UNIVERSITY OF TECHNOLOGY
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Deep Reinforcement Learning

Dynamic Programming

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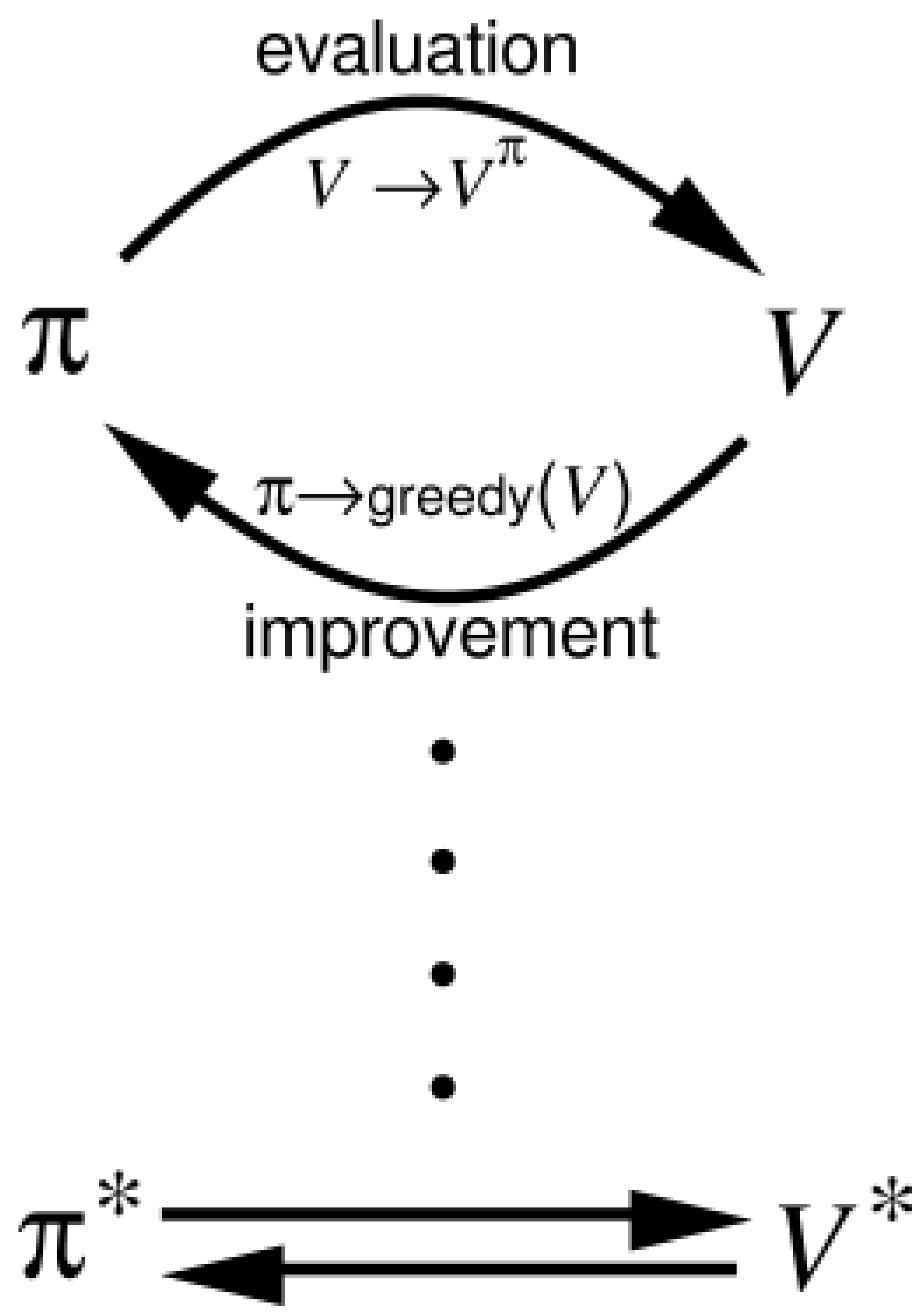
https://tu-chemnitz.de/informatik/KI/edu/deeprl

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 ne **better** policy π is derived.

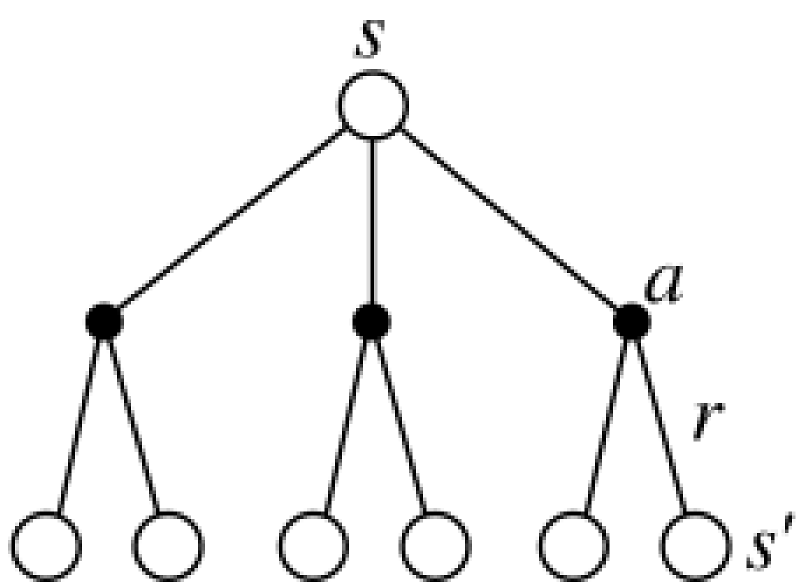
$$\pi' \leftarrow \text{Greedy}(V^\pi)$$

- 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):

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

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

- 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 (MRP), 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** $\mathbf{R}^{\pi}$:

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

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

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

Policy evaluation

- You can simply check that:

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

leads to the same equations as:

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

for all states s.

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

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

Policy evaluation

- The Bellman equations for all states s is:

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

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

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

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

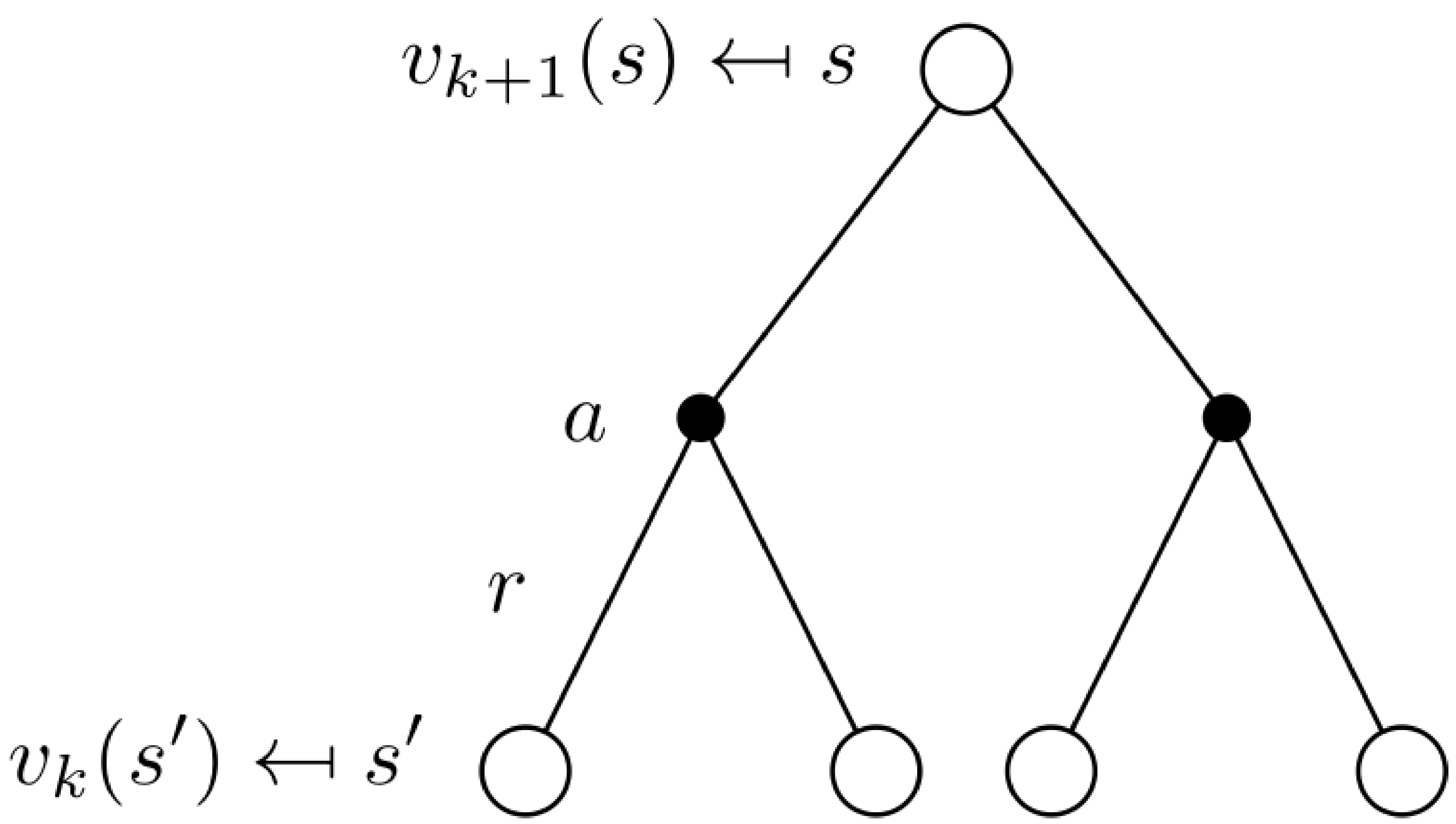
$$\mathbf{V}^\pi = (\mathbb{I} - \gamma \, \mathcal{P}^\pi)^{-1} \times \mathbf{R}^\pi$$

- 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:

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

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:

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

- 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:

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

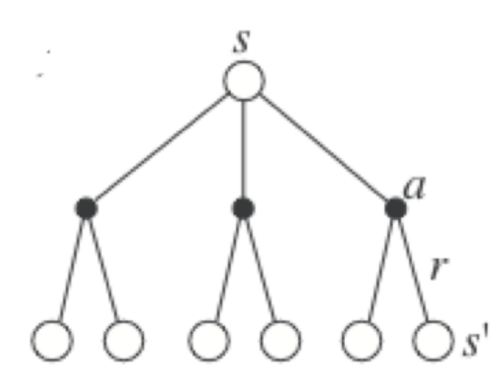
- The **contraction mapping theorem** ensures that $\mathcal{T}^\pi$ converges to an unique fixed point:
  - Existence and uniqueness of the solution of the Bellman equations.

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.

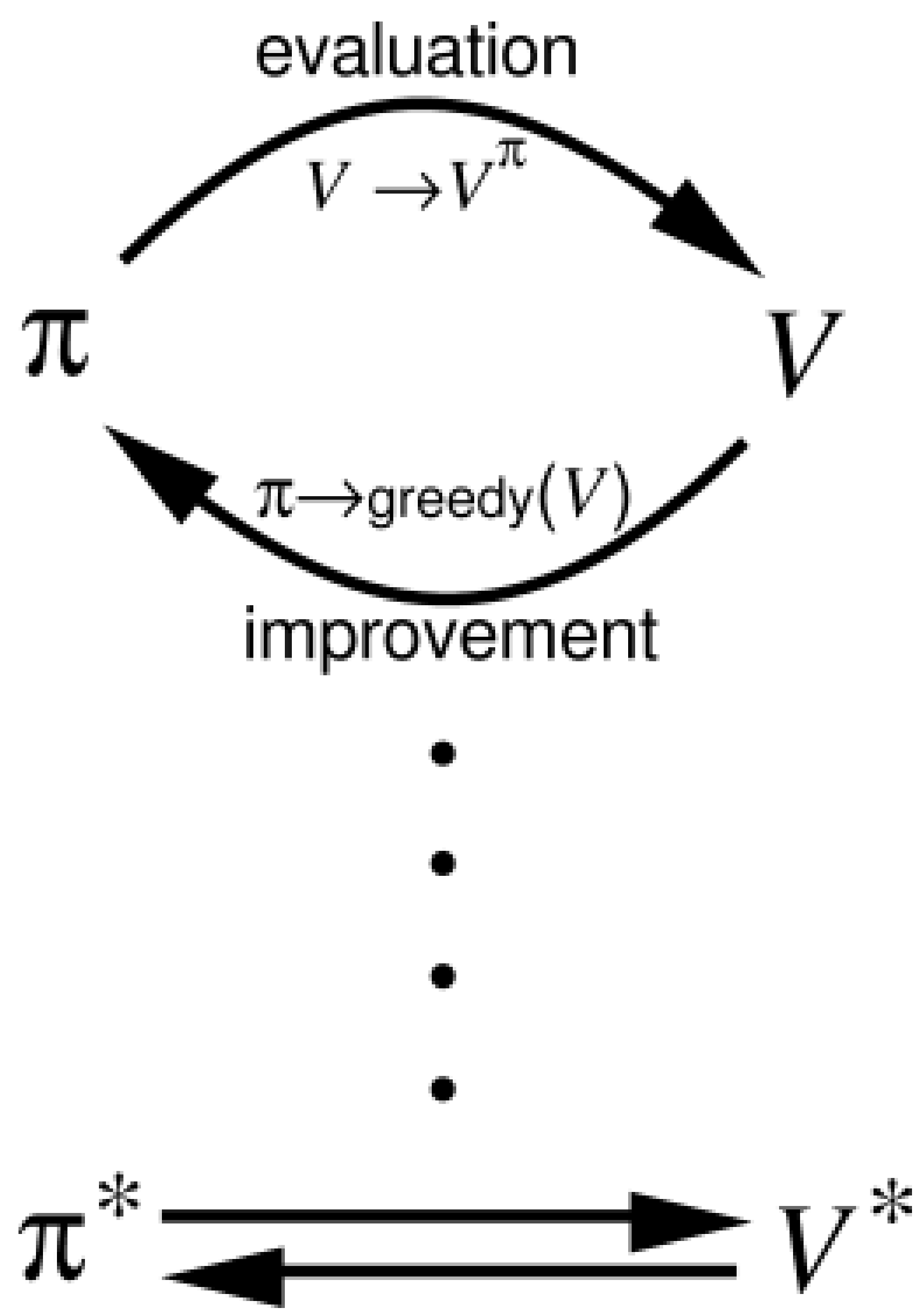
$$\mathbf{V}_{k+1} = \mathbf{R}^{\pi} + \gamma \, \mathcal{P}^{\pi} \, \mathbf{V}_k$$

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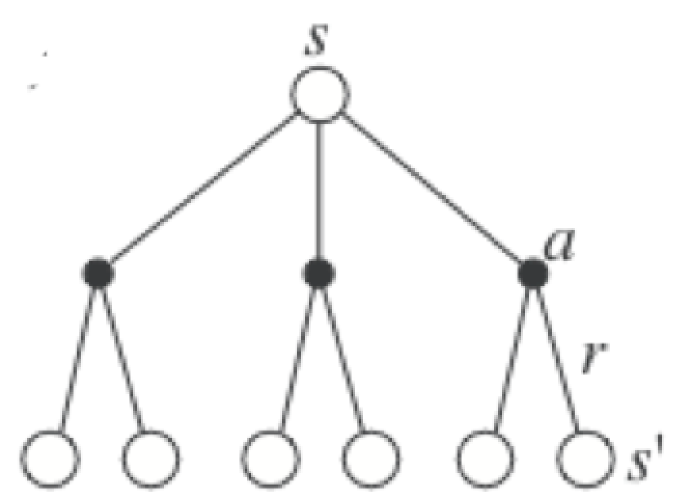
  2. **Policy improvement**
     - From the current estimated values $V^\pi(s)$ or $Q^\pi(s, a)$, a new **better** policy π is derived.

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.

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

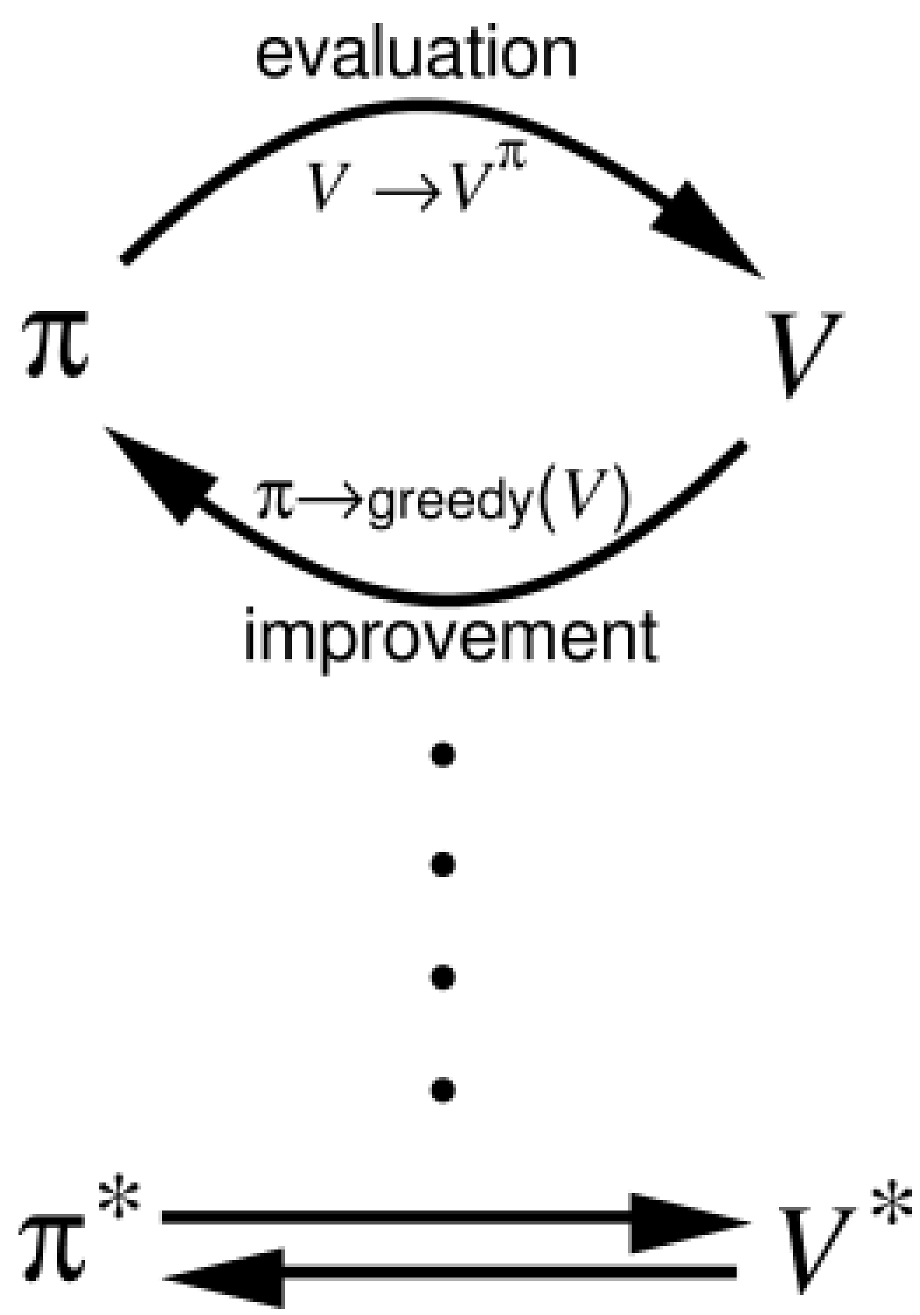
- This defines an **improved** policy π', where all states and actions have a higher value than previously.
- **Greedy action selection** over the state value function implements policy improvement:

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

Greedy policy improvement:

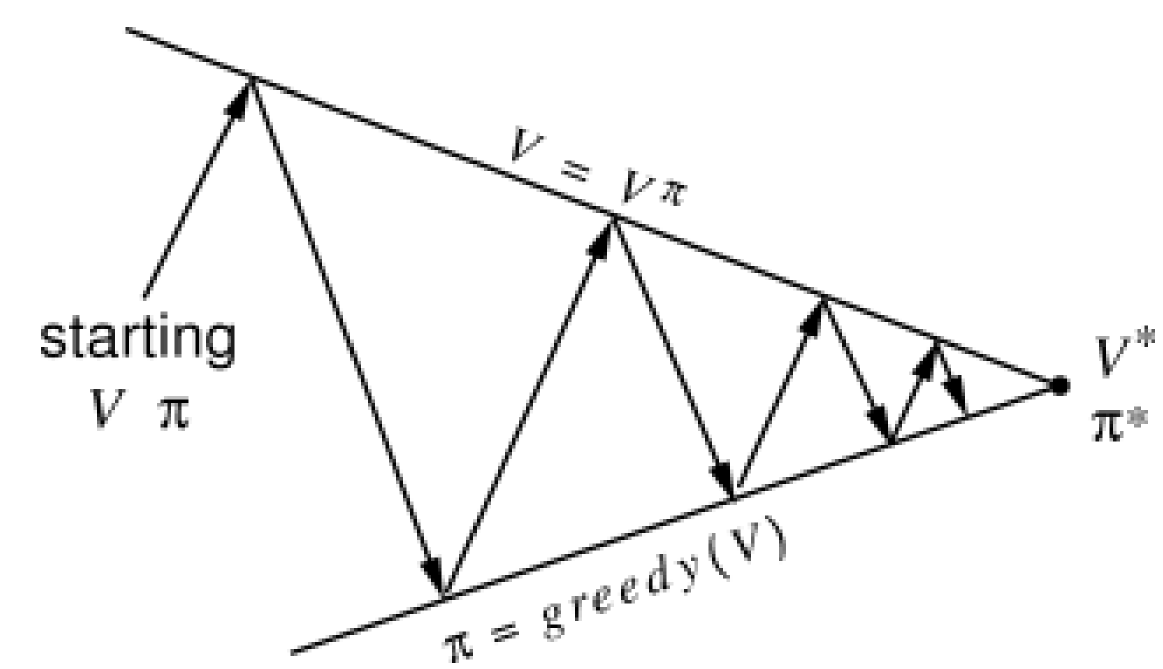
- **for** each state $s \in \mathcal{S}$:
  - $\pi(s) \leftarrow \text{argmax}_a \sum_{s' \in \mathcal{S}} p(s' | s, a) \, [r(s, a, s') + \gamma \, V^\pi (s')]$

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**

2 - Value iteration

Value iteration

- 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.

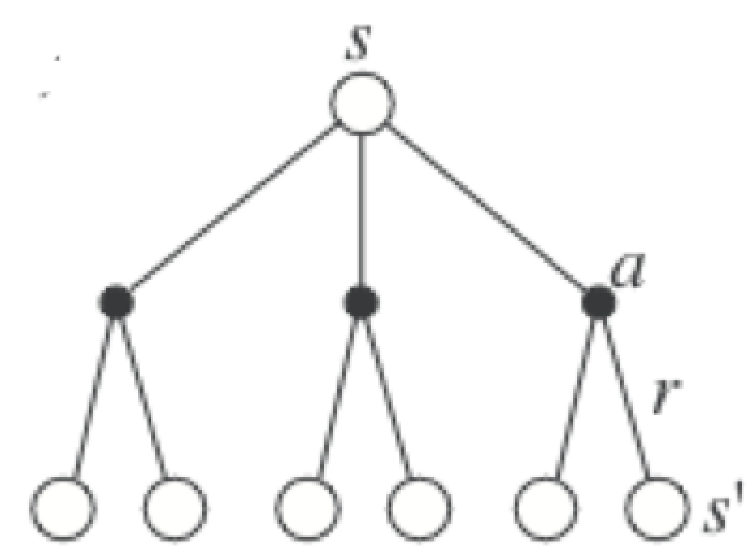
Value iteration

- 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

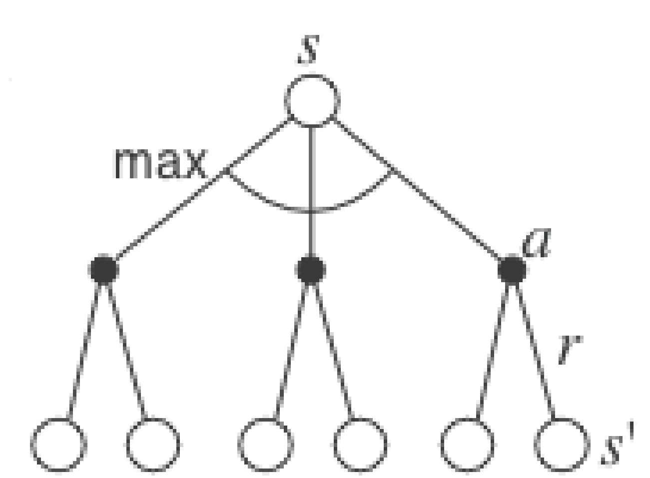
Full policy-evaluation backup

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



Full value-iteration backup

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



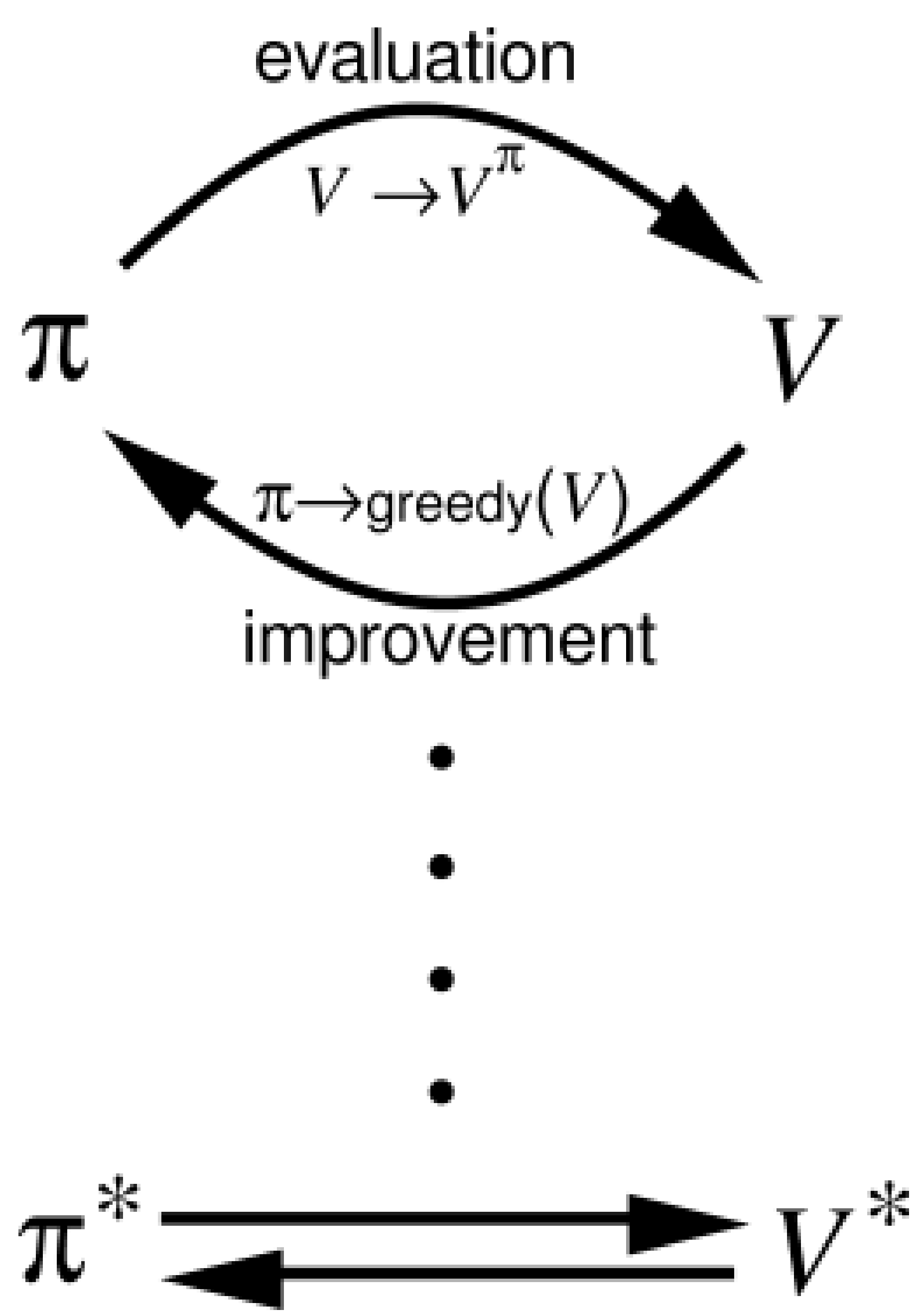
Asynchronous dynamic programming

- 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.

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

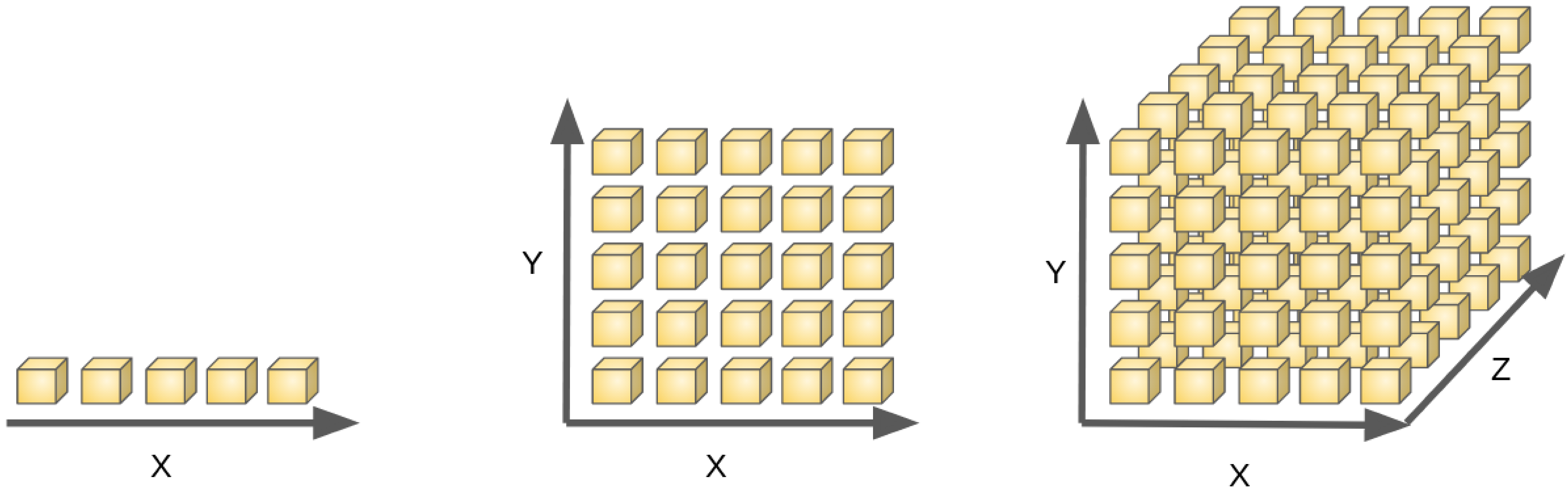
- We must still ensure that all states are visited, but their frequency and order is irrelevant.

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.