz.de/informatik/KI/edu/deeprl

Dynamic Programming (DP)



- Dynamic Programming (DP) iterates over two steps:
  1. **Policy evaluation**
     - For a given policy π, the value of all states $V^\pi(s)$ or all state action pairs $Q^\pi(s, a)$ is calculated based on the Bellman equations:

$$V^\pi(s) = \sum_{a \in \mathcal{A}(s)} \pi(s, a) \sum_{s' \in \mathcal{S}} p(s' | s, a) \, [r(s, a, s') + \gamma \, V^\pi(s'$$

  2. **Policy improvement**
     - From the current estimated values $V^\pi(s)$ or $Q^\pi(s, a)$, a new **better** policy π is derived.

- After enough iterations, the policy converges to the **optimal policy** (if the states are Markov).
- Two main algorithms: **policy iteration** and **value iteration**.

1 - Policy iteration

Policy evaluation

- Bellman equation for the state s and a fixed policy π:

$$V^{\pi}(s) = \sum_{a \in \mathcal{A}(s)} \pi(s, a) \sum_{s' \in \mathcal{S}} p(s' | s, a) \, [r(s, a, s') + \gamma \, V^{\pi}(s')]$$

- Let's note $\mathcal{P}_{ss'}^{\pi}$ the transition probability between s and s' (dependent on the policy π) and $\mathcal{R}_{s}^{\pi}$ the expected reward in s (also dependent):

$$\mathcal{P}_{ss'}^{\pi} = \sum_{a \in \mathcal{A}(s)} \pi(s, a) \sum_{s' \in \mathcal{S}} p(s' | s, a)$$

$$\mathcal{R}_{s}^{\pi} = \sum_{a \in \mathcal{A}(s)} \pi(s, a) \sum_{s' \in \mathcal{S}} p(s' | s, a) \, r(s, a, s')$$

- The Bellman equation becomes:

$$V^{\pi}(s) = \mathcal{R}_{s}^{\pi} + \gamma \sum_{s' \in \mathcal{S}} \mathcal{P}_{ss'}^{\pi} \, V^{\pi}(s')$$

- As we have a fixed policy during the evaluation (Markov Reward Process), the Bellman equation is simplified.

Policy evaluation

- Let's now put the Bellman equations in a matrix-vector form.

$$V^{\pi}(s) = \mathcal{R}_s^{\pi} + \gamma \sum_{s' \in \mathcal{S}} \mathcal{P}_{ss'}^{\pi} \, V^{\pi}(s')$$

- We first define the **vector of state values** $\mathbf{V}^{\pi}$:

$$\mathbf{V}^{\pi} = \begin{bmatrix} V^{\pi}(s_1) \\ V^{\pi}(s_2) \\ \vdots \\ V^{\pi}(s_n) \end{bmatrix}$$

- and the **vector of expected reward** $\mathcal{R}^{\pi}$:

$$\mathcal{R}^{\pi} = \begin{bmatrix} \mathcal{R}^{\pi}(s_1) \\ \mathcal{R}^{\pi}(s_2) \\ \vdots \\ \mathcal{R}^{\pi}(s_n) \end{bmatrix}$$

- The **state transition matrix** $\mathcal{P}^{\pi}$ is defined as:

$$\mathcal{P}^{\pi} = \begin{bmatrix} \mathcal{P}_{s_1 s_1}^{\pi} & \mathcal{P}_{s_1 s_2}^{\pi} & \dots & \mathcal{P}_{s_1 s_n}^{\pi} \\ \mathcal{P}_{s_2 s_1}^{\pi} & \mathcal{P}_{s_2 s_2}^{\pi} & \dots & \mathcal{P}_{s_2 s_n}^{\pi} \\ \vdots & \vdots & \vdots & \vdots \\ \mathcal{P}_{s_n s_1}^{\pi} & \mathcal{P}_{s_n s_2}^{\pi} & \dots & \mathcal{P}_{s_n s_n}^{\pi} \end{bmatrix}$$

Policy evaluation

- You can simply check that:

$$\begin{bmatrix} V^\pi(s_1) \\ V^\pi(s_2) \\ \vdots \\ V^\pi(s_n) \end{bmatrix} = \begin{bmatrix} \mathcal{R}^\pi(s_1) \\ \mathcal{R}^\pi(s_2) \\ \vdots \\ \mathcal{R}^\pi(s_n) \end{bmatrix} + \gamma \begin{bmatrix} \mathcal{P}_{s_1 s_1}^\pi & \mathcal{P}_{s_1 s_2}^\pi & \ldots & \mathcal{P}_{s_1 s_n}^\pi \\ \mathcal{P}_{s_2 s_1}^\pi & \mathcal{P}_{s_2 s_2}^\pi & \ldots & \mathcal{P}_{s_2 s_n}^\pi \\ \vdots & \vdots & \vdots & \vdots \\ \mathcal{P}_{s_n s_1}^\pi & \mathcal{P}_{s_n s_2}^\pi & \ldots & \mathcal{P}_{s_n s_n}^\pi \end{bmatrix} \times \begin{bmatrix} V^\pi(s_1) \\ V^\pi(s_2) \\ \vdots \\ V^\pi(s_n) \end{bmatrix}$$

leads to the same equations as:

$$V^\pi(s) = \mathcal{R}_s^\pi + \gamma \sum_{s' \in \mathcal{S}} \mathcal{P}_{ss'}^\pi \, V^\pi(s')$$

for all states s.

- The Bellman equations for all states s can therefore be written with a matrix-vector notation as:

$$\mathbf{V}^\pi = \mathcal{R}^\pi + \gamma \, \mathcal{P}^\pi \, \mathbf{V}^\pi$$

Policy evaluation

- The Bellman equations for all states s is:

$$\mathbf{V}^\pi = \mathcal{R}^\pi + \gamma \, \mathcal{P}^\pi \, \mathbf{V}^\pi$$

- If we know $\mathcal{P}^\pi$ and $\mathcal{R}^\pi$ (dynamics of the MDP for the policy π), we can simply obtain the state values:

$$(\mathbb{I} - \gamma \, \mathcal{P}^\pi) \times \mathbf{V}^\pi = \mathcal{R}^\pi$$

where $\mathbb{I}$ is the identity matrix, what gives:

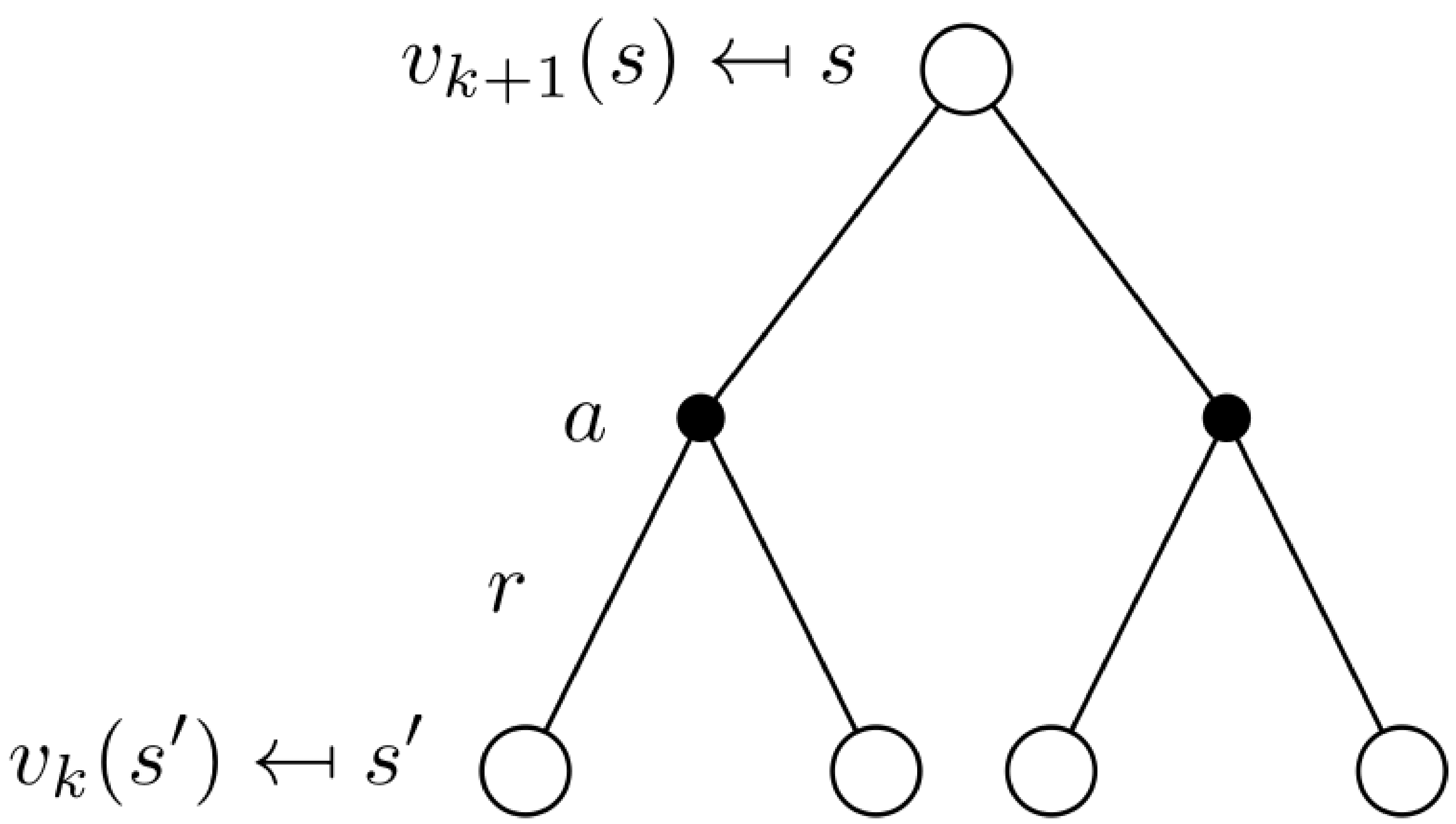
$$\mathbf{V}^\pi = (\mathbb{I} - \gamma \, \mathcal{P}^\pi)^{-1} \times \mathcal{R}^\pi$$

- Done!
- **But**, if we have n states, the matrix $\mathcal{P}^\pi$ has n^2 elements.
- Inverting $\mathbb{I} - \gamma \, \mathcal{P}^\pi$ requires at least $\mathcal{O}(n^{2.37})$ operations.
- Forget it if you have more than a thousand states ($1000^{2.37} \approx 13$ million operations).
- In **dynamic programming**, we will use **iterative methods** to estimate $\mathbf{V}^\pi$.

Iterative policy evaluation

- The idea of **iterative policy evaluation** (IPE) is to consider a sequence of consecutive state-value functions which should converge from initially wrong estimates $V_0(s)$ towards the real state-value function $V^\pi(s)$.

$$V_0 \rightarrow V_1 \rightarrow V_2 \rightarrow \ldots \rightarrow V_k \rightarrow V_{k+1} \rightarrow \ldots \rightarrow V^\pi$$



- The value function at step $k+1$ $V_{k+1}(s)$ is computed using the previous estimates $V_k(s)$ and the Bellman equation transformed into an **update rule**.
- In vector notation:

$$\mathbf{V}_{k+1} = \mathcal{R}^\pi + \gamma \, \mathcal{P}^\pi \, \mathbf{V}_k$$

Source: David Silver.
http://www0.cs.ucl.ac.uk/staff/d.silver/web/Teaching.html

Iterative policy evaluation

- Let's start with dummy (e.g. random) initial estimates $V_0(s)$ for the value of every state s.
- We can obtain new estimates $V_1(s)$ which are slightly less wrong by applying once the **Bellman operator**:

$$V_1(s) \leftarrow \sum_{a \in \mathcal{A}(s)} \pi(s, a) \sum_{s' \in \mathcal{S}} p(s' | s, a) \, [r(s, a, s') + \gamma \, V_0(s')] \quad \forall s \in \mathcal{S}$$

- Based on these estimates $V_1(s)$, we can obtain even better estimates $V_2(s)$ by applying again the Bellman operator:

$$V_2(s) \leftarrow \sum_{a \in \mathcal{A}(s)} \pi(s, a) \sum_{s' \in \mathcal{S}} p(s' | s, a) \, [r(s, a, s') + \gamma \, V_1(s')] \quad \forall s \in \mathcal{S}$$

- Generally, state-value function estimates are improved iteratively through:

$$V_{k+1}(s) \leftarrow \sum_{a \in \mathcal{A}(s)} \pi(s, a) \sum_{s' \in \mathcal{S}} p(s' | s, a) \, [r(s, a, s') + \gamma \, V_k(s')] \quad \forall s \in \mathcal{S}$$

- $V_\infty = V^\pi$ is a fixed point of this update rule because of the uniqueness of the solution to the Bellman equation.

Bellman operator

- The **Bellman operator** $\mathcal{T}^\pi$ is a mapping between two vector spaces:

$$\mathcal{T}^\pi (\mathbf{V}) = \mathcal{R}^\pi + \gamma \, \mathcal{P}^\pi \, \mathbf{V}$$

- If you apply repeatedly the Bellman operator on any initial vector $\mathbf{V}_0$, it converges towards the solution of the Bellman equations $\mathbf{V}^\pi$.
- Mathematically speaking, $\mathcal{T}^\pi$ is a γ-contraction, i.e. it makes value functions closer by at least γ:

$$|| \mathcal{T}^\pi (\mathbf{V}) - \mathcal{T}^\pi (\mathbf{U})||_\infty \leq \gamma \, ||\mathbf{V} - \mathbf{U} ||_\infty$$

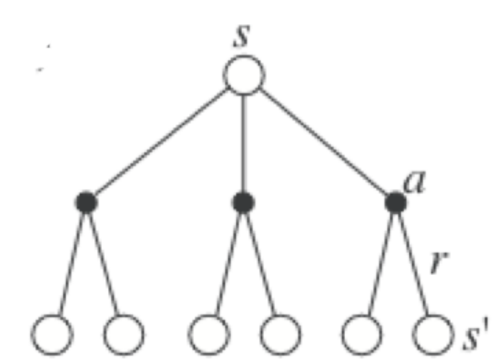
- The **contraction mapping theorem** ensures that $\mathcal{T}^\pi$ converges to an unique fixed point:
  - existence and uniqueness of the solution of the Bellman equations.

Backup diagram of IPE

- Iterative Policy Evaluation relies on **full backups**: it backs up the value of ALL possible successive states into the new value of a state.

$$V_{k+1}(s) \leftarrow \sum_{a \in \mathcal{A}(s)} \pi(s, a) \sum_{s' \in \mathcal{S}} p(s' | s, a) \, [r(s, a, s') + \gamma \, V_k(s')] \quad \forall s \in \mathcal{S}$$

- **Backup diagram:** which other values do you need to know in order to update one value?



- The backups are **synchronous**: all states are backed up in parallel.

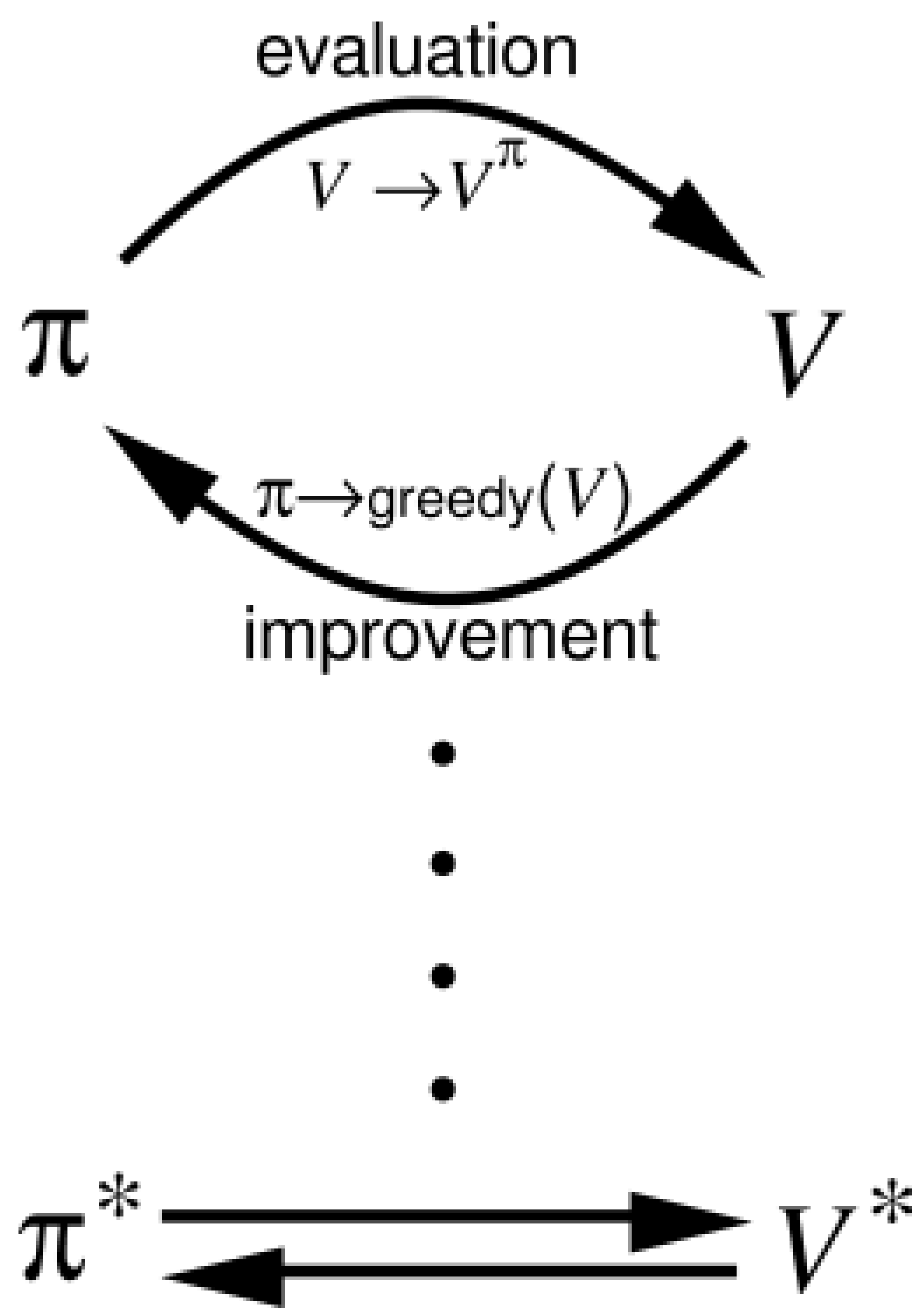
$$\mathbf{V}_{k+1} = \mathcal{R}^\pi + \gamma \, \mathcal{P}^\pi \, \mathbf{V}_k$$

- The termination of iterative policy evaluation has to be controlled by hand, as the convergence of the algorithm is only at the limit.
- It is good practice to look at the variations on the values of the different states, and stop the iteration when this variation falls below a predefined threshold.

Iterative policy evaluation

- For a fixed policy π, initialize $V(s) = 0 \; \forall s \in \mathcal{S}$.
- **while** not converged:
    - **for** all states s:
        - $V_\text{target}(s) = \sum_{a \in \mathcal{A}(s)} \pi(s, a) \, \sum_{s' \in \mathcal{S}} p(s' | s, a) \, [r(s, a, s') + \gamma \, V(s')]$
    - $\delta = 0$
    - **for** all states s:
        - $\delta = \max(\delta, |V(s) - V_\text{target}(s)|)$
        - $V(s) = V_\text{target}(s)$
    - **if** $\delta < \delta_\text{threshold}$:
        - converged = True

Dynamic Programming (DP)



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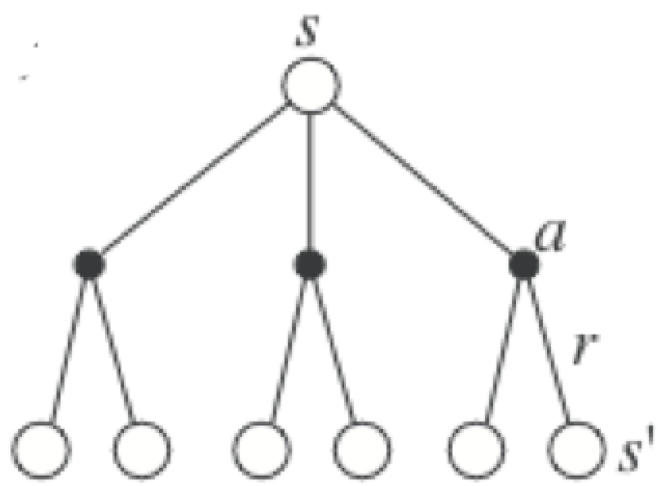
  2. **Policy improvement**
     - From the current estimated values $V^\pi(s)$ or $Q^\pi(s, a)$, a ne **better** policy π is derived.

Policy improvement

- For each state s, we would like to know if we should deterministically choose an action $a \neq \pi(s)$ or not in order to improve the policy.

- The value of an action a in the state s for the policy π is given by:



$$Q^{\pi}(s, a) = \sum_{s' \in \mathcal{S}} p(s'|s, a) \, [r(s, a, s') + \gamma \, V^{\pi}(s')]$$

- If the Q-value of an action a is higher than the one currently selected by the **deterministic** policy:

$$Q^{\pi}(s, a) > Q^{\pi}(s, \pi(s)) = V^{\pi}(s)$$

then it is better to select a once in s and thereafter follow π.

- If there is no better action, we keep the previous policy for this state.
- This corresponds to a **greedy** action selection over the Q-values, defining a **deterministic** policy $\pi(s)$:

$$\pi(s) \leftarrow \text{argmax}_a \, Q^{\pi}(s, a) = \sum_{s' \in \mathcal{S}} p(s'|s, a) \, [r(s, a, s') + \gamma \, V^{\pi}(s')]$$

Policy improvement

- After the policy improvement, the Q-value of each deterministic action $\pi(s)$ has increased or stayed the same.

$$\text{argmax}_a Q^\pi (s, a) = \sum_{s' \in \mathcal{S}} p(s' | s, a) \, [r(s, a, s') + \gamma \, V^\pi(s')] \geq Q^\pi(s, \pi(s))$$

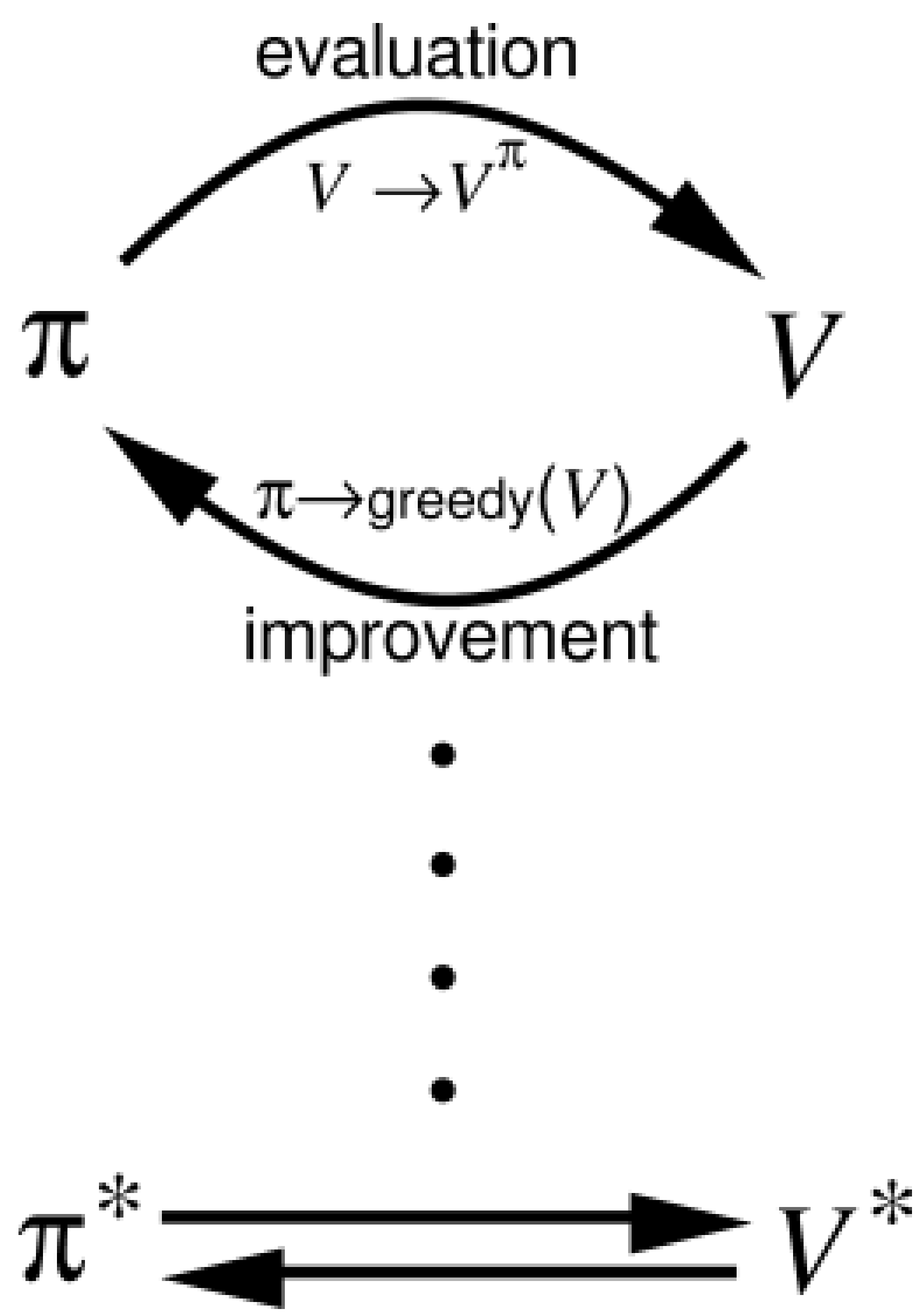
- This defines an **improved** policy π', where all states and actions have a higher value than previously.
- **Greedy action selection** over the state value function implements policy improvement:

$$\pi' \leftarrow \text{Greedy}(V^\pi)$$

Greedy policy improvement:

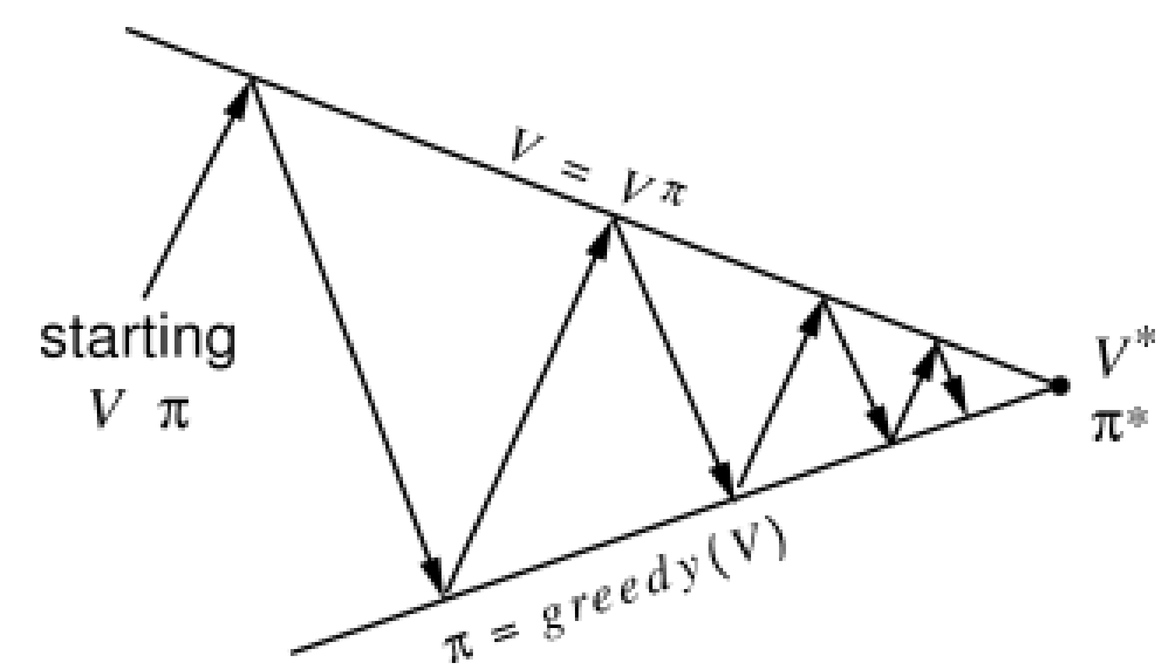
- **for** each state $s \in \mathcal{S}$:
  - $\pi(s) \leftarrow \text{argmax}_a \sum_{s' \in \mathcal{S}} p(s' | s, a) \, [r(s, a, s') + \gamma \, V^\pi(s')]$

Policy iteration



- Once a policy π has been improved using V^{π} to yield a better policy π', we can then compute $V^{\pi'}$ and improve it again to yield an even better policy π''.
- The algorithm **policy iteration** successively uses **policy evaluation** and **policy improvement** to find the optimal policy.

$$\pi_0 \xrightarrow{E} V^{\pi_0} \xrightarrow{I} \pi_1 \xrightarrow{E} V^{\pi^1} \xrightarrow{I} ... \xrightarrow{I} \pi^* \xrightarrow{E} V^*$$

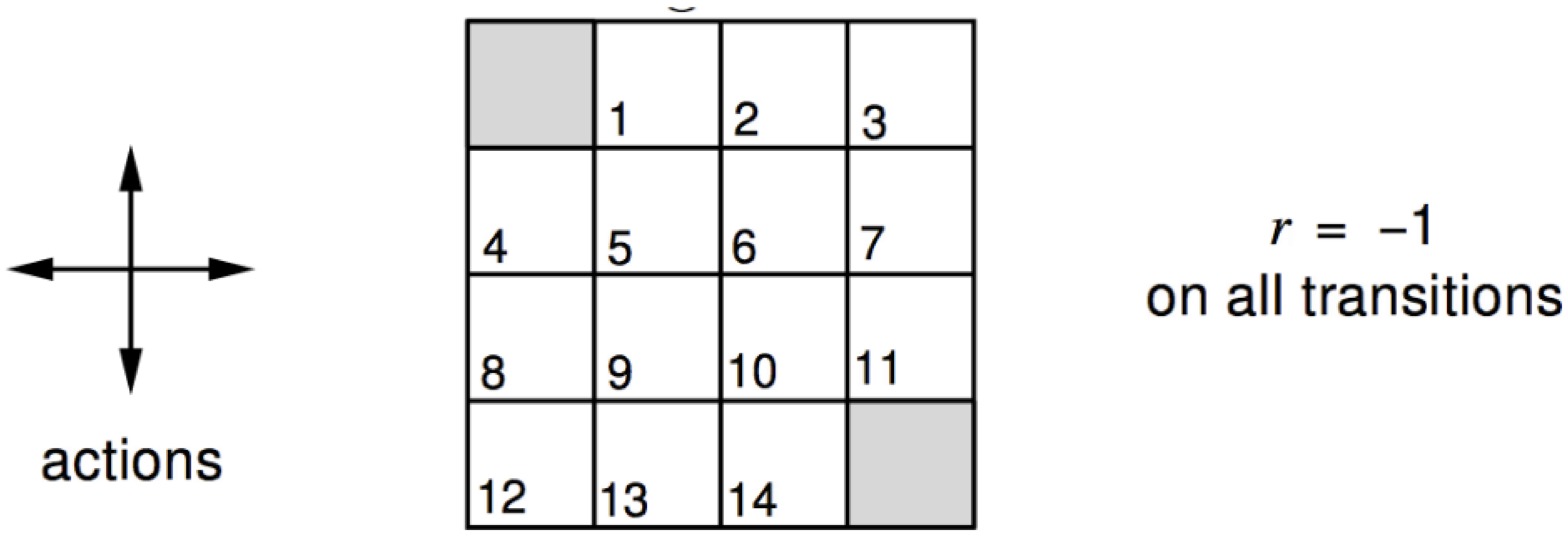


- The **optimal policy** being deterministic, policy improvement can be greedy over the state values.
- If the policy does not change after policy improvement, the optimal policy has been found.

Policy iteration

- Initialize a deterministic policy $\pi(s)$ and set $V(s) = 0 \; \forall s \in \mathcal{S}$.
- **while** π is not optimal:
  - **while** not converged: # Policy evaluation
    - **for** all states s:
      - $V_\text{target}(s) = \sum_{a \in \mathcal{A}(s)} \pi(s, a) \, \sum_{s' \in \mathcal{S}} p(s' | s, a) \, [r(s, a, s') + \gamma \, V(s')]$
    - **for** all states s:
      - $V(s) = V_\text{target}(s)$
  - **for** each state $s \in \mathcal{S}$: # Policy improvement
    - $\pi(s) \leftarrow \text{argmax}_a \sum_{s' \in \mathcal{S}} p(s' | s, a) \, [r(s, a, s') + \gamma \, V^{\pi}(s')]$
  - **if** π has not changed: **break**

Small Gridworld example

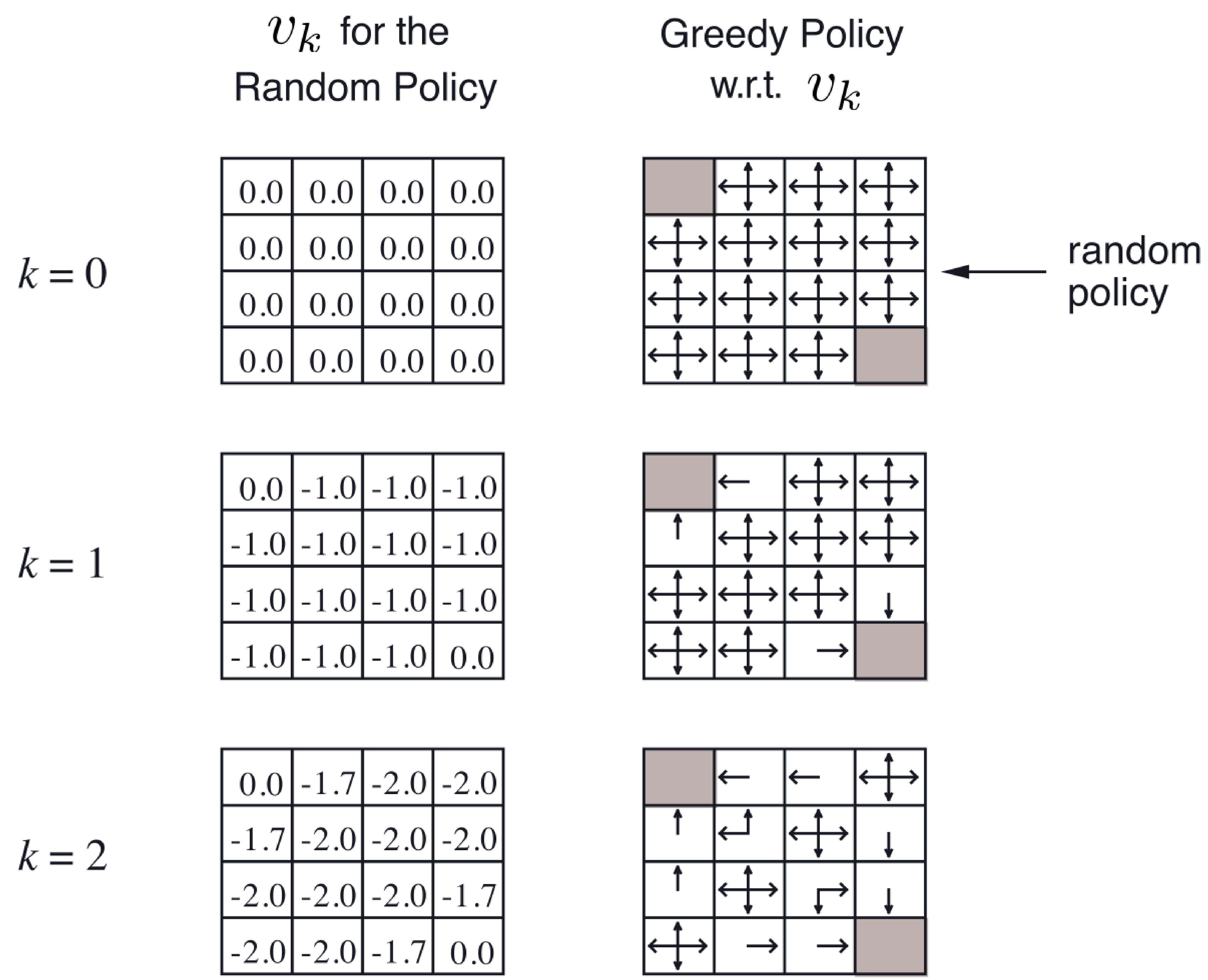


Source: David Silver. http://www0.cs.ucl.ac.uk/staff/d.silver/web/Teaching.html

- **Gridworld** is an undiscounted MDP (we can take $\gamma = 1$).
- The states are the position in the grid, the actions are up, down, left, right. Transitions to a wall leave in the same state.
- The reward is always -1, except after being in the terminal states in gray ($r = 0$).
- The initial policy is random:

$$\pi(s, \text{up}) = \pi(s, \text{down}) = \pi(s, \text{left}) = \pi(s, \text{right}) = 0.25$$

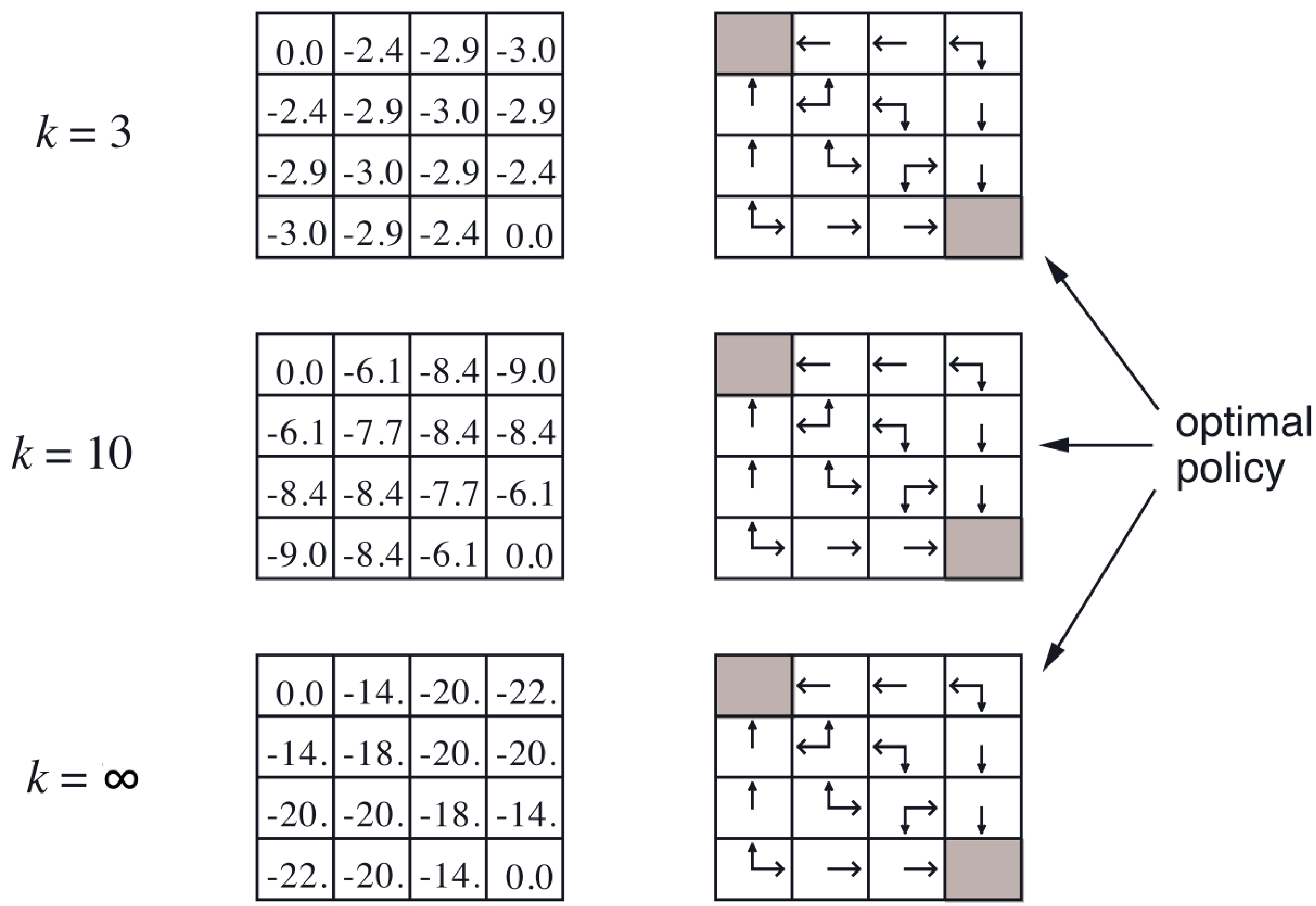
Small Gridworld example



- $k = 0$:
  - The initial values V_0 are set to 0 as the initial policy is random.
- $k = 1$:
  - The random policy is evaluated: all states get the value of the average immediate reward in that state. -1, except the terminal states (0).
  - The greedy policy is already an improvement over the random policy: adjacent states to the terminal states would decide to go there systematically, as the value is 0 instead of -1.

- $k = 2$: The previous estimates propagate: states adjacent to the terminal states get a higher value, as there will be less punishments after these states.

Small Gridworld example



- $k = 3$:
  - The values continue to propagate.
  - The greedy policy at that step of policy evaluation is already optimal.
- $k > 3$:
  - The values continue to converge towards the true values.
  - The greedy policy does not change. In this simple example, it is already the optimal policy.

- Two things to notice:
  - There is no actually no need to wait until the end of policy evaluation to improve the policy, as the greedy policy might already be optimal.
  - There can be more than one optimal policy: some actions may have the same Q-value: choosing one or other is equally optimal.

2 - Value iteration

Value iteration

- **Policy iteration** can converge in a surprisingly small number of iterations.
- One drawback of *policy iteration* is that it uses a full policy evaluation, which can be computationally exhaustive as the convergence of V_k is only at the limit and the number of states can be huge.
- The idea of **value iteration** is to interleave policy evaluation and policy improvement, so that the policy is improved after EACH iteration of policy evaluation, not after complete convergence.
- As policy improvement returns a deterministic greedy policy, updating of the value of a state is then simpler:

$$V_{k+1}(s) = \max_a \sum_{s'} p(s'|s, a)[r(s, a, s') + \gamma \, V_k(s')]$$

- Note that this is equivalent to turning the **Bellman optimality equation** into an update rule.
- Value iteration converges to V^*, faster than policy iteration, and should be stopped when the values do not change much anymore.

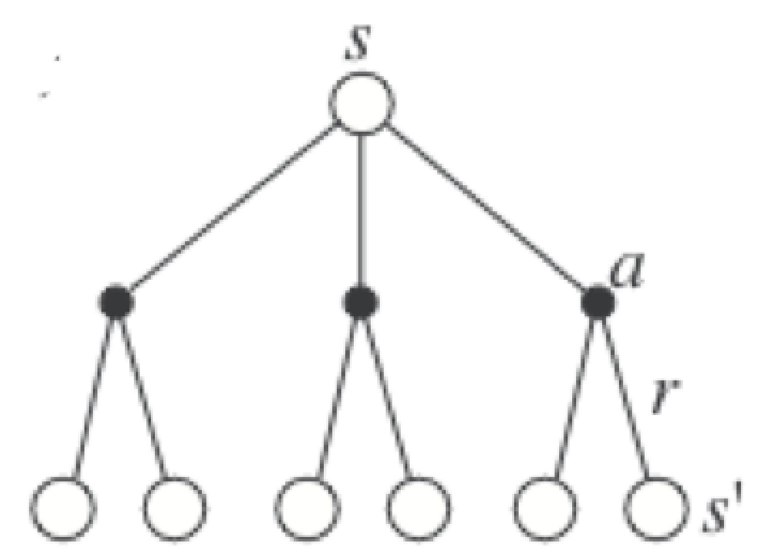
Value iteration

- Initialize a deterministic policy $\pi(s)$ and set $V(s) = 0 \; \forall s \in \mathcal{S}$.
- **while** not converged:
    - **for** all states s:
        - $V_\text{target}(s) = \max_a \; \sum_{s' \in \mathcal{S}} p(s' | s, a) \, [r(s, a, s') + \gamma \, V(s')]$
    - $\delta = 0$
    - **for** all states s:
        - $\delta = \max(\delta, |V(s) - V_\text{target}(s)|)$
        - $V(s) = V_\text{target}(s)$
    - **if** $\delta < \delta_\text{threshold}$:
        - converged = True

Comparison of Policy- and Value-iteration

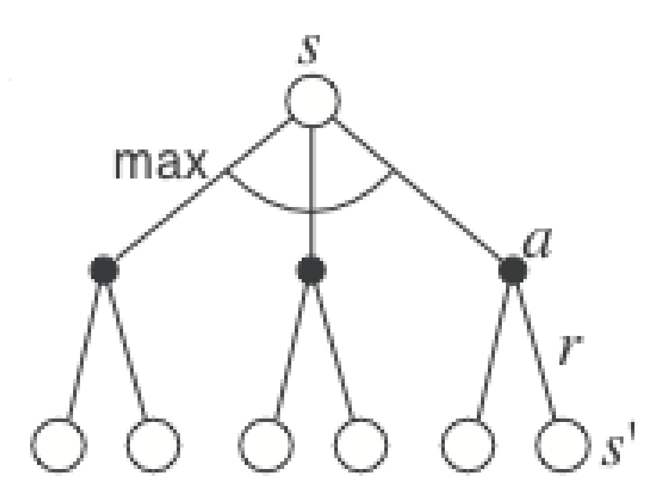
Full policy-evaluation backup

$$V_{k+1}(s) \leftarrow \sum_{a \in \mathcal{A}(s)} \pi(s,a) \sum_{s' \in \mathcal{S}} p(s'|s,a)\left[r(s,a,s') + \gamma\, V_k(s')\right]$$



Full value-iteration backup

$$V_{k+1}(s) \leftarrow \max_{a \in \mathcal{A}(s)} \sum_{s' \in \mathcal{S}} p(s'|s,a)\left[r(s,a,s') + \gamma\, V_k(s')\right]$$



Asynchronous dynamic programming

- Synchronous DP requires exhaustive sweeps of the entire state set (**synchronous backups**).
    - **while** not converged:
        - **for** all states s:
            - $V_\text{target}(s) = \max_a \, \sum_{s' \in \mathcal{S}} p(s' | s, a) \, [r(s, a, s') + \gamma \, V(s')]$
        - **for** all states s:
            - $V(s) = V_\text{target}(s)$
- Asynchronous DP updates instead each state independently and asynchronously (**in-place**):
    - **while** not converged:
        - Pick a state s randomly (or following a heuristic).
        - Update the value of this state.

$$V(s) = \max_a \, \sum_{s' \in \mathcal{S}} p(s' | s, a) \, [r(s, a, s') + \gamma \, V(s')]$$

- We must still ensure that all states are visited, but their frequency and order is irrelevant.

Asynchronous dynamic programming

- Is it possible to select the states to backup intelligently?
- **Prioritized sweeping** selects in priority the states with the largest remaining **Bellman error**:

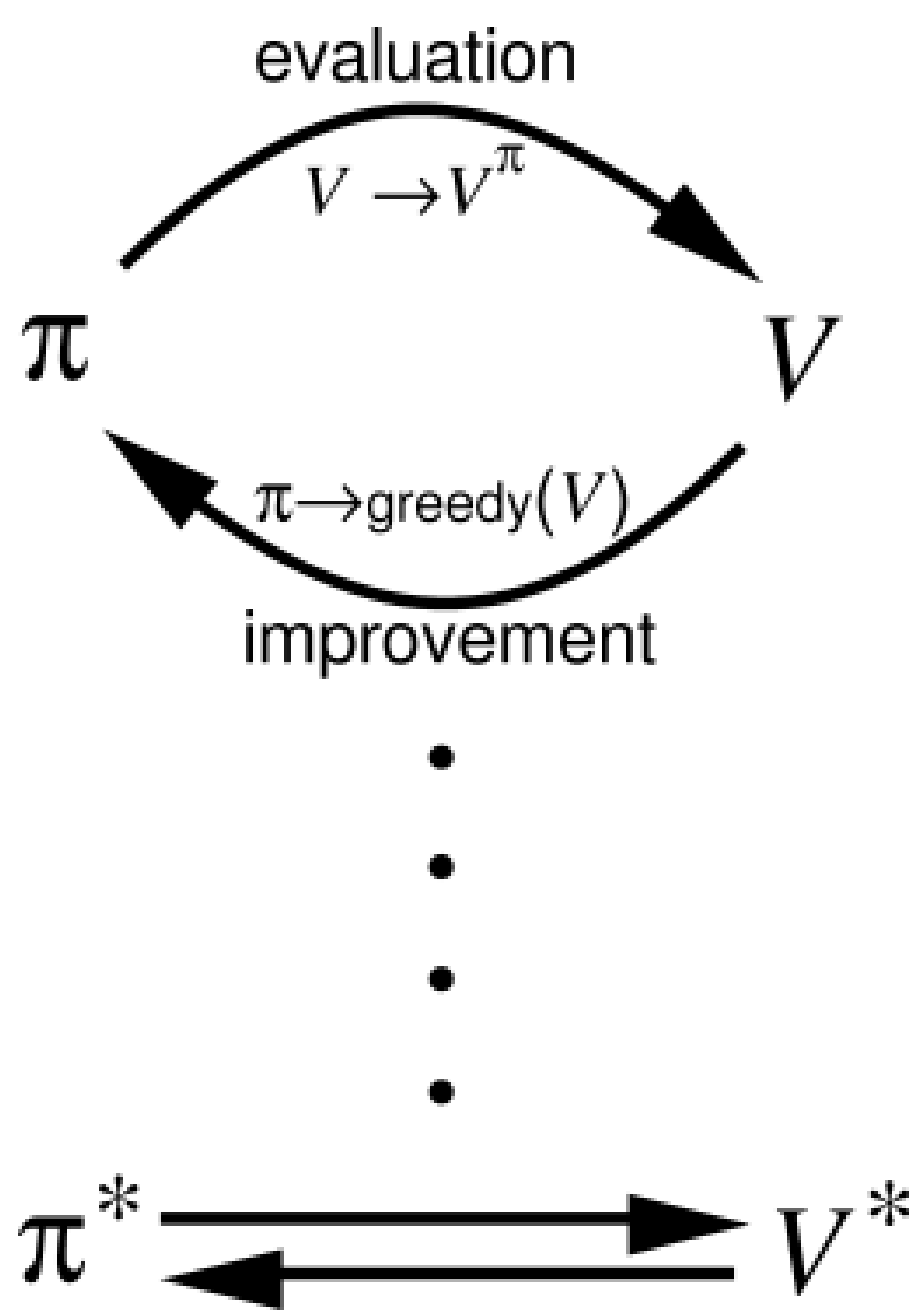
$$\delta = | \max_a \sum_{s' \in \mathcal{S}} p(s' | s, a) \, [r(s, a, s') + \gamma \, V(s')] - V(s) |$$

- A large Bellman error means that the current estimate $V(s)$ is very different from the **target** y:

$$y = \max_a \sum_{s' \in \mathcal{S}} p(s' | s, a) \, [r(s, a, s') + \gamma \, V(s')]$$

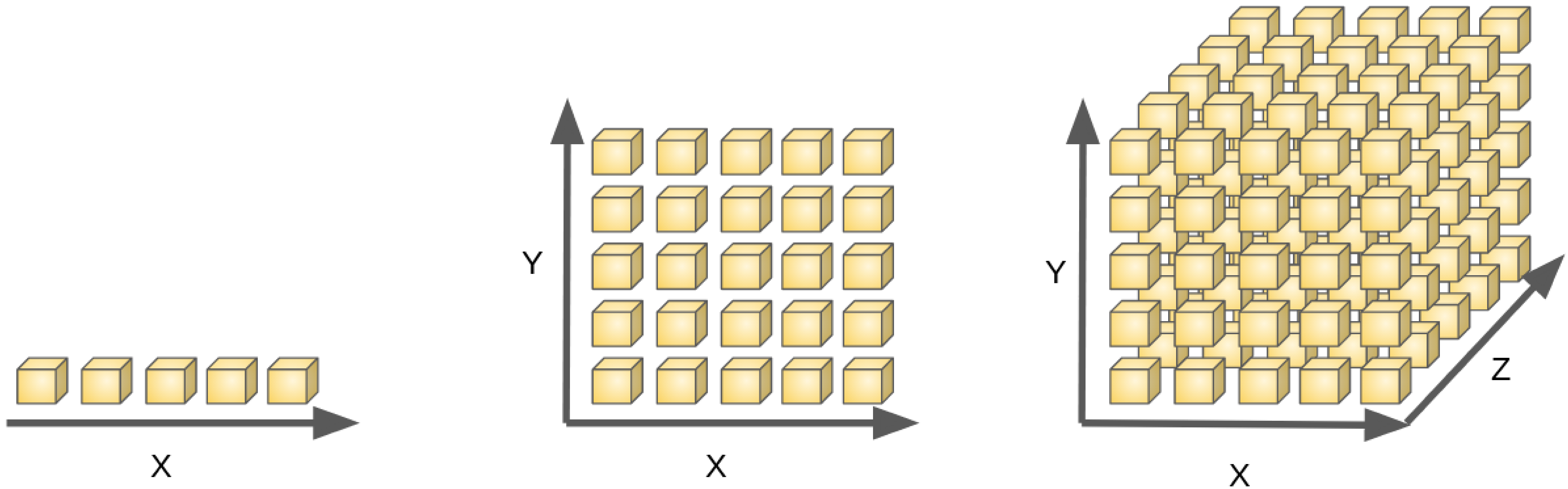
- States with a high Bellman error should be updated in priority.
- If the Bellman error is small, this means that the current estimate $V(s)$ is already close to what it should be, there is no hurry in evaluating this state.
- The main advantage is that the DP algorithm can be applied as the agent is actually experiencing its environment (no need for the dynamics of environment to be fully known).

Efficiency of Dynamic Programming



- Policy-iteration and value-iteration consist of alternations between policy evaluation and policy improvement, although at different frequencies.
- This principle is called **Generalized Policy Iteration** (GPI).
- Finding an optimal policy is polynomial in the number of states and actions: $\mathcal{O}(n^2\, m)$ (n is the number of states, m the number of actions).
- However, the number of states is often astronomical, e.g., often growing exponentially with the number of state variables (what Bellman called **"the curse of dimensionality"**).
- In practice, classical DP can only be applied to problems with a few millions of states.

Curse of dimensionality



Source: https://medium.com/diogo-menezes-borges/give-me-the-antidote-for-the-curse-of-dimensionality-b14bce4bf4d2

- If one variable can be represented by 5 discrete values:
  - 2 variables necessitate 25 states,
  - 3 variables need 125 states, and so on…
- The number of states explodes exponentially with the number of dimensions of the problem.