UNIVERSITY OF TECHNOLOGY
IN THE EUROPEAN CAPITAL OF CULTURE
CHEMNITZ

Deep Reinforcement Learning

Bandits

Julien Vitay

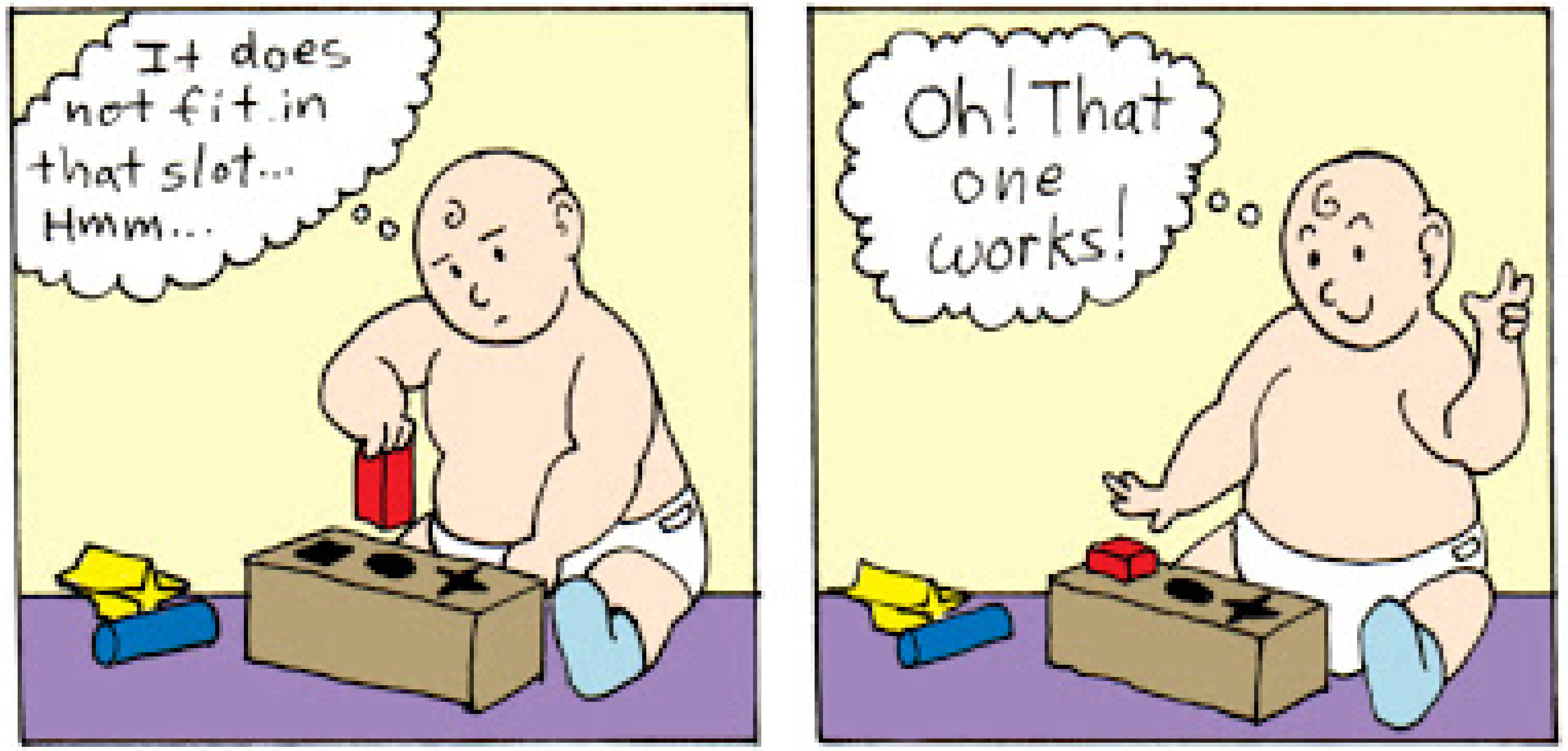
Professur für Künstliche Intelligenz - Fakultät für Informatik

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

Outline

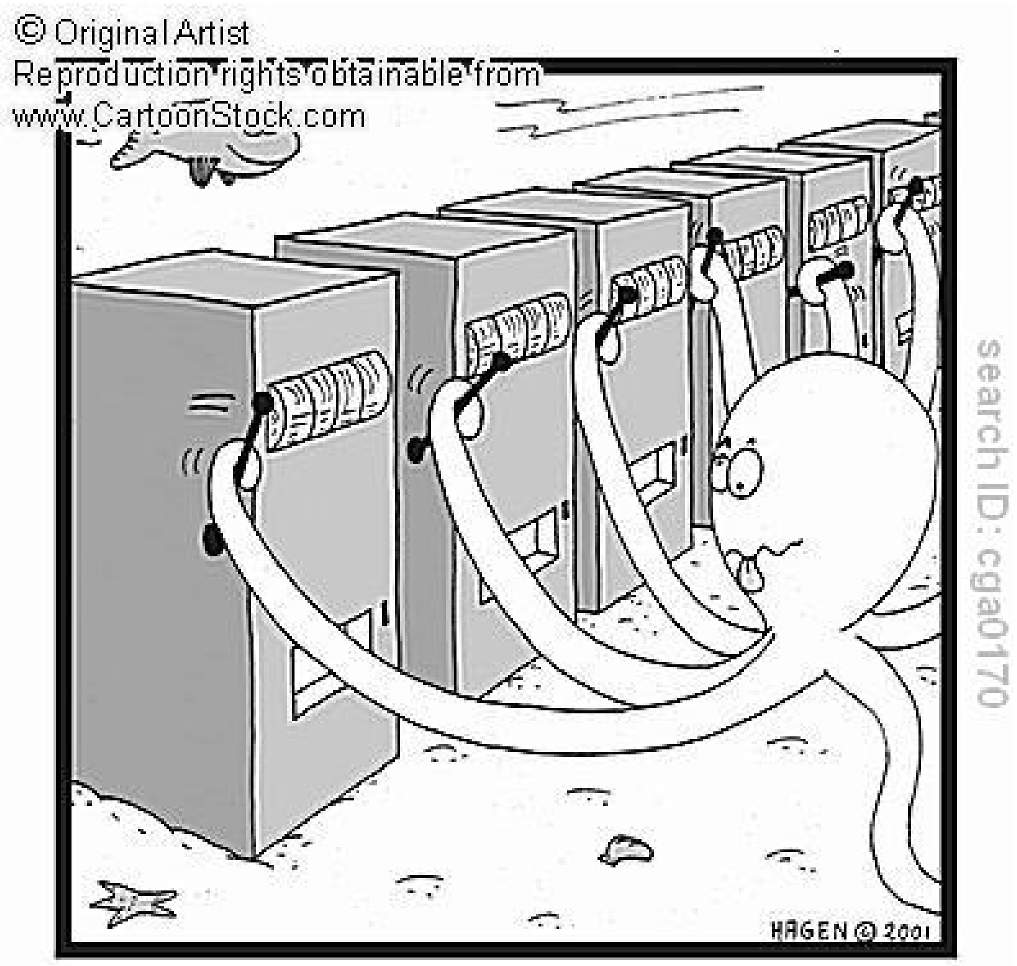
1 - n-armed bandits

Evaluative Feedback



- RL evaluates actions through **trial-and-error** rather than comparing its predictions to the correct actions.
  - RL: **evaluative feedback** depends completely on the action taken.
  - SL: **instructive feedback** depends not at all on the action taken.
- Evaluative feedback indicates how good the action is, but not whether it is the best or worst action possible.
  - **Associative learning**: inputs are mapped to the best possible outputs (general RL).
  - **Non-associative learning**: finds one best output, regardless of the current state or past history (bandits).

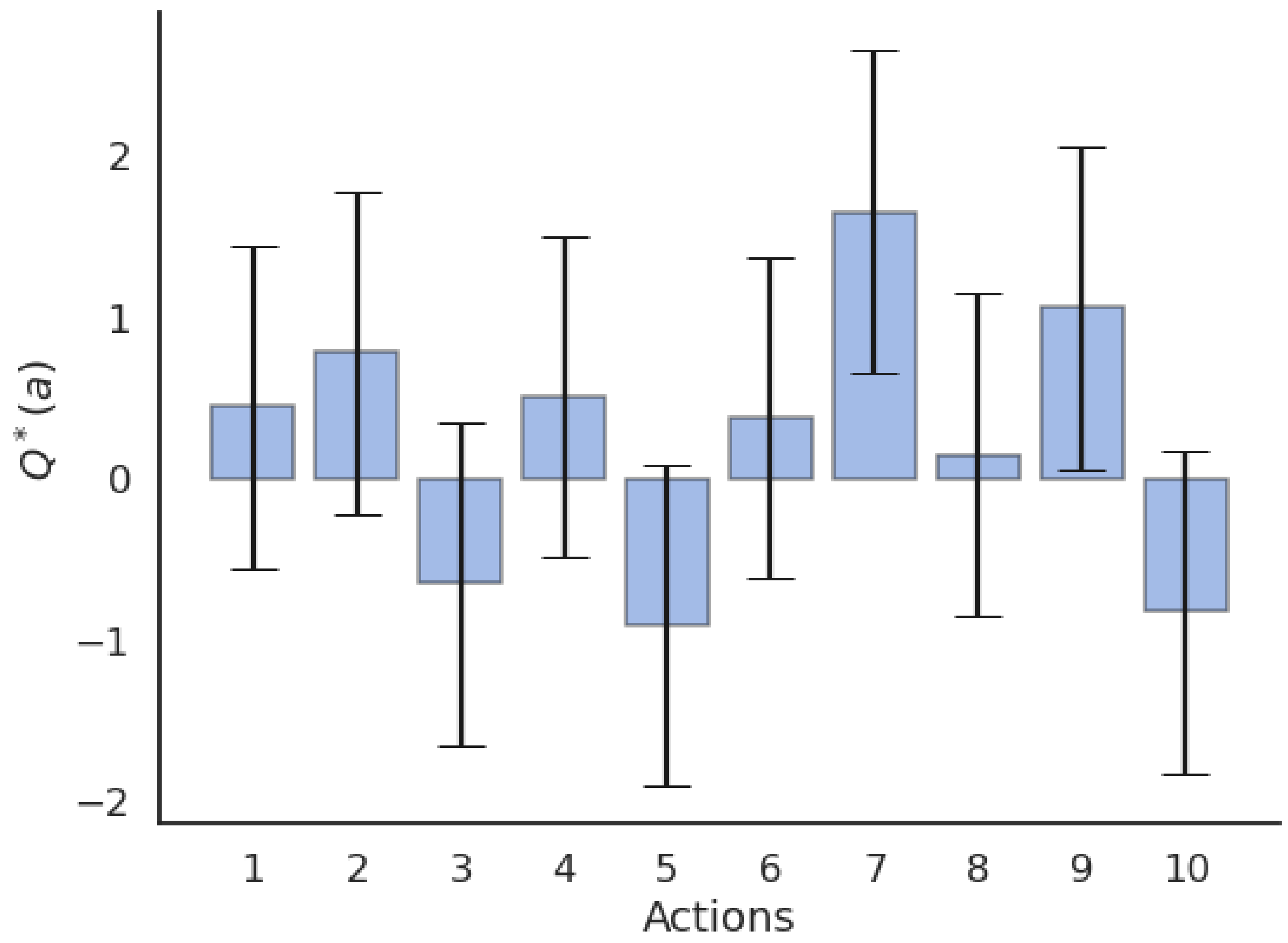
n-armed bandits



Compulsive gambling

- The **n-armed bandit** (or multi-armed bandit) is a non-associative evaluative feedback procedure.
- Learning and action selection take place in the same single state.
- The n actions have different reward distributions.
- The goal is to find out through trial and error which action provides the most reward on average.

n-armed bandits



- We have the choice between N different actions $(a_1, ..., a_N)$.
- Each action a taken at time t provides a **reward** r_t drawn from the action-specific probability distribution $r(a)$.
- The mathematical expectation of that distribution is the **expected reward**, called the **true value** of the action $Q^*(a)$.

$$Q^*(a) = \mathbb{E}[r(a)]$$

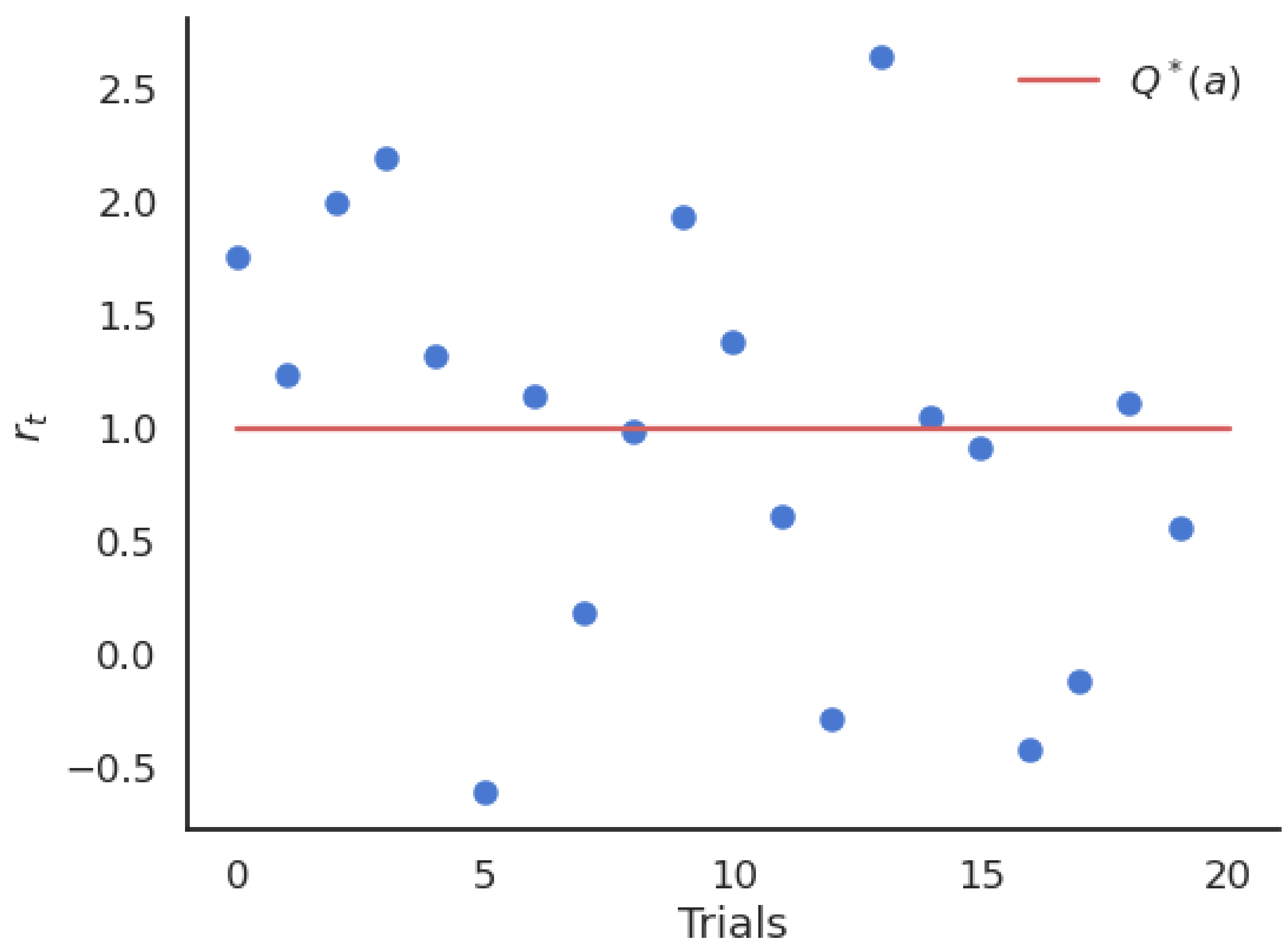
- The reward distribution also has a **variance**: we usually ignore it in RL, as all we care about is the **optimal action** a^* (but see distributional RL later).

$$a^* = \text{argmax}_a \, Q^*(a)$$

- If we take the optimal action an infinity of times, we maximize the reward intake **on average**.

n-armed bandits

- The question is how to find out the optimal action through **trial and error**, i.e. without knowing the exact reward distribution $r(a)$.



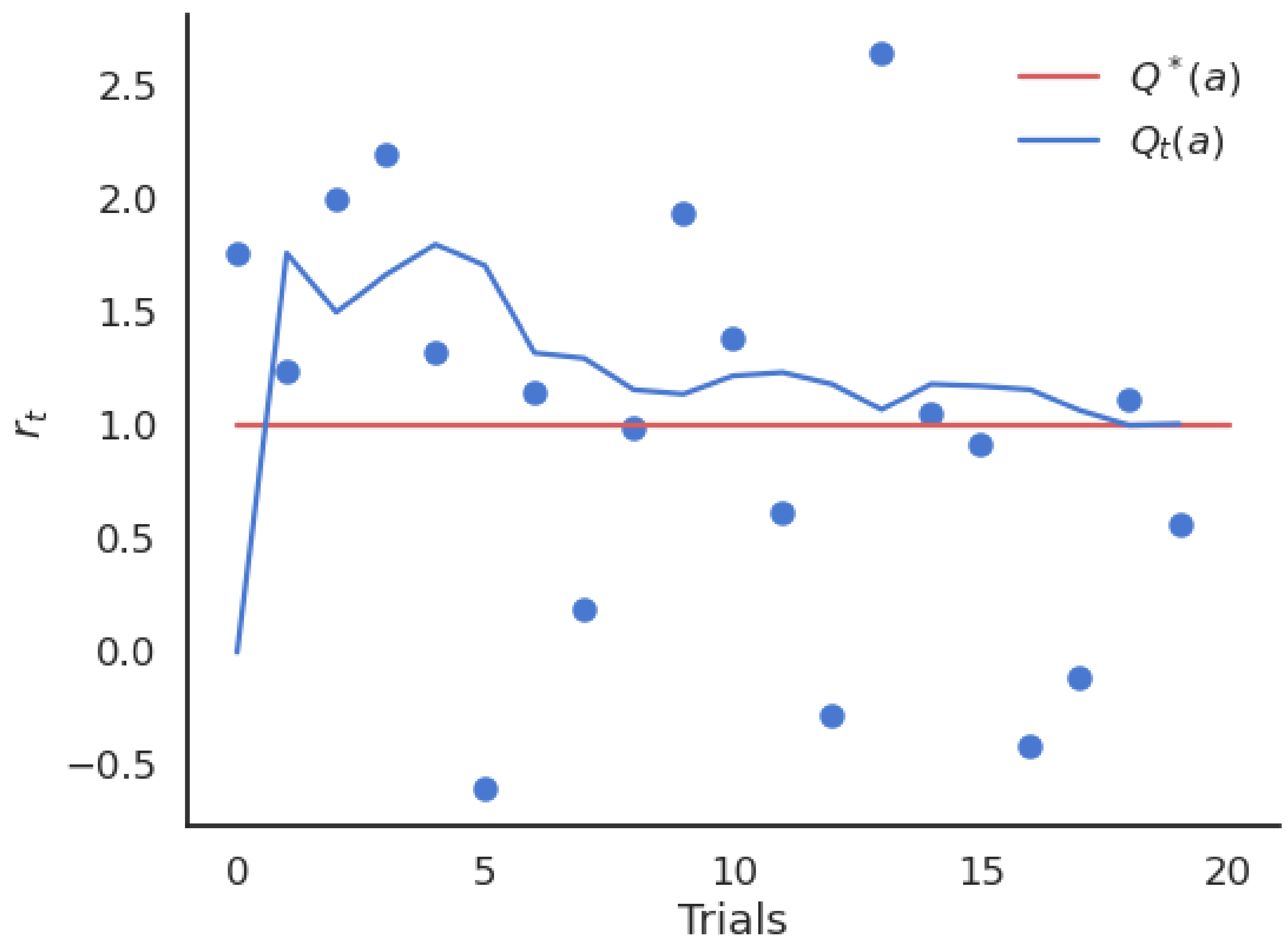
- We only have access to **samples** of $r(a)$ by taking the action a at time t (a **trial**, **play** or **step**).

$$r_t \sim r(a)$$

- The received rewards r_t vary around the true value over time.
- We need to build **estimates** $Q_t(a)$ of the value of each action based on the samples.
- These estimates will be very wrong at the beginning, but should get better over time.

2 - Sampling-based evaluation

Sampling-based evaluation



- The expectation of the reward distribution can be approximated by the **mean** of its samples:

$$\mathbb{E}[r(a)] \approx \frac{1}{N} \sum_{t=1}^{N} r_t|_{a_t=a}$$

- Suppose that the action a had been selected t times, producing rewards

$$(r_1, r_2, \ldots, r_t)$$

- The estimated value of action a at play t is then:

$$Q_t(a) = \frac{r_1 + r_2 + \ldots + r_t}{t}$$

- Over time, the estimated action-value converges to the true action-value:

$$\lim_{t \to \infty} Q_t(a) = Q^*(a)$$

Online evaluation

- The drawback of maintaining the mean of the received rewards is that it consumes a lot of memory:

$$Q_t(a) = \frac{r_1 + r_2 + ... + r_t}{t} = \frac{1}{t} \sum_{i=1}^{t} r_i$$

- It is possible to update an estimate of the mean in an **online** or incremental manner:

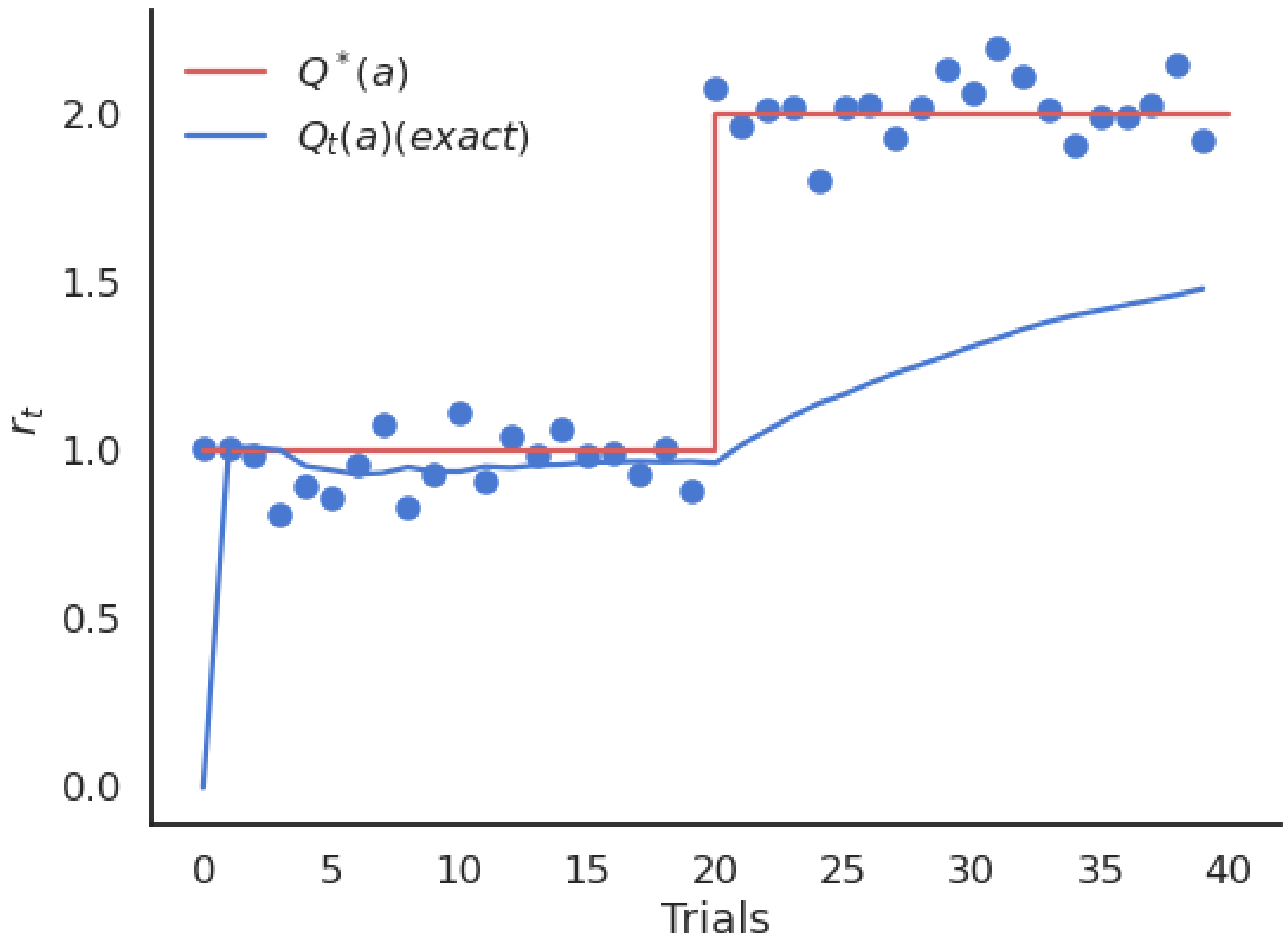
$$\begin{aligned}
Q_{t+1}(a) &= \frac{1}{t+1} \sum_{i=1}^{t+1} r_i = \frac{1}{t+1} \, (r_{t+1} + \sum_{i=1}^{t} r_i) \\
&= \frac{1}{t+1} \, (r_{t+1} + t \, Q_t(a)) \\
&= \frac{1}{t+1} \, (r_{t+1} + (t+1) \, Q_t(a) - Q_t(a))
\end{aligned}$$

- The estimate at time $t+1$ depends on the previous estimate at time t and the last reward r_{t+1}:

$$Q_{t+1}(a) = Q_t(a) + \frac{1}{t+1} \, (r_{t+1} - Q_t(a))$$

Online evaluation

- The problem with the exact mean is that it is only exact when the reward distribution is **stationary**, i.e. when the probability distribution does not change over time.
- If the reward distribution is **non-stationary**, the $\frac{1}{t+1}$ term will become very small and prevent rapid updates of the mean.



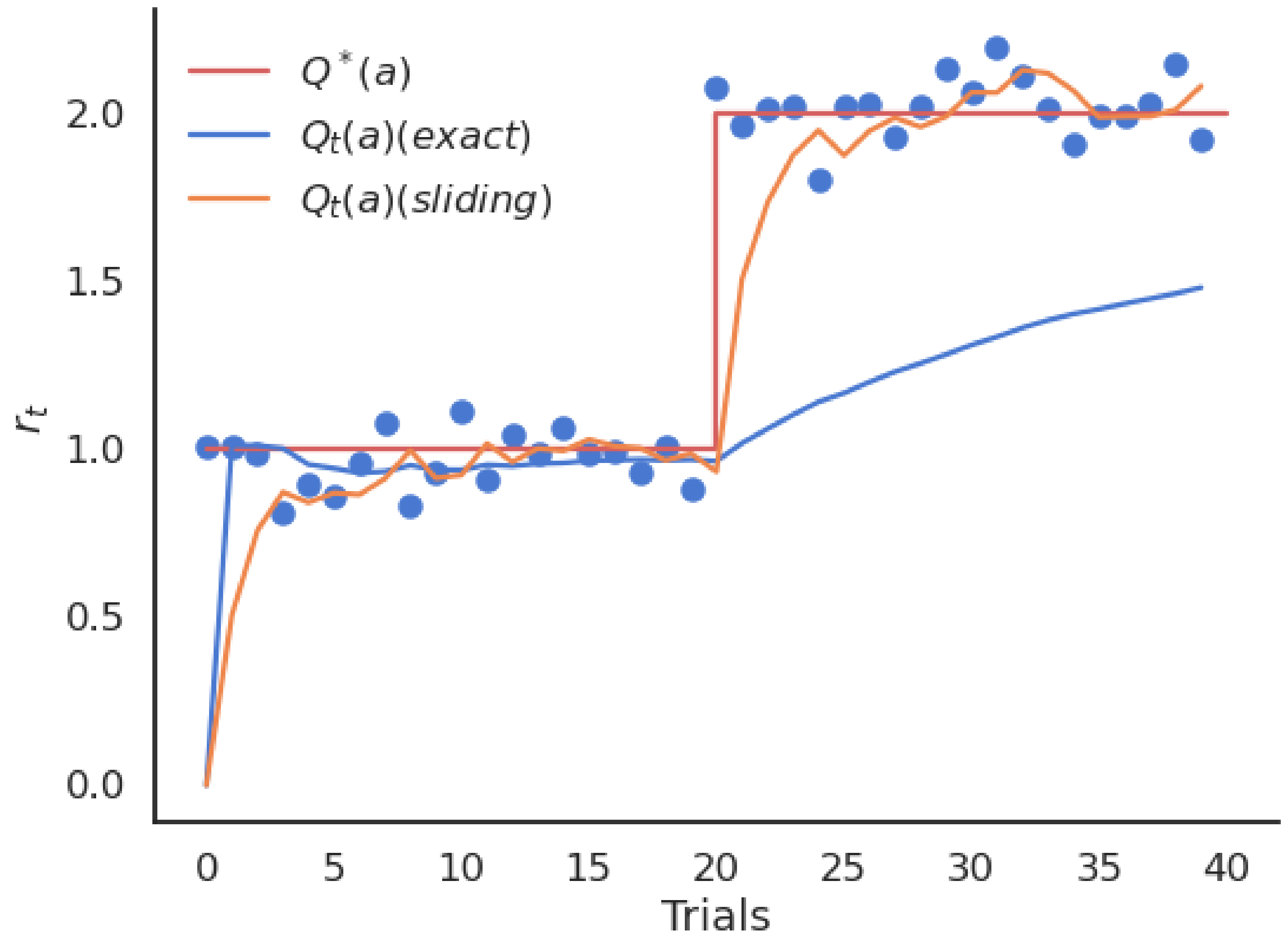
Online evaluation

- The solution is to replace $\frac{1}{t+1}$ with a fixed parameter called the **learning rate** (or **step size**) α:

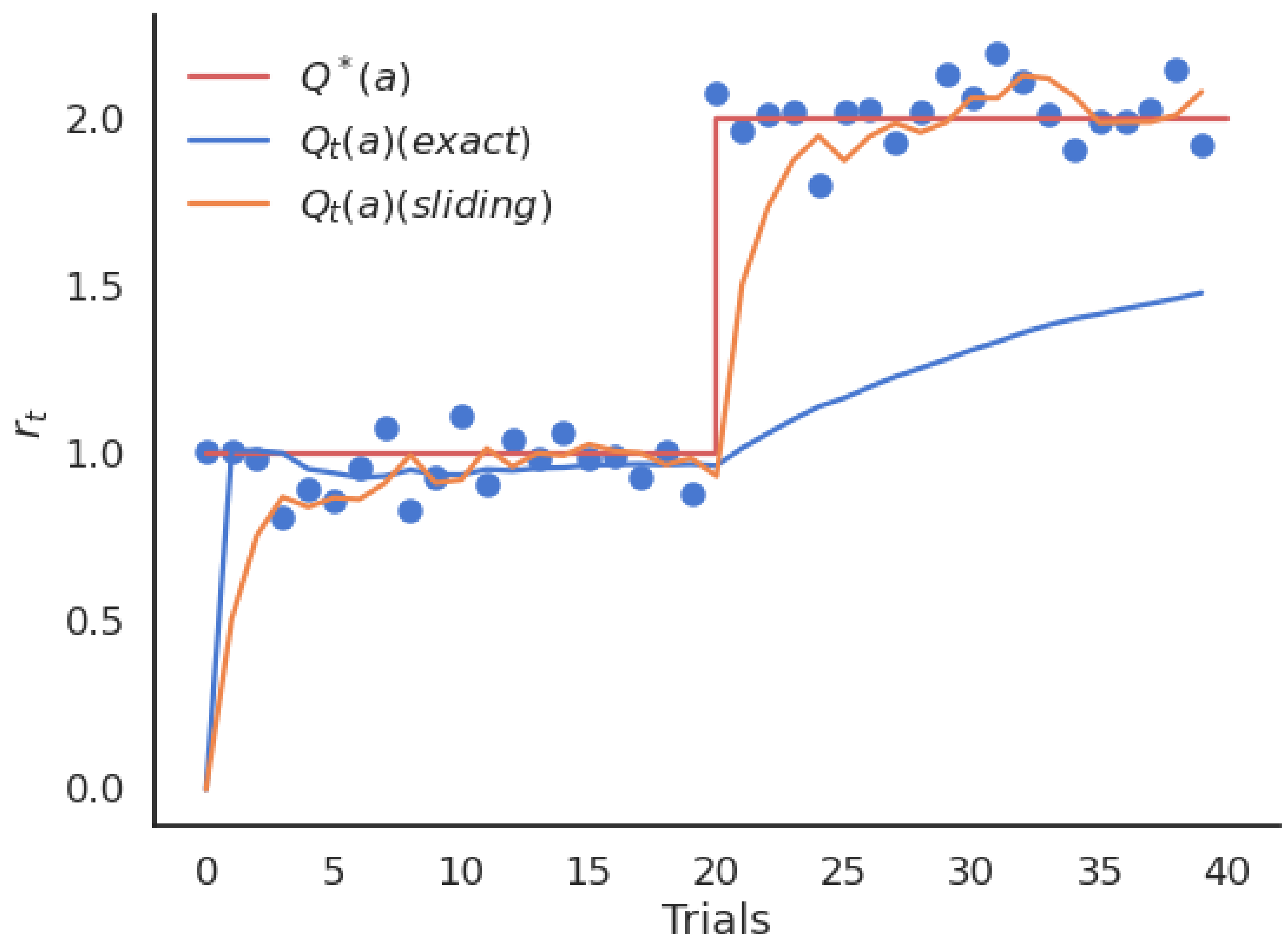
$$Q_{t+1}(a) = Q_t(a) + \alpha \, (r_{t+1} - Q_t(a))$$

$$= (1 - \alpha) \, Q_t(a) + \alpha \, r_{t+1}$$

- The computed value is called a **moving average** (or sliding average), as if one used only a small window of the past history.



Online evaluation



- Moving average:

$$Q_{t+1}(a) = Q_t(a) + \alpha \, (r_{t+1} - Q_t(a))$$

or:

$$\Delta Q(a) = \alpha \, (r_{t+1} - Q_t(a))$$

- The moving average adapts very fast to changes in the reward distribution and should be used in **non-stationary problems**.
- It is however not exact and sensible to noise.
- Choosing the right value for α can be difficult.

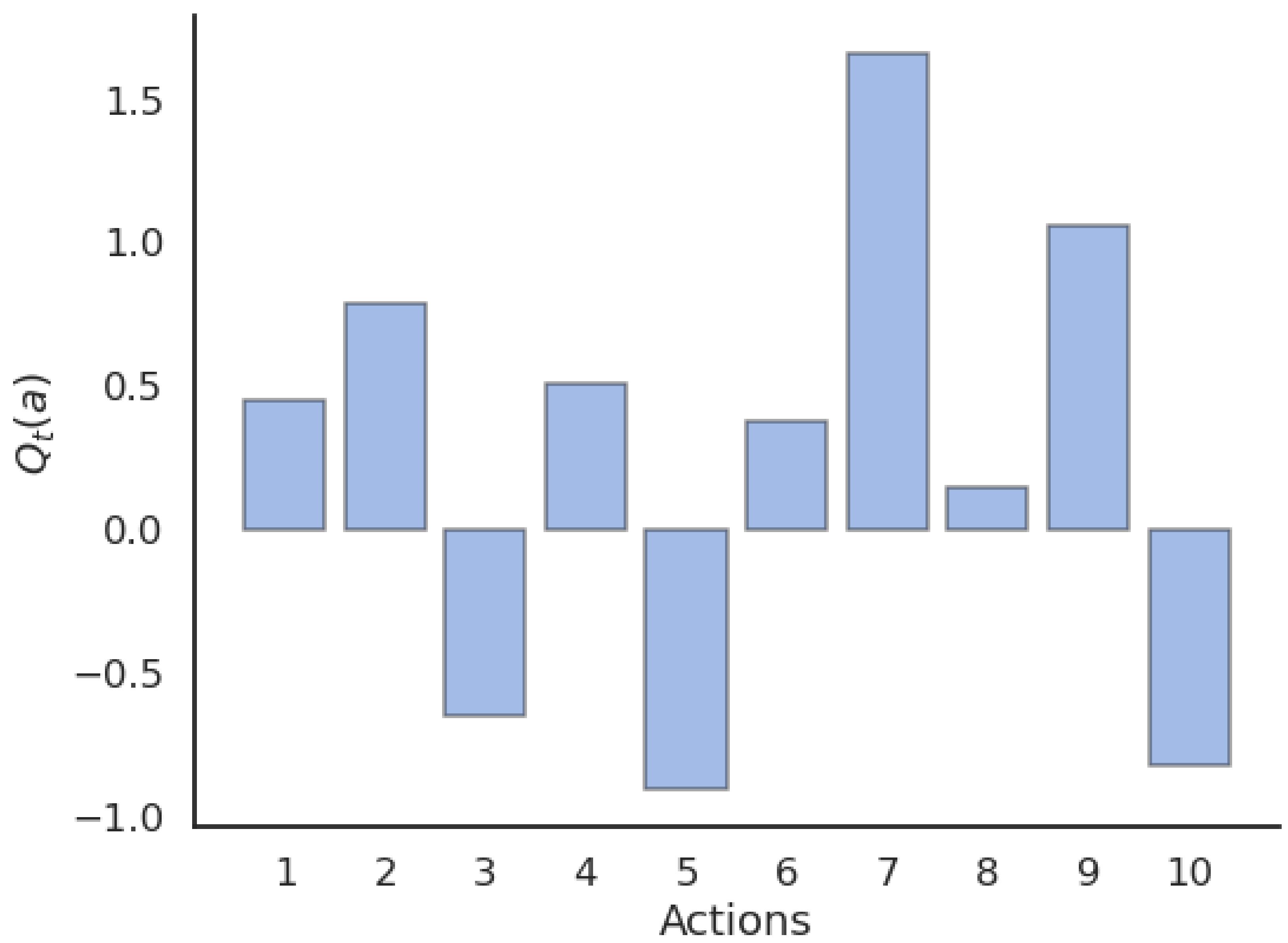
- The form of this **update rule** is very important to remember:

$$\text{new estimate} = \text{current estimate} + \alpha \, (\text{target} - \text{current estimate})$$

- Estimates following this update rule track the mean of their sampled target values.
- $\text{target} - \text{current estimate}$ is the **prediction error** between the target and the estimate.

3 - Action selection

Action selection

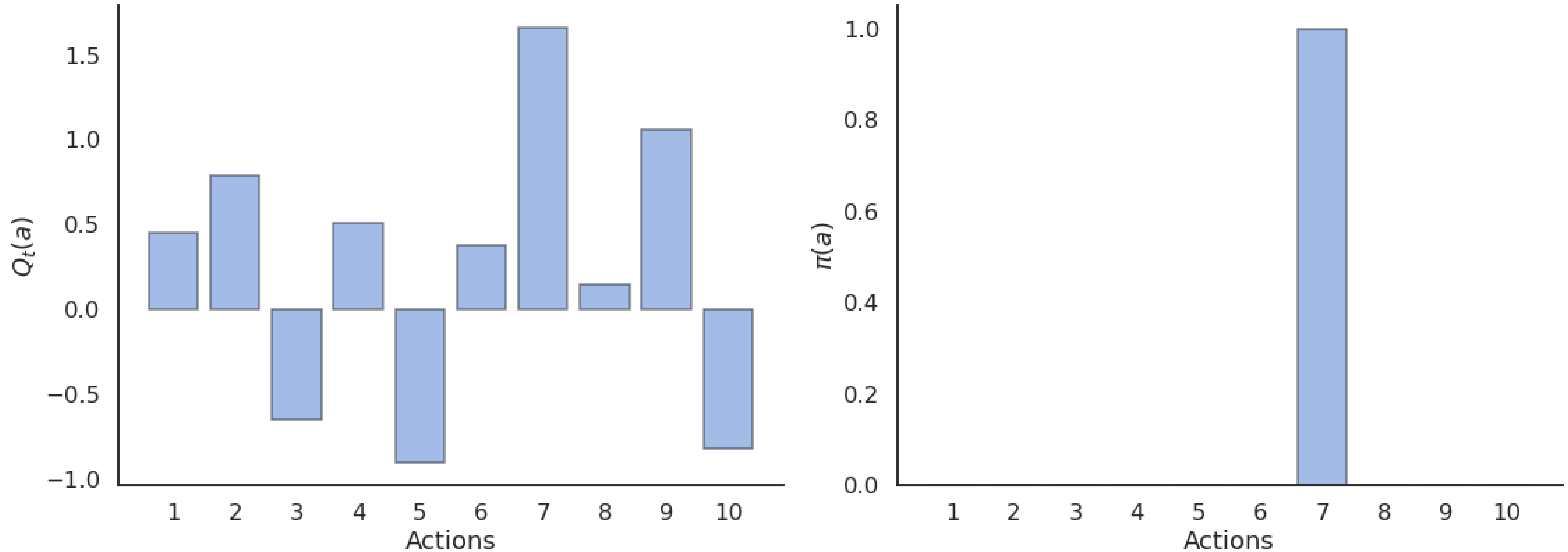


- Let's suppose we have formed reasonable estimates of the Q-values $Q_t(a)$ at time t.
- Which action should we do next?
- If we select the next action a_{t+1} randomly (**random agent**), we do not maximize the rewards we receive, but we can continue learning the Q-values.
- Choosing the action to perform next is called **action selection** and several schemes are possible.

Action selection

1. Greedy action selection
2. ϵ-greedy action selection
3. Softmax action selection
4. Optimistic initialization
5. Reinforcement comparison
6. Gradient bandit algorithm
7. Upper-Confidence-Bound action selection

Greedy action selection

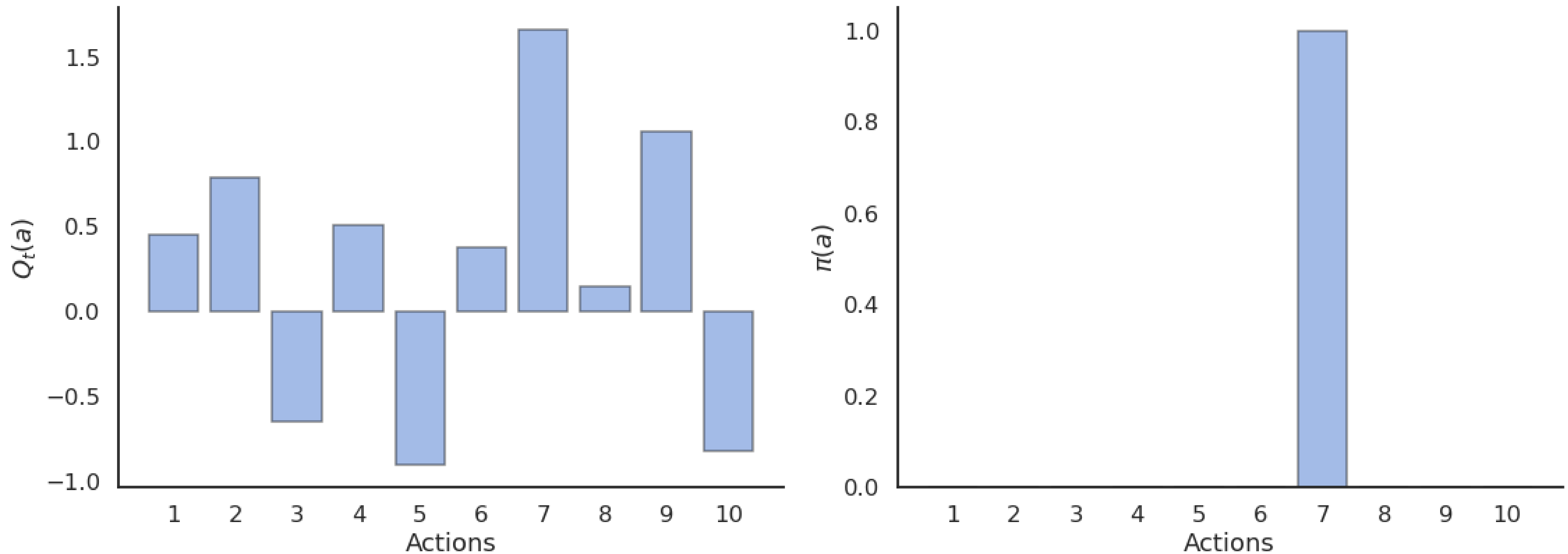


- The **greedy action** is the action whose estimated value is **maximal** at time t based on our current estimates:

$$a^*_t = \text{argmax}_a Q_t(a)$$

- If our estimates Q_t are correct (i.e. close from Q^*), the greedy action is the **optimal action** and we maximize the rewards on average.
- If our estimates are wrong, the agent will perform **sub-optimally**.

Greedy action selection



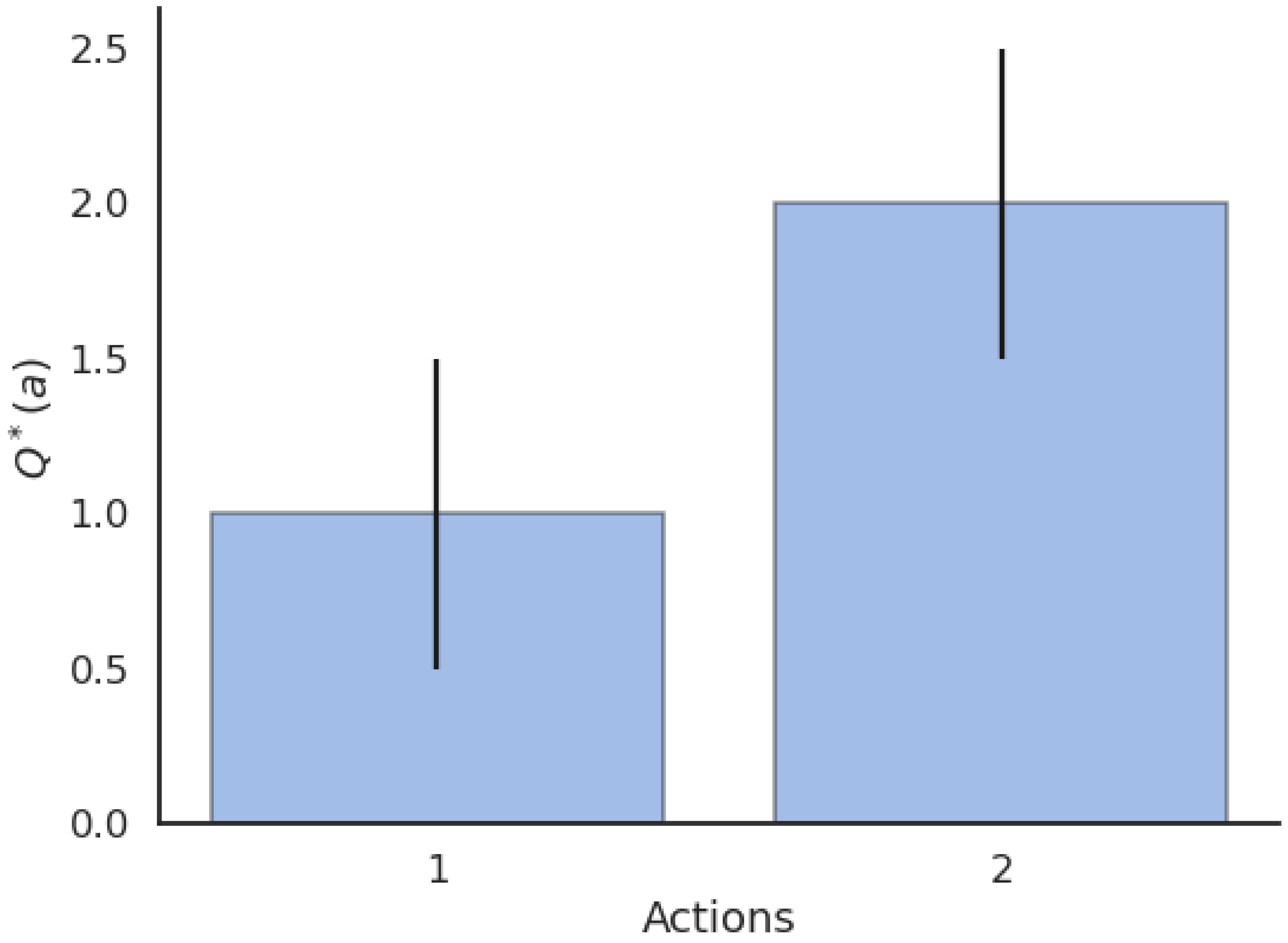
- This defines the **greedy policy**, where the probability of taking the greedy action is 1 and the probability of selecting another action is 0:

$$\pi(a) = \begin{cases} 1 \text{ if } a = a_t^* \\ 0 \text{ otherwise.} \end{cases}$$

- The greedy policy is **deterministic**: the action taken is always the same for a fixed Q_t.

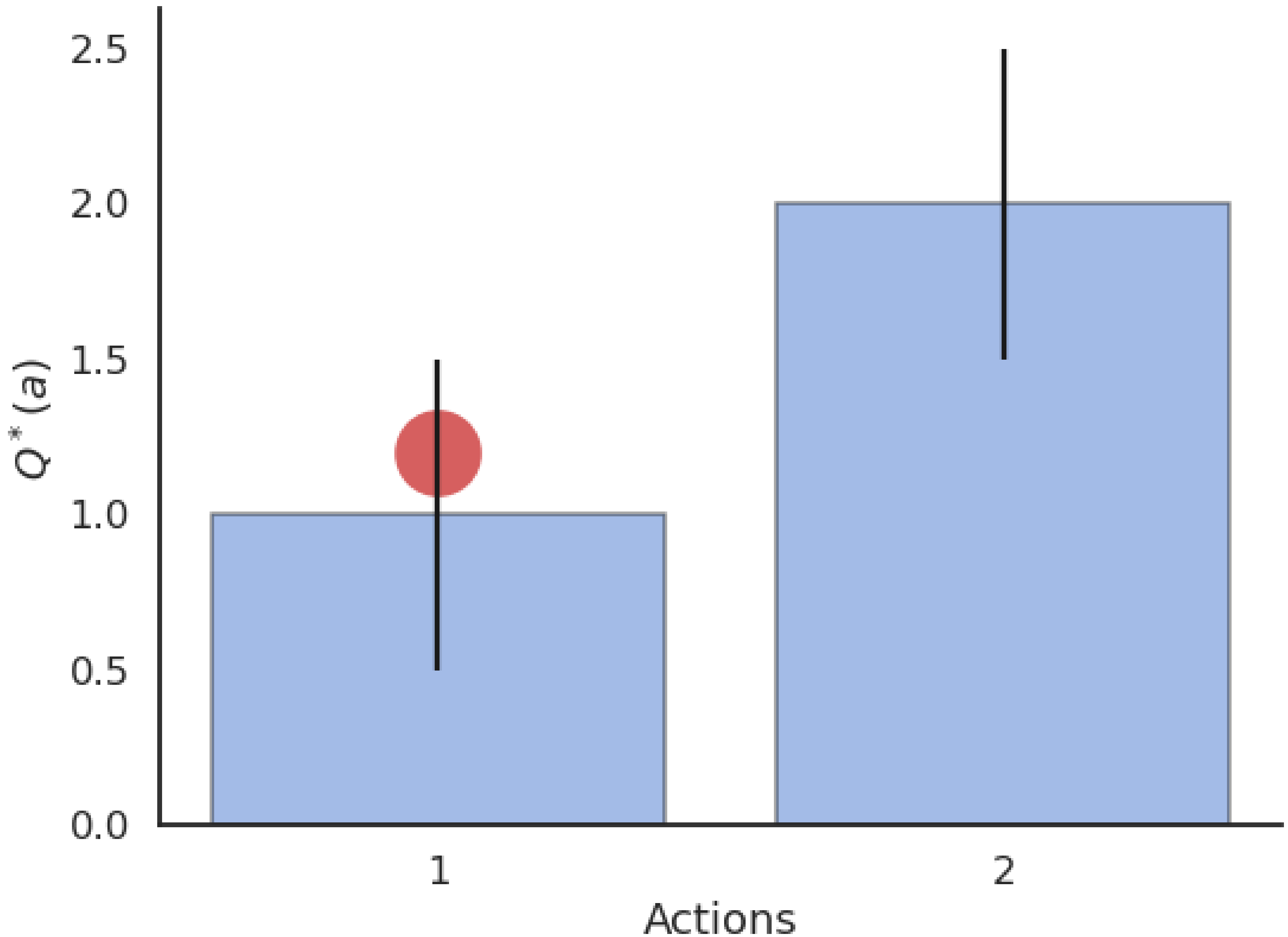
Problem with greedy action selection

- Greedy action selection only works when the estimates are good enough.



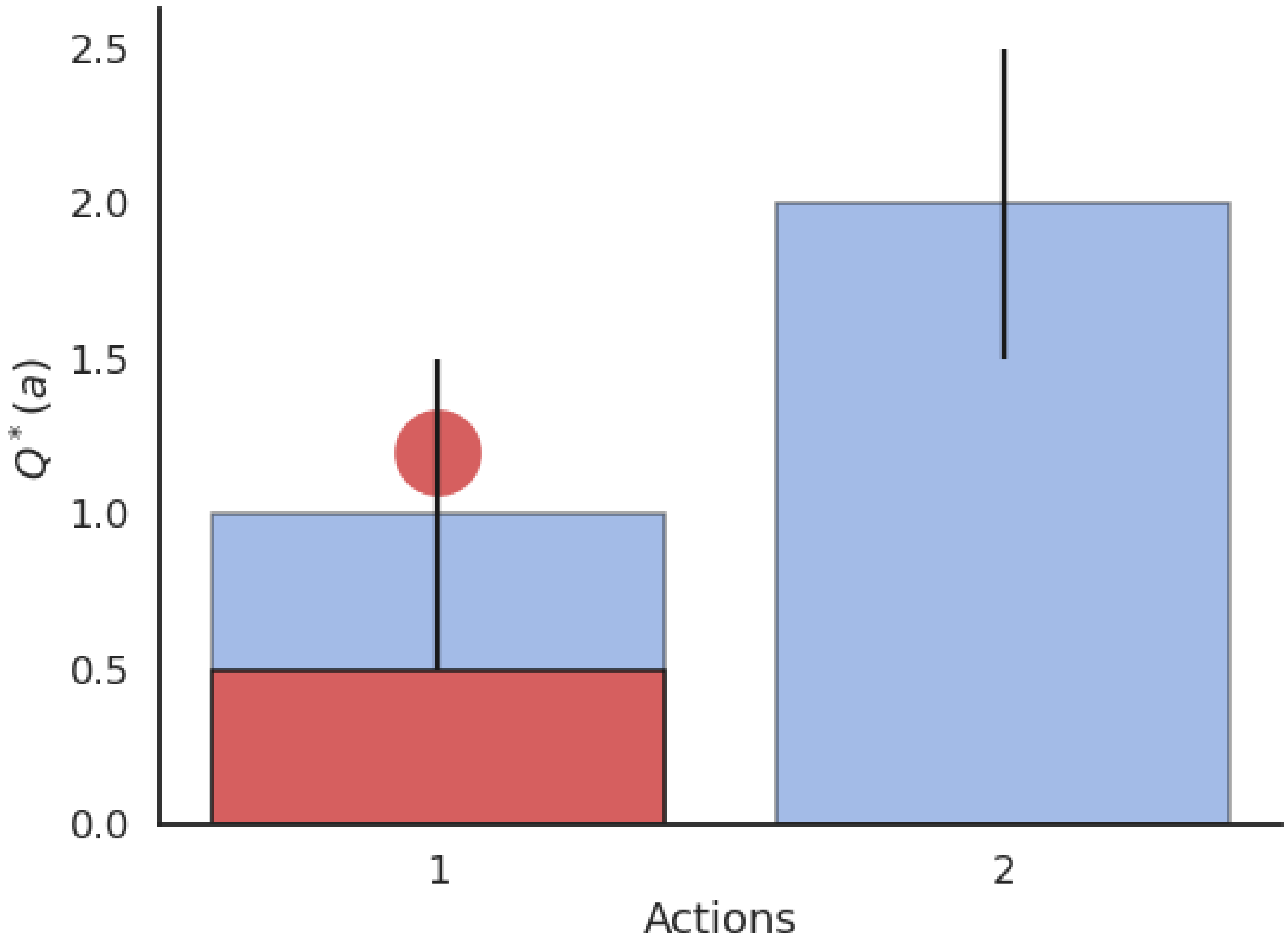
Problem with greedy action selection

- Estimates are initially bad (e.g. 0 here), so an action is sampled randomly and a reward is received.



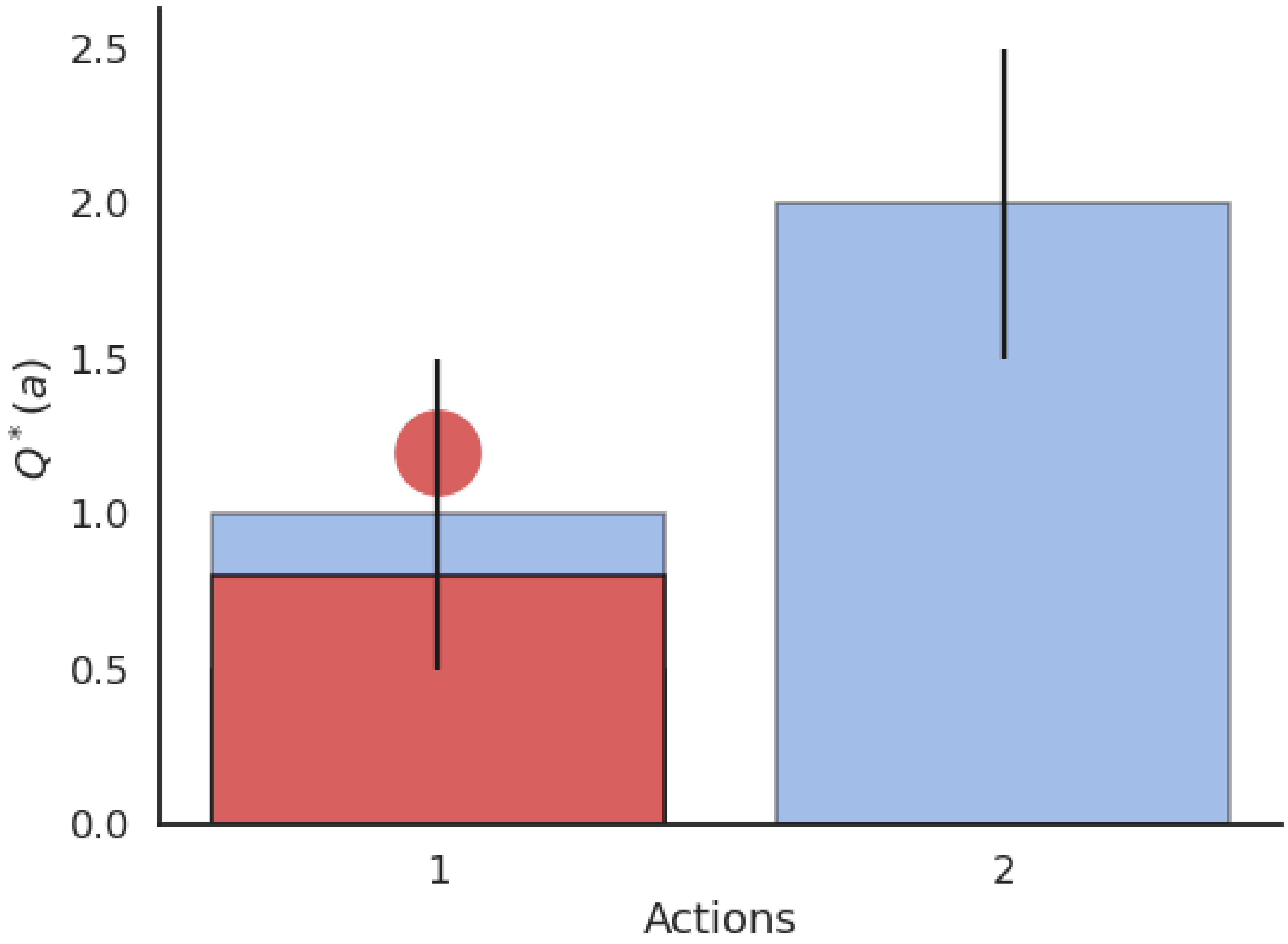
Problem with greedy action selection

- The Q-value of that action becomes positive, so it becomes the greedy action.

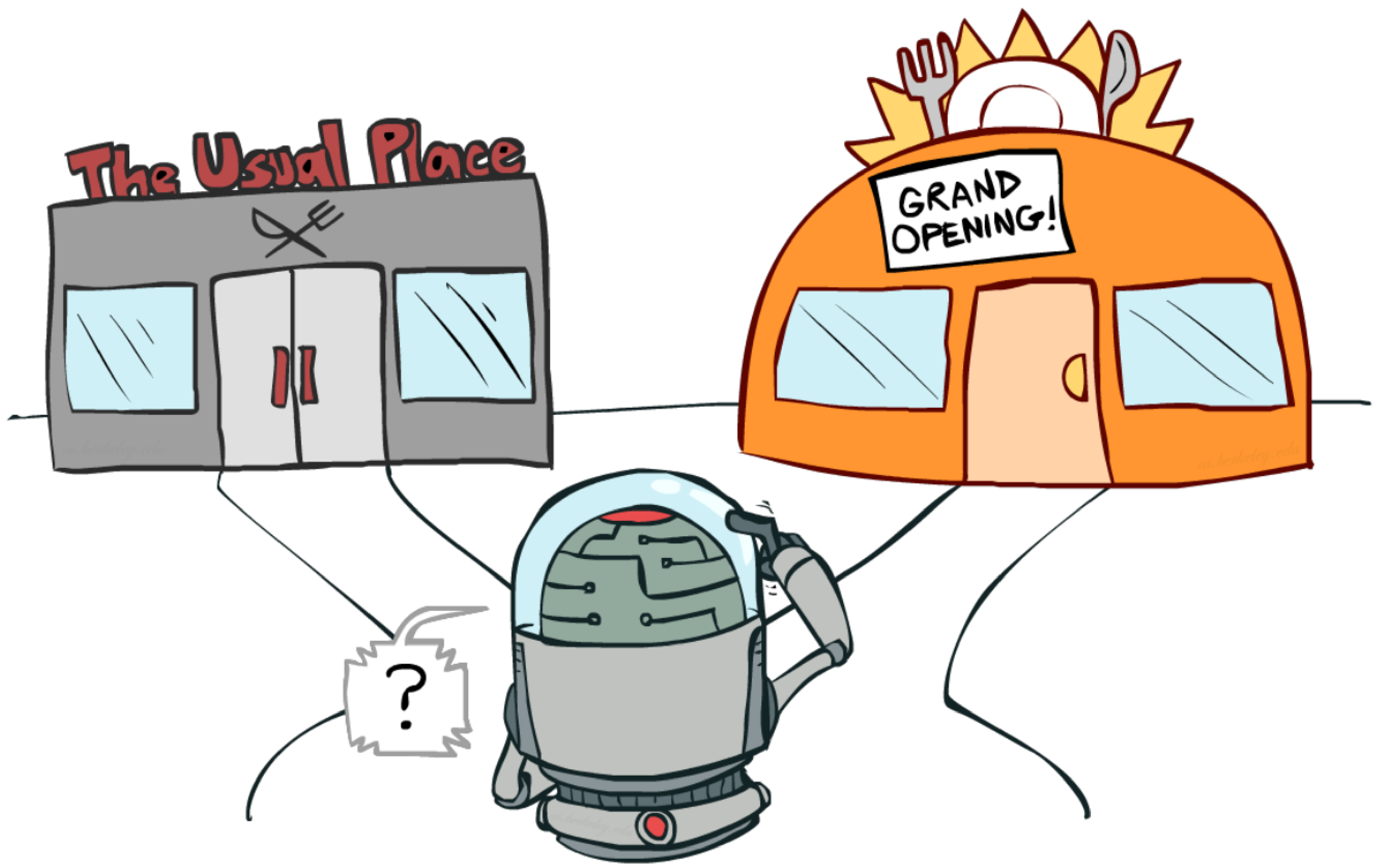


Problem with greedy action selection

- Greedy action selection will always select that action, although the second one would have been better.

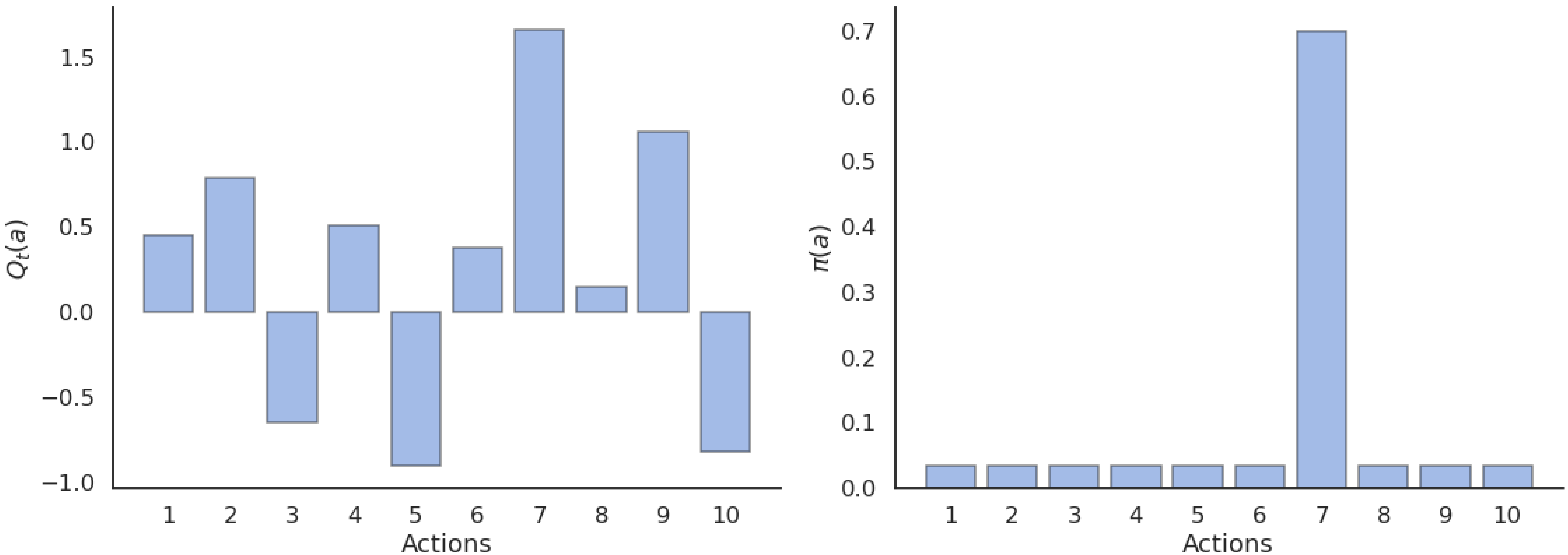


Exploration-exploitation dilemma



- This **exploration-exploitation** dilemma is the hardest problem in RL:
  - **Exploitation** is using the current estimates to select an action: they might be wrong!
  - **Exploration** is selecting non-greedy actions in order to improve their estimates: they might not be optimal!
- One has to balance exploration and exploitation over the course of learning:
  - More exploration at the beginning of learning, as the estimates are initially wrong.
  - More exploitation at the end of learning, as the estimates get better.

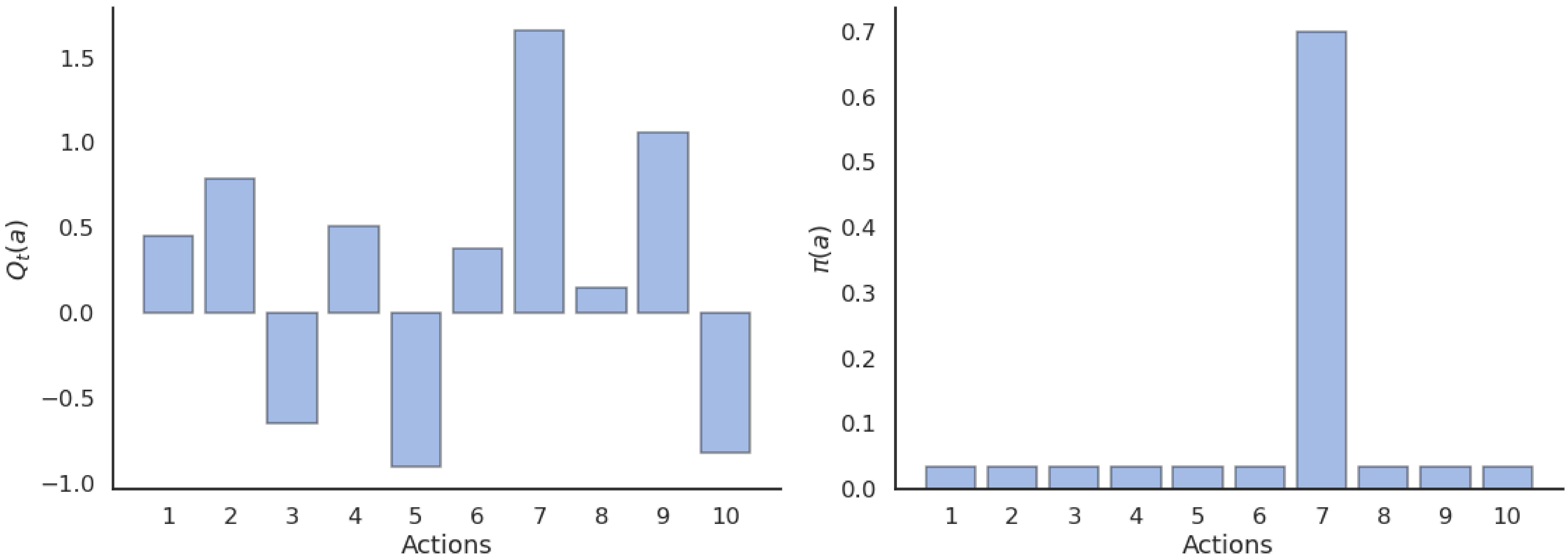
ϵ-greedy action selection



- **ϵ-greedy action selection** ensures a trade-off between exploitation and exploration.
- The greedy action is selected with probability $1 - \epsilon$ (with $0 < \epsilon < 1$), the others with probability ϵ:

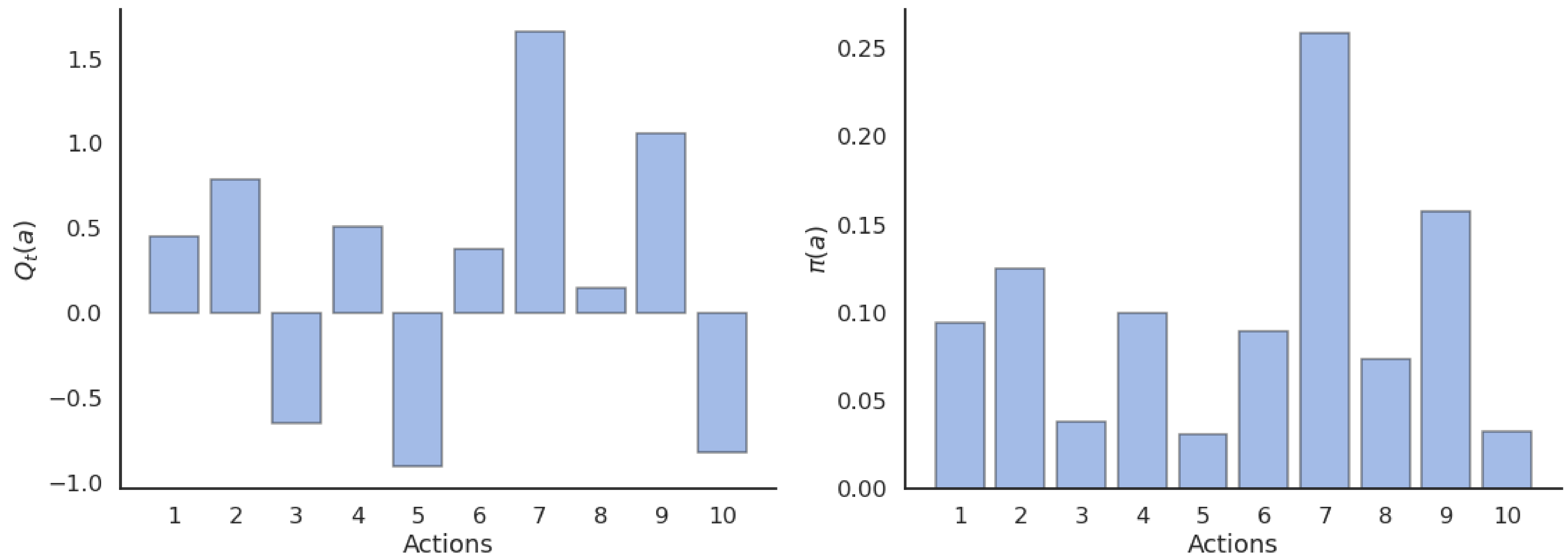
$$\pi(a) = \begin{cases} 1 - \epsilon \; \text{if} \; a = a_t^* \\ \frac{\epsilon}{|\mathcal{A}| - 1} \; \text{otherwise.} \end{cases}$$

ϵ-greedy action selection



- The parameter ϵ controls the level of exploration: the higher ϵ, the more exploration.
- One can set ϵ high at the beginning of learning and progressively reduce it to exploit more.
- However, it chooses equally among all actions: the worst action is as likely to be selected as the next-to-best action.

Softmax action selection

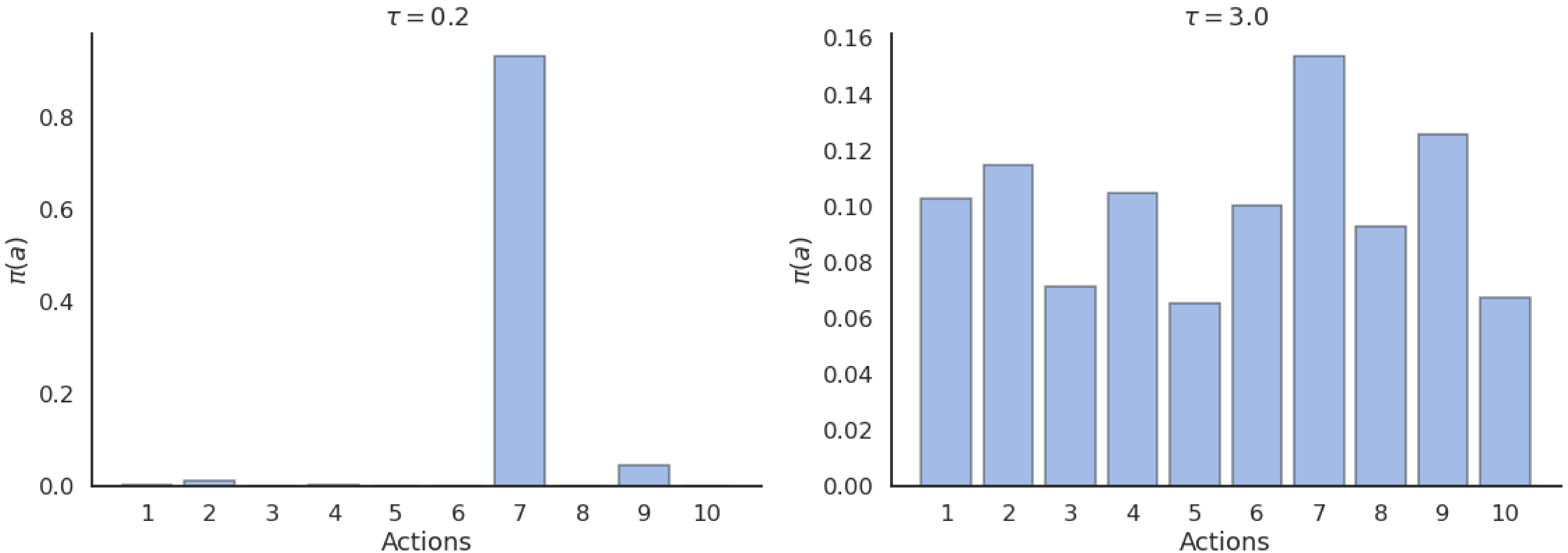


- **Softmax action selection** defines the probability of choosing an action using all estimated value.
- It represents the policy using a Gibbs (or Boltzmann) distribution:

$$\pi(a) = \frac{\exp \dfrac{Q_t(a)}{\tau}}{\displaystyle\sum_{a'} \exp \dfrac{Q_t(a')}{\tau}}$$

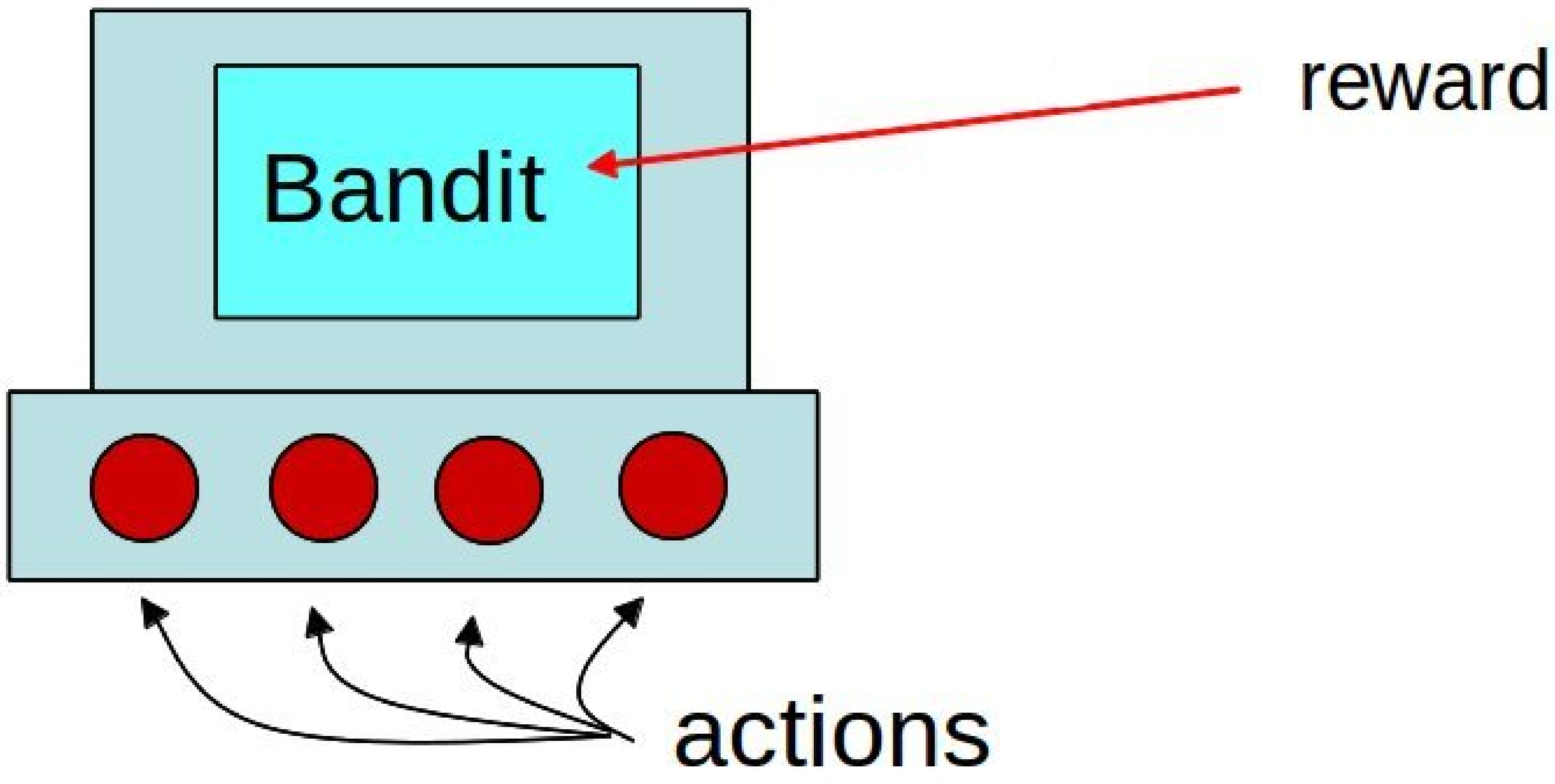
where τ is a positive parameter called the **temperature**.

Softmax action selection



- Just as ϵ, the temperature τ controls the level of exploration:
  - High temperature causes the actions to be nearly equiprobable (**random agent**).
  - Low temperature causes the greediest actions only to be selected (**greedy agent**).

Example of action selection for the 10-armed bandit

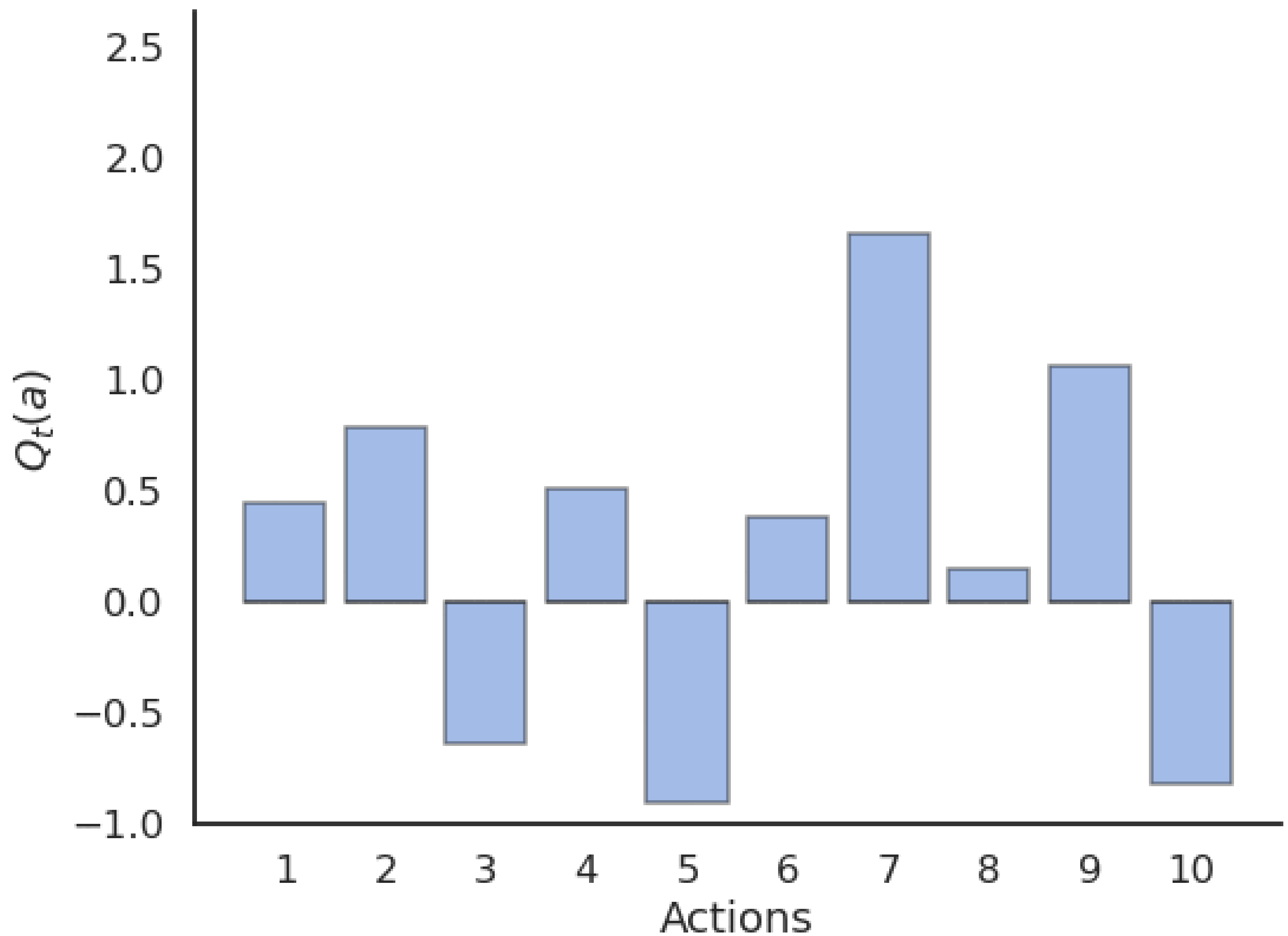


Procedure as in (Sutton and Barto, 2017):

- N = 10 possible actions with Q-values $Q^*(a_1), ..., Q^*(a_{10})$ randomly chosen in $\mathcal{N}(0, 1)$.
- Each reward r_t is drawn from a normal distribution $\mathcal{N}(Q^*(a), 1)$ depending on the selected action.
- Estimates $Q_t(a)$ are initialized to 0.
- The algorithms run for 1000 plays, and the results are averaged 200 times.

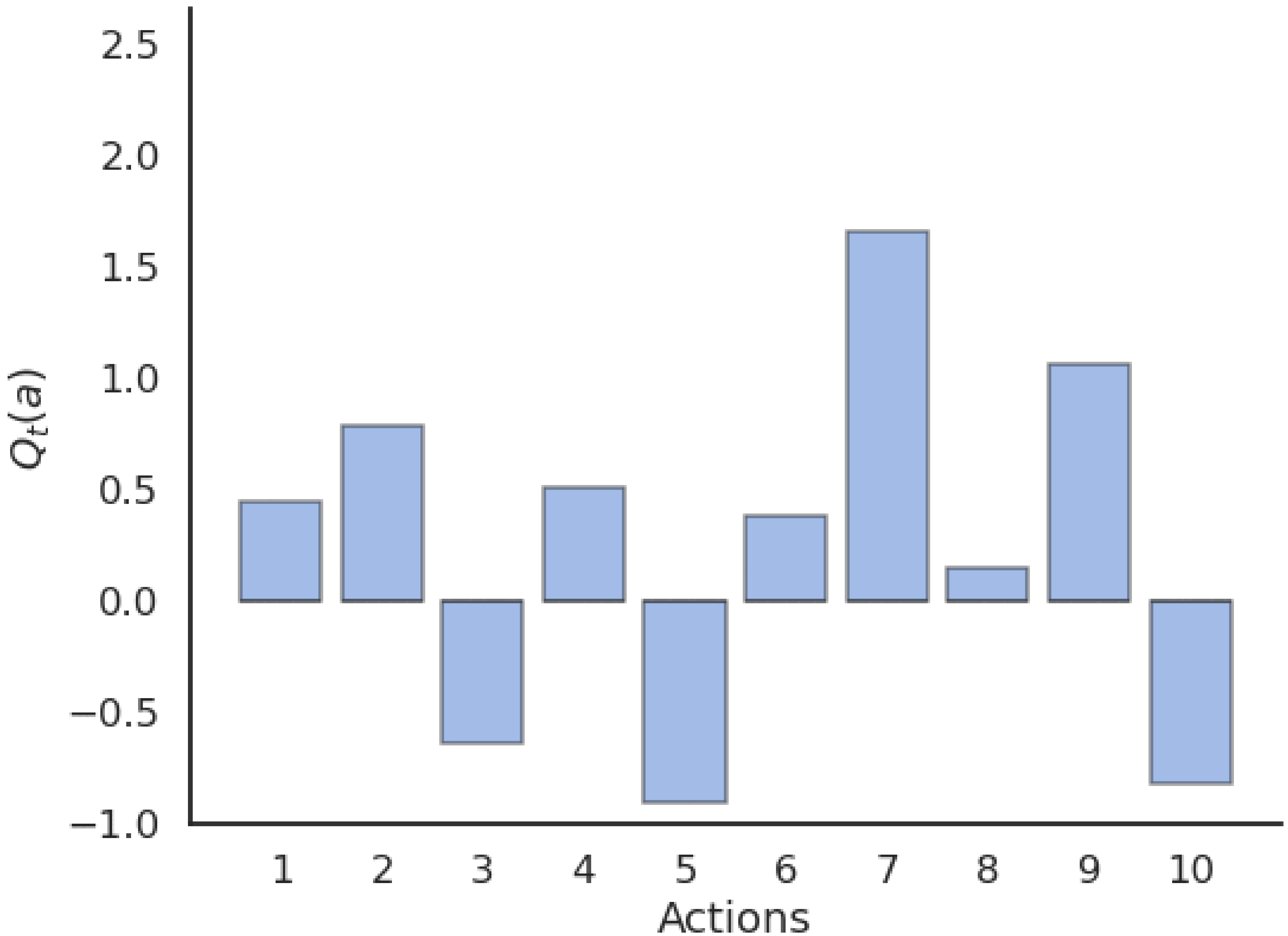
Greedy action selection

- Greedy action selection allows to get rid quite early of the actions with negative rewards.
- However, it may stick with the first positive action it founds, probably not the optimal one.
- The more actions you have, the more likely you will get stuck in a **suboptimal policy**.



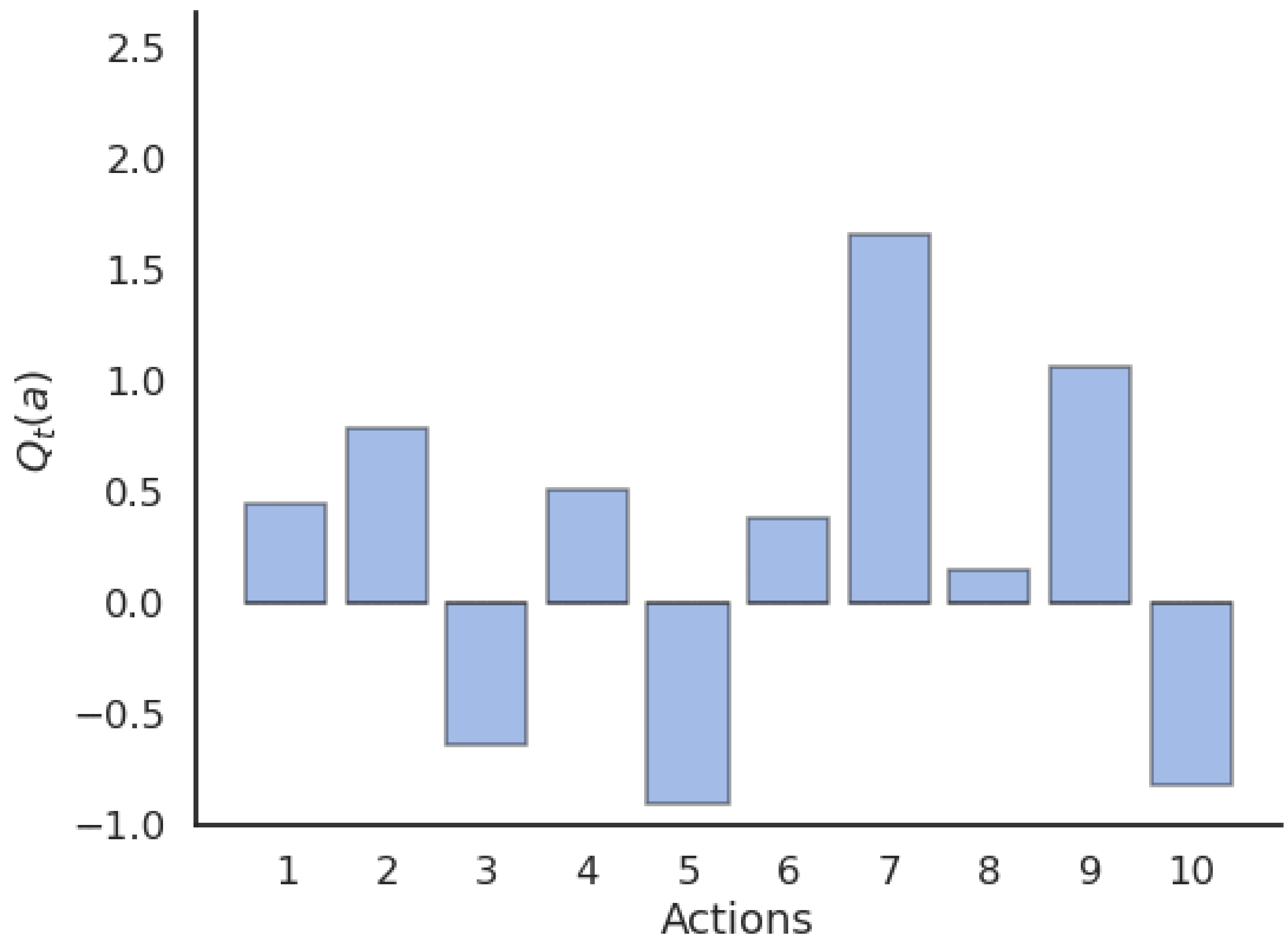
ϵ-greedy action selection

- ϵ-greedy action selection continues to explore after finding a good (but often suboptimal) action.
- It is not always able to recognize the optimal action (it depends on the variance of the rewards).

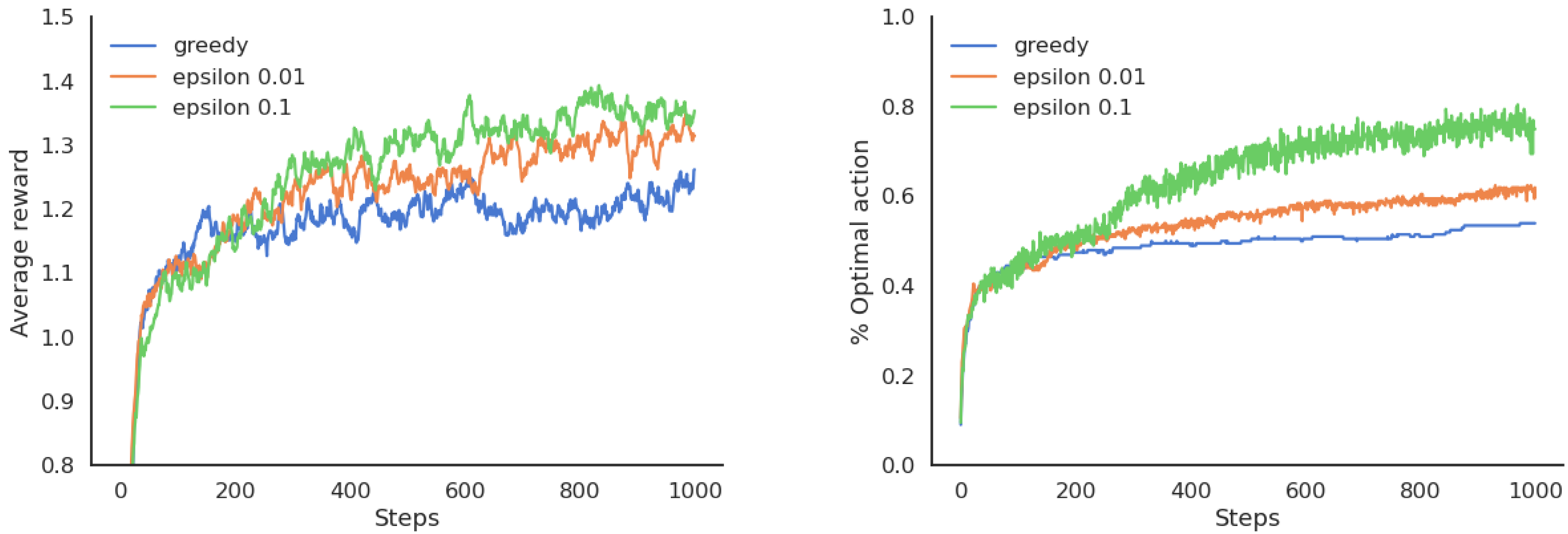


Softmax action selection

- Softmax action selection explores more consistently the available actions.
- The estimated Q-values are much closer to the true values than with (ϵ-)greedy methods.

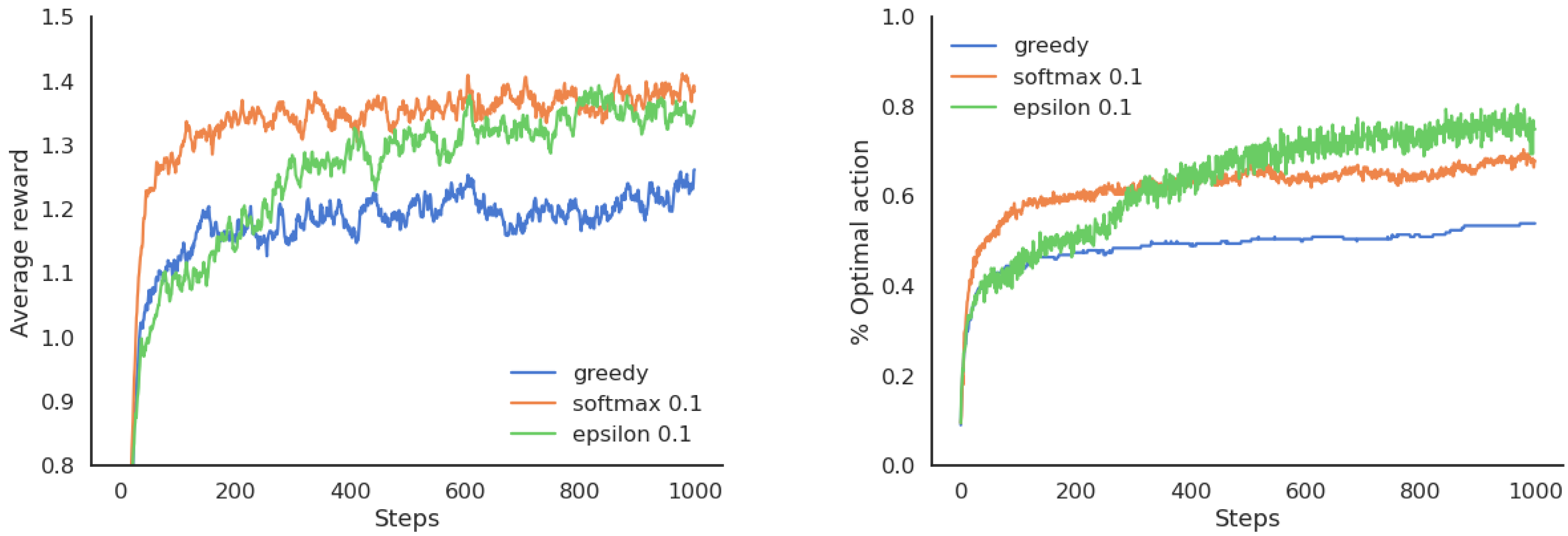


Greedy vs. ϵ-greedy



- The **greedy** method learns faster at the beginning, but get stuck in the long-term by choosing **suboptimal** actions (50% of trials).
- ϵ-greedy methods perform better on the long term, because they continue to explore.
- High values for ϵ provide more exploration, hence find the optimal action earlier, but also tend to deselect it more often: with a limited number of plays, it may collect less reward than smaller values of ϵ.

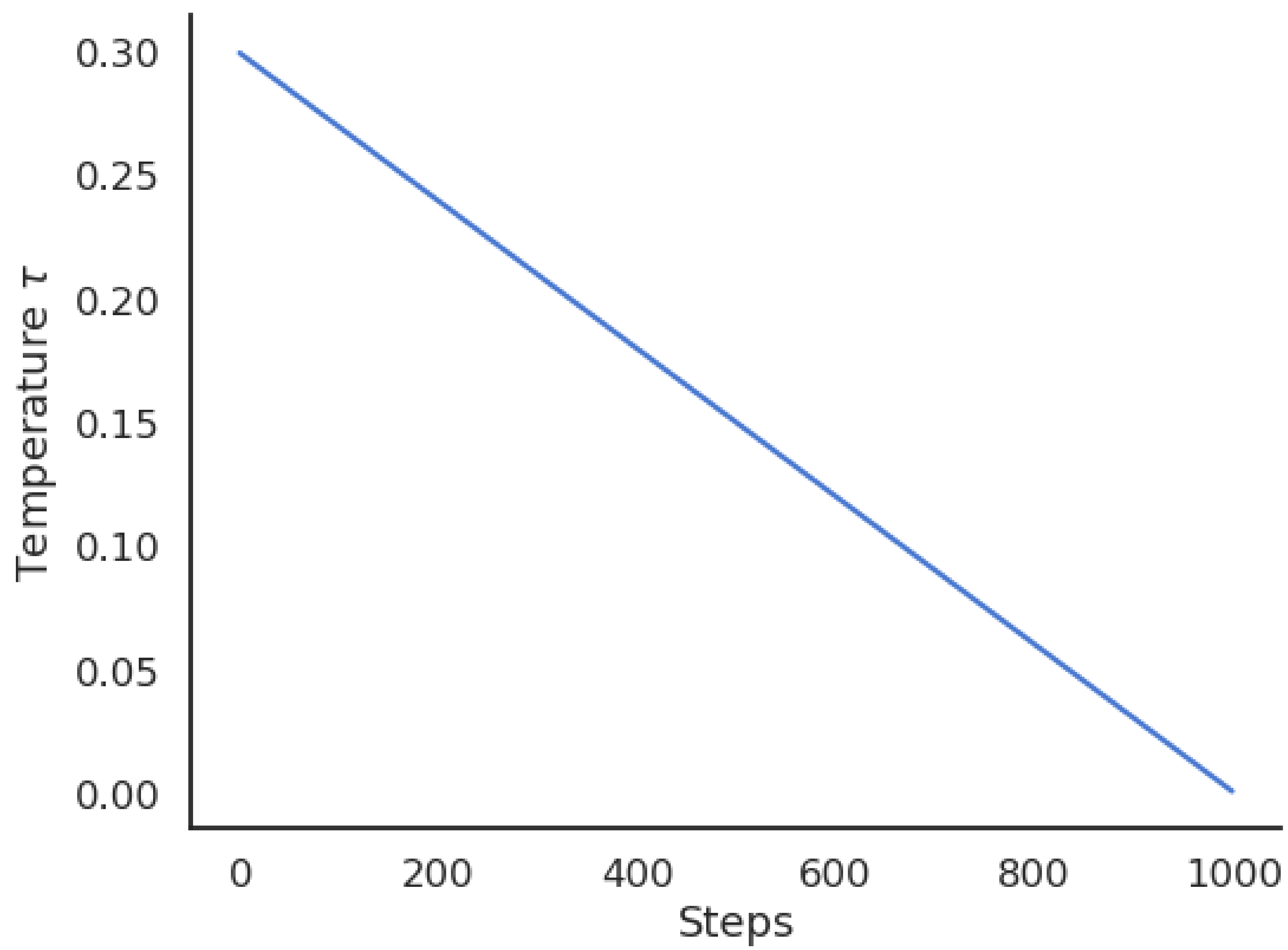
Softmax vs. ϵ-greedy



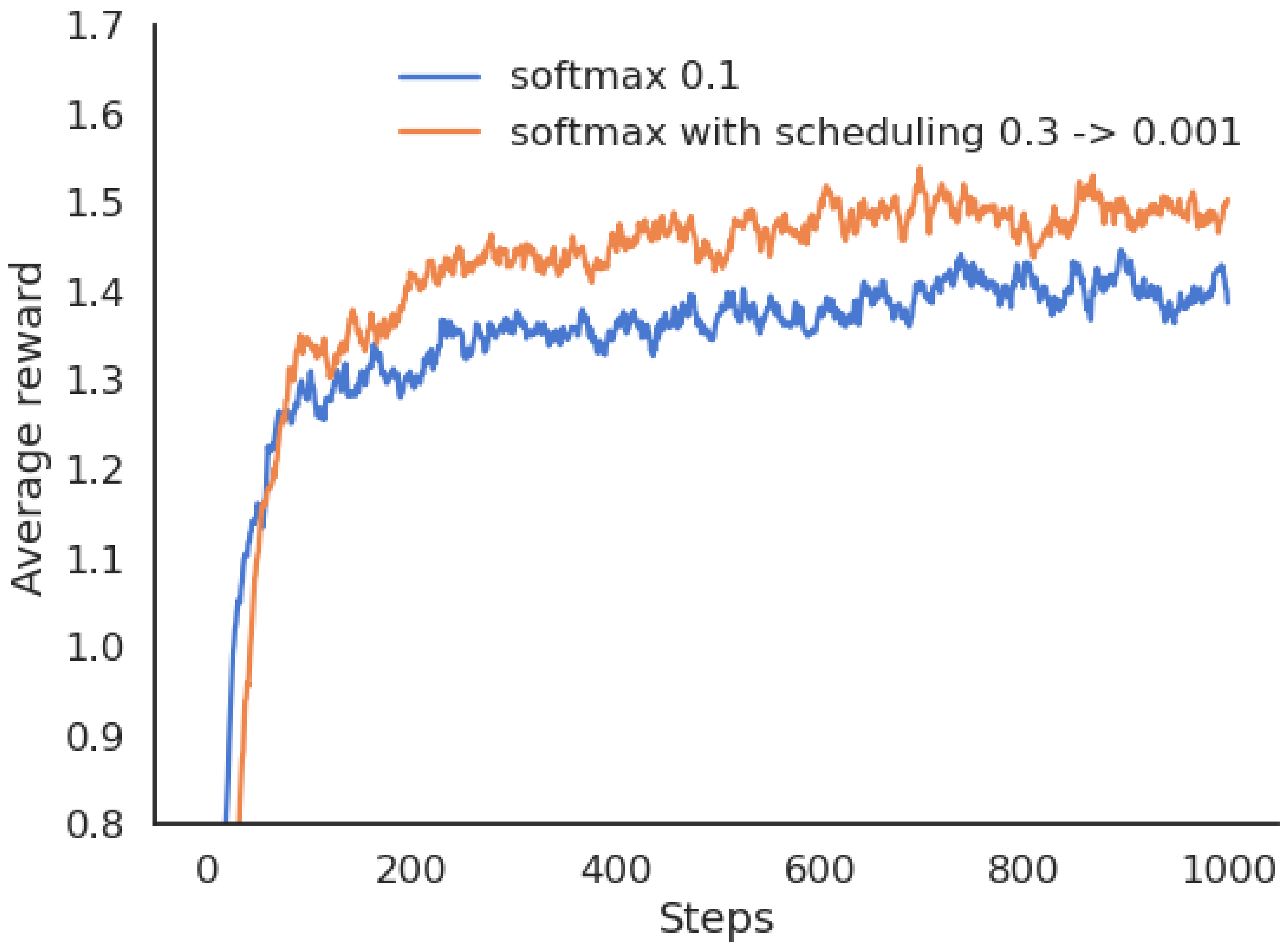
- The softmax does not necessarily find a better solution than ϵ-greedy, but it tends to find it **faster** (depending on ϵ or τ), as it does not lose time exploring obviously bad solutions.
- ϵ-greedy or softmax methods work best when the variance of rewards is high.
- If the variance is zero (always the same reward value), the greedy method would find the optimal action more rapidly: the agent only needs to try each action once.

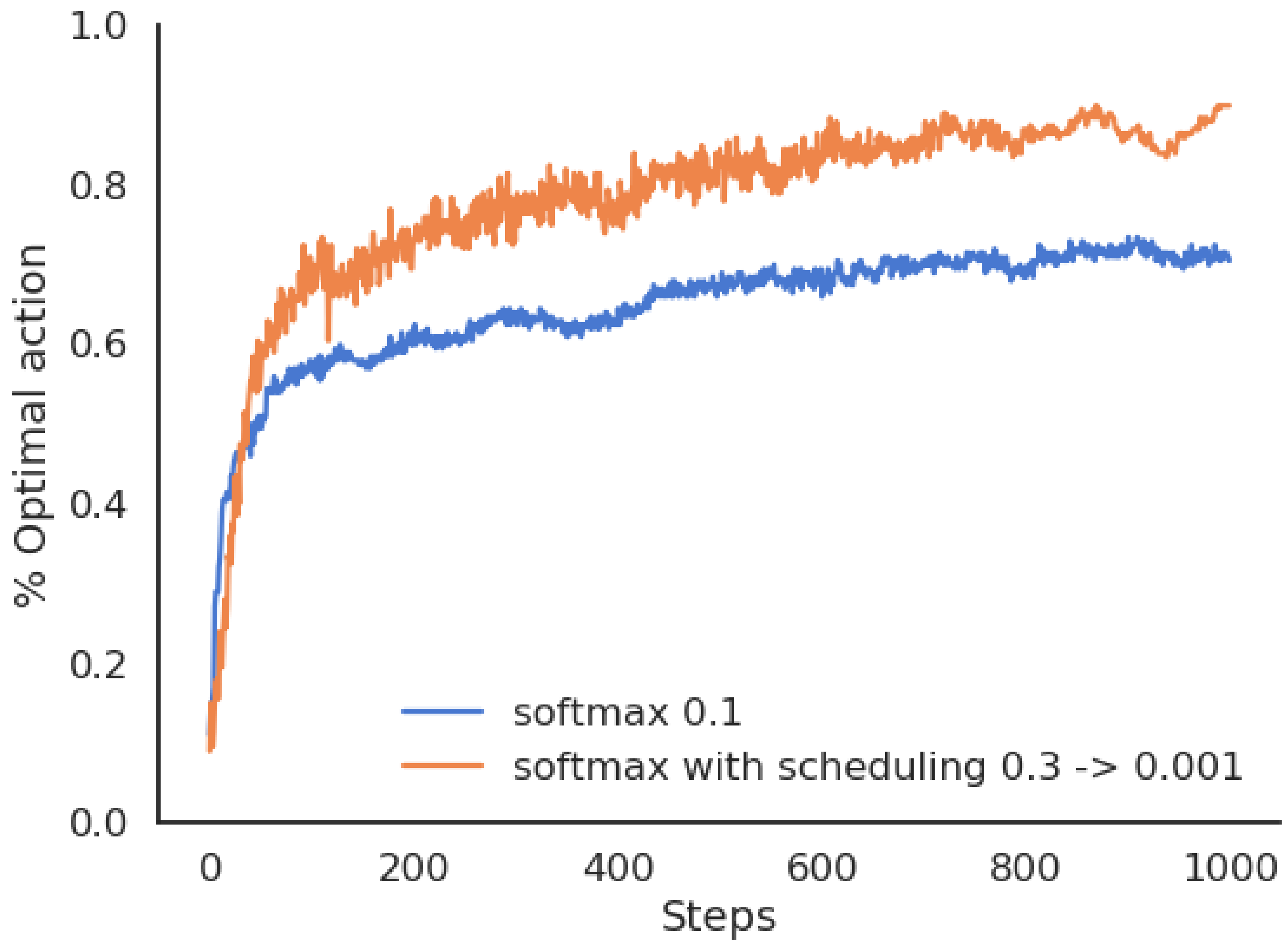
Exploration schedule

- A useful technique to cope with the **exploration-exploitation dilemma** is to slowly decrease the value of ϵ or τ with the number of plays.
- This allows for more exploration at the beginning of learning and more exploitation towards the end.
- It is however hard to find the right **decay rate** for the exploration parameters.



Exploration schedule





- The performance is worse at the beginning, as the agent explores with a high temperature.
- But as the agent becomes greedier and greedier, the performance become more **optimal** than with a fixed temperature.

Optimistic initial values

- The problem with online evaluation is that it depends a lot on the initial estimates Q_0.
  - If the initial estimates are already quite good (expert knowledge), the Q-values will converge very fast.
  - If the initial estimates are very wrong, we will need a lot of updates to correctly estimate the true values.

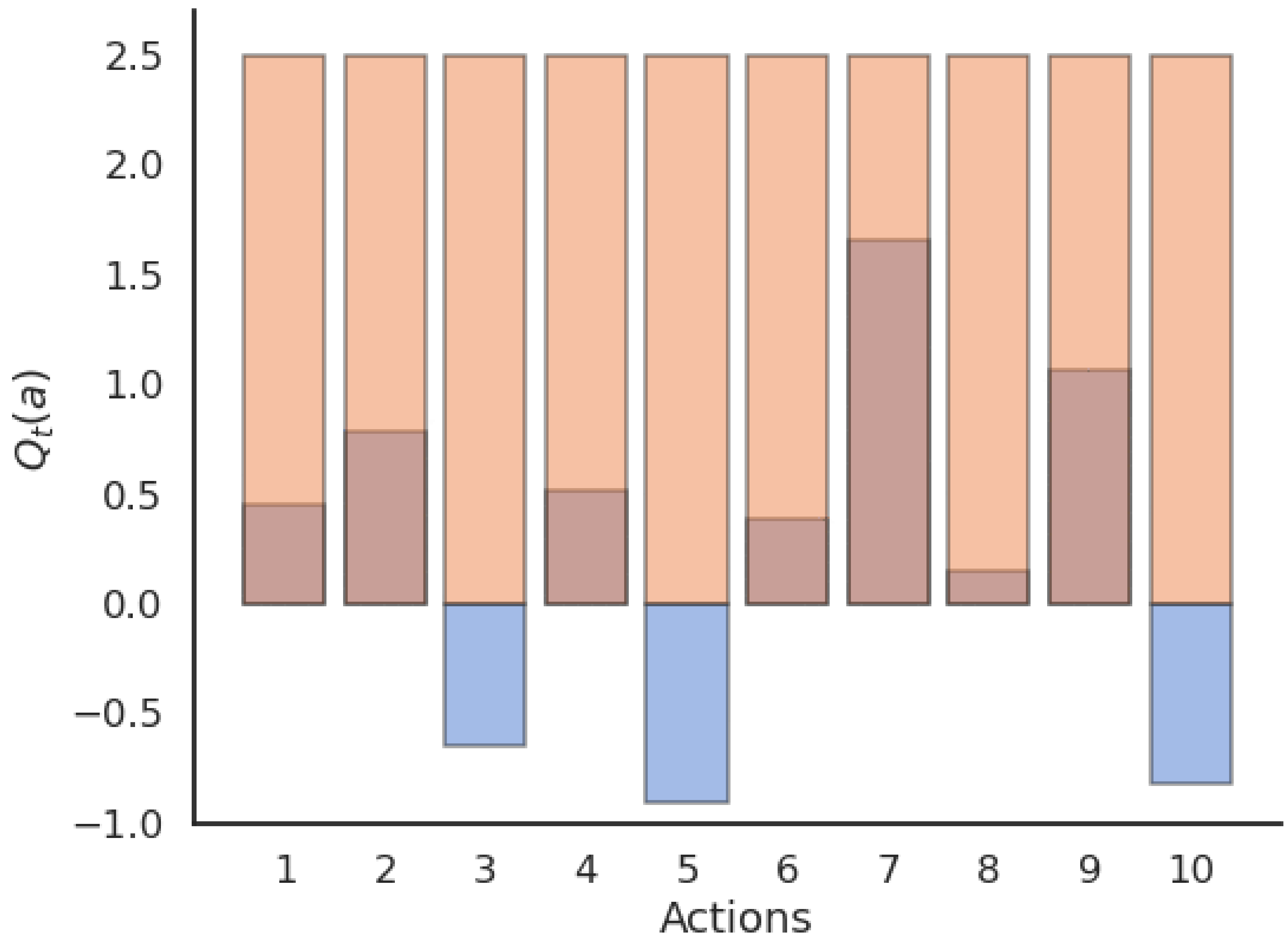
$$Q_{t+1}(a) = (1 - \alpha) \, Q_t(a) + \alpha \, r_{t+1}$$

$$\begin{aligned} &\rightarrow Q_1(a) = (1 - \alpha) \, Q_0(a) + \alpha \, r_1 \\ &\rightarrow Q_2(a) = (1 - \alpha) \, Q_1(a) + \alpha \, r_2 = (1 - \alpha)^2 \, Q_0(a) + (1 - \alpha)\alpha \, r_1 + \alpha r_2 \end{aligned}$$

- The influence of Q_0 on Q_t **fades** quickly with $(1 - \alpha)^t$, but that can be lost time or lead to a suboptimal policy.
- However, we can use this at our advantage with **optimistic initialization**.

Optimistic initial values

- By choosing very high initial values for the estimates (they can only decrease), one can ensure that all possible actions will be selected during learning by the greedy method, solving the **exploration problem**.
- This leads however to an **overestimation** of the value of other actions.



Reinforcement comparison

- Actions followed by large rewards should be made more likely to recur, whereas actions followed by small rewards should be made less likely to recur.
- But what is a large/small reward? Is a reward of 5 large or small?
- **Reinforcement comparison** methods only maintain a **preference** $p_t(a)$ for each action, which is not exactly its Q-value.
- The preference for an action is updated after each play, according to the update rule:

$$p_{t+1}(a_t) = p_t(a_t) + \beta \, (r_t - \tilde{r}_t)$$

where $\tilde{r}_t$ is the moving average of the recently received rewards (regardless the action):

$$\tilde{r}_{t+1} = \tilde{r}_t + \alpha \, (r_t - \tilde{r}_t)$$

- If an action brings more reward than usual (**good surprise**), we increase the preference for that action.
- If an action brings less reward than usual (**bad surprise**), we decrease the preference for that action.
- $\beta > 0$ and $0 < \alpha < 1$ are two constant parameters.

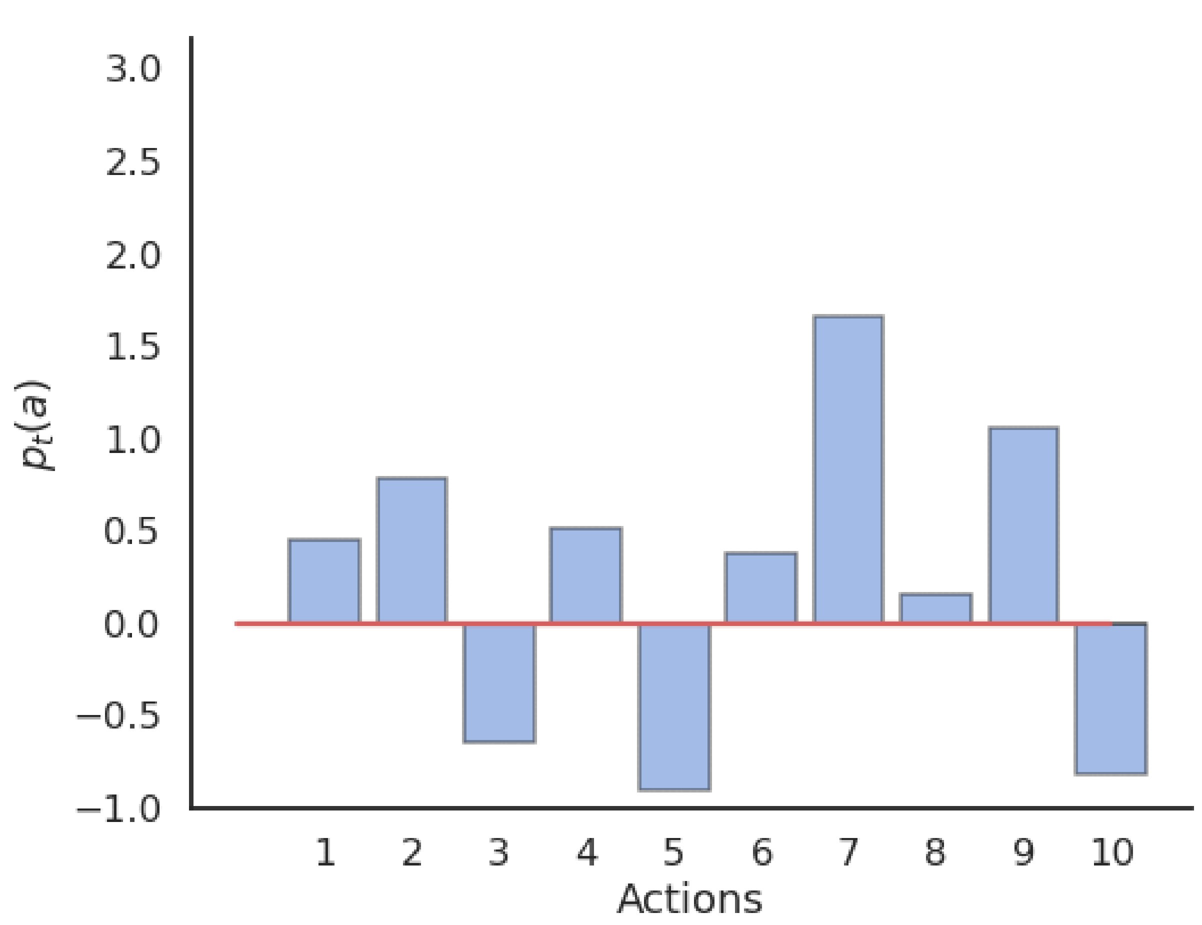
Reinforcement comparison

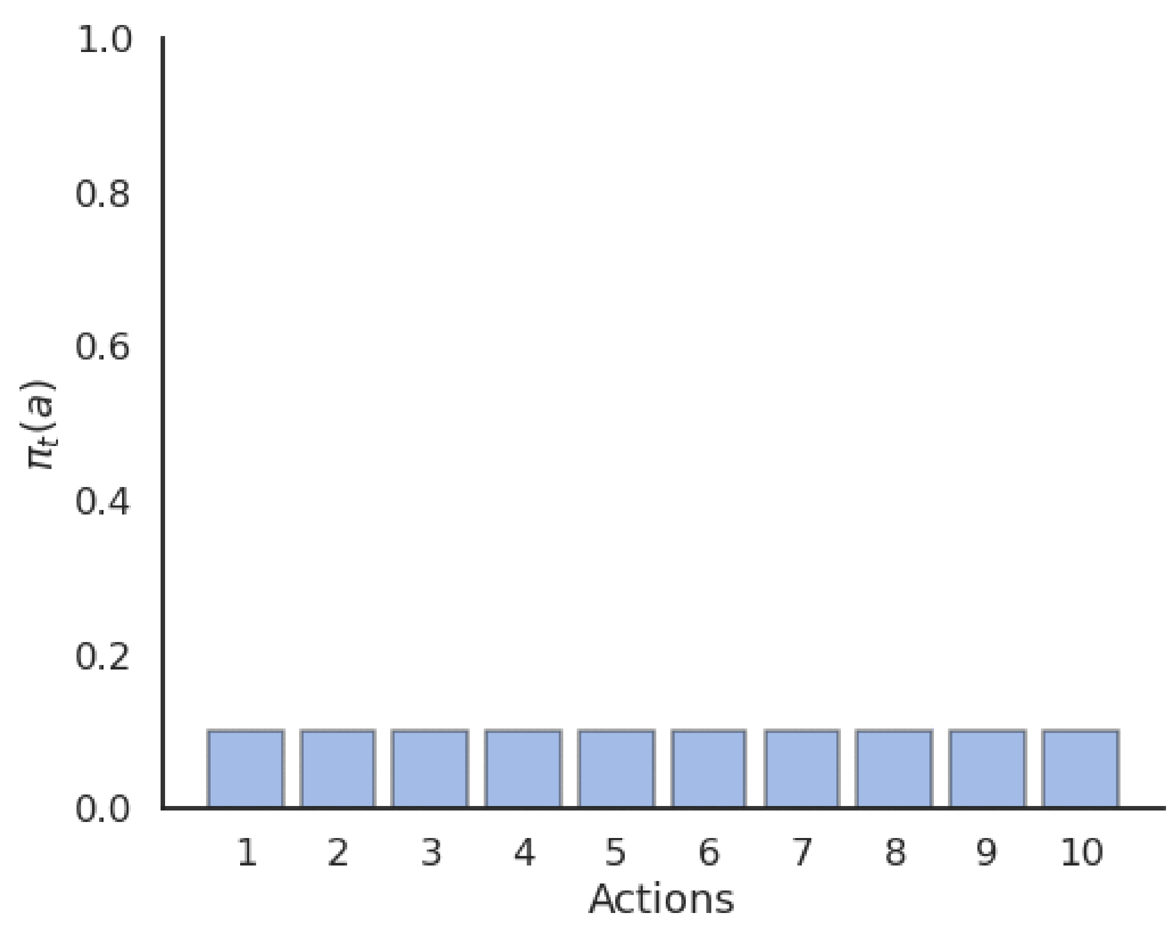
- Preferences are updated by replacing the action-dependent Q-values by a baseline $\tilde{r}_t$:

$$p_{t+1}(a_t) = p_t(a_t) + \beta \, (r_t - \tilde{r}_t)$$

- The preferences can be used to select the action using the softmax method just as the Q-values (without temperature):

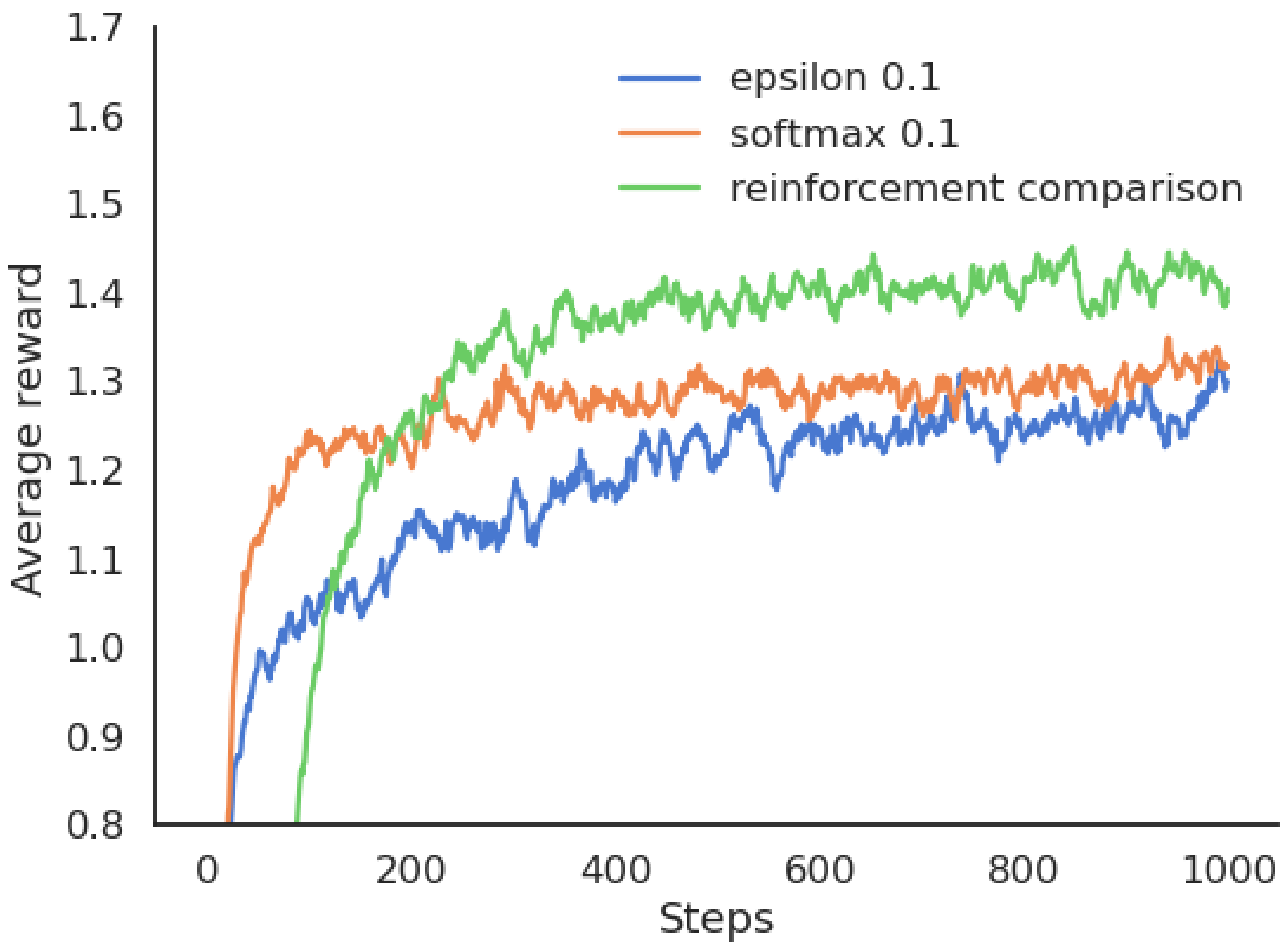
$$\pi_t(a) = \frac{\exp p_t(a)}{\sum_{a'} \exp p_t(a')}$$

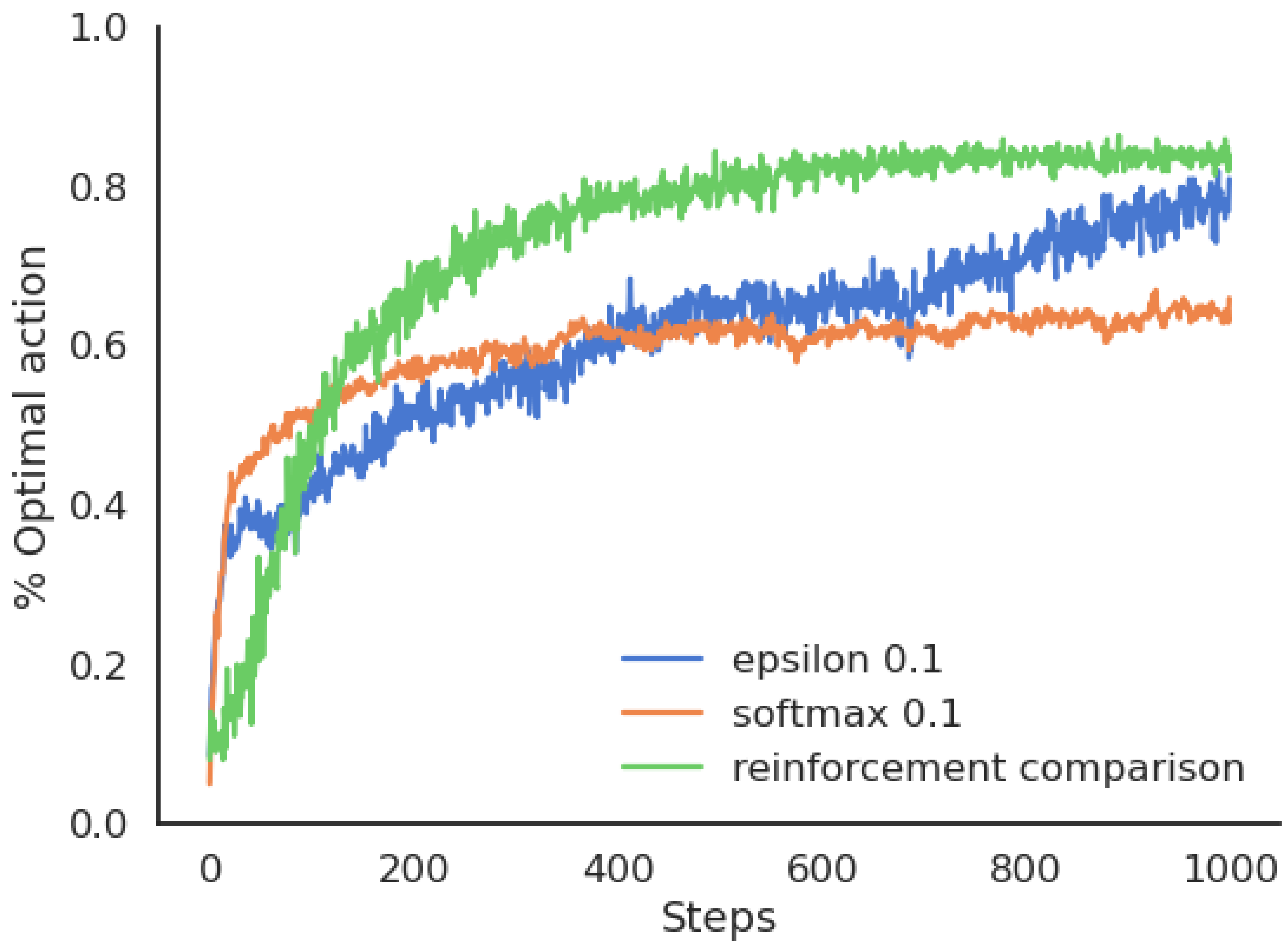




Reinforcement comparison

- Reinforcement comparison can be very effective, as it does not rely only on the rewards received, but also on their comparison with a **baseline**, the average reward.
- This idea is at the core of **actor-critic** architectures which we will see later.
- The initial average reward $\tilde{r}_0$ can be set optimistically to encourage exploration.





Gradient bandit algorithm

- Instead of only increasing the preference for the executed action if it brings more reward than usual, we could also decrease the preference for the other actions.
- The preferences are used to select an action a_t *via* softmax:

$$\pi_t(a) = \frac{\exp p_t(a)}{\displaystyle\sum_{a'} \exp p_t(a')}$$

- Update rule for the **action taken** a_t:

$$p_{t+1}(a_t) = p_t(a_t) + \beta \, (r_t - \tilde{r}_t) \, (1 - \pi_t(a_t))$$

- Update rule for the **other actions** $a \neq a_t$:

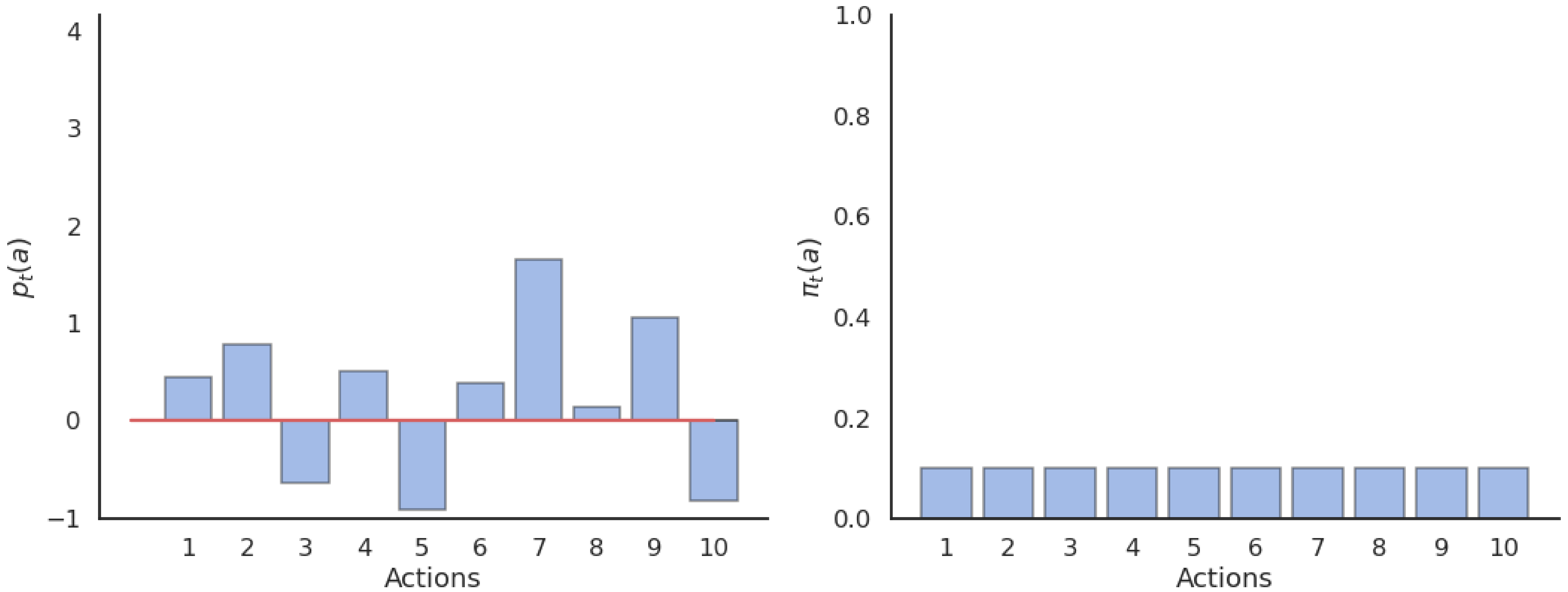
$$p_{t+1}(a) = p_t(a) - \beta \, (r_t - \tilde{r}_t) \, \pi_t(a)$$

- Update of the reward **baseline**:

$$\tilde{r}_{t+1} = \tilde{r}_t + \alpha \, (r_t - \tilde{r}_t)$$

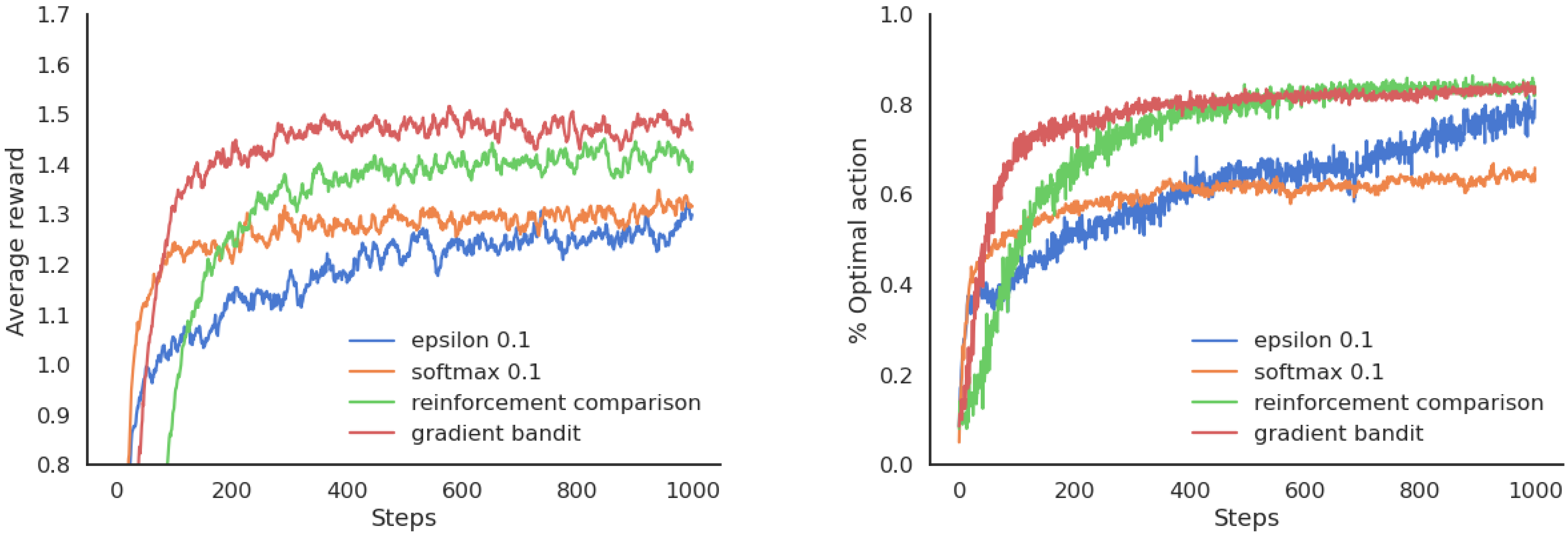
Gradient bandit algorithm

- The preference can increase become quite high, making the policy greedy towards the end.
- No need for a temperature parameter!



Gradient bandit algorithm

- Gradient bandit is not always better than reinforcement comparison, but learns initially faster (depending on the parameters α and β).



Upper-Confidence-Bound action selection

- In the previous methods, **exploration** is controlled by an external parameter (ϵ or τ) which is **global** to each action an must be scheduled.
- A much better approach would be to decide whether to explore an action based on the **uncertainty** about its Q-value:
  - If we are certain about the value of an action, there is no need to explore it further, we only have to exploit it if it is good.
- The **central limit theorem** tells us that the variance of a sampling estimator decreases with the number of samples:
  - The distribution of sample averages is normally distributed with mean μ and variance $\frac{\sigma^2}{N}$.

$$S_N \sim \mathcal{N}(\mu, \frac{\sigma}{\sqrt{N}})$$

- The more you explore an action a, the smaller the variance of $Q_t(a)$, the more certain you are about the estimation, the less you need to explore it.

Upper-Confidence-Bound action selection

- **Upper-Confidence-Bound** (UCB) action selection is a **greedy** action selection method that uses an **exploration** bonus:

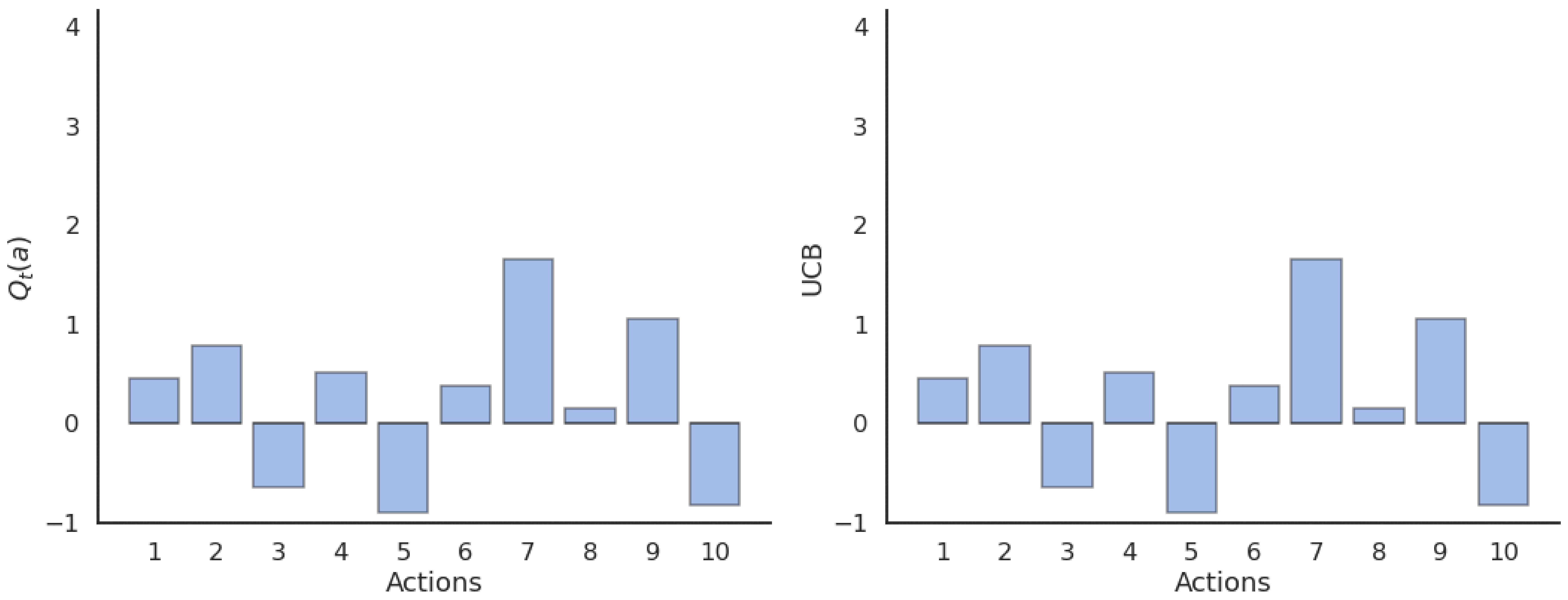
$$a^*_t = \text{argmax}_{a} \left[Q_t(a) + c \, \sqrt{\frac{\ln t}{N_t(a)}} \right]$$

- $Q_t(a)$ is the current estimated value of a and $N_t(a)$ is the number of times the action a has already been selected.
- It realizes a balance between trusting the estimates $Q_t(a)$ and exploring uncertain actions which have not been explored much yet.
- The term $\sqrt{\frac{\ln t}{N_t(a)}}$ is an estimate of the variance of $Q_t(a)$. The sum of both terms is an **upper-bound** of the true value $\mu + \sigma$.
- When an action has not been explored much yet, the uncertainty term will dominate and the action be explored, although its estimated value might be low.
- When an action has been sufficiently explored, the uncertainty term goes to 0 and we greedily follow $Q_t(a)$.

Upper-Confidence-Bound action selection

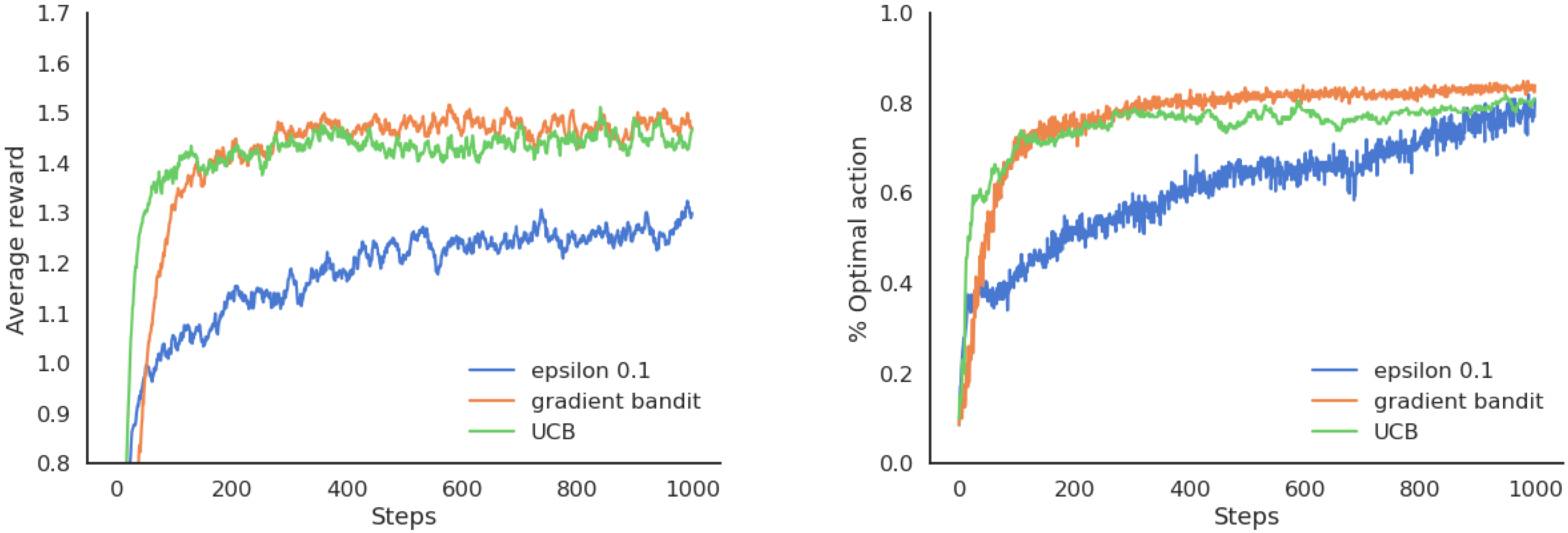
- The **exploration-exploitation** trade-off is automatically adjusted by counting visits to an action.

$$a^*_t = \text{argmax}_a \left[Q_t(a) + c \, \sqrt{\frac{\ln t}{N_t(a)}} \right]$$



Upper-Confidence-Bound action selection

- The “smart” exploration of UCB allows to find the optimal action faster.



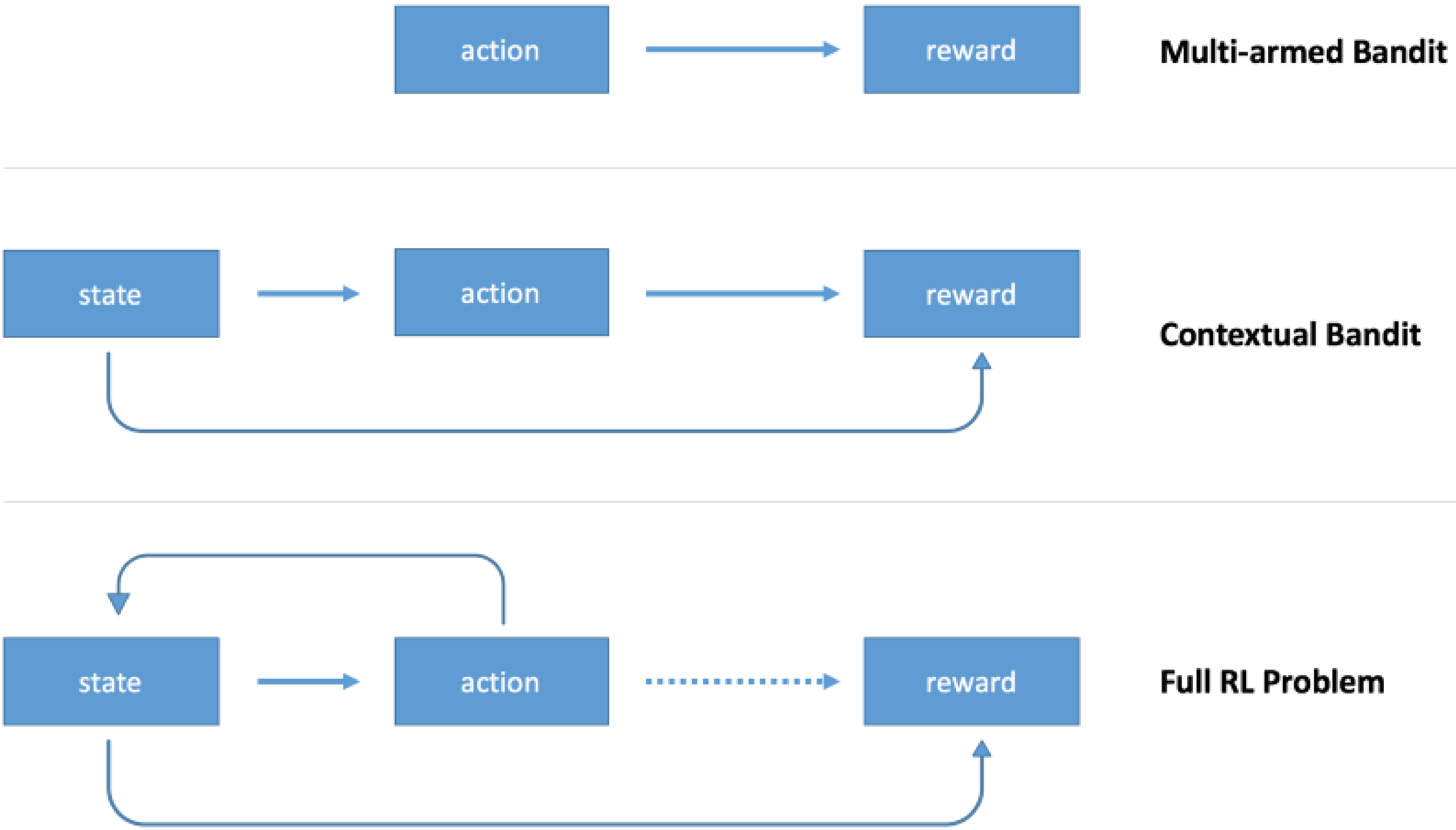
Summary of evaluative feedback methods

- Greedy, ϵ-greedy, softmax, reinforcement comparison, gradient bandit and UCB all have their own advantages and disadvantages depending on the type of problem: stationary or not, high or low reward variance, etc…
- These simple techniques are the most useful ones for bandit-like problems: more sophisticated ones exist, but they either make too restrictive assumptions, or are computationally intractable.
- Take home messages:

  1. RL tries to **estimate values** based on sampled rewards.
  2. One has to balance **exploitation and exploration** throughout learning with the right **action selection scheme**.
  3. Methods exploring more find **better policies**, but are initially slower.

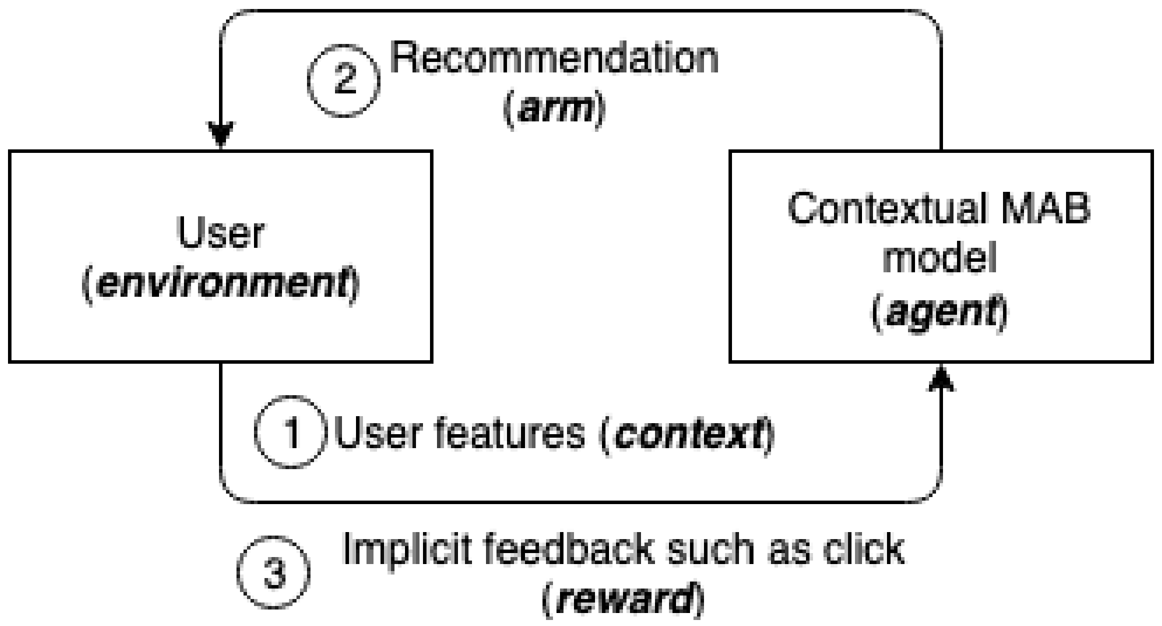
4 - Contextual bandits

Contextual bandits



Source: https://medium.com/emergent-future/simple-reinforcement-learning-with-tensorflow-part-1-5-contextual-bandits-bff01d1aad9c

Contextual bandits



Source: https://aws.amazon.com/blogs/machine-learning/power-contextual-bandits-using-continual-learning-with-amazon-sagemaker-rl/

Recommender systems:

- Actions: advertisements.
- Context: user features / identity.
- Reward: user clicked on the ad.

- In contextual bandits, the obtained rewards do not only depend on the action a, but also on the **state** or **context** s:

$$r_{t+1} \sim r(s, a)$$

- For example, the n-armed bandit could deliver rewards with different probabilities depending on:
  - who plays.
  - the time of the year.
  - the availability of funds in the casino.
- The problem is simply to estimate $Q(s, a)$ instead of $Q(a)$…

- Some efficient algorithms have been developed recently, for example:

> Agarwal, A., Hsu, D., Kale, S., Langford, J., Li, L., and Schapire, R. E. (2014). Taming the Monster: A Fast and Simple Algorithm for Contextual Bandits. in Proceedings of the 31 st International Conference on Machine Learning (Beijing, China), 9. http://proceedings.mlr.press/v32/agarwalb14.pdf