UNIVERSITY OF TECHNOLOGY
IN THE EUROPEAN CAPITAL OF CULTURE
CHEMNITZ

Deep Reinforcement Learning

Sampling and Bandits

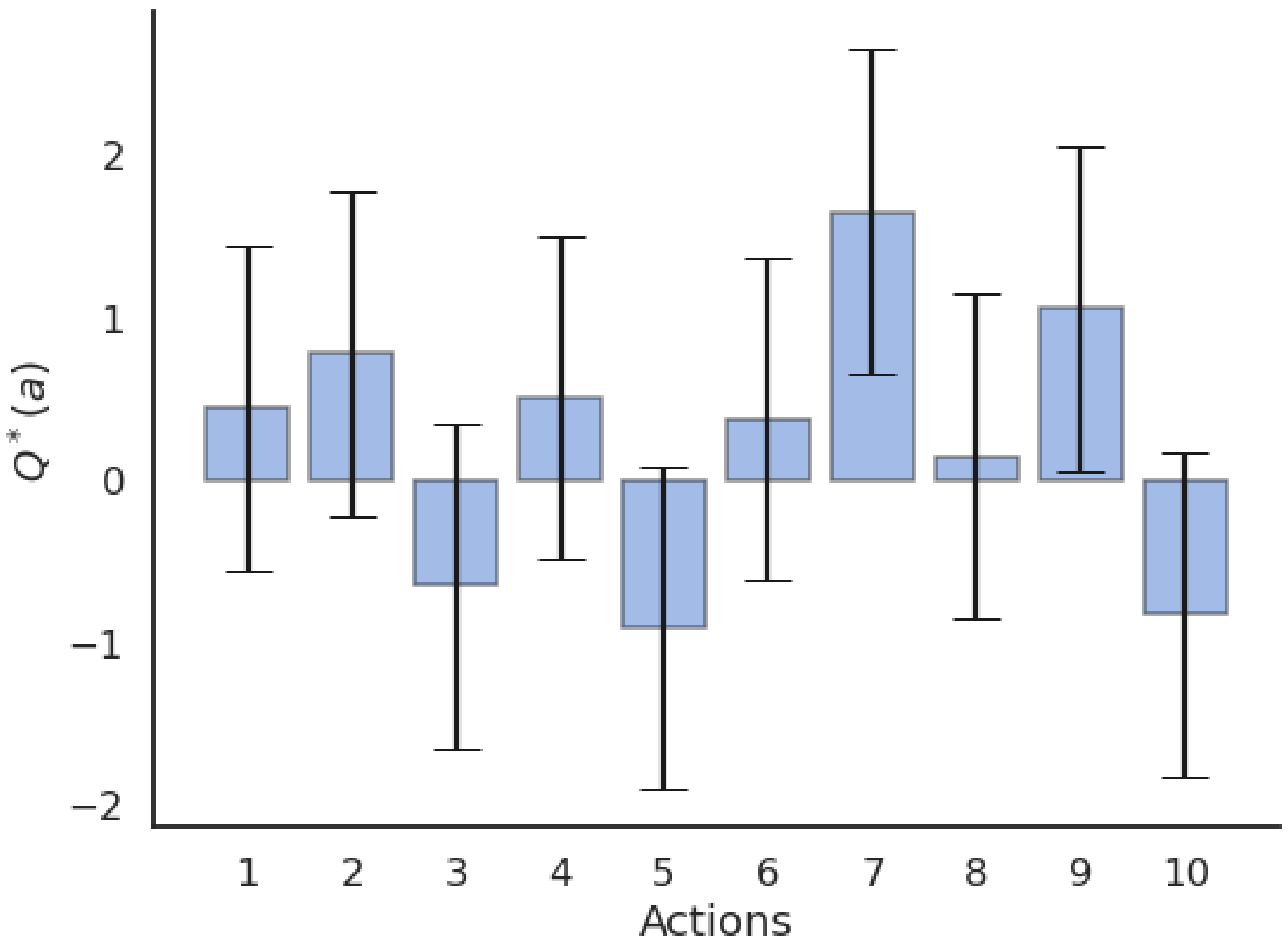
Julien Vitay
Professur für Künstliche Intelligenz - Fakultät für Informatik

1 - n-armed bandits

n-armed bandits

- The **n-armed bandit** (or multi-armed bandit) is the simplest form of learning by trial and error.
- Learning and action selection take place in the same single state.
- The n actions have different reward distributions: the reward varies around a mean value but is not always the same.
- 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 $Q^*(a)$.

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

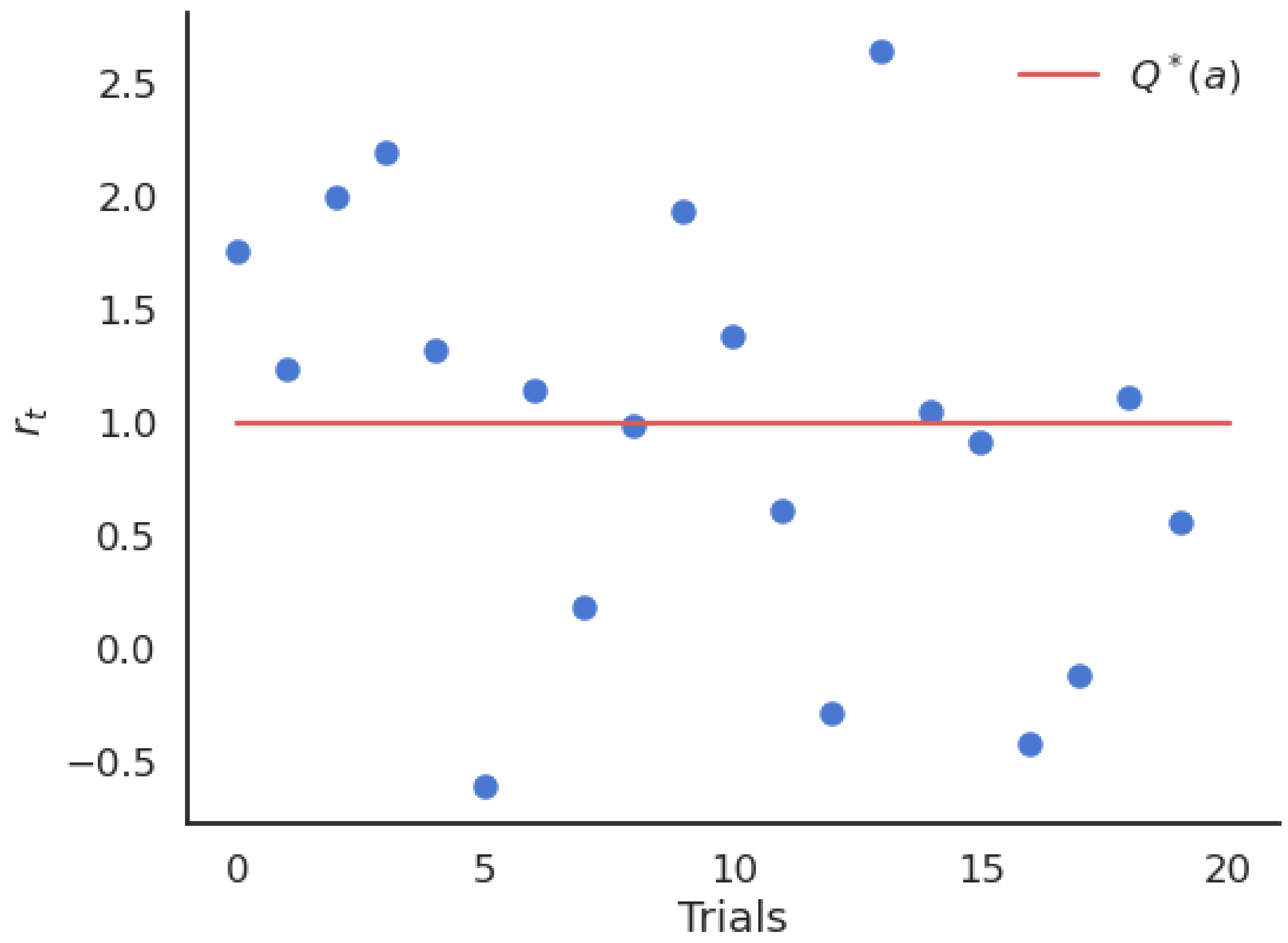
- The reward distribution also has a **variance**: we usually ignore it in RL, as all we care about is the **optimal action** a^* (but see distributional RL later).

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

- 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**).

$$r_t \sim r(a)$$

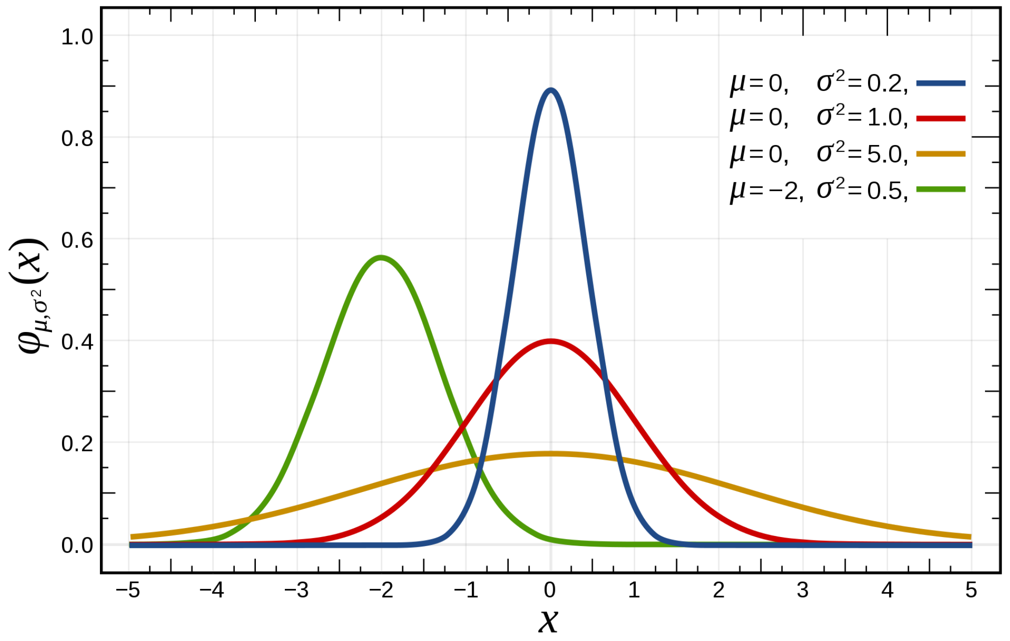
- The received rewards r_t vary around the true value over time.
- We need to build **estimates** $Q_t(a)$ of the value of each action based on the samples.
- These estimates will be very wrong at the beginning, but should get better over time.

2 - Random sampling

Mathematical expectation

- An important metric for a random variable is its **mathematical expectation** or expected value.
- For discrete distributions, it is the “mean” realization / outcome weighted by the corresponding probabilities:

$$\mathbb{E}[X] = \sum_{i=1}^{n} P(X = x_i)\, x_i$$



Source:
https://en.wikipedia.org/wiki/Normal_distribution

- For continuous distributions, one needs to integrate the **probability density function** (pdf) instead of the probabilities:

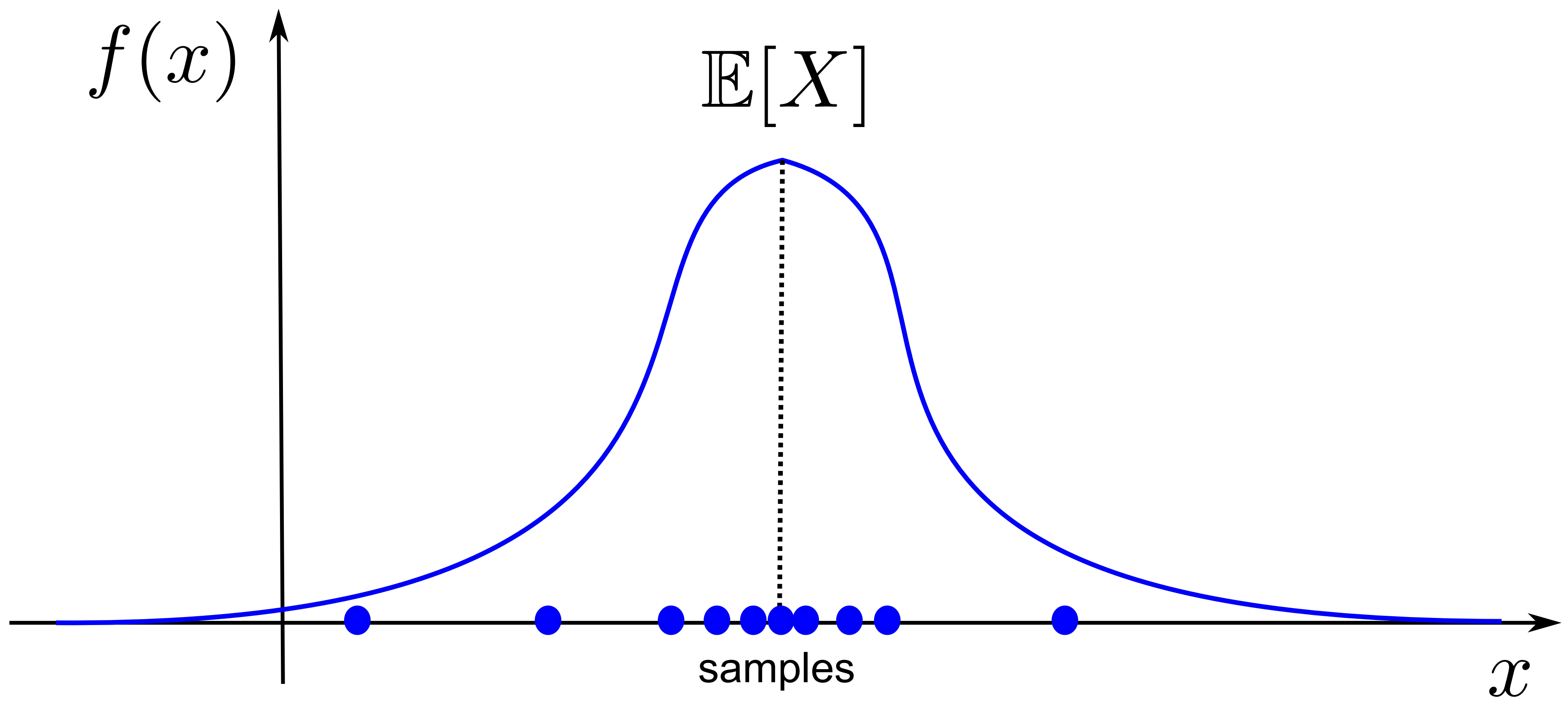
$$\mathbb{E}[X] = \int_{x \in \mathcal{D}_X} f(x)\, x \, dx$$

- One can also compute the expectation of a function of a random variable:

$$\mathbb{E}[g(X)] = \int_{x \in \mathcal{D}_X} f(x)\, g(x)\, dx$$

Random sampling / Monte Carlo sampling

- In ML and RL, we deal with random variables whose exact probability distribution is unknown, but we are interested in their expectation or variance anyway.



- **Random sampling** or **Monte Carlo sampling** (MC) consists of taking N samples x_i out of the distribution X (discrete or continuous) and computing the **sample average**:

$$\mathbb{E}[X] = \mathbb{E}_{x \sim X} [x] \approx \frac{1}{N} \sum_{i=1}^N x_i$$

- More samples will be obtained where $f(x)$ is high (x is probable), so the average of the sampled data will be close to the expected value of the distribution.

Random sampling / Monte Carlo sampling

Law of big numbers

> As the number of identically distributed, randomly generated variables increases, their sample mean (average) approaches their theoretical mean.

- MC estimates are only correct when:
    - the samples are **i.i.d** (independent and identically distributed):
        - independent: the samples must be unrelated with each other.
        - identically distributed: the samples must come from the same distribution X.
    - the number of samples is large enough.

Monte Carlo sampling

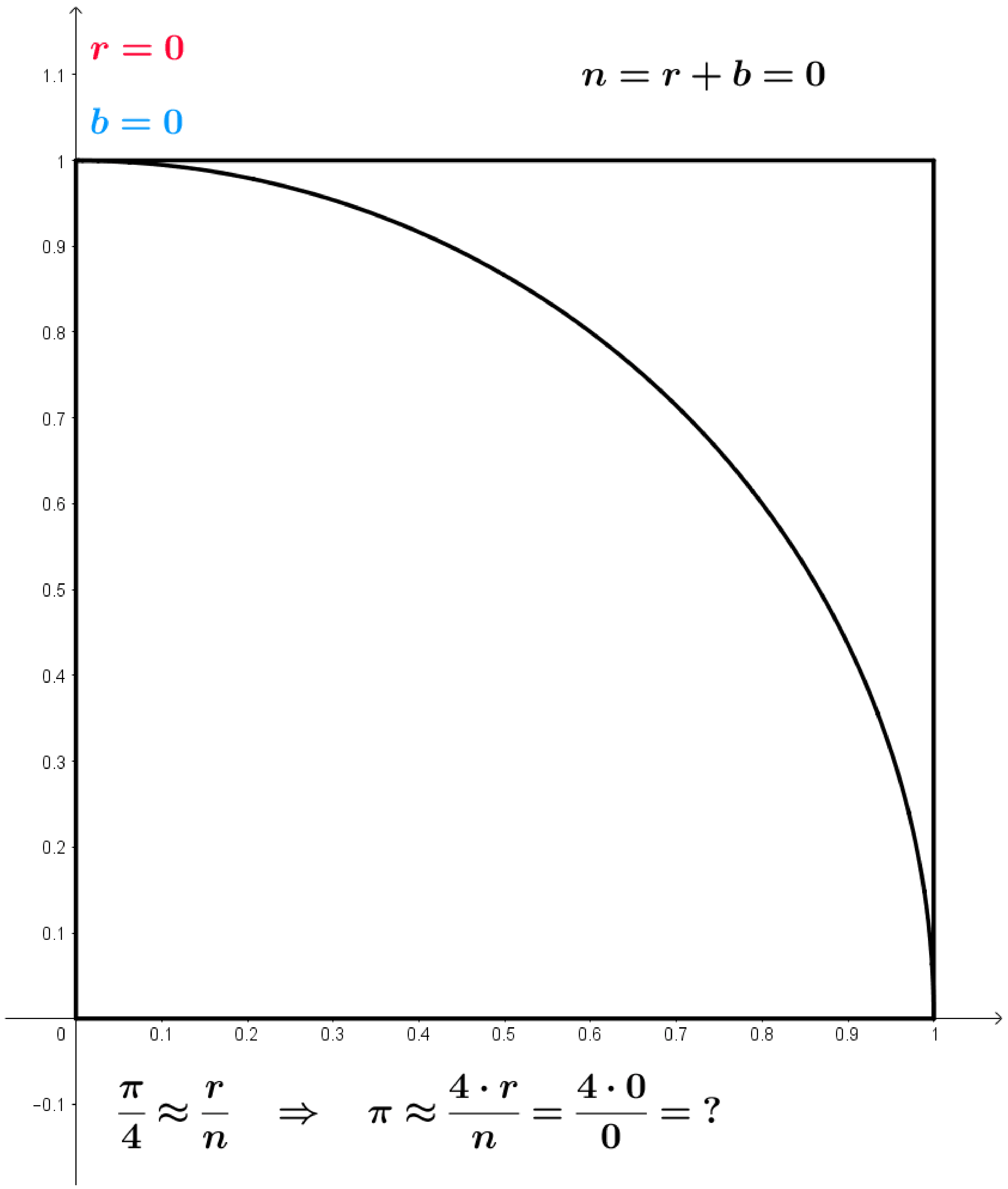
- One can estimate any function of the random variable with random sampling:

$$\mathbb{E}[f(X)] = \mathbb{E}_{x \sim X}[f(x)] \approx \frac{1}{N} \sum_{i=1}^{N} f(x_i)$$

- Example of Monte Carlo sampling to estimate $\pi/4$:

1. Sample a 2D point $\mathbf{x}_i$ inside the unit square using the uniform distribution $\mathcal{U}(0, 1)$.
2. The point is inside the circle ($||\mathbf{x}_i|| \leq 1$) with a probability $\dfrac{\pi}{4}$.
3. Update the estimation of π:

$$\pi \approx 4 \, \frac{\text{number of red points}}{\text{total number of points}}$$



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Central limit theorem

- Suppose we have an unknown distribution X with expected value $\mu = \mathbb{E}[X]$ and variance σ^2.
- We can take randomly N samples from X to compute the sample average:

$$S_N = \frac{1}{N} \sum_{i=1}^{N} x_i$$

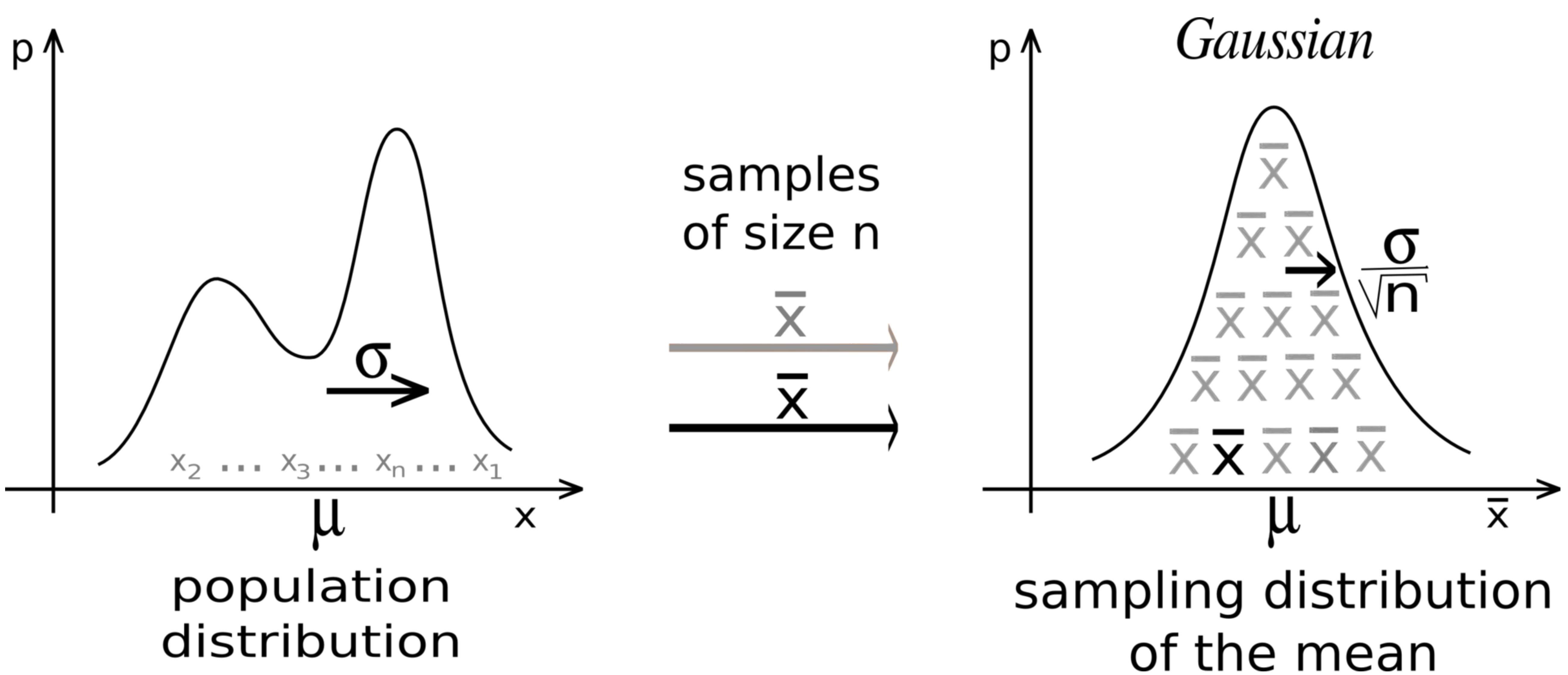
- The **Central Limit Theorem** (CLT) states that:

> The distribution of sample averages is normally distributed with mean μ and variance $\frac{\sigma^2}{N}$.

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

Central limit theorem

- If we perform the sampling multiple times, even with few samples, the average of the sampling averages will be very close to the expected value.
- The more samples we get, the smaller the variance of the estimates.
- Although the distribution X can be anything, the sampling averages are normally distributed.



Source:: https://en.wikipedia.org/wiki/Central_limit_theorem

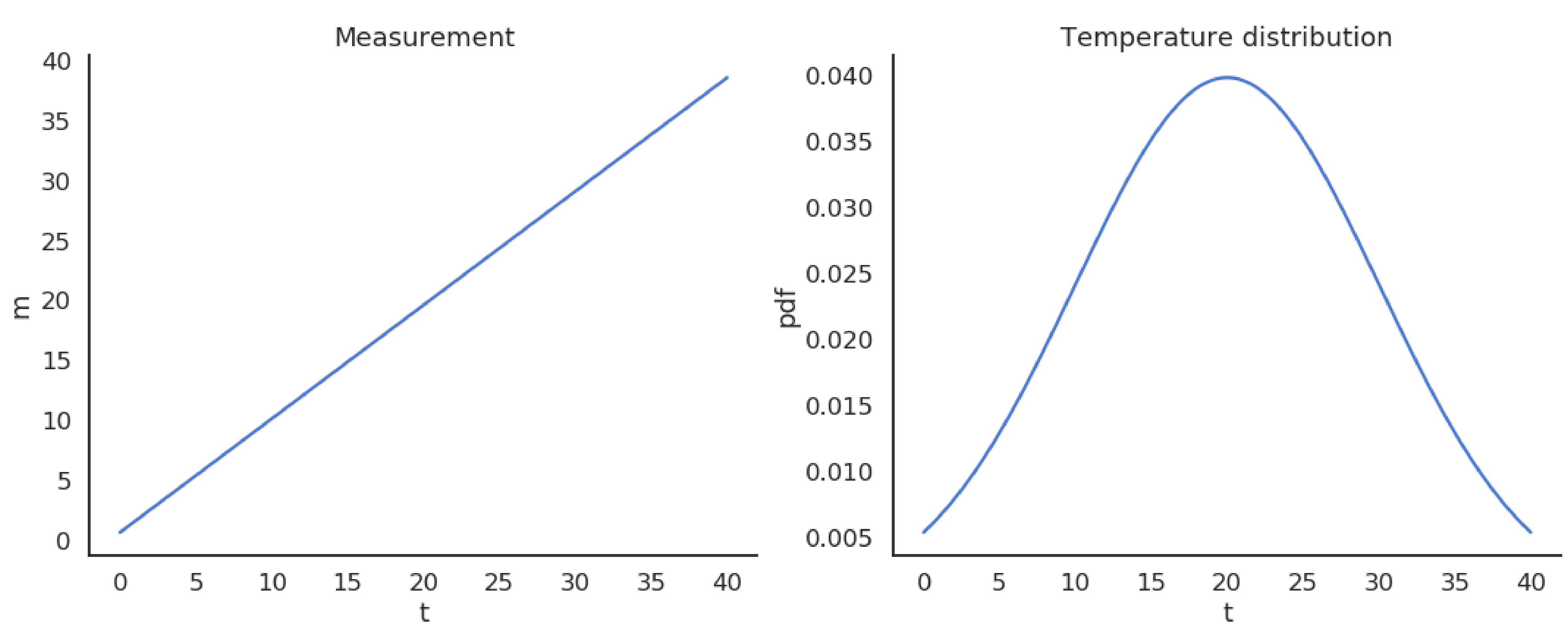
Estimators

- CLT shows that the sampling average is an **unbiased estimator** of the expected value of a distribution:

$$\mathbb{E}(S_N) = \mathbb{E}(X)$$

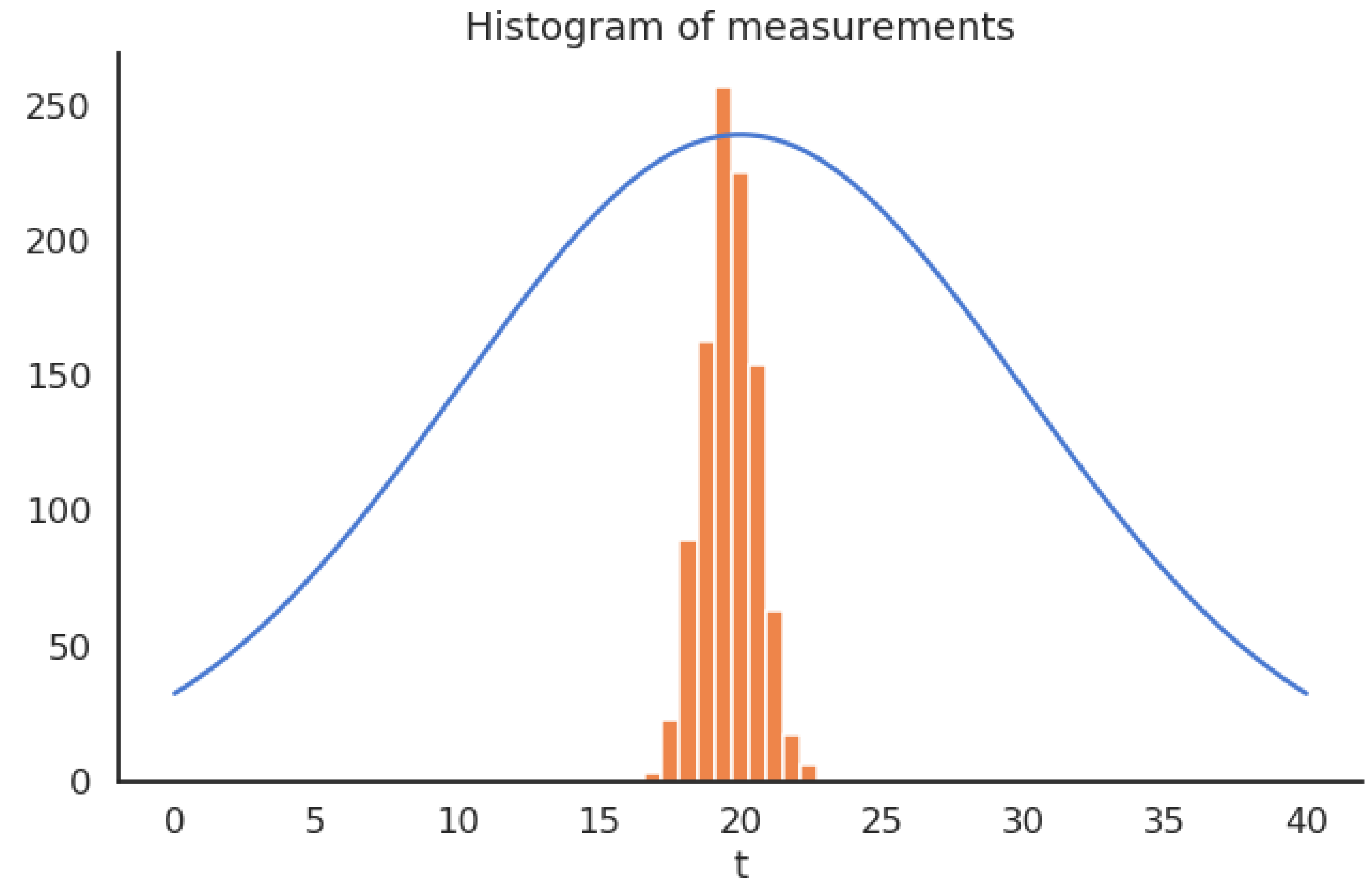
- An estimator is a random variable used to measure parameters of a distribution (e.g. its expectation). The problem is that estimators can generally be **biased**.
- Take the example of a thermometer M measuring the temperature T. T is a random variable (normally distributed with $\mu = 20$ and $\sigma = 10$) and the measurements M relate to the temperature with the relation:

$$M = 0.95\,T + 0.65$$



Estimators

- The thermometer is not perfect, but do random measurements allow us to estimate the expected value of the temperature?
- We could repeatedly take 100 random samples of the thermometer and see how the distribution of sample averages look like:



- But, as the expectation is linear, we actually have:

$$\mathbb{E}[M] = \mathbb{E}[0.95\,T + 0.65] = 0.95\,\mathbb{E}[T] + 0.65 = 19.65 \neq \mathbb{E}[T]$$

- The thermometer is a **biased estimator** of the temperature.

Estimators

- Let’s note θ a parameter of a probability distribution X that we want to estimate (it does not have to be its mean).
- An **estimator** $\hat{\theta}$ is a random variable mapping the sample space of X to a set of sample estimates.
- The **bias** of an estimator is the mean error made by the estimator:

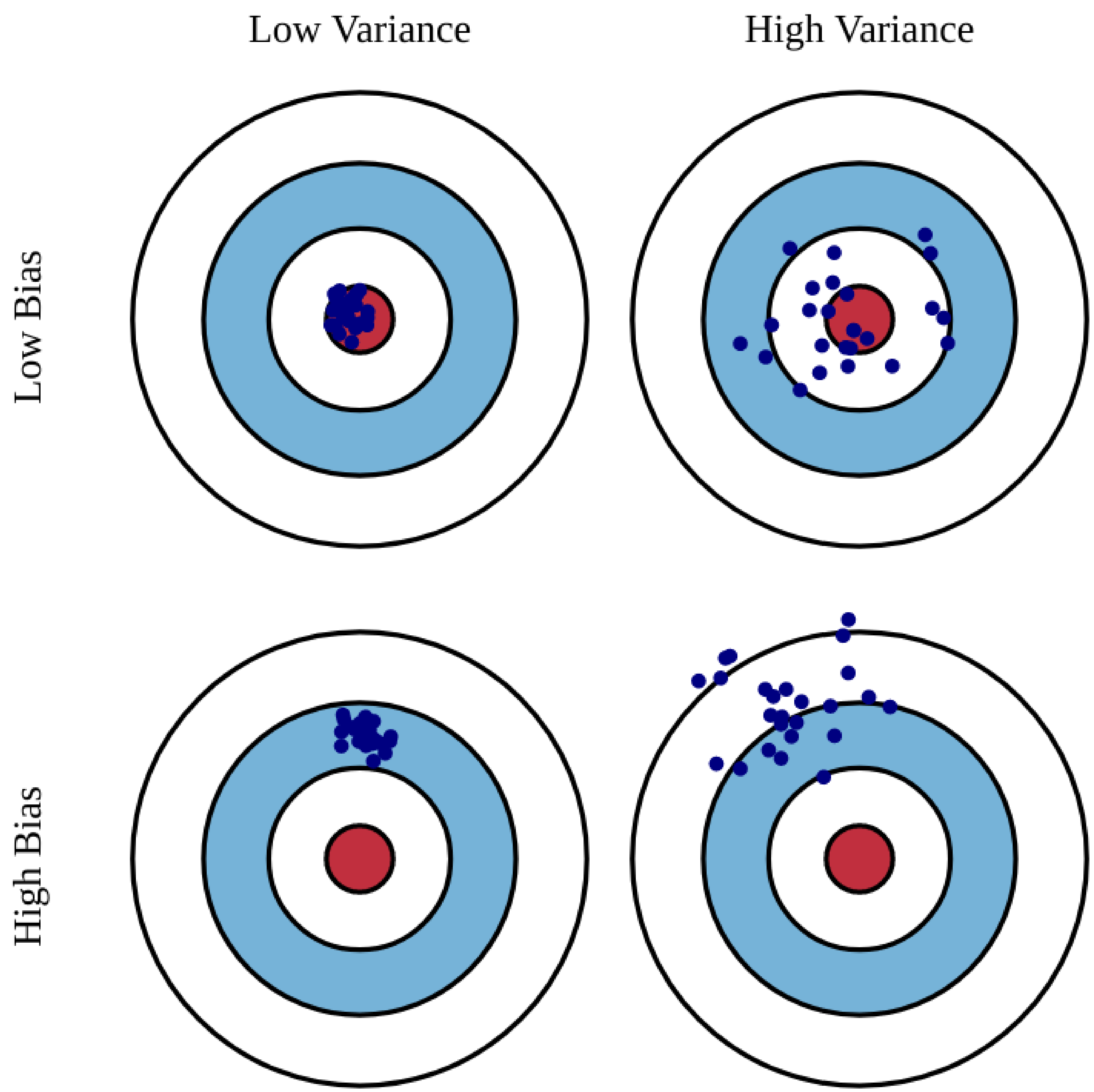
$$\mathcal{B}(\hat{\theta}) = \mathbb{E}[\hat{\theta} - \theta] = \mathbb{E}[\hat{\theta}] - \theta$$

- The **variance** of an estimator is the deviation of the samples around the expected value:

$$\text{Var}(\hat{\theta}) = \mathbb{E}[(\hat{\theta} - \mathbb{E}[\hat{\theta}])^2]$$

- Ideally, we would like estimators with:
  - **low bias**: the estimations are correct on average (= equal to the true parameter).
  - **low variance**: we do not need many estimates to get a correct estimate (CLT: $\frac{\sigma}{\sqrt{N}}$)

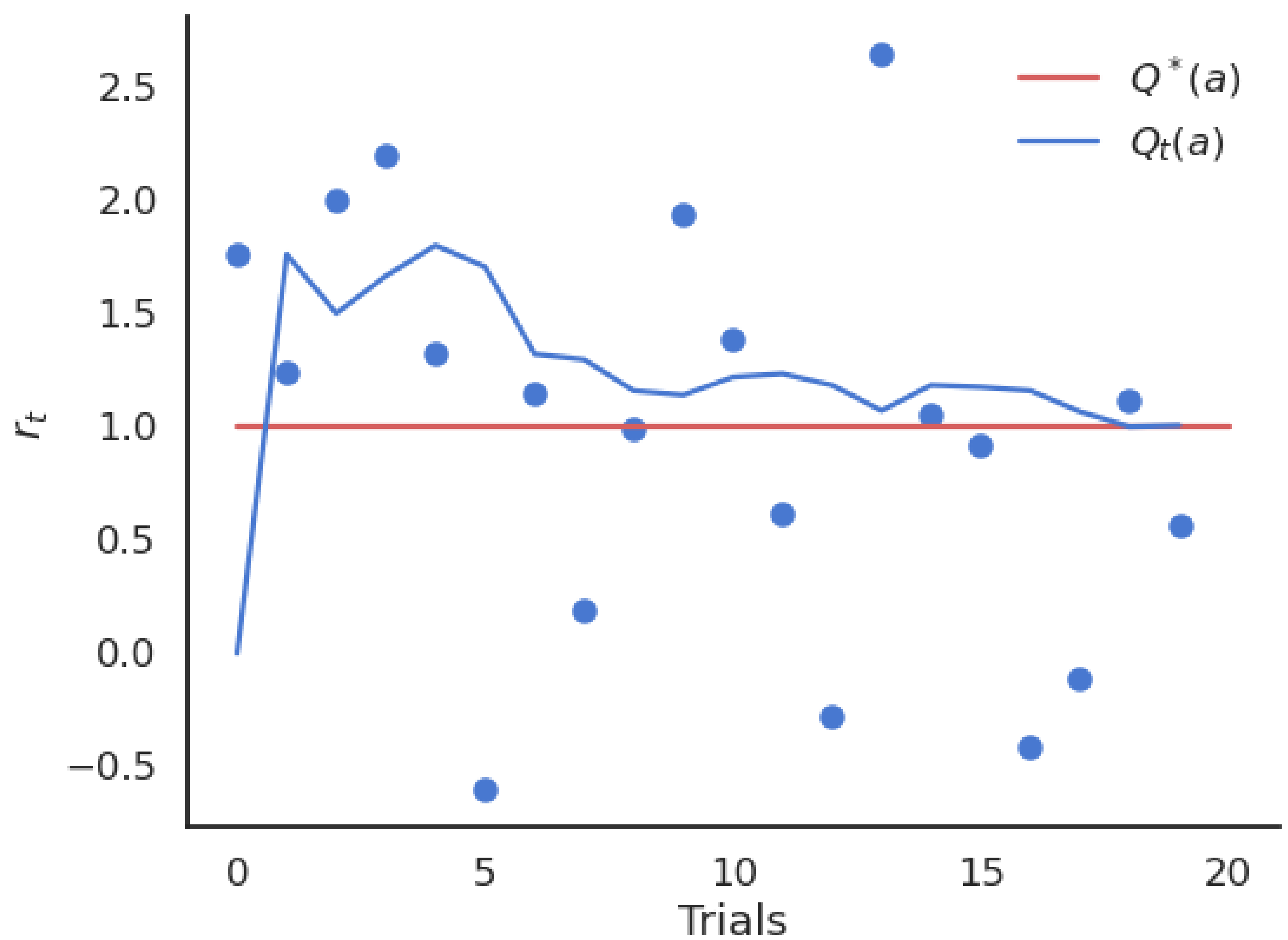
Estimators: bias and variance



- Unfortunately, the perfect estimator does not exist.
- Estimators will have a bias and a variance:
  - **Bias**: the estimated values will be wrong, and the policy not optimal.
  - **Variance**: we will need a lot of samples (trial and error) to have correct estimates.
- One usually talks of a **bias/variance** trade-off: if you have a small bias, you will have a high variance, or vice versa.
- In machine learning, bias corresponds to underfitting, variance to overfitting.

3 - 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

$$(r_1, r_2, ..., r_t)$$

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

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

- 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:

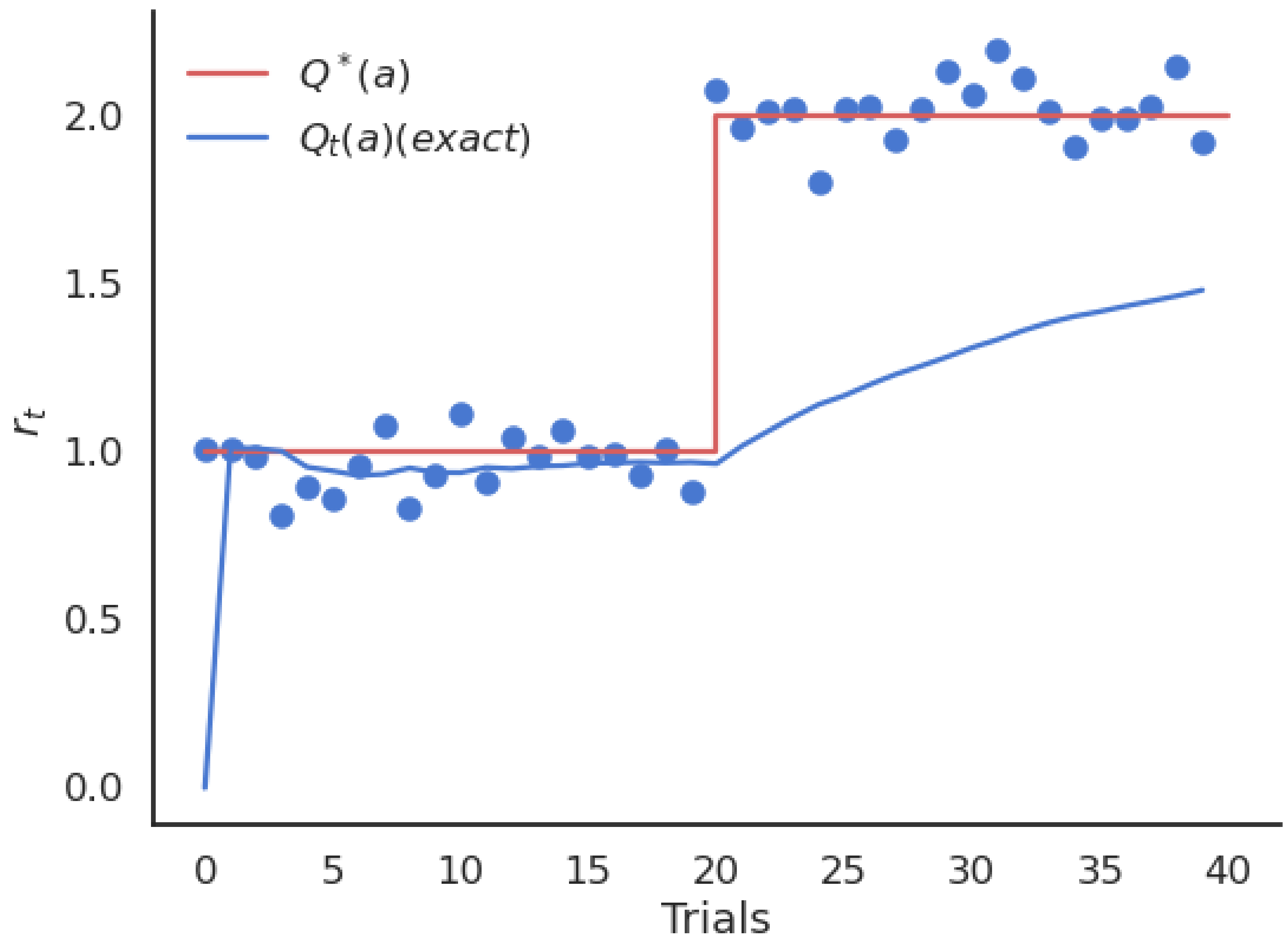
$$\begin{aligned}
Q_{t+1}(a) &= \frac{1}{t+1} \sum_{i=1}^{t+1} r_i = \frac{1}{t+1} \, (r_{t+1} + \sum_{i=1}^{t} r_i) \\
&= \frac{1}{t+1} \, (r_{t+1} + t \, Q_t(a)) \\
&= \frac{1}{t+1} \, (r_{t+1} + (t+1) \, Q_t(a) - Q_t(a))
\end{aligned}$$

- 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.



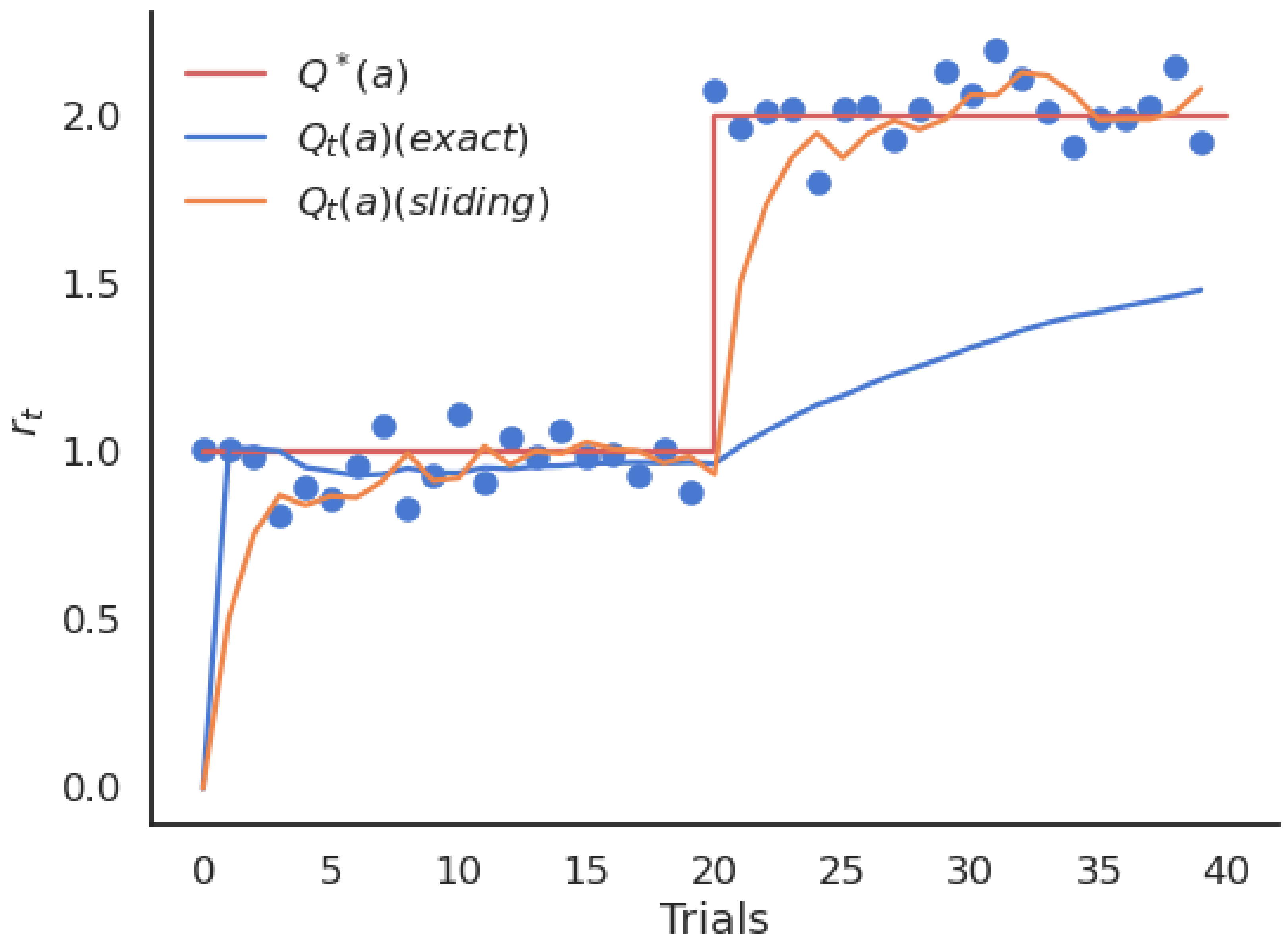
Online evaluation

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

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

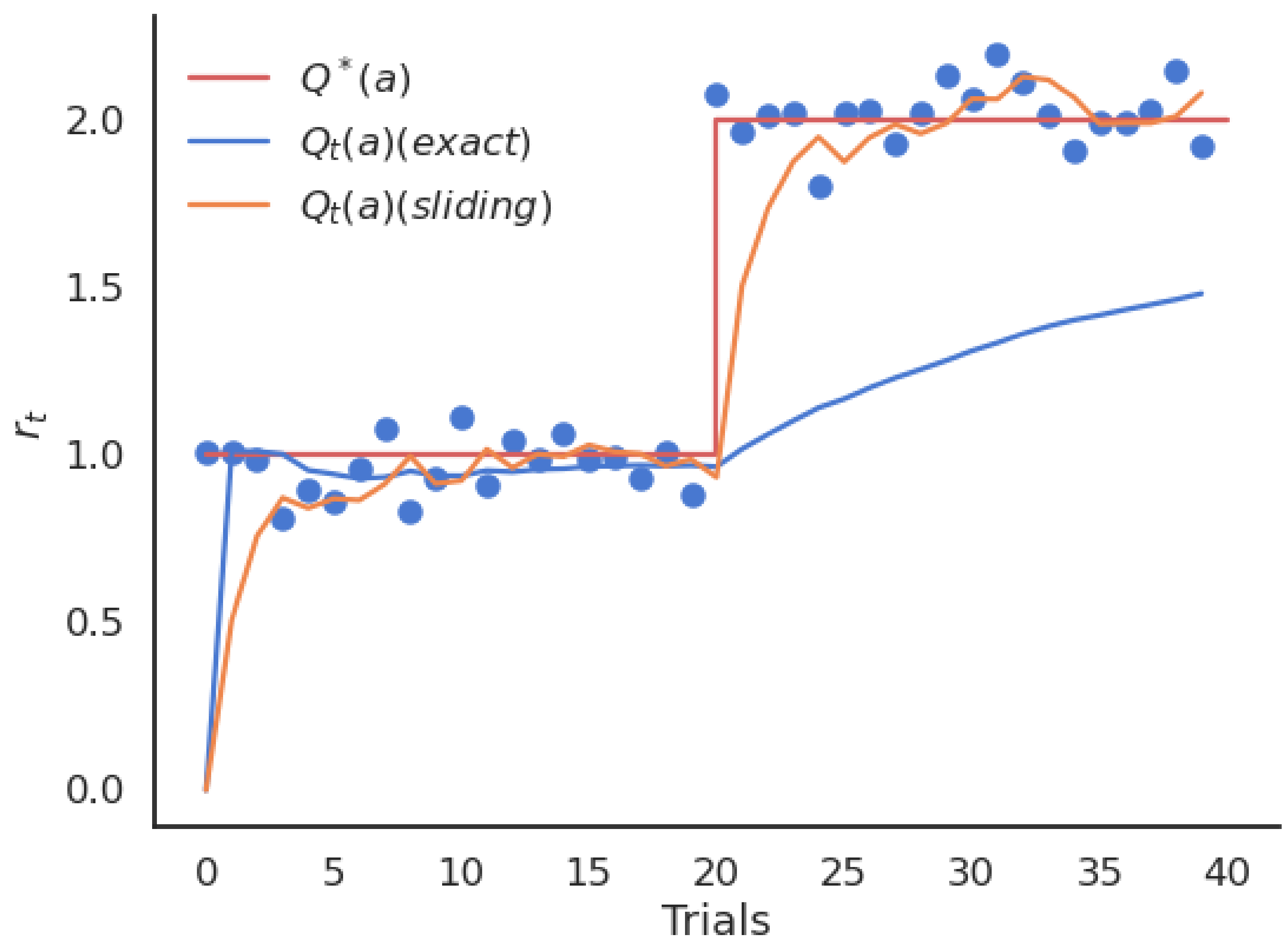
- Equivalent formulation:

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



- The computed value is called an **exponentially 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:

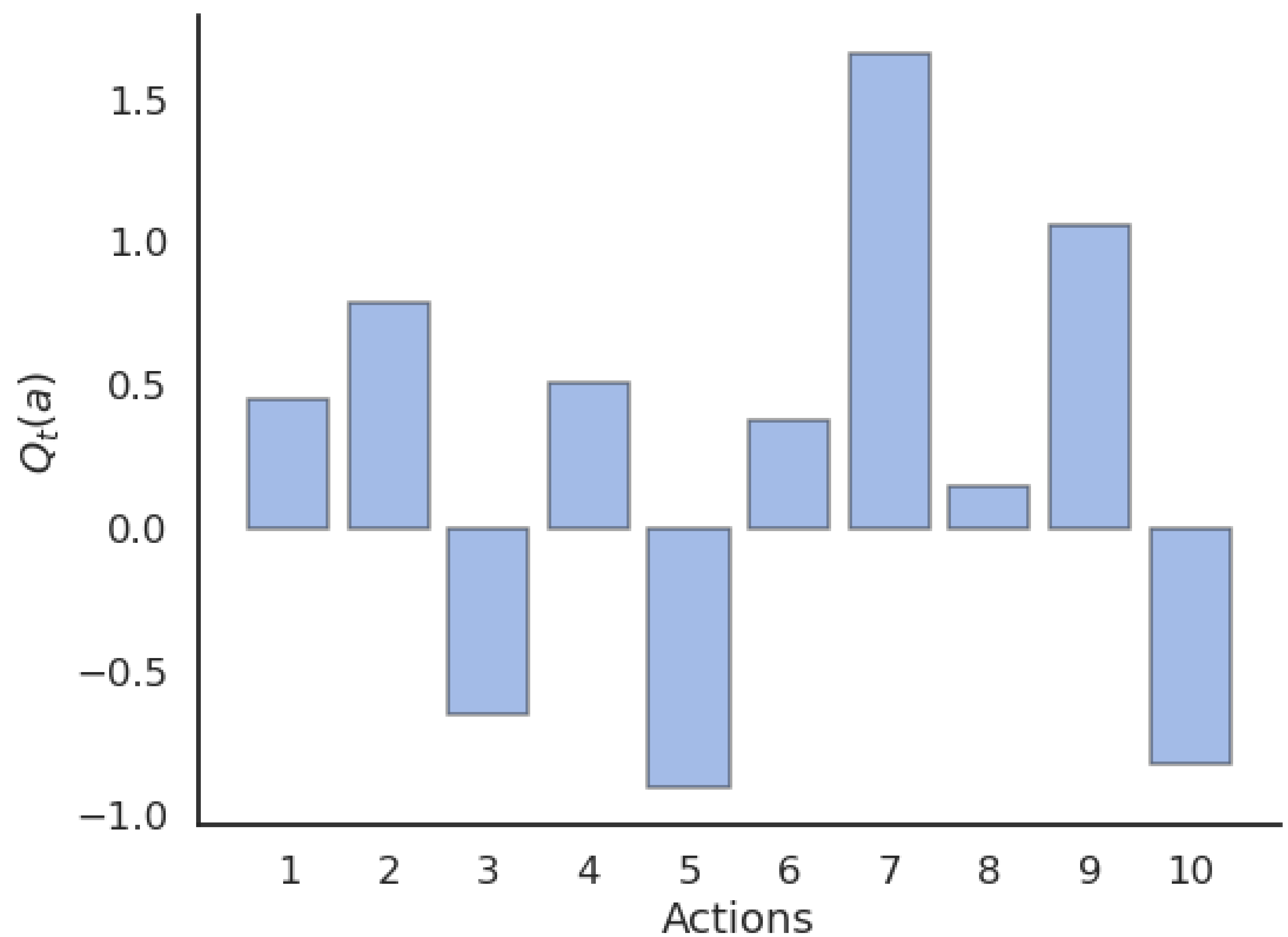
$$\text{new estimate} = \text{current estimate} + \alpha \, (\text{target} - \text{current estimate})$$

- 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.

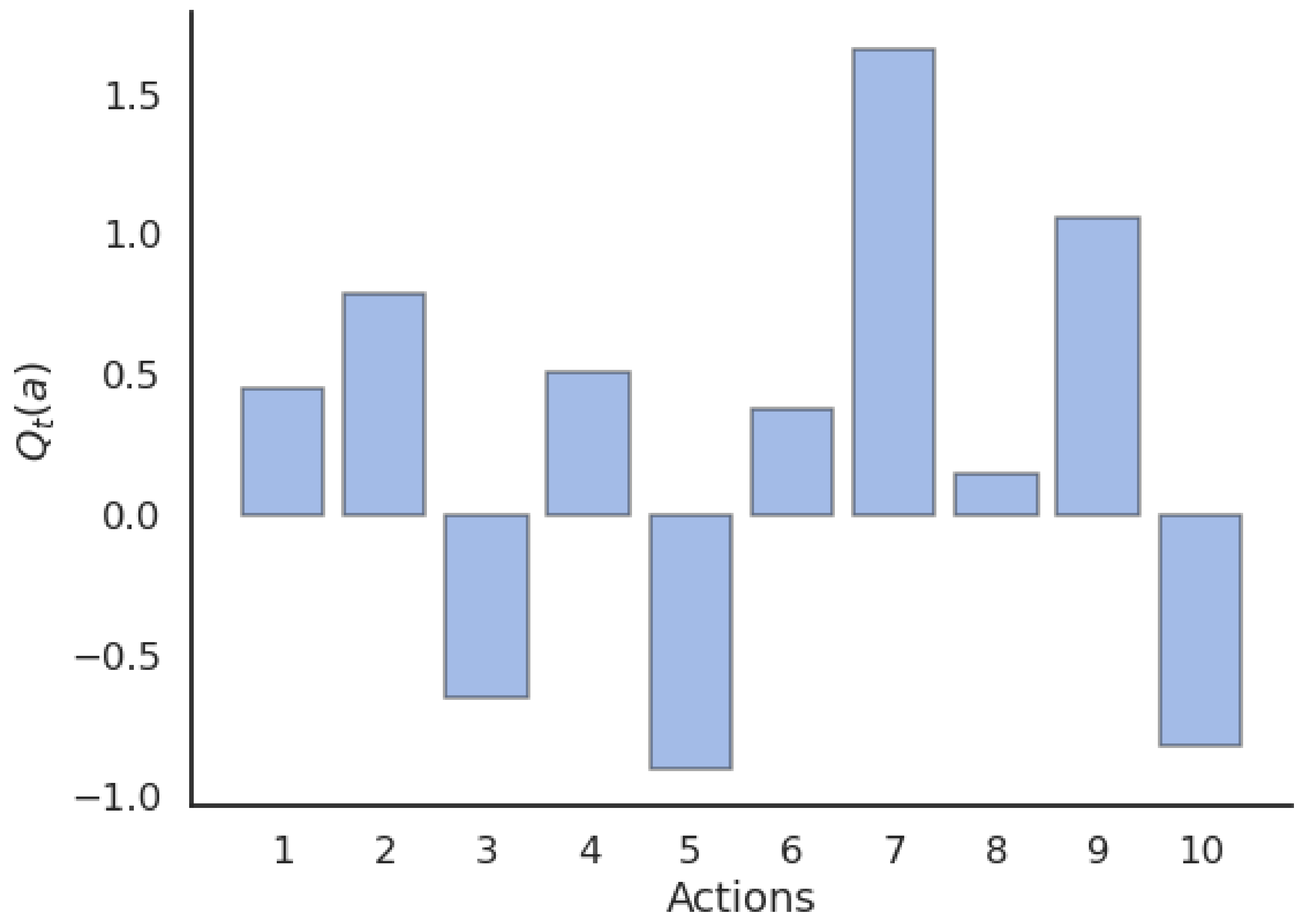


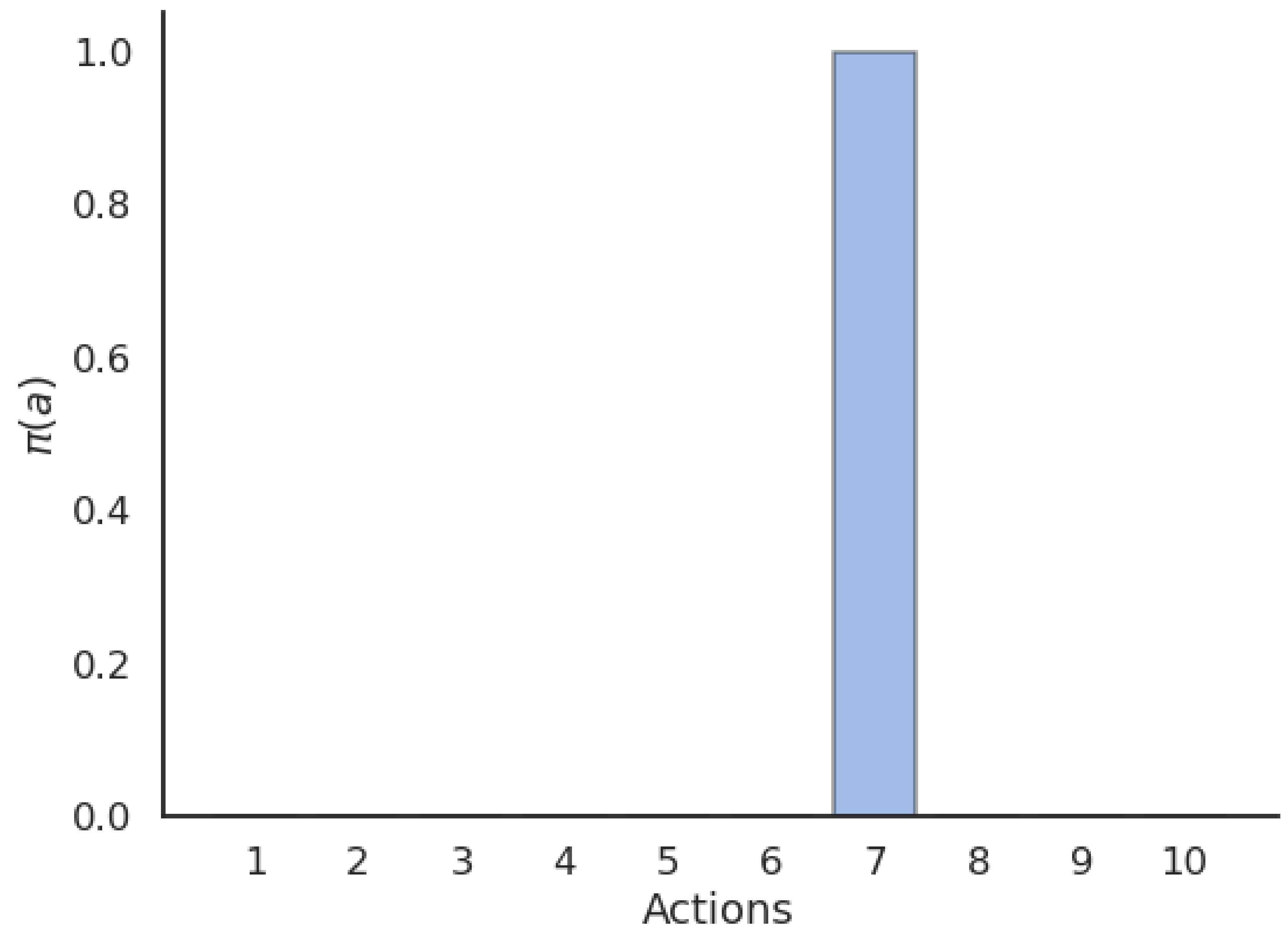
Greedy action selection

- 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**.



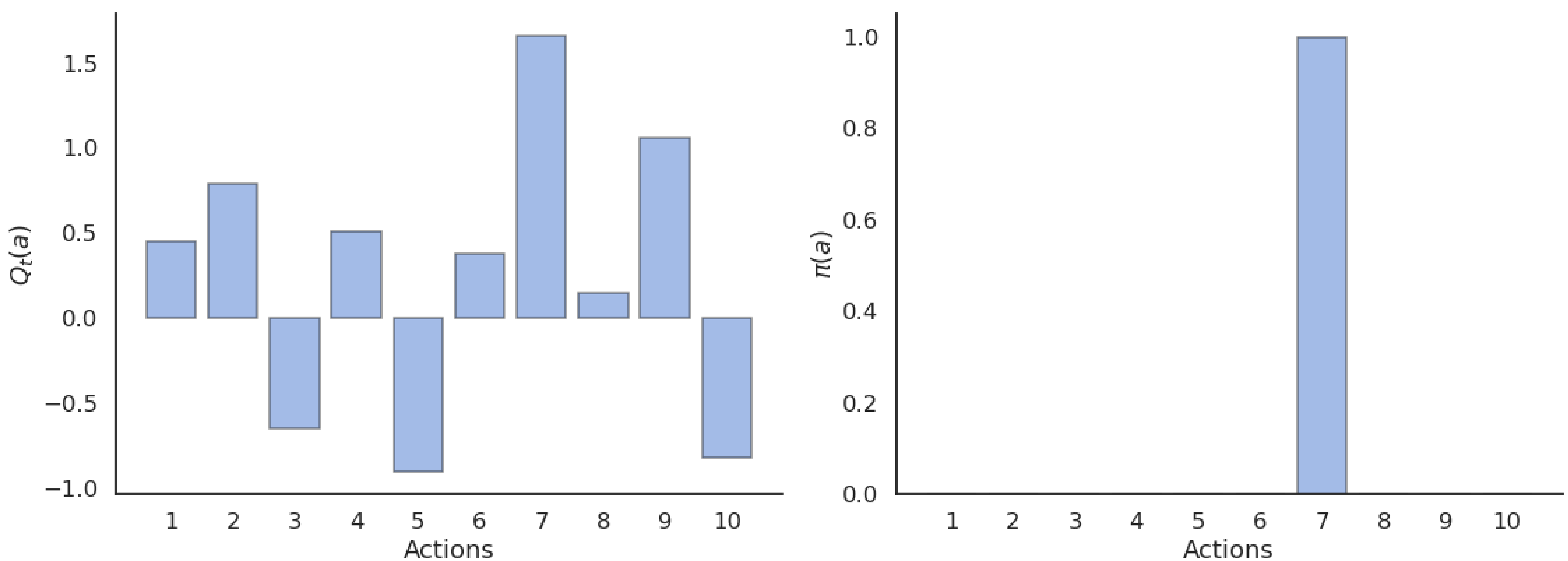


Greedy action selection

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

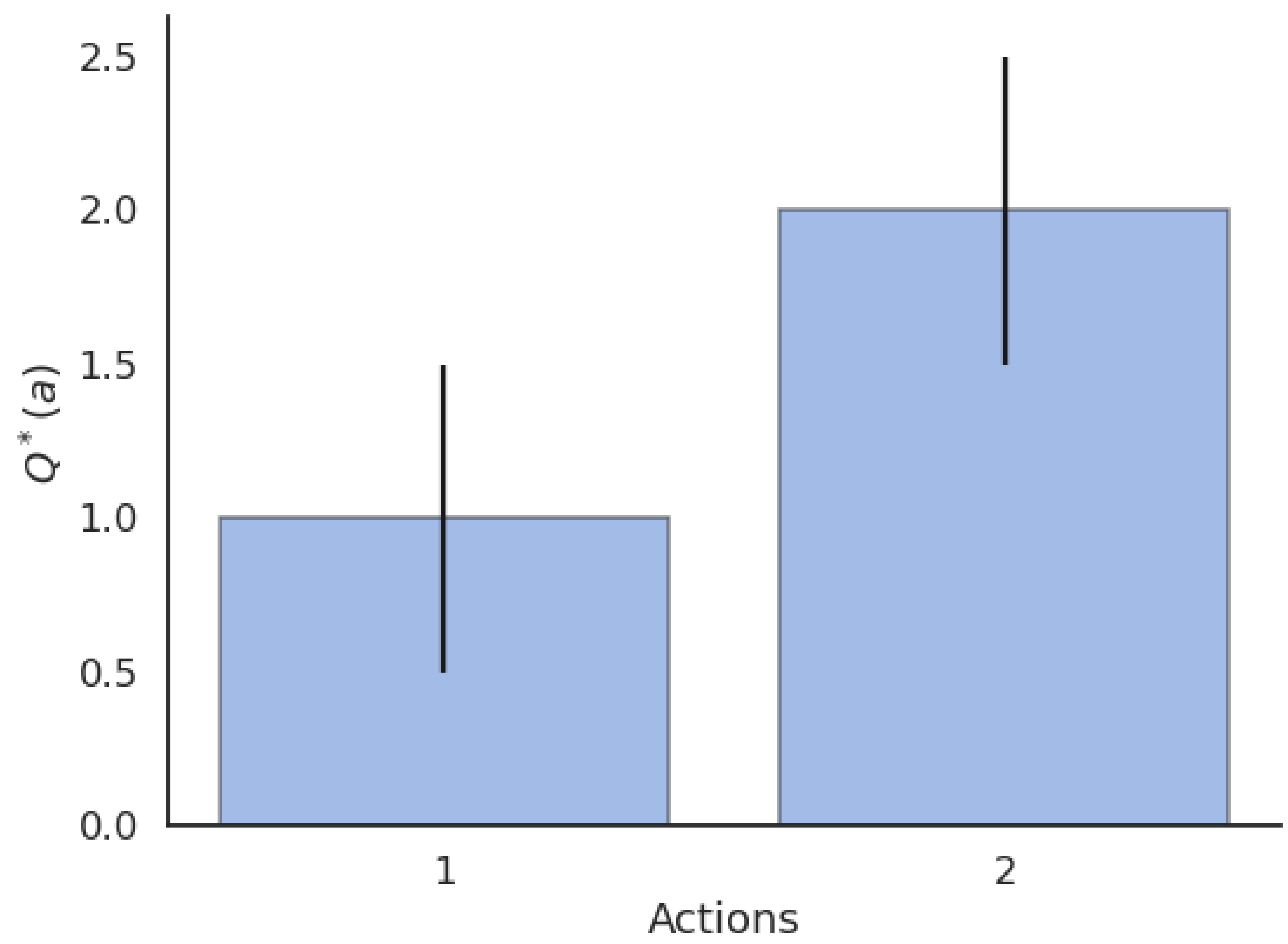
$$\pi(a) = \begin{cases} 1 \text{ if } a = a_t^* \\ 0 \text{ otherwise.} \end{cases}$$

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



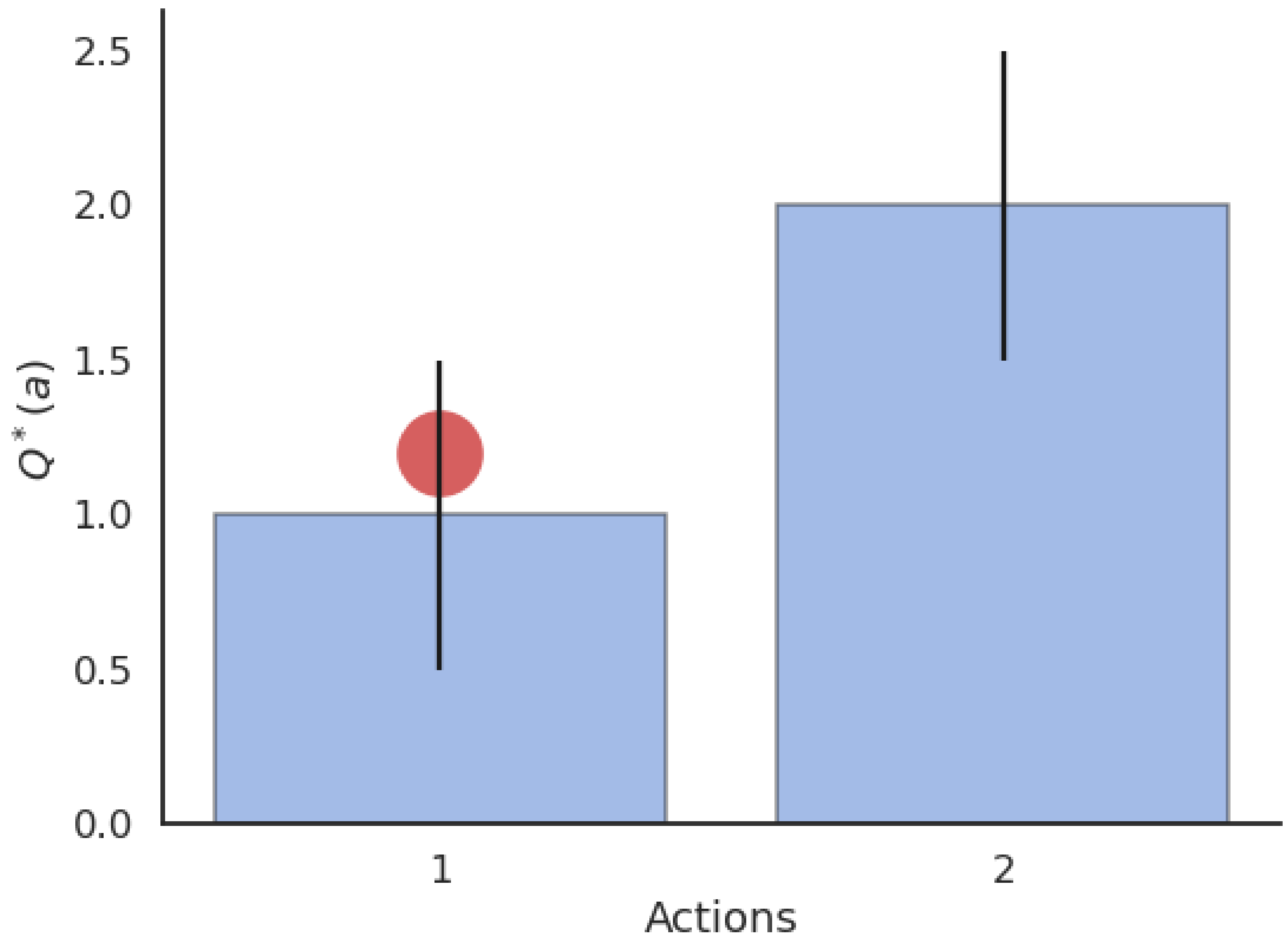
Problem with greedy action selection

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



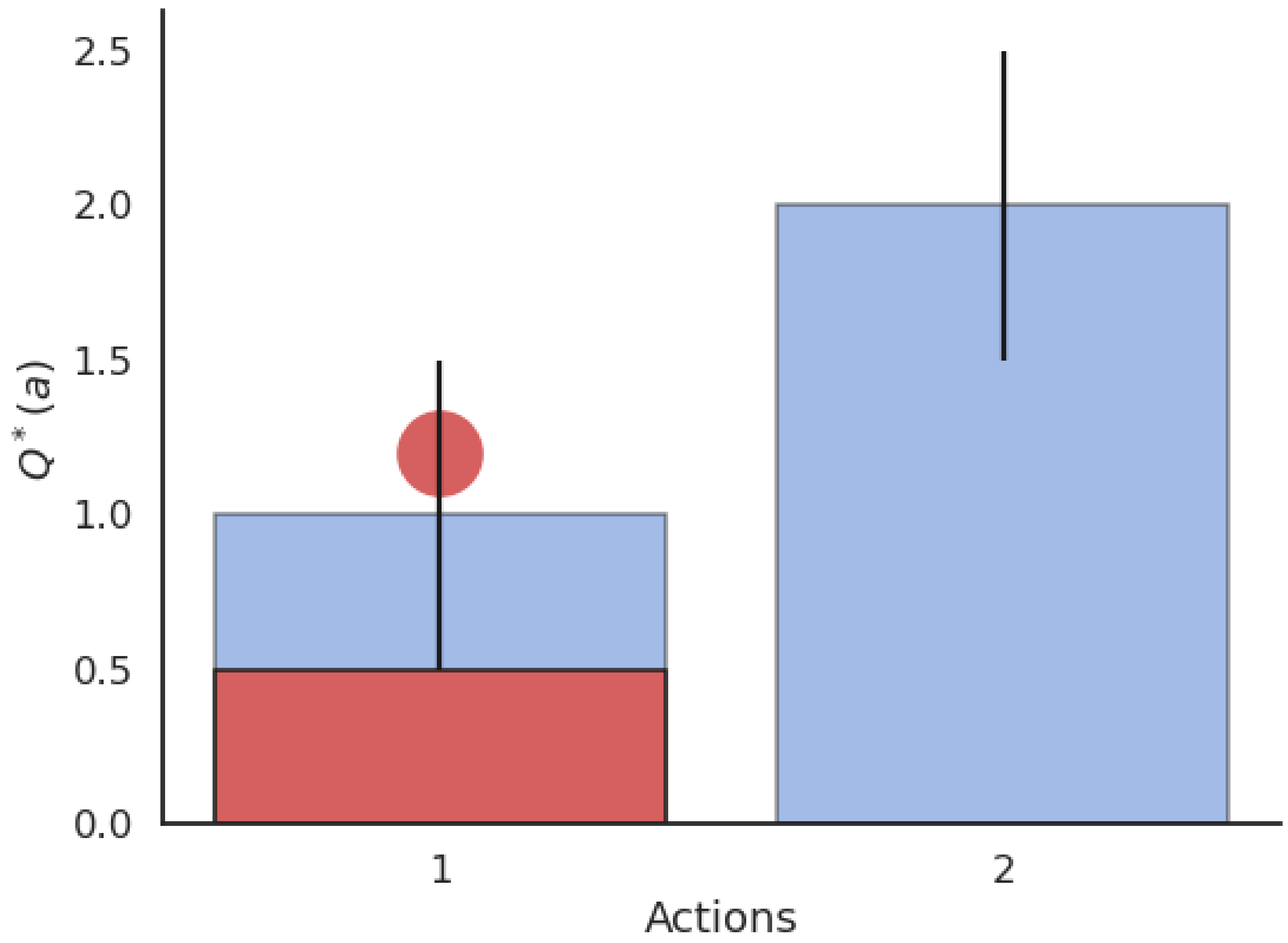
Problem with greedy action selection

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



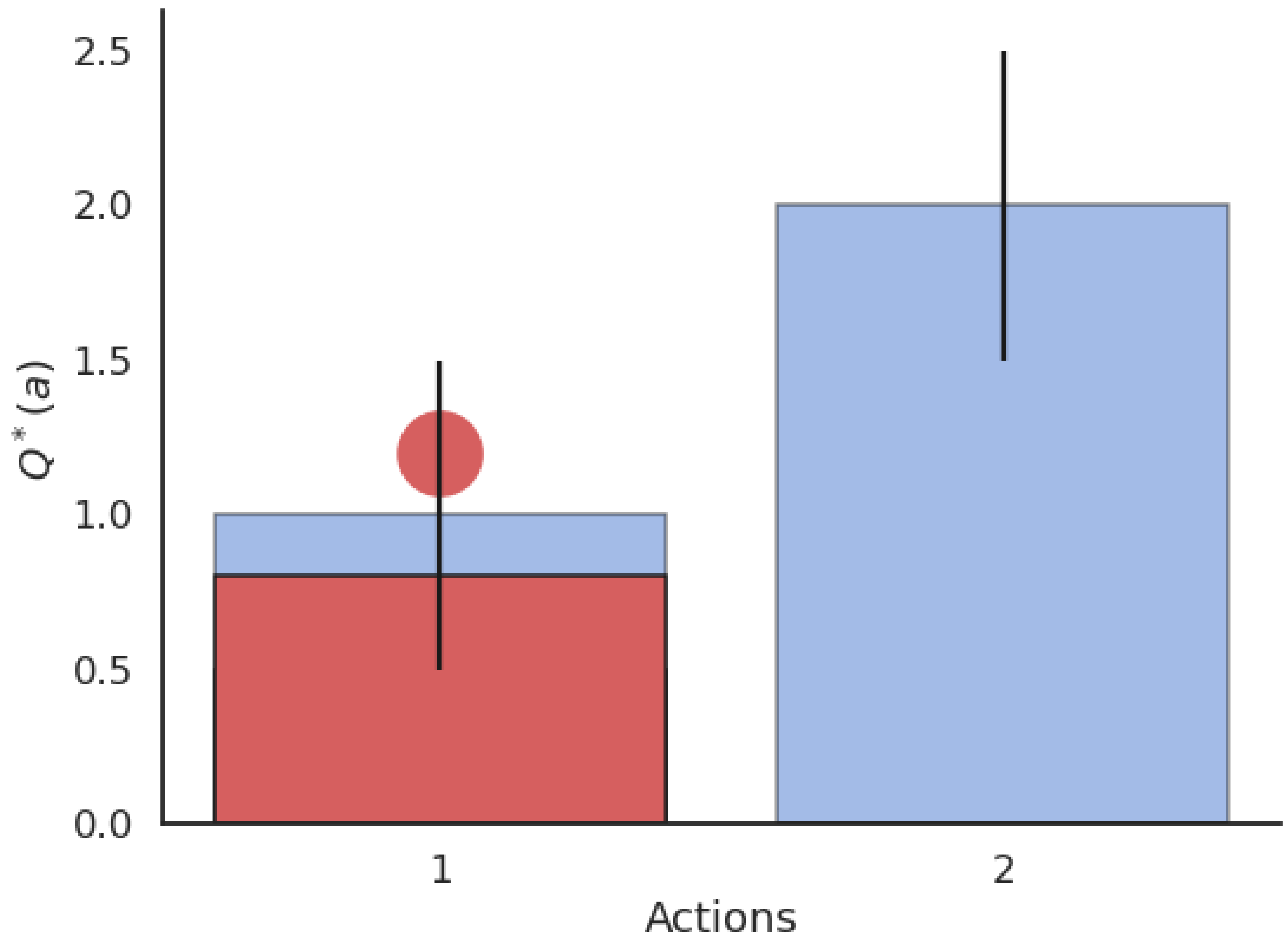
Problem with greedy action selection

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



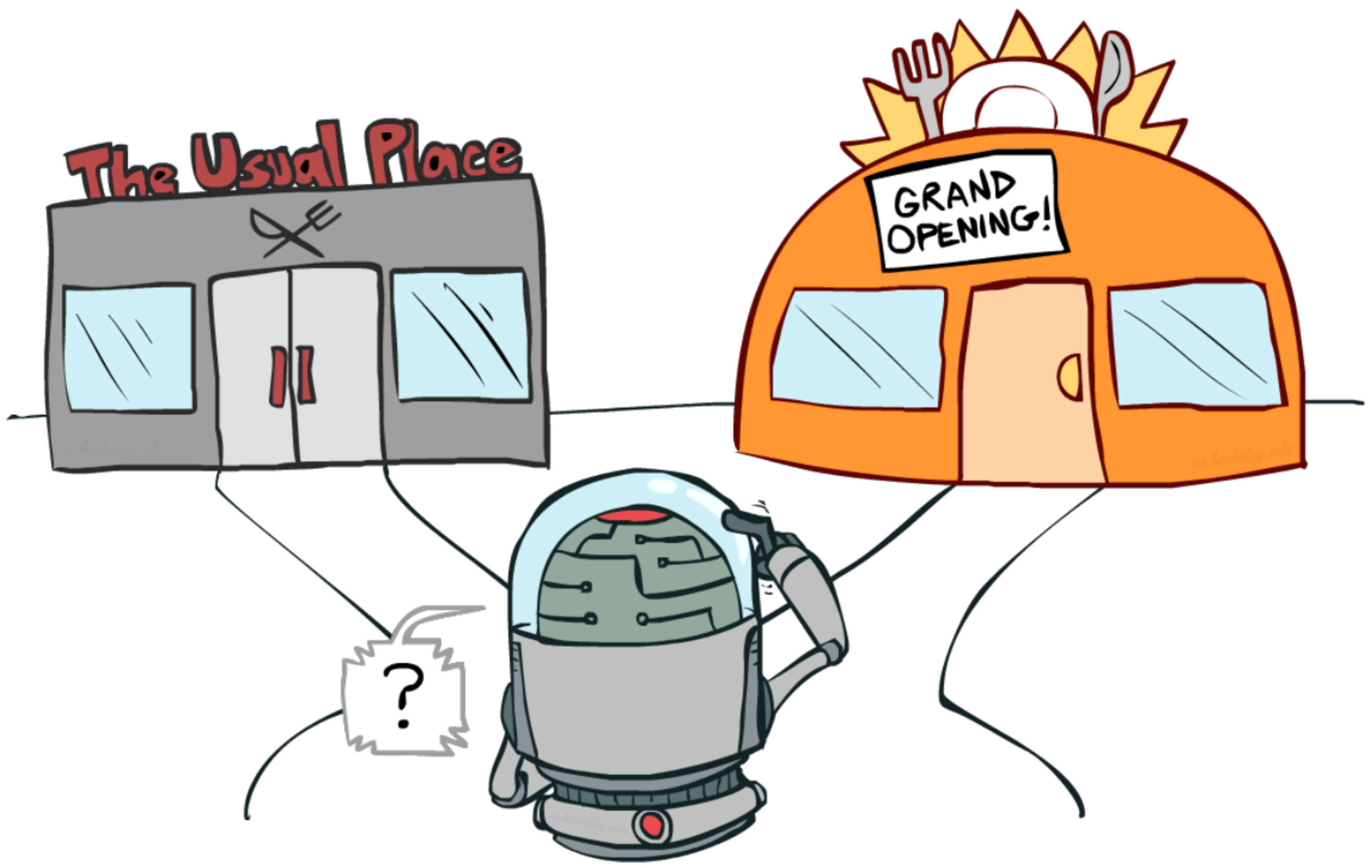
Problem with greedy action selection

- 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.

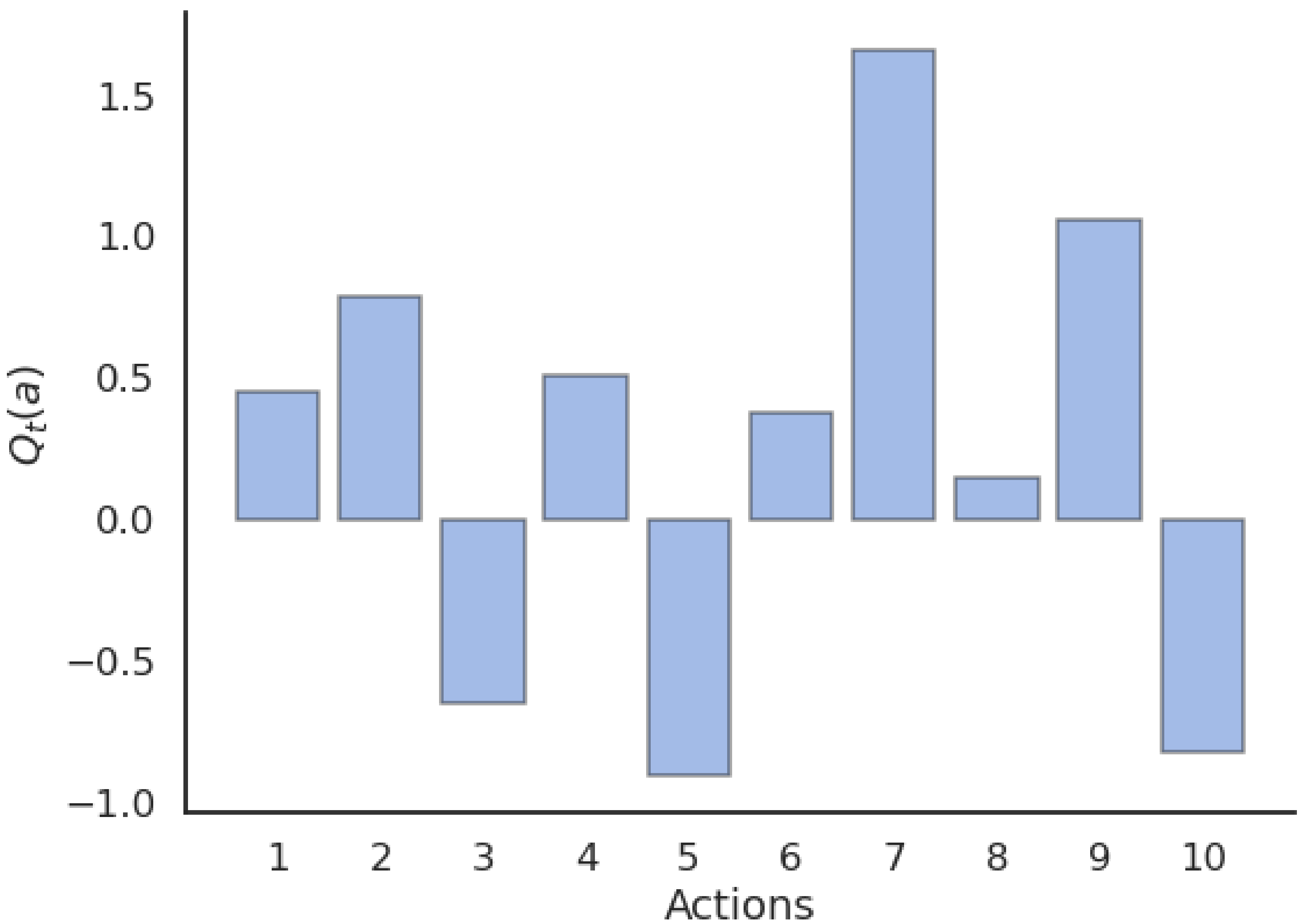


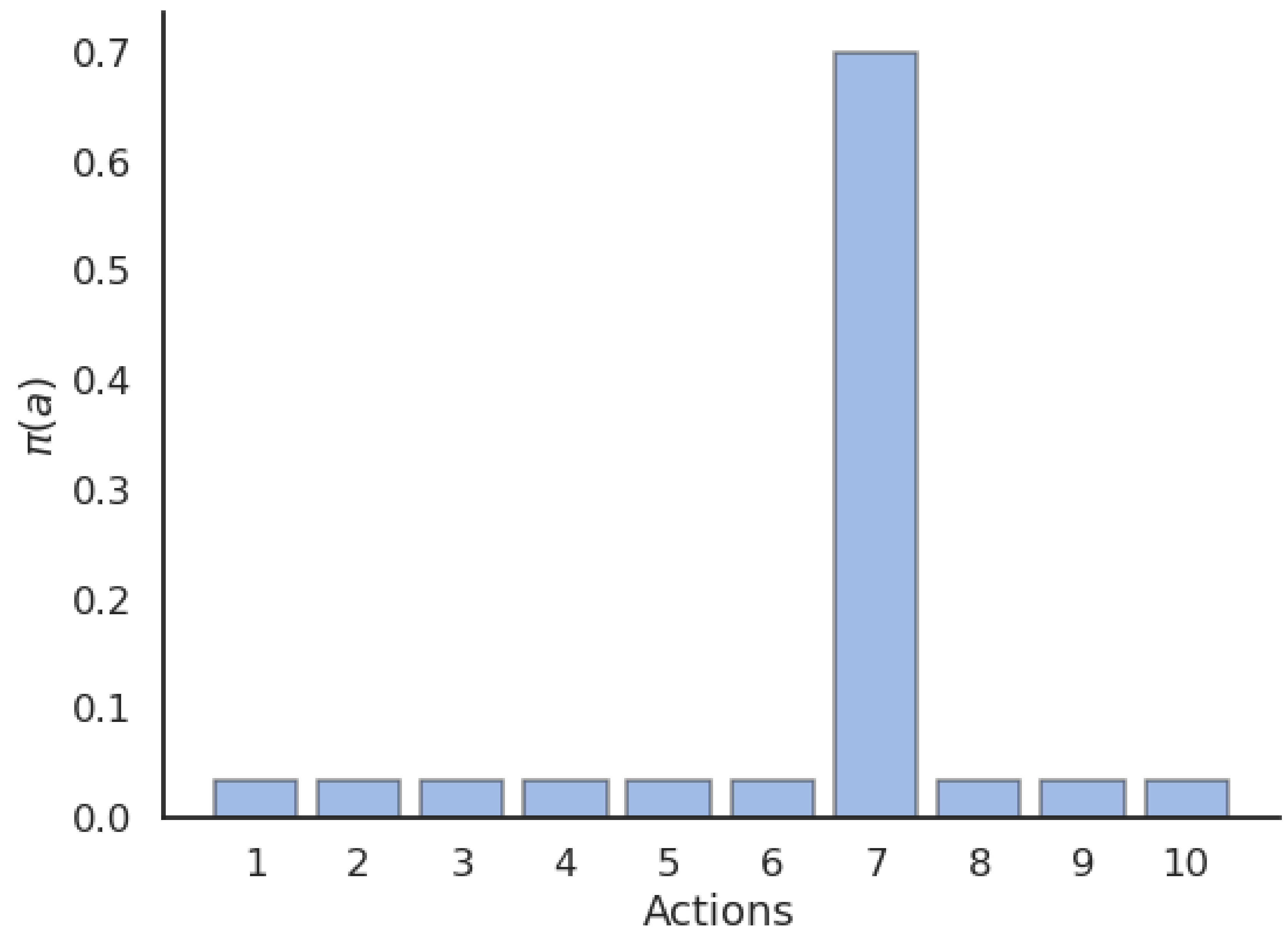
Source: UC Berkeley AI course slides, lecture 11

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:

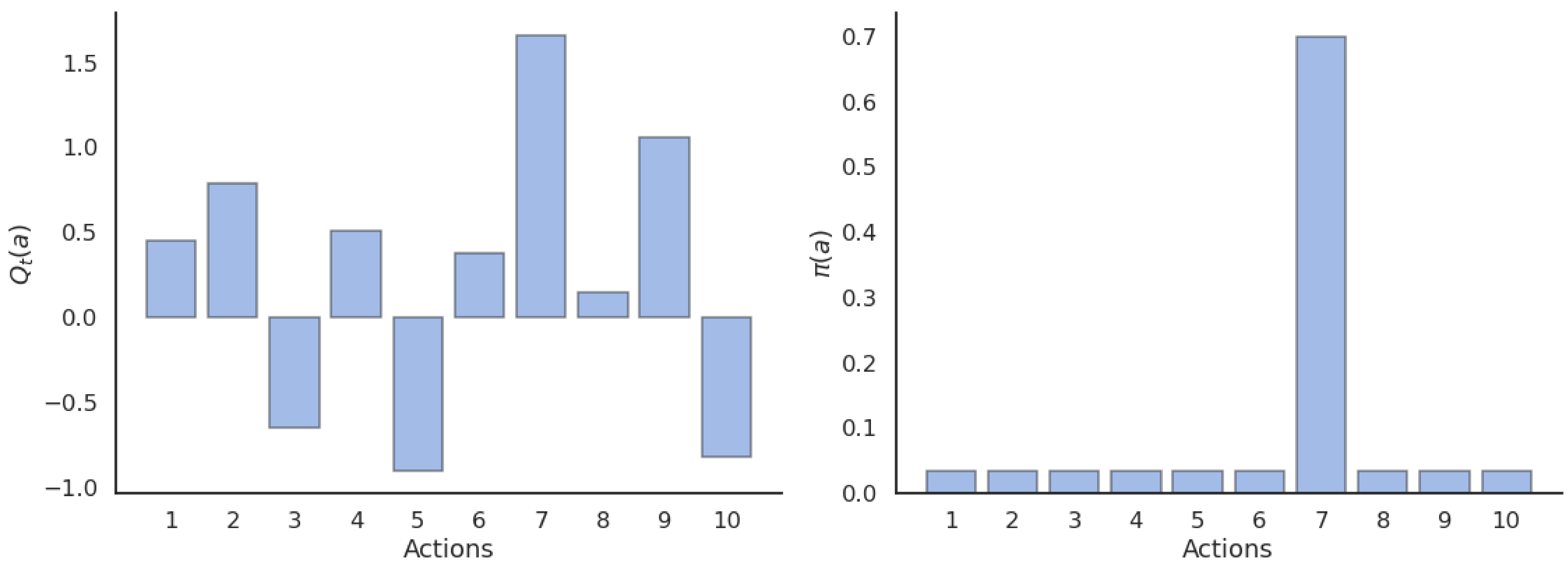
$$\pi(a) = \begin{cases} 1 - \epsilon \; \text{if} \; a = a_t^* \\ \frac{\epsilon}{|\mathcal{A}| - 1} \; \text{otherwise.} \end{cases}$$





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.

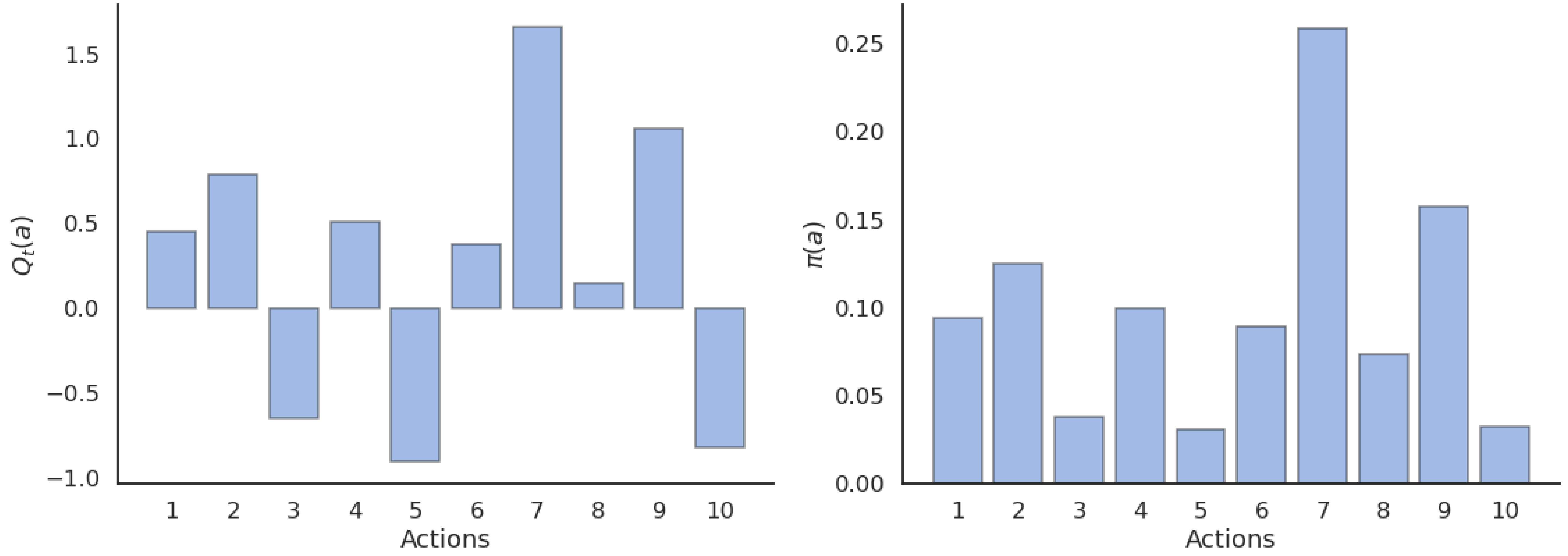


Softmax action selection

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

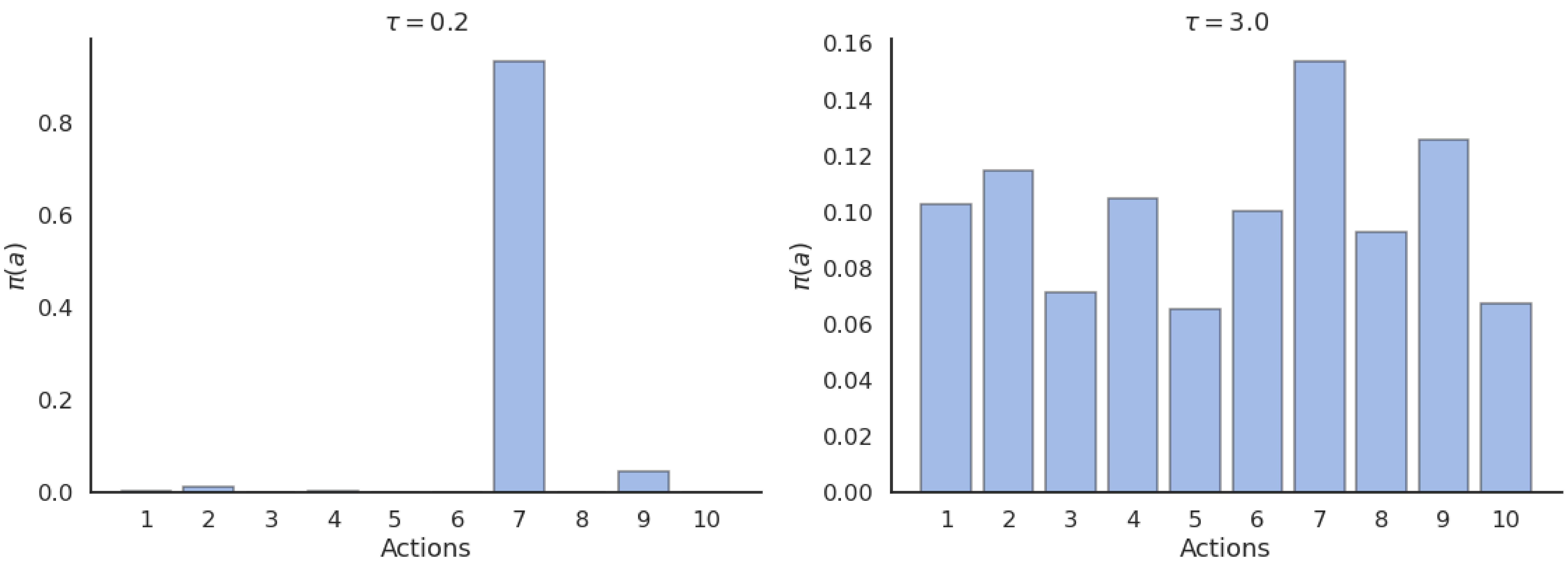
$$\pi(a) = \frac{\exp \frac{Q_t(a)}{\tau}}{\sum_{a'} \exp \frac{Q_t(a')}{\tau}}$$

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



Softmax action selection

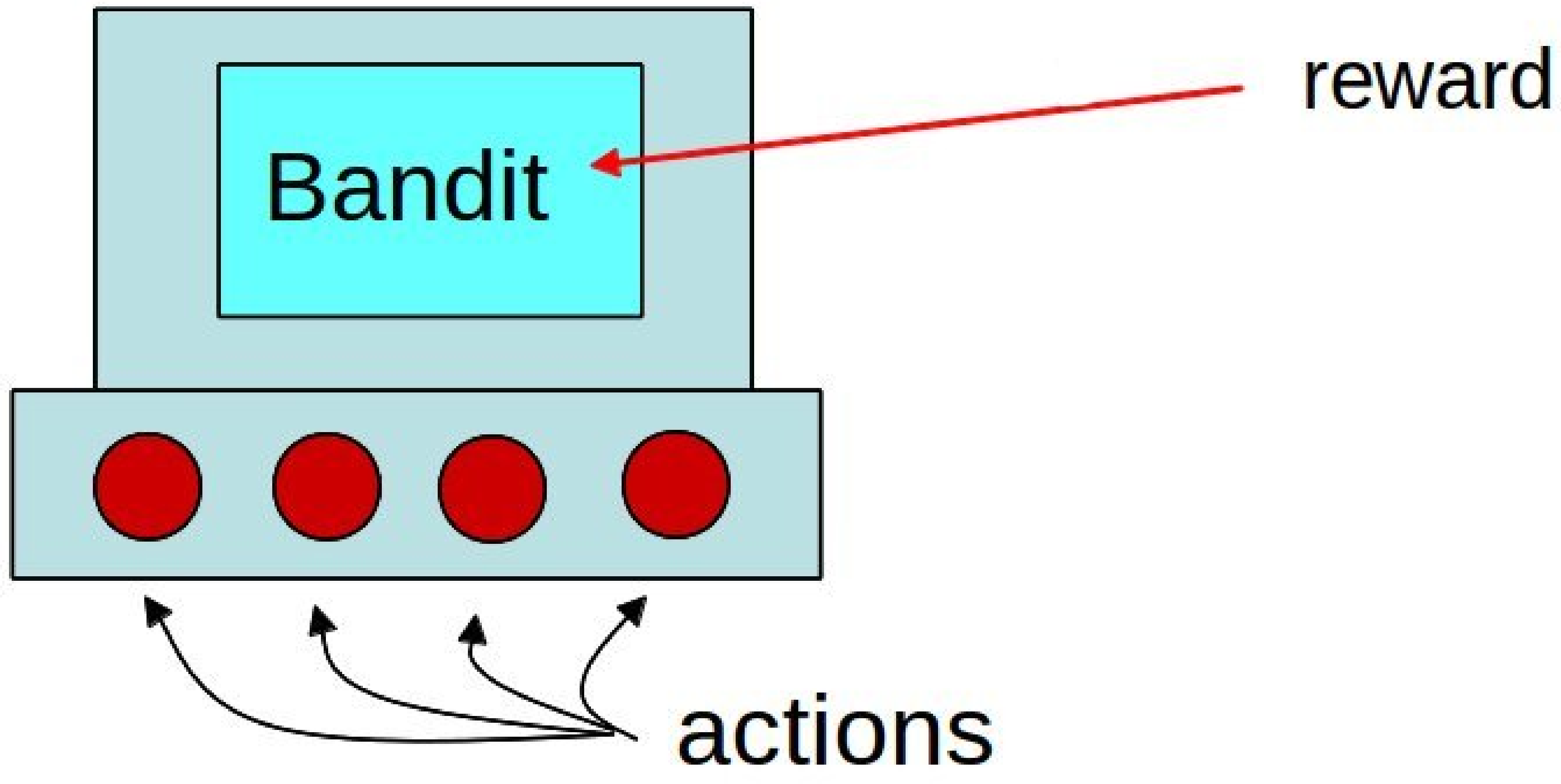
- Just as ϵ, the temperature τ controls the level of exploration:
  - High temperature causes the actions to be nearly equiprobable (**random agent**).
  - Low temperature causes the greediest actions only to be selected (**greedy agent**).



Example of action selection for the 10-armed bandit

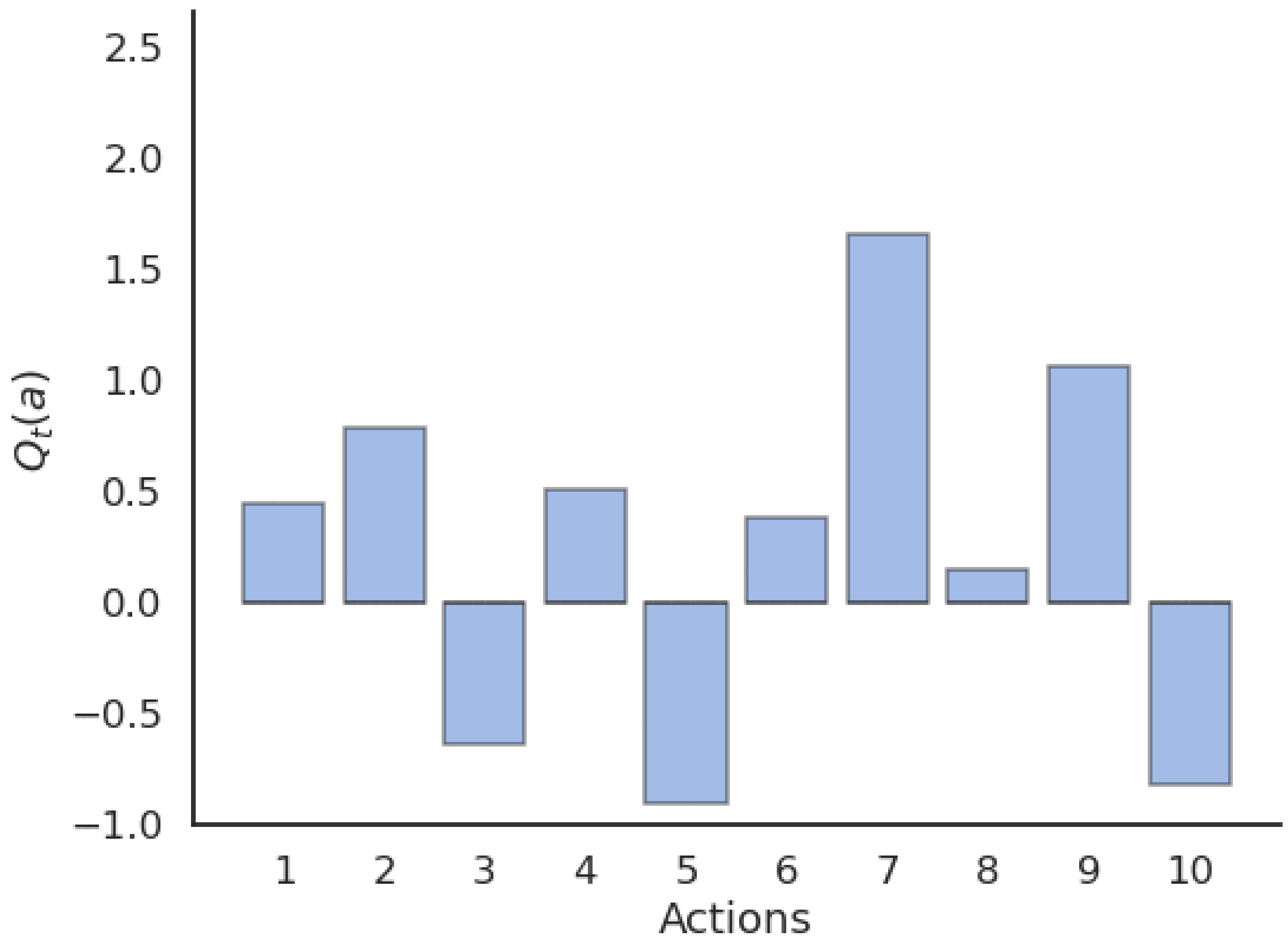
Procedure as in (Sutton and Barto, 2017):

- 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.



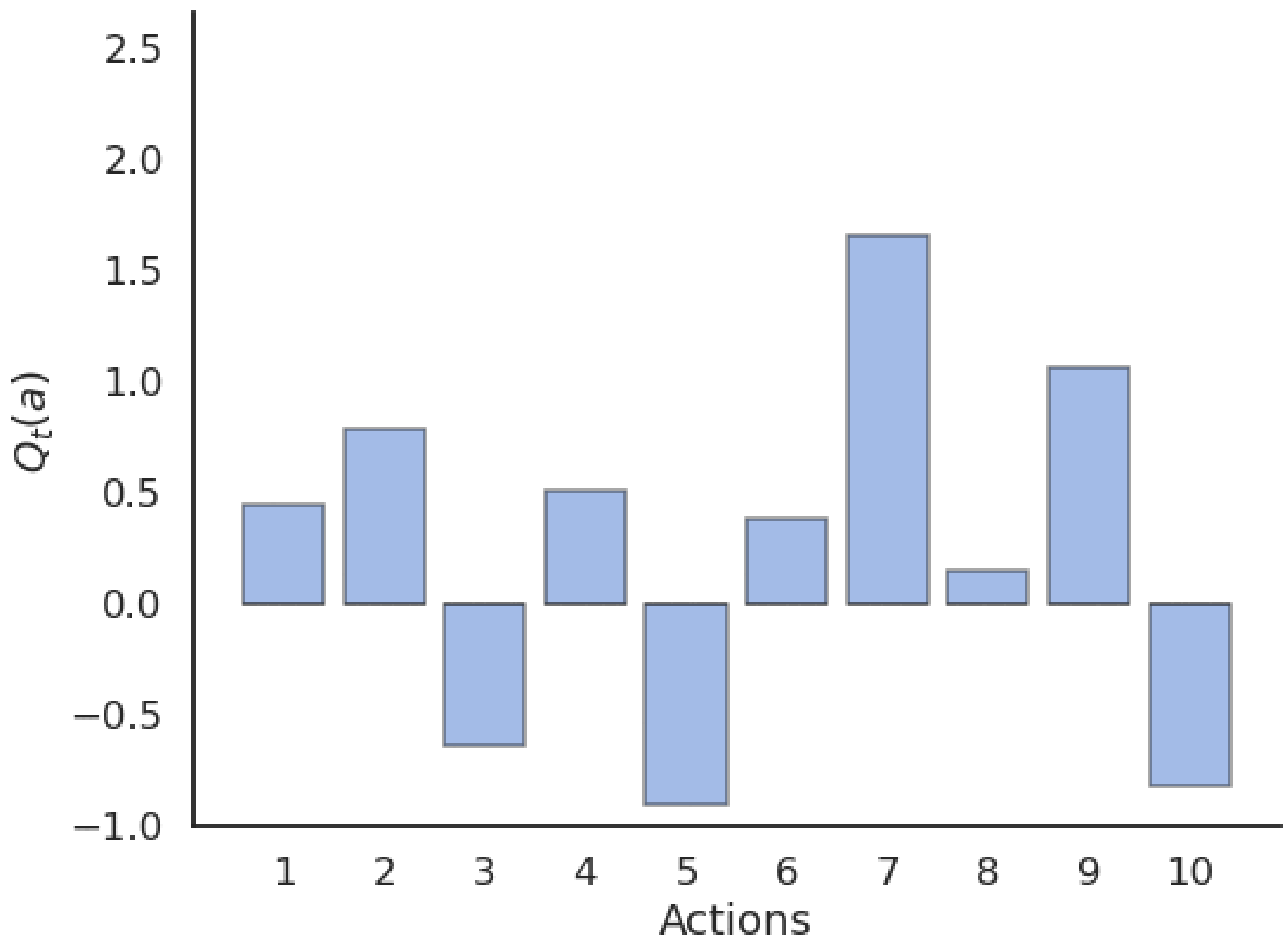
Greedy action selection

- 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**.



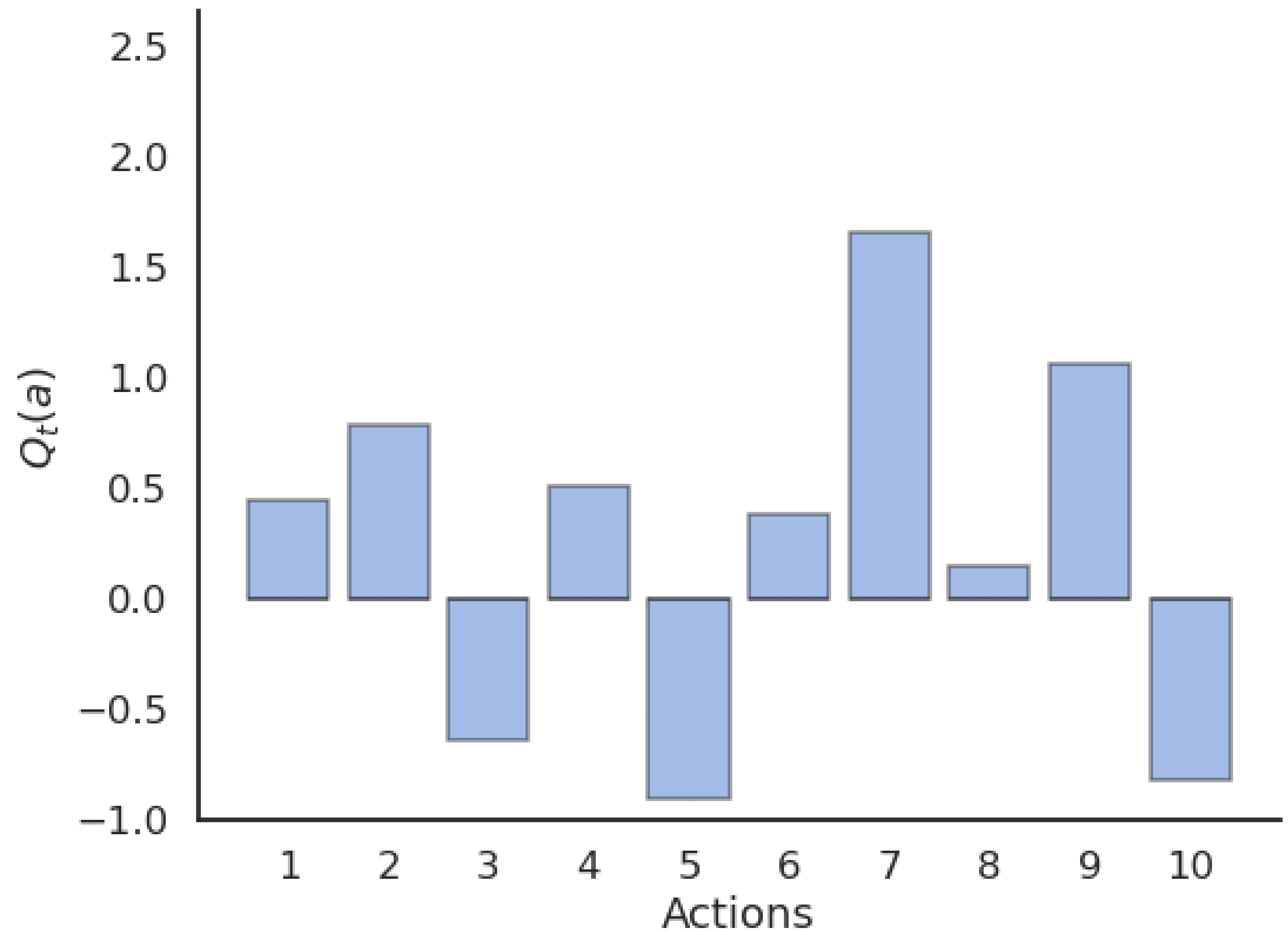
ϵ-greedy action selection

- 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).

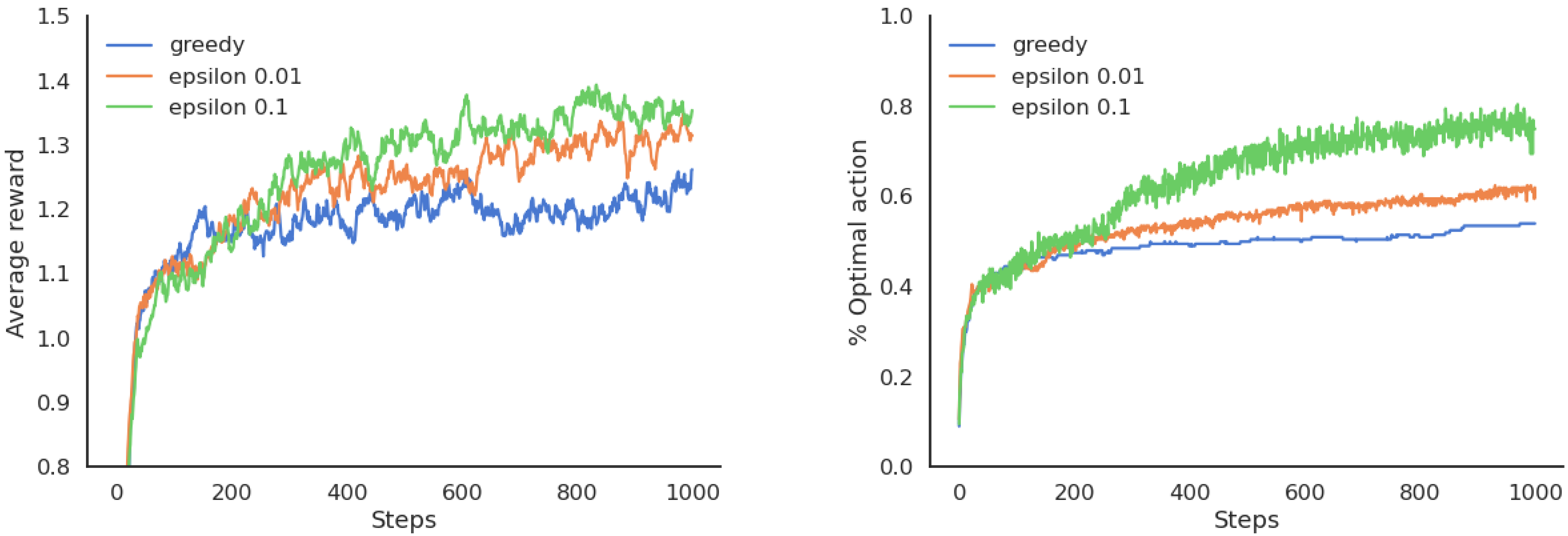


Softmax action selection

- 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.

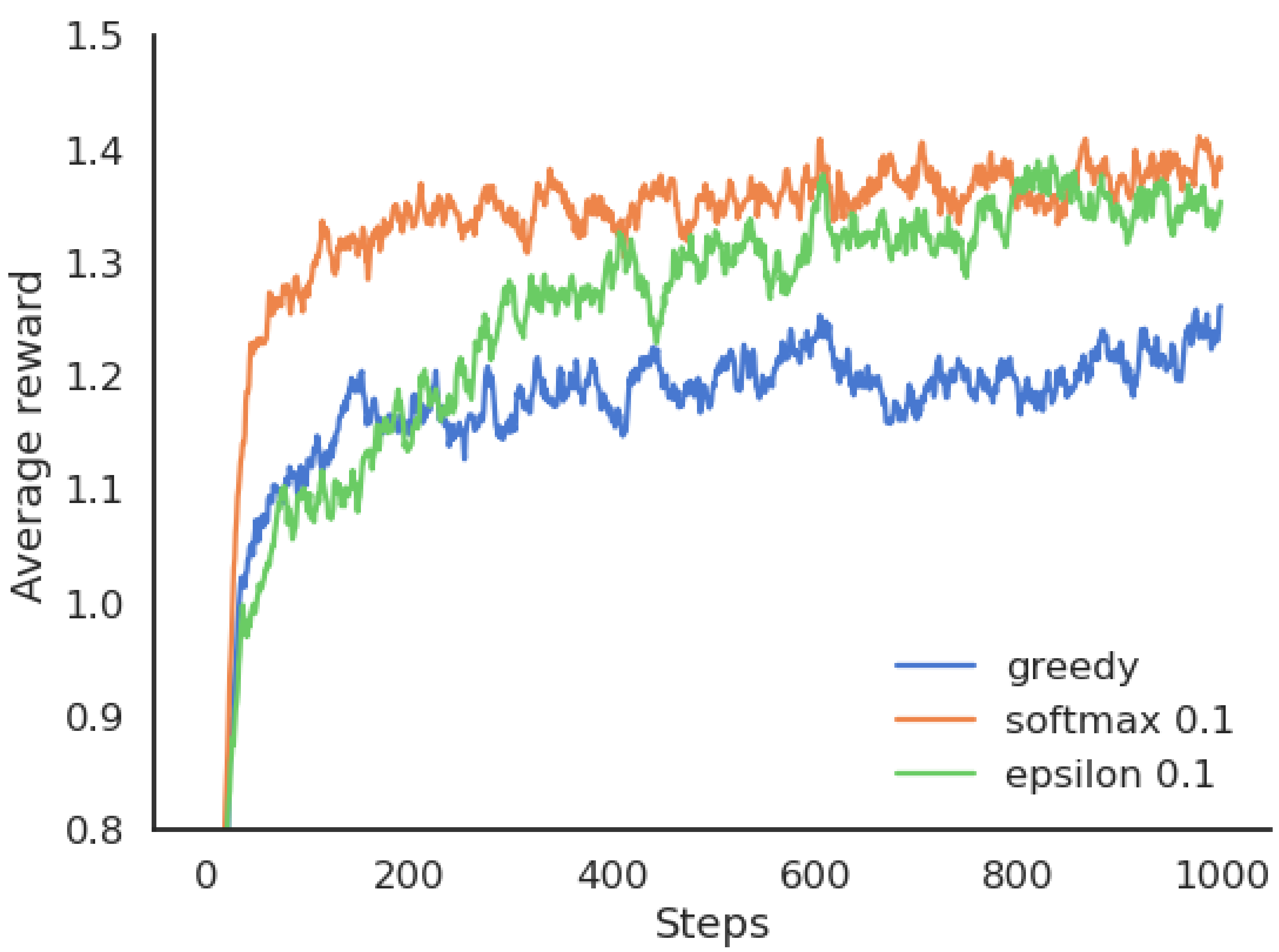


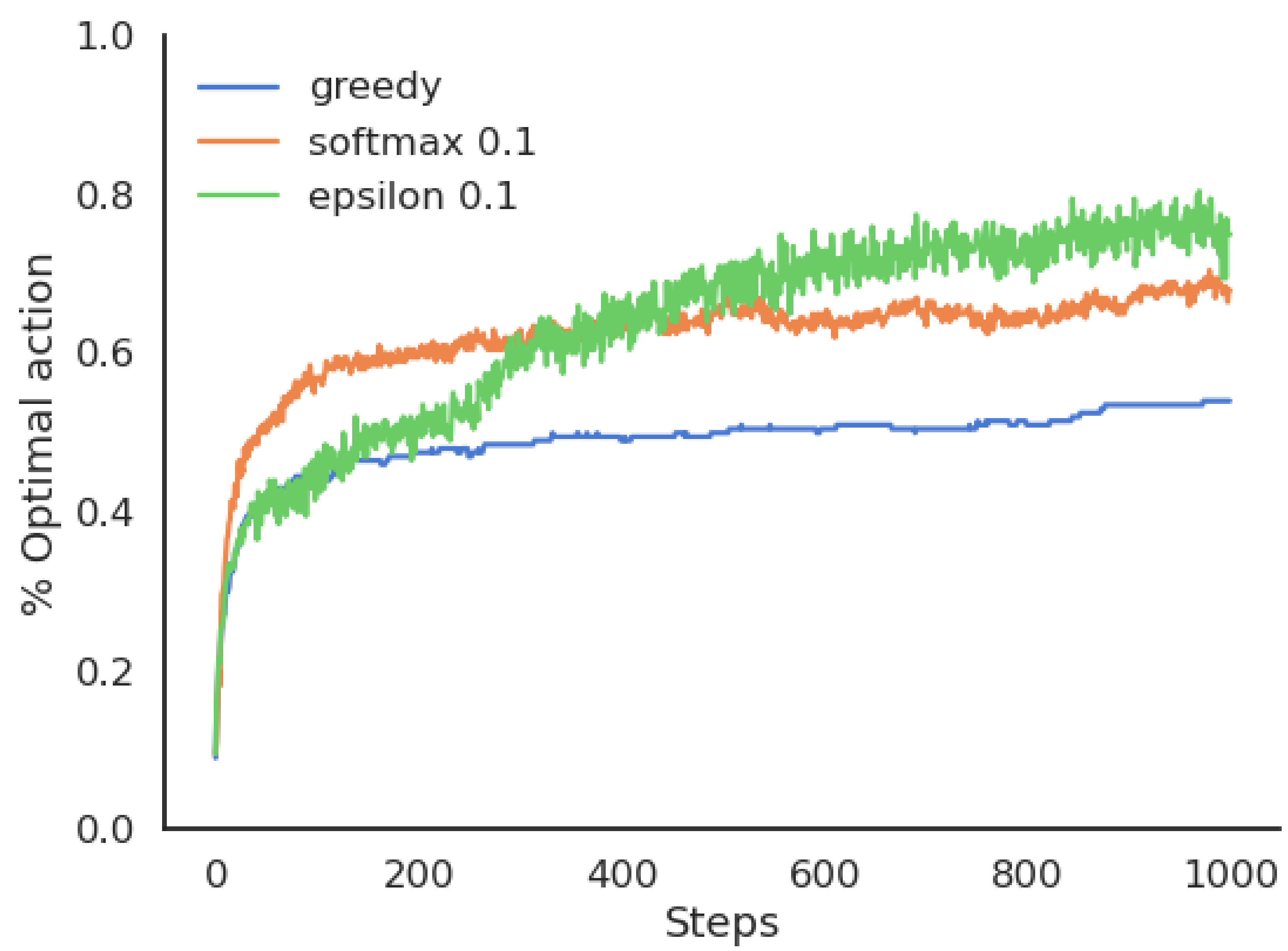
Greedy vs. ϵ-greedy



- 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

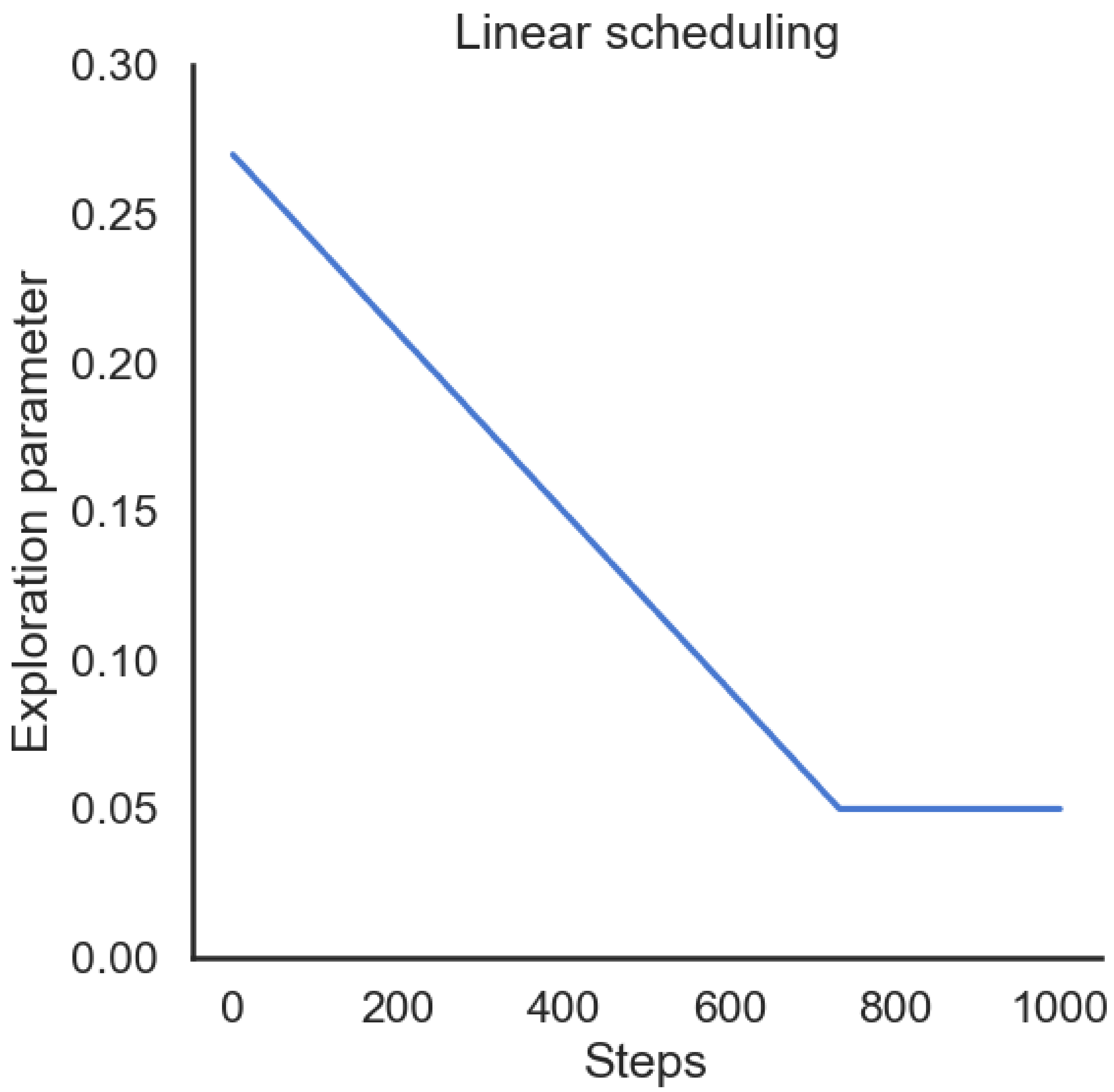


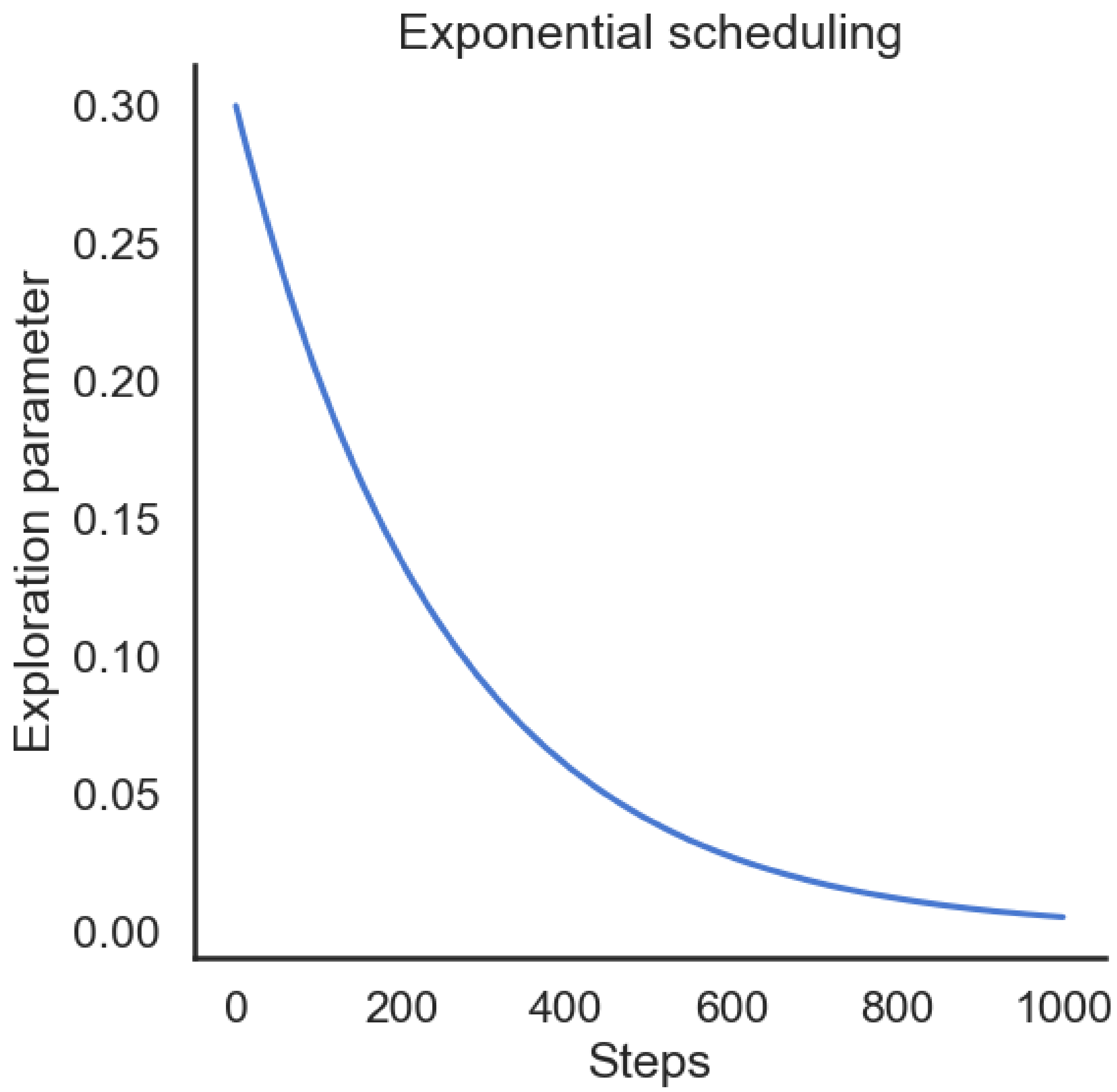


- The softmax does not necessarily find a better solution than ϵ-greedy, but it tends to find it **faster** (depending on ϵ or τ), as it does not lose time exploring obviously bad solutions.
- ϵ-greedy or softmax methods work best when the variance of rewards is high.
- If the variance is zero (always 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

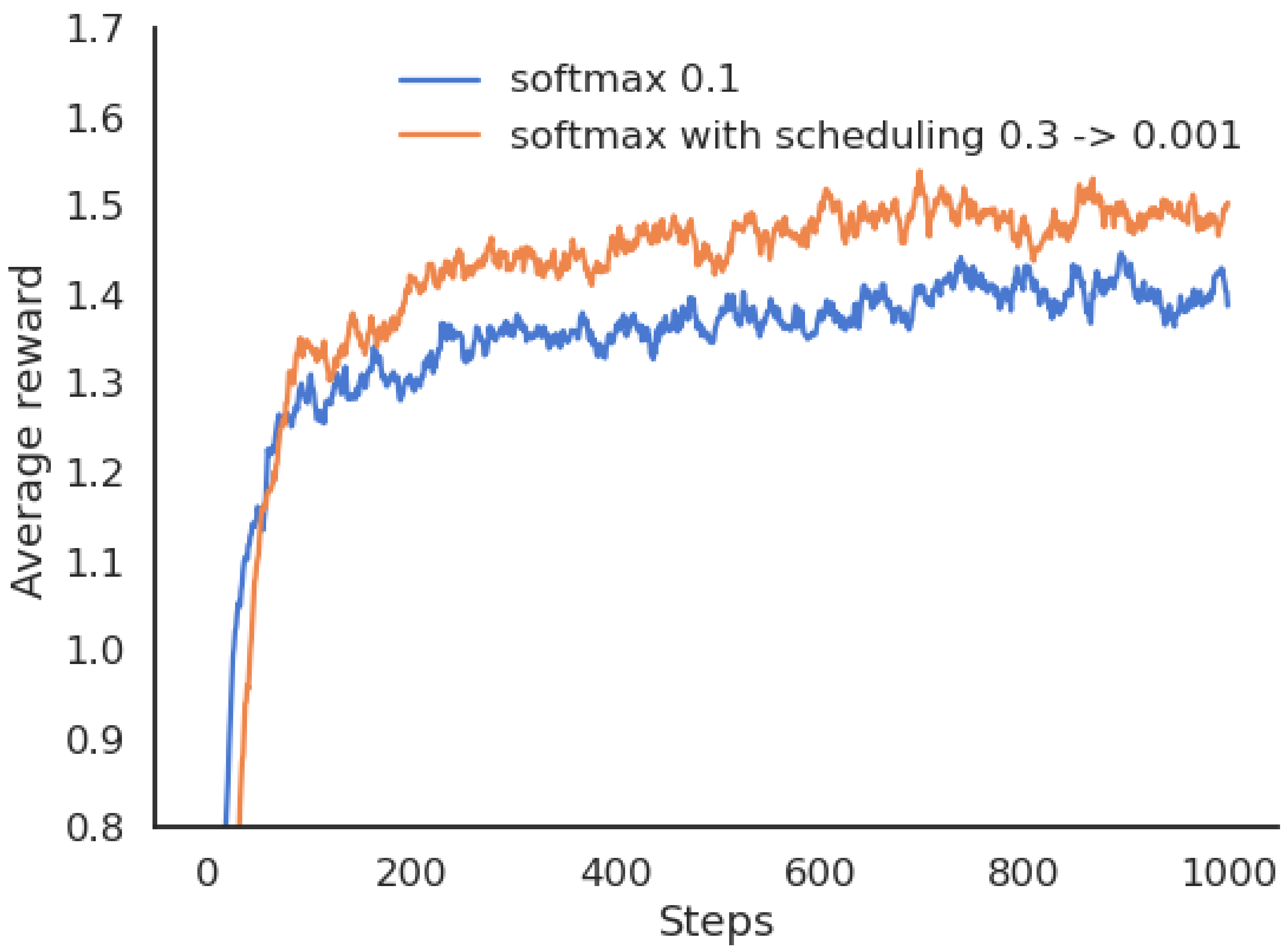
- A useful technique to cope with the **exploration-exploitation dilemma** is to slowly decrease the value of ϵ or τ with the number of plays.
- This allows for more exploration at the beginning of learning and more exploitation towards the end.
- It is however hard to find the right **decay rate** for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

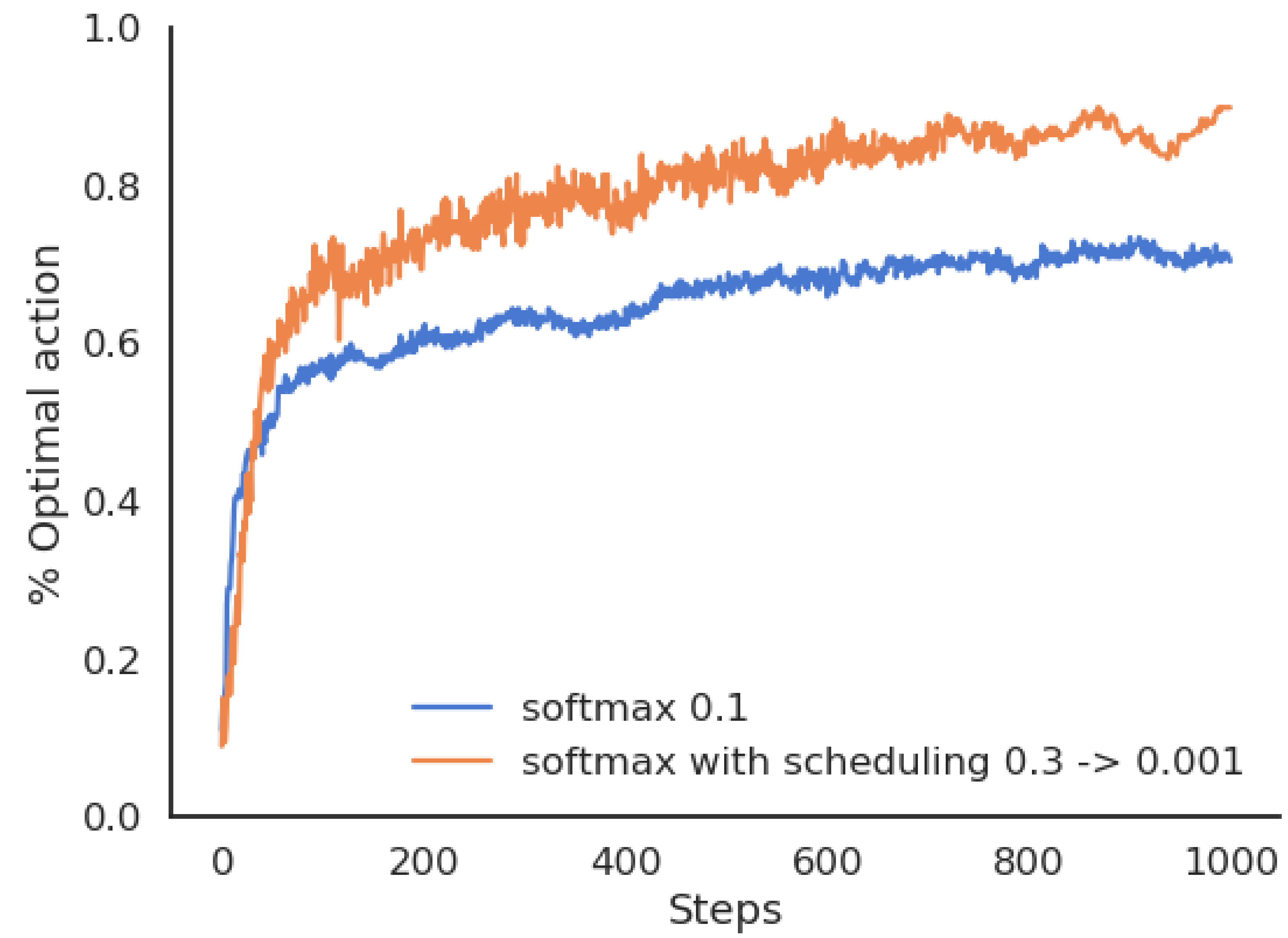




Exploration schedule

- 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.





Summary of evaluative feedback methods

- Other methods such as reinforcement comparison, gradient bandit and UCB exist, see (Sutton and Barto, 2017) and the second exercise on bandits.
- The methods 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.

References

Sutton, R. S., and Barto, A. G. (2017). *Reinforcement Learning: An Introduction*. 2nd ed. Cambridge, MA: MIT Press http://incompleteideas.net/book/the-book-2nd.html.