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# Deep Reinforcement Learning

Monte-Carlo methods

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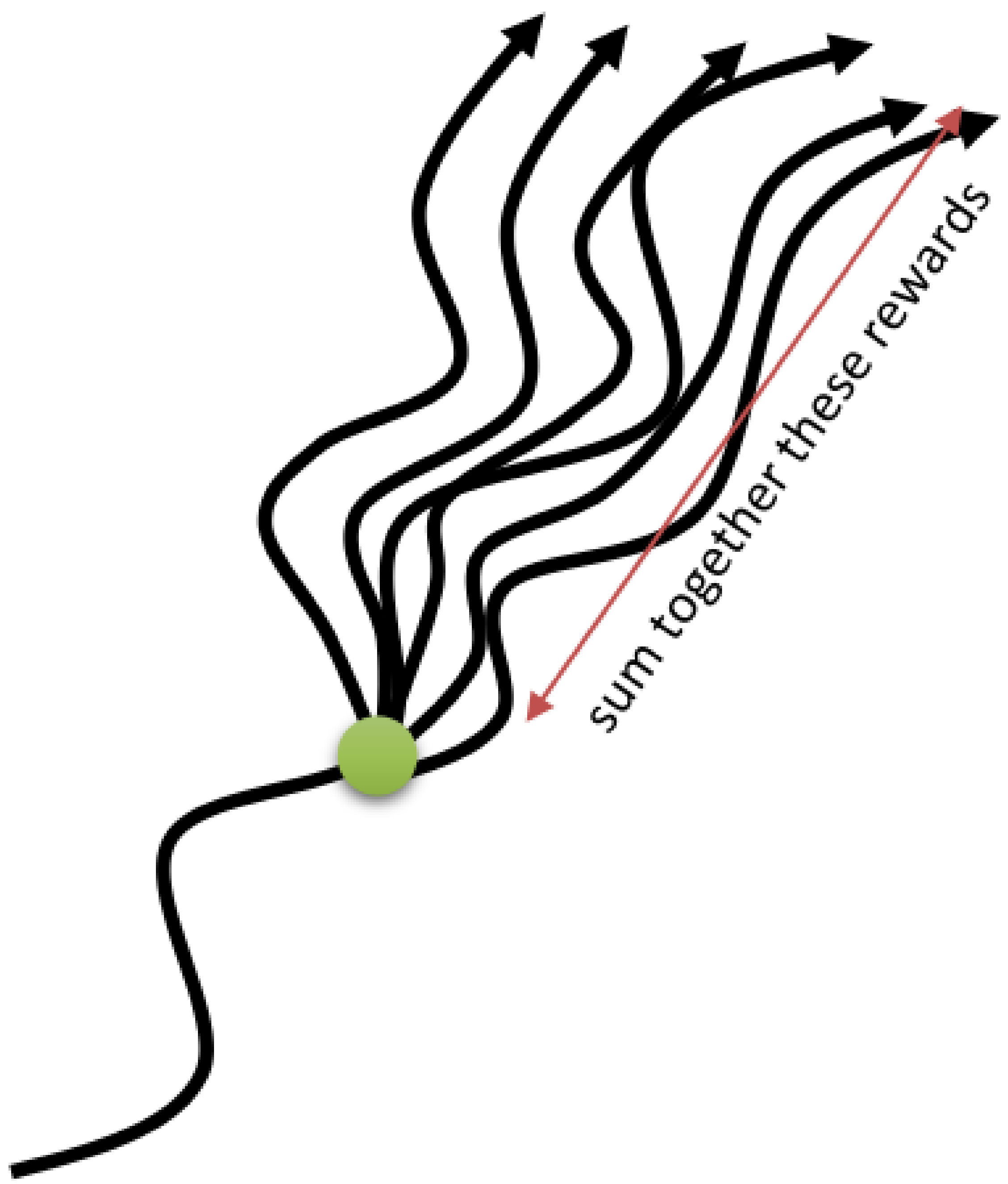
https://tu-chemnitz.de/informatik/KI/edu/deeprl

# Principle of Monte-Carlo (MC) methods




- The value of each state is defined as the mathematical expectation of the return obtained after that state and thereafter following the policy $\pi$:

$$V^\pi(s) = \mathbb{E}_{\rho_\pi}(R_t | s_t = s) = \mathbb{E}_{\rho_\pi}(\sum_{k=0}^\infty \gamma^k r_{t+k+1} | s_t = s)$$

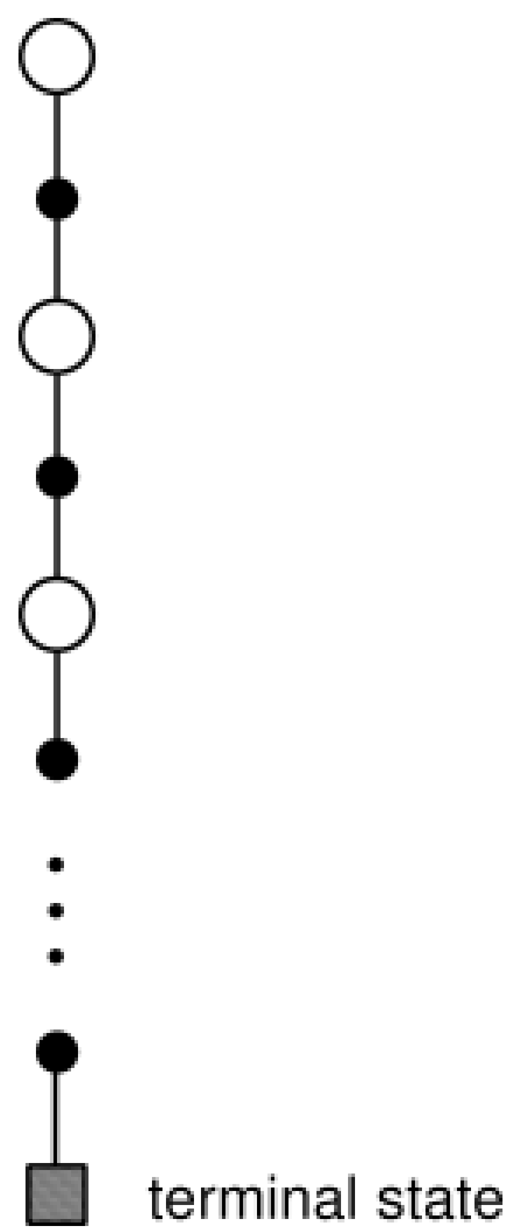
- **Monte-Carlo methods** (MC) approximate this mathematical expectation by **sampling** $M$ trajectories $\tau_i$ starting from $s$ and computing the sampling average of the obtained returns:

$$V^\pi(s) = \mathbb{E}_{\rho_\pi}(R_t | s_t = s) \approx \frac{1}{M} \sum_{i=1}^M R(\tau_i)$$

- If you have enough trajectories, the sampling average is an unbiased estimator of the value function.
- The advantage of Monte-Carlo methods is that they require only **experience**, not the complete dynamics $p(s' | s, a)$ and $r(s, a, s')$.

# Monte-Carlo policy evaluation

- The idea of MC policy evaluation is to repeatedly sample **episodes** starting from each possible state $s_0$ and maintain a **running average** of the obtained returns for each state:



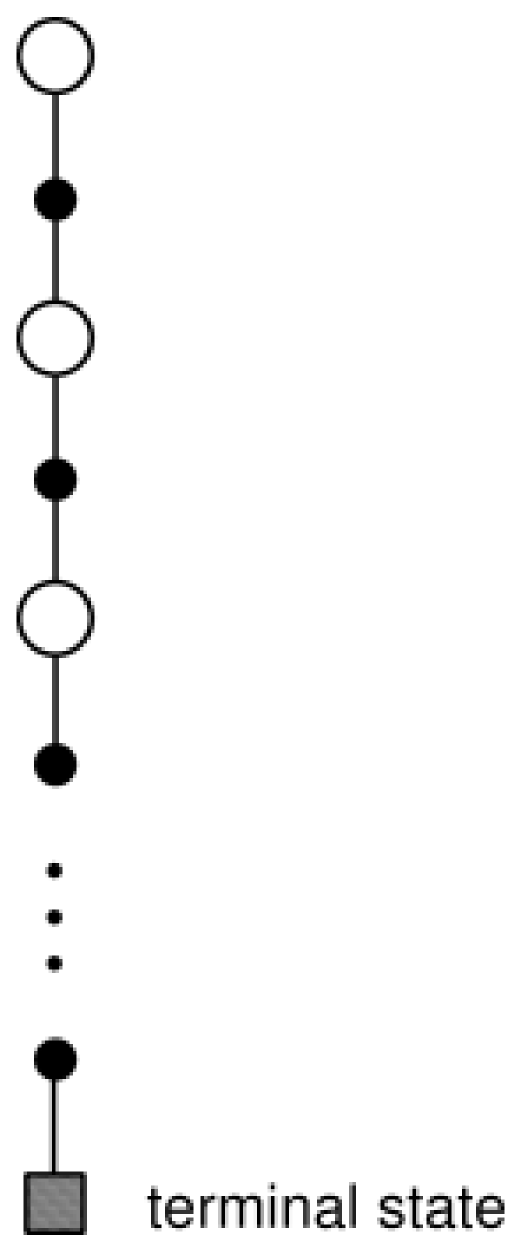

- **while** True:
  1. Start from an initial state $s_0$.
  2. Generate a sequence of transitions according to the current policy $\pi$ until a terminal state $s_T$ is reached.

$$\tau = (s_o, a_o, r_1, s_1, a_1, \ldots, s_T)$$

  3. Compute the return $R_t = \sum_{k=0}^{\infty} \gamma^k r_{t+k+1}$ for all encountered states $s_0, s_1, \ldots, s_T$ .
  4. Update the estimated state value $V(s_t)$ of all encountered states using the obtained return:

$$V(s_t) \leftarrow V(s_t) + \alpha \, (R_t - V(s_t))$$

# Monte-Carlo policy evaluation of action values




- The same method can be used to estimate Q-values.
- **while** True:
  1. Start from an initial state $s_0$.
  2. Generate a sequence of transitions according to the current policy $\pi$ until a terminal state $s_T$ is reached.

  $$\tau = (s_o, a_o, r_1, s_1, a_1, \ldots, s_T)$$

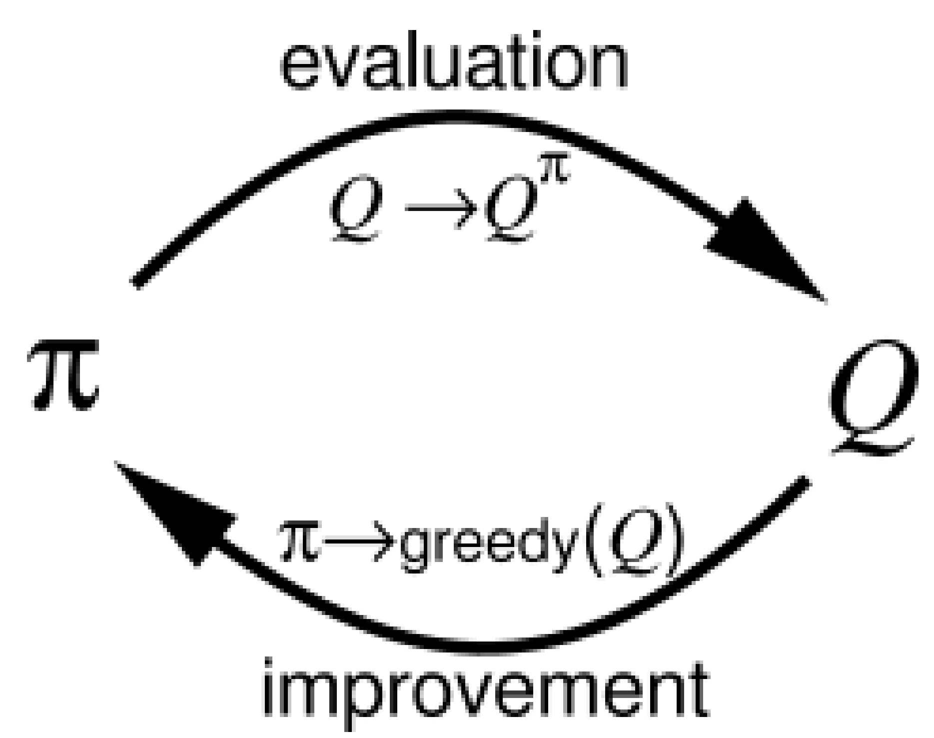
  3. Compute the return $R_t = \sum_{k=0}^{\infty} \gamma^k r_{t+k+1}$ for all encountered state-action pairs $(s_0, a_0), (s_1, a_1), \ldots, (s_{T-1}, a_{T-1})$.
  4. Update the estimated action value $Q(s_t, a_t)$ of all encountered state-action pairs using the obtained return:

  $$Q(s_t, a_t) = Q(s_t, a_t) + \alpha \, (R_t - Q(s_t, a_t))$$

- There are much more values to estimate (one per state-action pair), but the policy will be easier to derive.

# Monte-Carlo policy improvement

- After each episode, the state or action values of the visited $(s, a)$ pairs have changed, so the current policy might not be optimal anymore.




- As in DP, the policy can then be improved in a greedy manner:

$$\pi'(s) = \text{argmax}_a Q(s, a)$$

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

- Estimating the Q-values allows to act greedily, while estimating the V-values still requires the dynamics $p(s'|s, a)$ and $r(s, a, s')$.

# Monte-Carlo control

- **Monte-Carlo control** alternates between **MC policy evaluation** and **policy improvement** until the optimal policy is found: generalized policy iteration (GPI).
- **while** True:

1. Select an initial state $s_0$.
2. Generate a sequence of transitions according to the current policy $\pi$ until a terminal state $s_T$ is reached.

$$\tau = (s_o, a_o, r_1, s_1, a_1, \ldots, s_T)$$

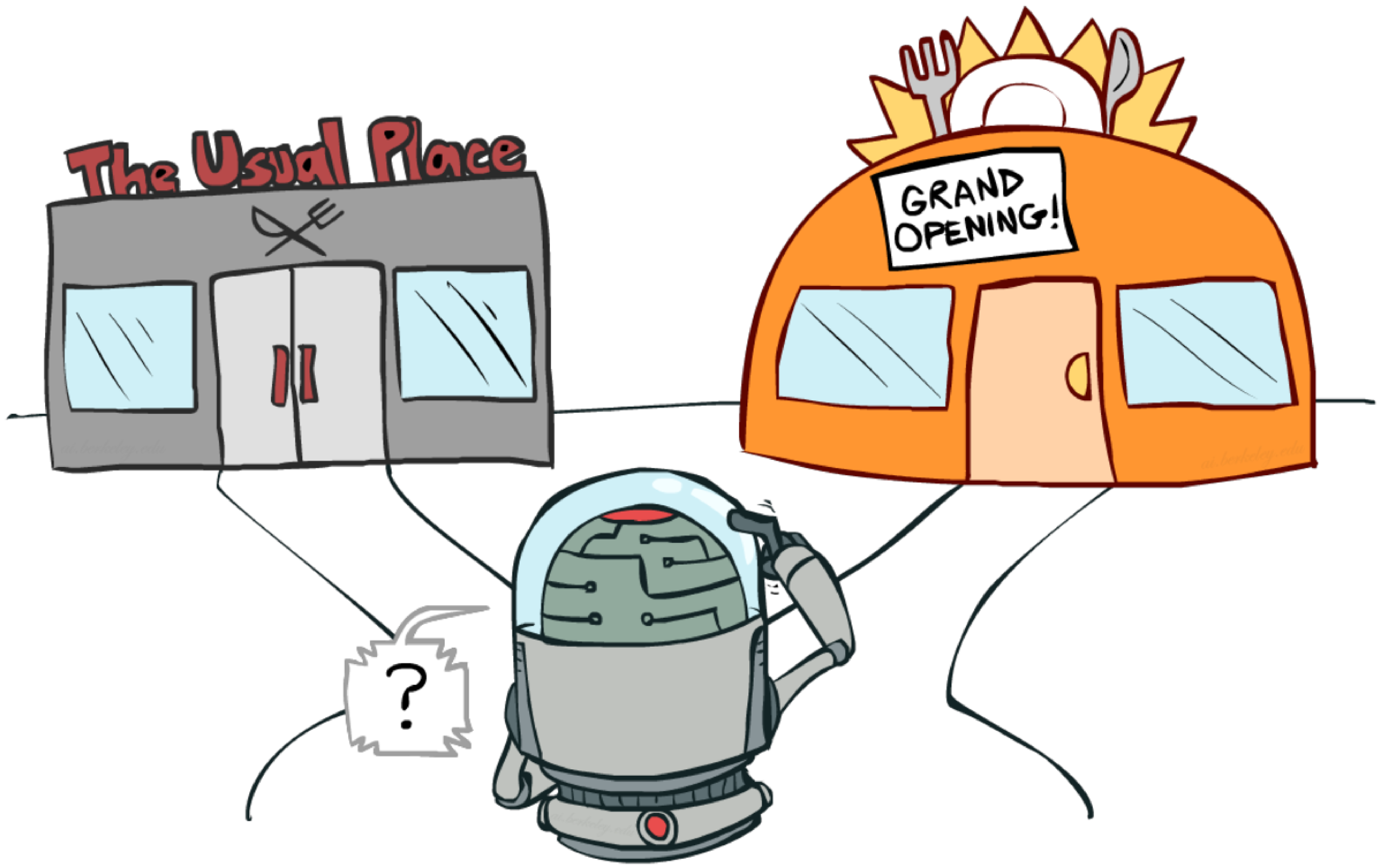
3. Compute the return $R_t = \sum_{k=0}^{\infty} \gamma^k r_{t+k+1}$ of all encountered state-action pairs.
4. Update the estimated action value $Q_k(s_t, a_t)$ of all encountered state-action pairs:

$$Q(s_t, a_t) = Q(s_t, a_t) + \alpha \, (R_t - Q(s_t, a_t))$$

5. For each state $s_t$ in the episode, **improve** the policy:

$$\pi(s_t, a) = \begin{cases} 1 \text{ if } a = \text{argmax} \, Q(s_t, a) \\ 0 \text{ otherwise.} \end{cases}$$

# How to generate the episodes?




Source: http://ai.berkeley.edu/lecture_slides.html

- The problem with MC control is that we need a policy to generate the sample episodes, but it is that policy that we want to learn.
- We have the same **exploration/exploitation** problem as in bandits:
  - If I trust my estimates too much (**exploitation**), I may miss more interesting solutions by keeping generating the same episodes.
  - If I act randomly (**exploration**), I will find more interesting solutions, but I won't keep doing them.

# Exploration/Exploitation dilemma

- **Exploitation** is using the current estimated values to select the greedy action:
  - The estimated values represent how good we think an action is, so we have to use this value to update the policy.
- **Exploration** is executing non-greedy actions to try to reduce our uncertainty about the true values:
  - The values are only estimates: they may be wrong so we can not trust them completely.
- If you only **exploit** your estimates, you may miss interesting solutions.
- If you only **explore**, you do not use what you know: you act randomly and do not obtain as much reward as you could.

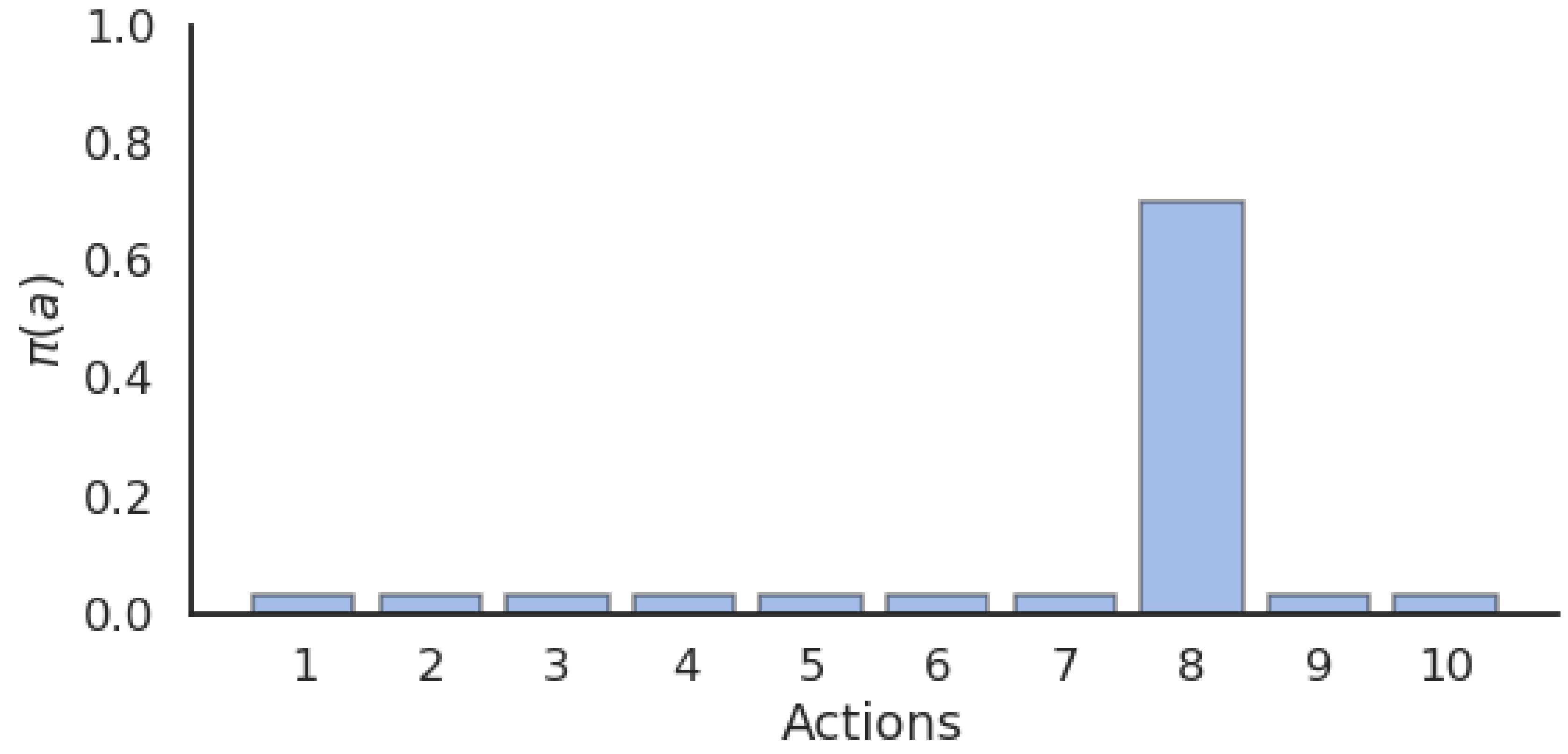
$\rightarrow$ **You can't exploit all the time; you can't explore all the time.**

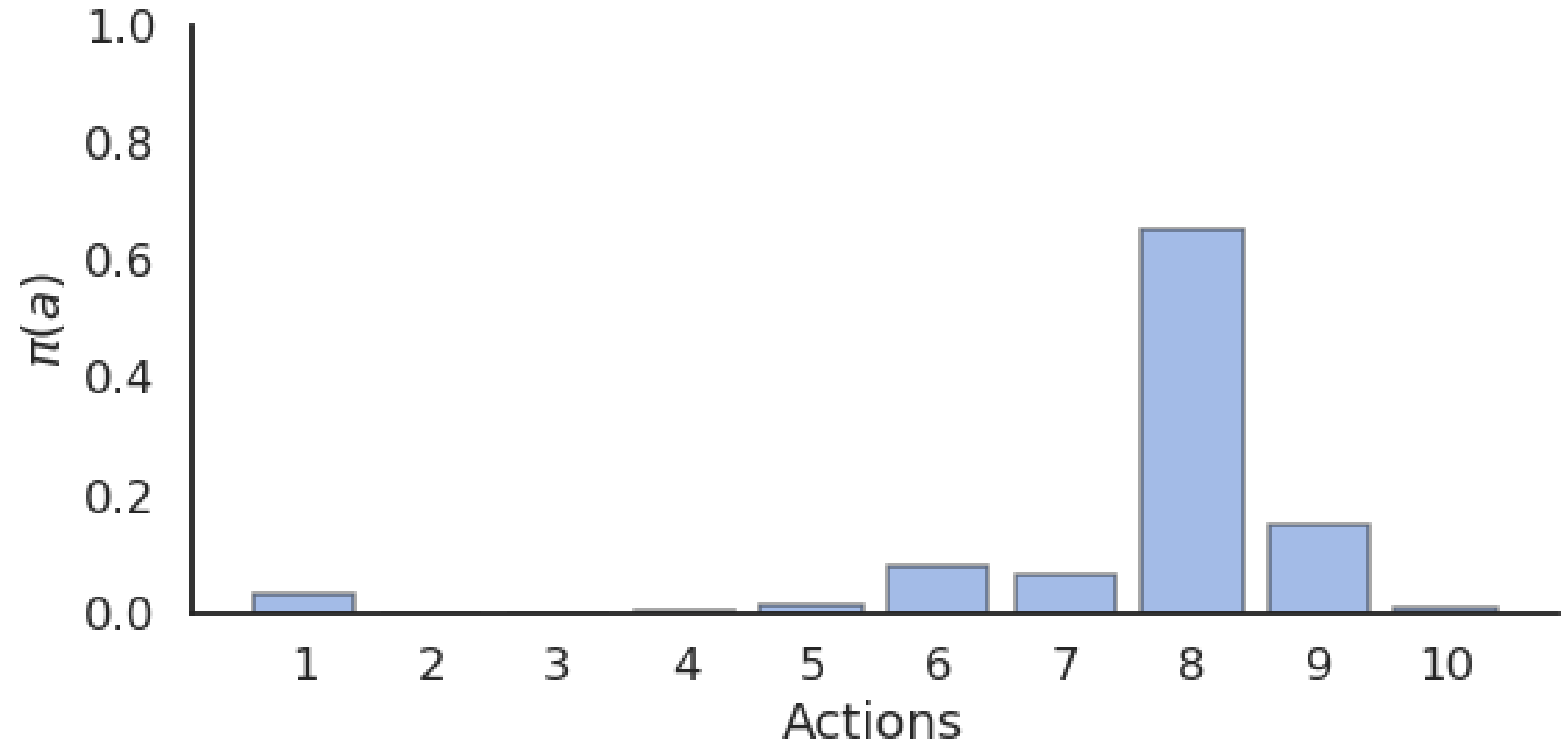
$\rightarrow$ You can never stop exploring; but you can reduce it if your performance is good enough.

- An easy solution to ensure exploration is to assume **exploring starts**, where every state-action pair has a non-zero probability to be selected as the start of an episode.

# Stochastic policies

- **Exploration** can be ensured by forcing the learned policy to be **stochastic**, aka $\epsilon$**-soft**.




- $\epsilon$**-Greedy action selection** randomly selects non-greedy actions with a small probability $\epsilon$:

$$\pi(s, a) = \begin{cases} 1 - \epsilon \; \text{if} \; a = \text{argmax}\, Q(s, a) \\ \frac{\epsilon}{|\mathcal{A}| - 1} \; \text{otherwise.} \end{cases}$$

- **Softmax action selection** uses a Gibbs (or Boltzmann) distribution to represent the probability of choosing the action $a$ in state $s$:

$$\pi(s, a) = \frac{\exp Q(s, a) / \tau}{\sum_b \exp Q(s, b) / \tau}$$

- $\epsilon$-greedy choses non-greedy actions randomly, while softmax favors the best alternatives.

# On-policy Monte-Carlo control

- In **on-policy** control methods, the learned policy has to be $\epsilon$-soft, which means all actions have a probability of at least $\frac{\epsilon}{|\mathcal{A}|}$ to be visited. $\epsilon$-greedy and softmax policies meet this criteria.
- Each sample episode is generated using this policy, which ensures exploration, while the control method still converges towards the optimal $\epsilon$-policy.
- **while** True:

  1. Generate an episode $\tau = (s_0, a_0, r_1, \dots, s_T)$ using the current **stochastic** policy $\pi$.
  2. For each state-action pair $(s_t, a_t)$ in the episode, update the estimated Q-value:

$$Q(s_t, a_t) = Q(s_t, a_t) + \alpha \, (R_t - Q(s_t, a_t))$$

  3. For each state $s_t$ in the episode, improve the policy (e.g. $\epsilon$-greedy):

$$\pi(s_t, a) = \begin{cases} 1 - \epsilon \; \text{if} \; a = \text{argmax}\, Q(s, a) \\ \frac{\epsilon}{|\mathcal{A}(s_t) - 1|} \; \text{otherwise.} \end{cases}$$

# Off-policy Monte-Carlo control

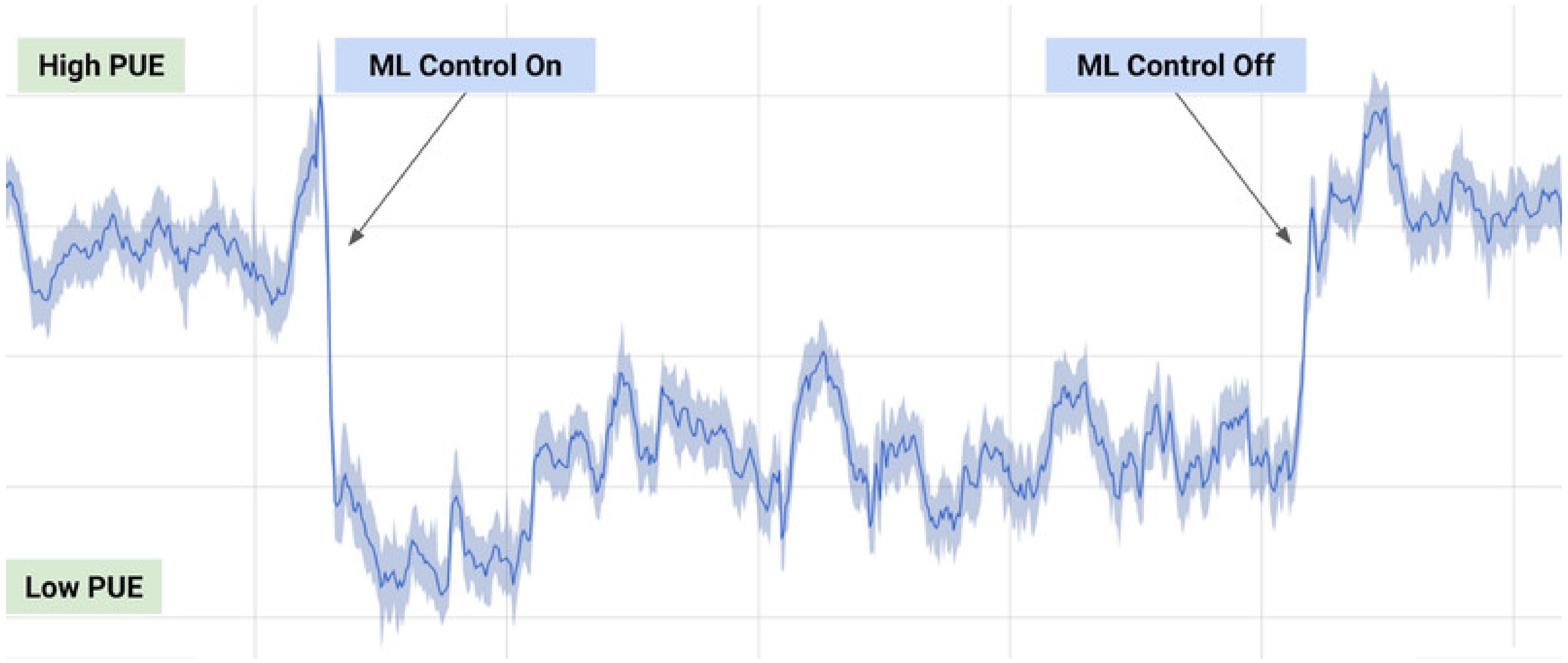
- Another option to ensure exploration is to generate the sample episodes using a policy $b(s, a)$ different from the current policy $\pi(s, a)$ of the agent.
- The **behavior policy** $b(s, a)$ used to generate the episodes is only required to select at least occasionally the same actions as the **learned policy** $\pi(s, a)$ (coverage assumption).

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

- There are mostly two choices regarding the behavior policy:

1. An $\epsilon$-soft behavior policy over the **Q-values** as in on-policy MC is often enough, while a deterministic (greedy) policy can be learned implictly.
2. The behavior policy could also come from **expert knowledge**, i.e. known episodes from the MDP generated by somebody else (human demonstrator, classical algorithm).

# Applications of RL: process control




Source: https://deepmind.com/blog/deepmind-ai-reduces-google-data-centre-cooling-bill-40/

- 40% reduction of energy consumption when using deep RL to control the cooling of Google's datacenters.
- The RL algorithm learned passively from the **behavior policy** (expert decisions) what the optimal policy should be.

# Importance sampling

- But are we mathematically allowed to do this?
- We search for the optimal policy that maximizes in expectation the return of each **trajectory** (episode) possible under the learned policy $\pi$:

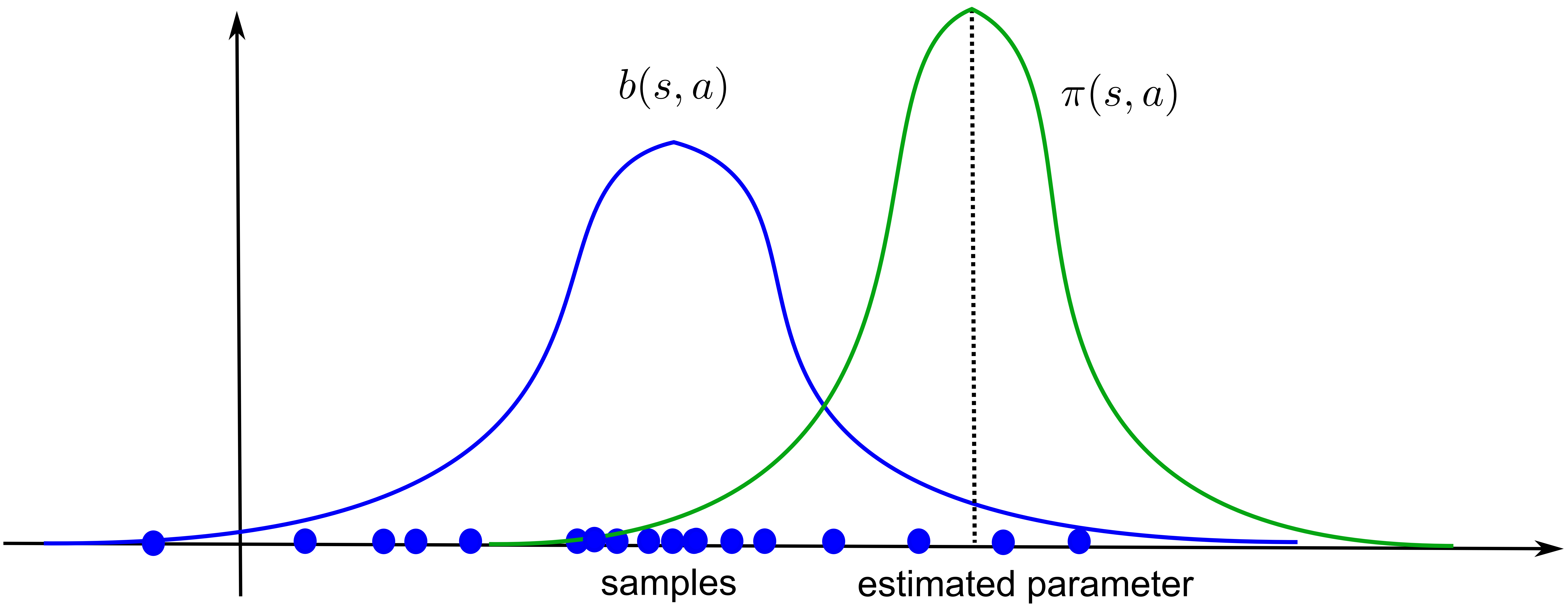
$$\mathcal{J}(\pi) = \mathbb{E}_{\tau \sim \rho_\pi} [R(\tau)]$$

- $\rho_\pi$ denotes the probability distribution of trajectories achievable using the policy $\pi$.
- If we generate the trajectories from the behavior policy $b(s, a)$, we end up maximizing something else:

$$\mathcal{J}'(\pi) = \mathbb{E}_{\tau \sim \rho_b} [R(\tau)]$$

- The policy that maximizes $\mathcal{J}'(\pi)$ is **not** the optimal policy of the MDP.

## Importance sampling




- If you try to estimate a parameter of a random distribution $\pi$ using samples of another distribution $b$, the sample average will have a strong **bias**.
- We need to **correct** the samples from $b$ in order to be able to estimate the parameters of $\pi$ correctly:
  - **importance sampling** (IS).

# Importance sampling

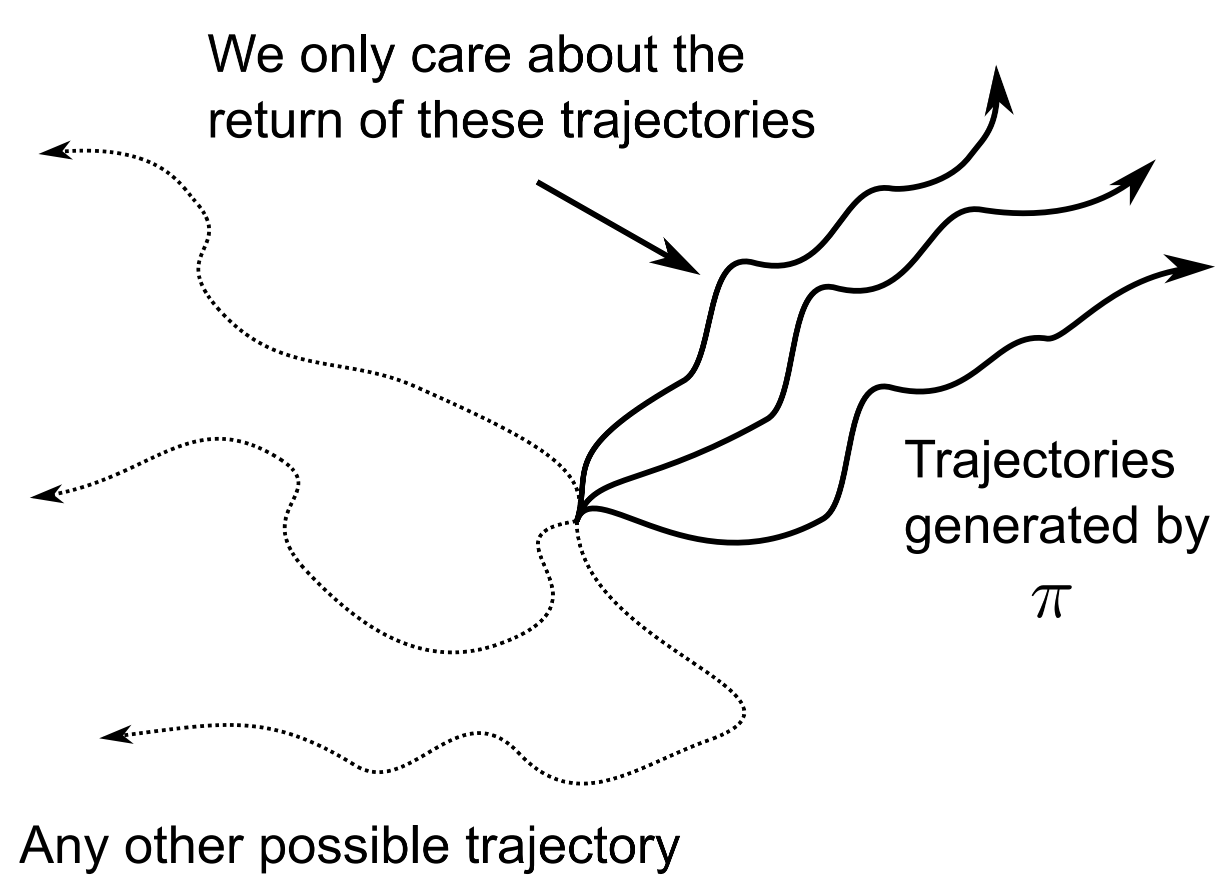
- We want to estimate the expected return of the trajectories generated by the policy $\pi$:

$$\mathcal{J}(\pi) = \mathbb{E}_{\tau \sim \rho_\pi} [R(\tau)]$$

- We start by using the definition of the mathematical expectation:

$$\mathcal{J}(\pi) = \int_\tau \rho_\pi(\tau) \, R(\tau) \, d\tau$$

- The expectation is the integral over all possible trajectories of their return $R(\tau)$, weighted by the likelihood $\rho_\pi(\tau)$ that a trajectory $\tau$ is generated by the policy $\pi$.



# Importance sampling

- The trick is to introduce the behavior policy $b$ in what we want to estimate:

$$\mathcal{J}(\pi) = \int_\tau \frac{\rho_b(\tau)}{\rho_b(\tau)} \, \rho_\pi(\tau) \, R(\tau) \, d\tau$$

- $\rho_b(\tau)$ is the likelihood that a trajectory $\tau$ is generated by the behavior policy $b$.
- We shuffle a bit the terms:

$$\mathcal{J}(\pi) = \int_\tau \rho_b(\tau) \, \frac{\rho_\pi(\tau)}{\rho_b(\tau)} \, R(\tau) \, d\tau$$

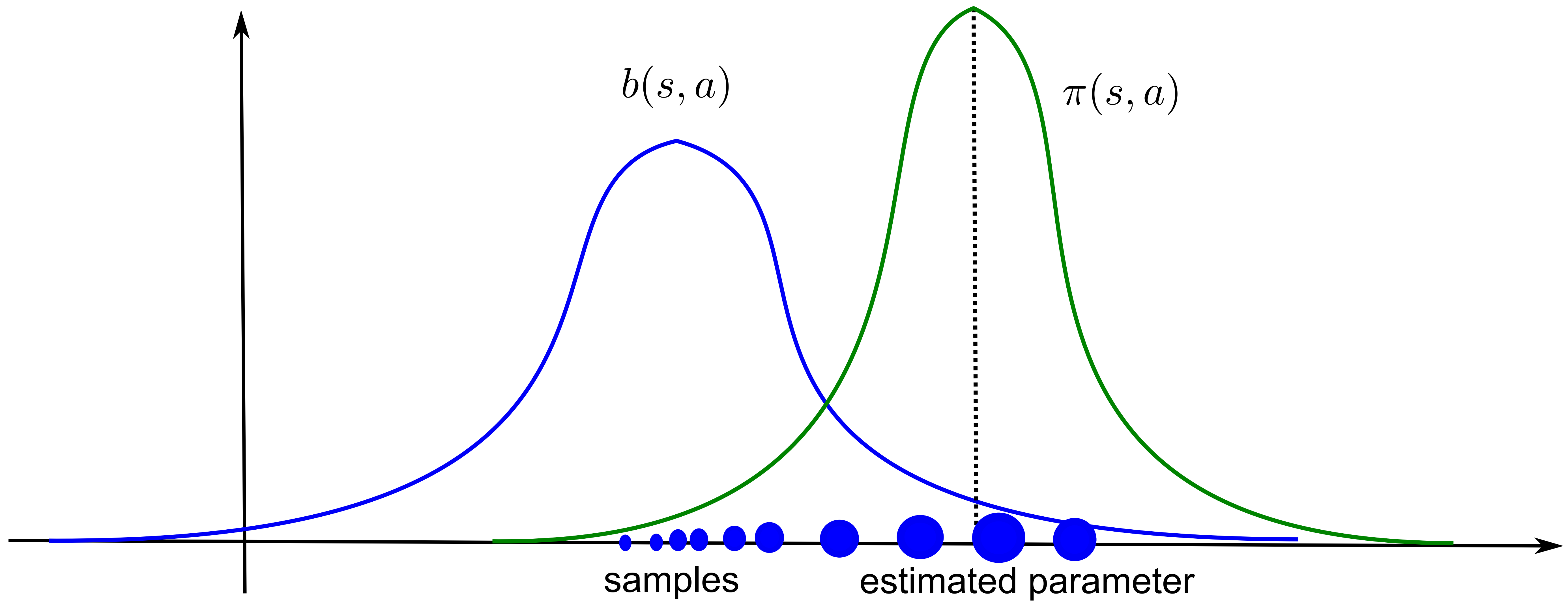
and notice that it has the form of an expectation over trajectories generated by $b$:

$$\mathcal{J}(\pi) = \mathbb{E}_{\tau \sim \rho_b} [\frac{\rho_\pi(\tau)}{\rho_b(\tau)} \, R(\tau)]$$

- This means that we can sample trajectories from $b$, but we need to **correct** the observed return by the **importance sampling weight** $\dfrac{\rho_\pi(\tau)}{\rho_b(\tau)}$.

# Importance sampling

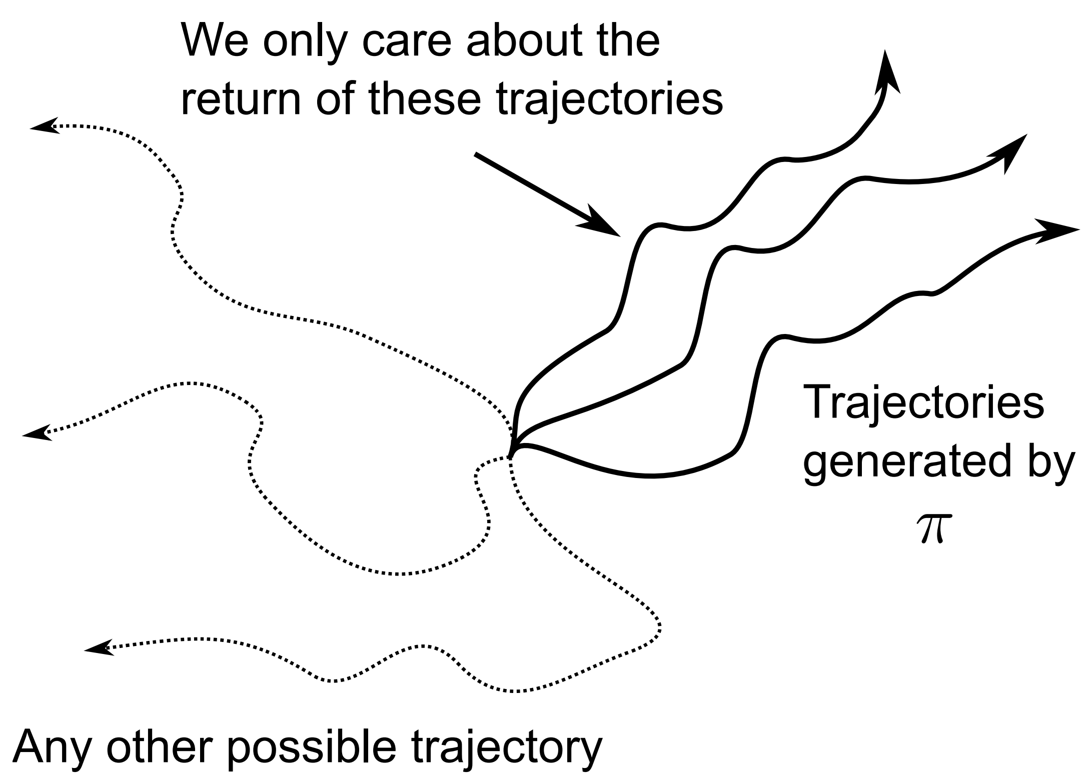
- The importance sampling weight corrects the mismatch between $\pi$ and $b$.



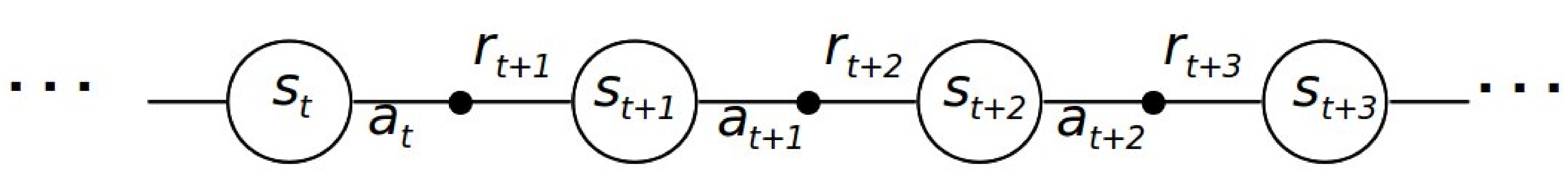

- If the two distributions are the same (on-policy), the IS weight is 1, no need to correct the return.
- If a sample is likely under $b$ but not under $\pi$, we should not care about its return: $\frac{\rho_\pi(\tau)}{\rho_b(\tau)} << 1$
- If a sample is likely under $\pi$ but not much under $b$, we increase its importance in estimating the return: $\frac{\rho_\pi(\tau)}{\rho_b(\tau)} >> 1$
- The sampling average of the corrected samples will be closer from the true estimate (unbiased).

# Importance sampling

- Great, but how do we compute these probability distributions $\rho_\pi(\tau)$ and $\rho_b(\tau)$ for a trajectory $\tau$?




- A trajectory $\tau$ is a sequence of state-action transitions $(s_0, a_0, s_1, a_1, \ldots, s_T)$ whose probability depends on:
  - the probability of choosing an action $a_t$ in state $s_t$: the **policy** $\pi(s, a)$.
  - the probability of arriving in the state $s_{t+1}$ from the state $s_t$ with the action $a_t$: the **transition probability** $p(s_{t+1}|s_t, a_t)$.



# Importance sampling

- The **likelihood** of a trajectory $\tau = (s_0, a_0, s_1, a_1, \ldots, s_T)$ under a policy $\pi$ depends on the policy and the transition probabilities (Markov property):

$$\rho_\pi(\tau) = p_\pi(s_0, a_0, s_1, a_1, \ldots, s_T) = p(s_0) \prod_{t=0}^{T-1} \pi_\theta(s_t, a_t) \, p(s_{t+1} | s_t, a_t)$$

- $p(s_0)$ is the probability of starting an episode in $s_0$, we do not have control over it.
- What is interesting is that the transition probabilities disappear when calculating the **importance sampling weight**:

$$\rho_{0:T-1} = \frac{\rho_\pi(\tau)}{\rho_b(\tau)} = \frac{p_0(s_0) \, \prod_{t=0}^{T-1} \pi(s_t, a_t) p(s_{t+1} | s_t, a_t)}{p_0(s_0) \, \prod_{t=0}^{T} b(s_t, a_t) p(s_{t+1} | s_t, a_t)} = \frac{\prod_{t=0}^{T-1} \pi(s_t, a_t)}{\prod_{t=0}^{T} b(s_t, a_t)} = \prod_{t=0}^{T-1} \frac{\pi(s_t, a_t)}{b(s_t, a_t)}$$

- The importance sampling weight is simply the product over the length of the episode of the ratio between $\pi(s_t, a_t)$ and $b(s_t, a_t)$.

# Off-policy Monte-Carlo control

- In **off-policy MC control**, we generate episodes using the behavior policy $b$ and update **greedily** the learned policy $\pi$.
- For the state $s_t$, the obtained returns just need to be weighted by the relative probability of occurrence of the **rest of the episode** following the policies $\pi$ and $b$:

$$\rho_{t:T-1} = \prod_{k=t}^{T-1} \frac{\pi(s_k, a_k)}{b(s_k, a_k)}$$

$$V^\pi(s_t) = \mathbb{E}_{\tau \sim \rho_b} [\rho_{t:T-1} \, R_t]$$

- This gives us the updates:

$$V(s_t) = V(s_t) + \alpha \, \rho_{t:T-1} \, (R_t - V(s_t))$$

and:

$$Q(s_t, a_t) = Q(s_t, a_t) + \alpha \, \rho_{t:T-1} \, (R_t - Q(s_t, a_t))$$

- Unlikely episodes under $\pi$ are barely used for learning, likely ones are used a lot.

# Off-policy Monte-Carlo control

- **while** True:
    1. Generate an episode $\tau = (s_0, a_0, r_1, \dots, s_T)$ using the **behavior** policy $b$.
    2. For each state-action pair $(s_t, a_t)$ in the episode, update the estimated Q-value:

$$\rho_{t:T-1} = \prod_{k=t}^{T-1} \frac{\pi(s_k, a_k)}{b(s_k, a_k)}$$

$$Q(s_t, a_t) = Q(s_t, a_t) + \alpha \, \rho_{t:T-1} \, (R_t - Q(s_t, a_t))$$

    3. For each state $s_t$ in the episode, update the **learned** deterministic policy (greedy):

$$\pi(s_t, a) = \begin{cases} 1 \text{ if } a = \text{argmax} \, Q(s_t, a) \\ 0 \text{ otherwise.} \end{cases}$$

# Off-policy Monte-Carlo control

- **Problem 1:** if the learned policy is greedy, the IS weight becomes quickly 0 for a non-greedy action $a_t$:

$$\pi(s_t, a_t) = 0 \rightarrow \rho_{0:T-1} = \prod_{k=0}^{T-1} \frac{\pi(s_k, a_k)}{b(s_k, a_k)} = 0$$

Off-policy MC control only learns from the last greedy actions, what is slow at the beginning.

**Solution:** $\pi$ and $b$ should not be very different. Usually $\pi$ is greedy and $b$ is a softmax (or $\epsilon$-greedy) over it.

- **Problem 2:** if the learned policy is stochastic, the IS weights can quickly **vanish** to 0 or **explode** to infinity:

$$\rho_{t:T-1} = \prod_{k=t}^{T-1} \frac{\pi(s_k, a_k)}{b(s_k, a_k)}$$

If $\frac{\pi(s_k, a_k)}{b(s_k, a_k)}$ is smaller than 1, the products go to 0. If it is bigger than 1, it grows to infinity.

**Solution:** one can normalize the IS weight between different episodes (see Sutton and Barto) or **clip** it (e.g. restrict it to [0.9, 1.1], see PPO later in this course).

# Off-policy Monte-Carlo control

Initialize, for all $s \in \mathcal{S}$, $a \in \mathcal{A}(s)$:

$Q(s, a) \leftarrow$ arbitrary

$N(s, a) \leftarrow 0$ ; Numerator and

$D(s, a) \leftarrow 0$ ; Denominator of $Q(s, a)$

$\pi \leftarrow$ an arbitrary deterministic policy

Repeat forever:

(a) Select a policy $\pi'$ and use it to generate an episode:

$$s_0, a_0, r_1, s_1, a_1, r_2, \ldots, s_{T-1}, a_{T-1}, r_T, s_T$$

(b) $\tau \leftarrow$ latest time at which $a_\tau \neq \pi(s_\tau)$

(c) For each pair $s, a$ appearing in the episode after $\tau$:

$t \leftarrow$ the time of first occurrence (after $\tau$) of $s, a$

$w \leftarrow \prod_{k=t+1}^{T-1} \frac{1}{\pi'(s_k, a_k)}$

$N(s, a) \leftarrow N(s, a) + wR_t$

$D(s, a) \leftarrow D(s, a) + w$

$Q(s, a) \leftarrow \frac{N(s,a)}{D(s,a)}$

(d) For each $s \in \mathcal{S}$:

$\pi(s) \leftarrow \arg\max_a Q(s, a)$

# Advantages of off-policy methods

- The main advantage of **off-policy** strategies is that you can learn from other's actions, you don't have to rely on your initially wrong policies to discover the solution by chance.
    - Example: learning to play chess by studying thousands/millions of plays by chess masters.
- In a given state, only a subset of the possible actions are actually executed by experts: the others may be too obviously wrong.
- The exploration is then guided by this expert knowledge, not randomly among all possible actions.
- Off-policy methods greatly reduce the number of transitions needed to learn a policy: very stupid actions are not even considered, but the estimation policy learns an optimal strategy from the "classical" moves.
- Drawback: if a good move is not explored by the behavior policy, the learned policy will never try it.

# Properties of Monte-Carlo methods

- Monte-Carlo evaluation estimates value functions via **sampling** of entire episodes.
- Monte-Carlo control (evaluation-improvement) is a generalized policy iteration method.
- MC for action values is **model-free**: you do not need to know $p(s'|s, a)$ to learn the optimal policy, you just sample transitions (trial and error).
- MC only applies to **episodic tasks**: as you learn at the end of an episode, it is not possible to learn continuing tasks.
- MC suffers from the **exploration-exploitation** problem:
  - **on-policy** MC learns a stochastic policy ($\epsilon$-greedy, softmax) to ensure exploration.
  - **off-policy** MC learns a greedy policy, but explores via a behavior policy (importance sampling).
- Monte-Carlo methods have:
  - a **small bias**: with enough sampled episodes, the estimated values converge to the true values.
  - a **huge variance**: the slightest change of the policy can completely change the episode and its return. You will need a lot of samples to form correct estimates: **sample complexity**.