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CHEMNITZ

Deep Reinforcement Learning

Policy gradient

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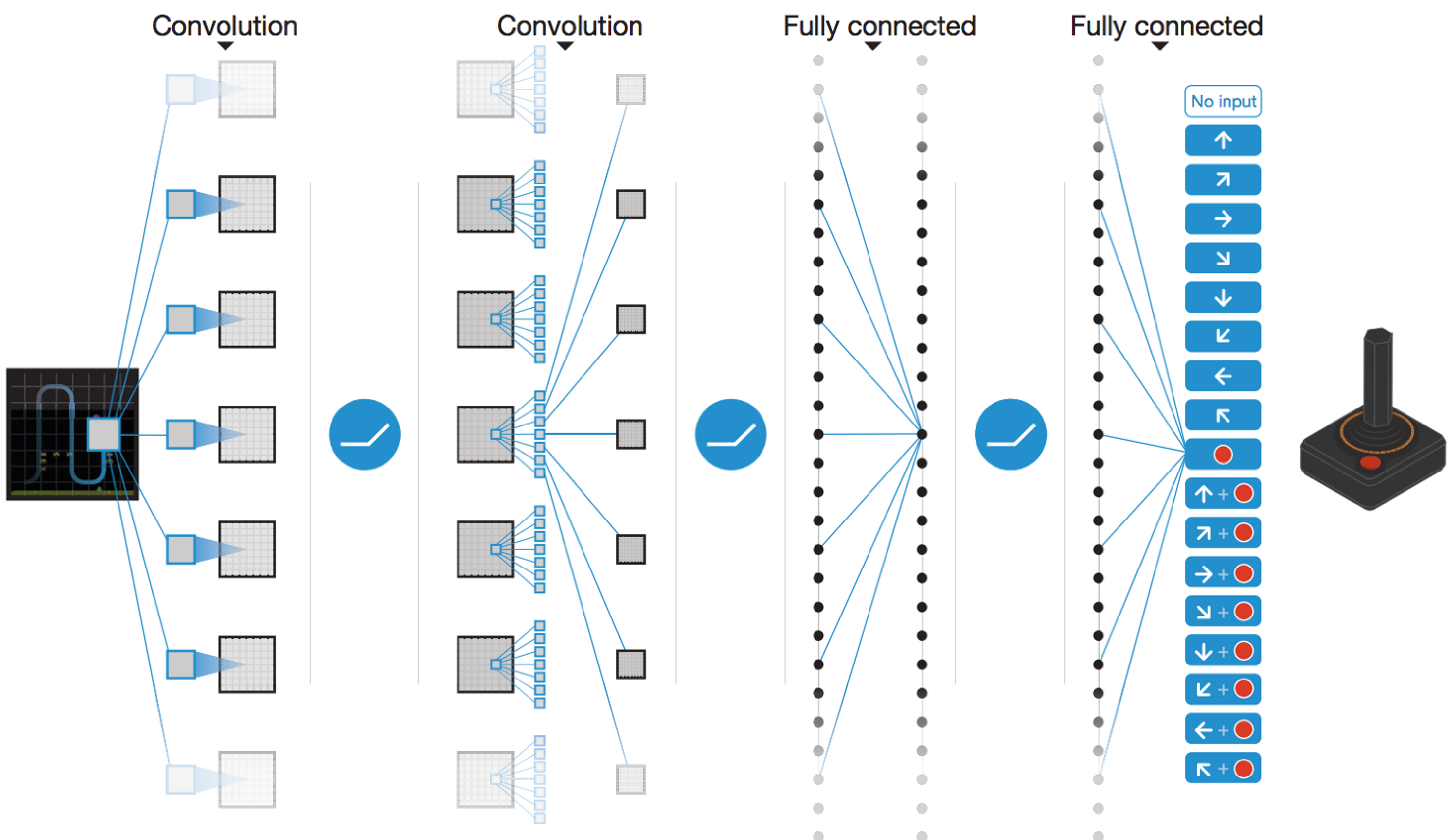
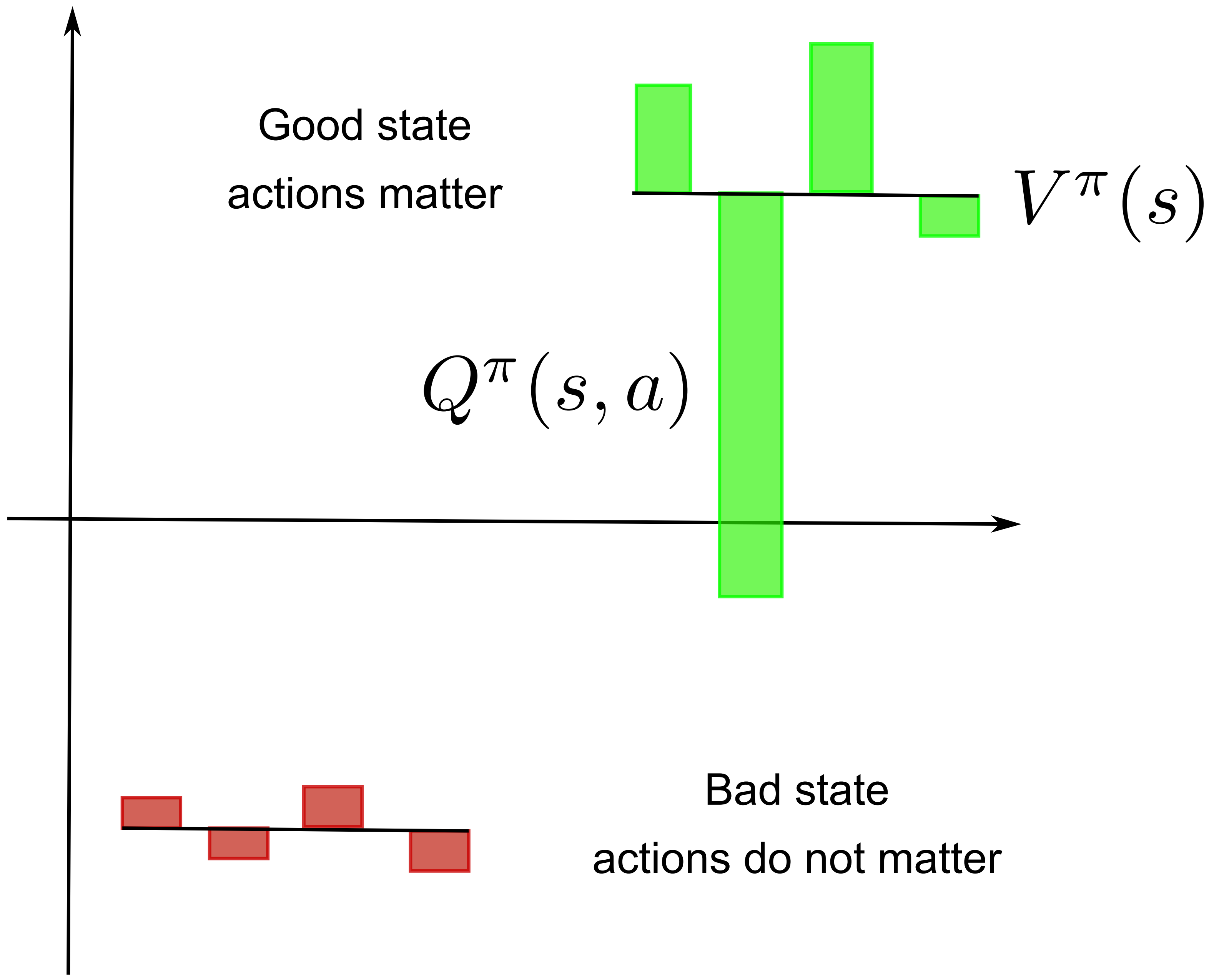
1 - Policy Search

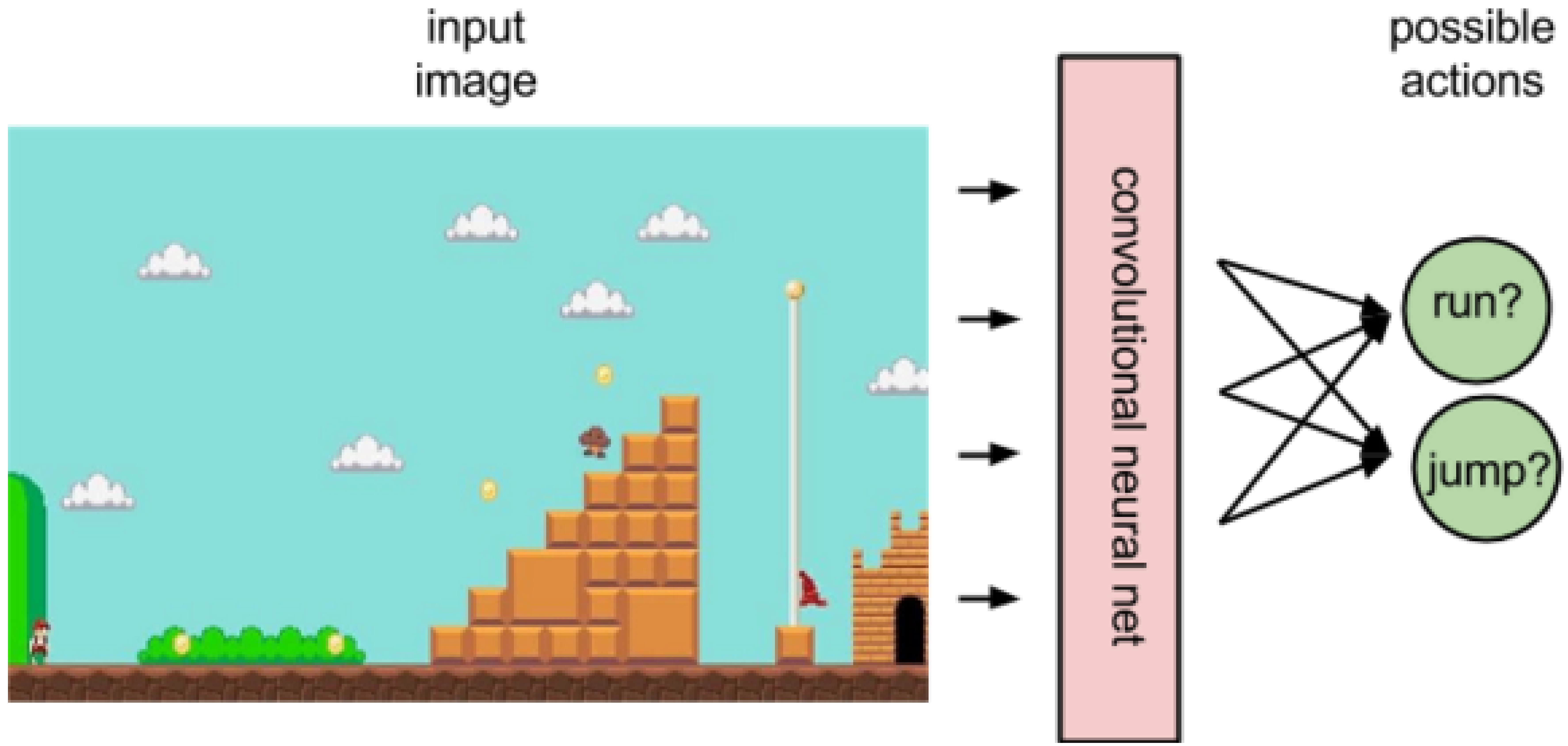
Policy search





- Learning directly the Q-values in value-based methods (DQN) suffers from many problems:
  - The Q-values are **unbounded**: they can take any value (positive or negative), so the output layer must be linear.
  - The Q-values have a **high variability**: some (s, a) pairs have very negative values, others have very positive values. Difficult to learn for a NN.
  - Works only for small **discrete action spaces**: need to iterate over all actions to find the greedy action.

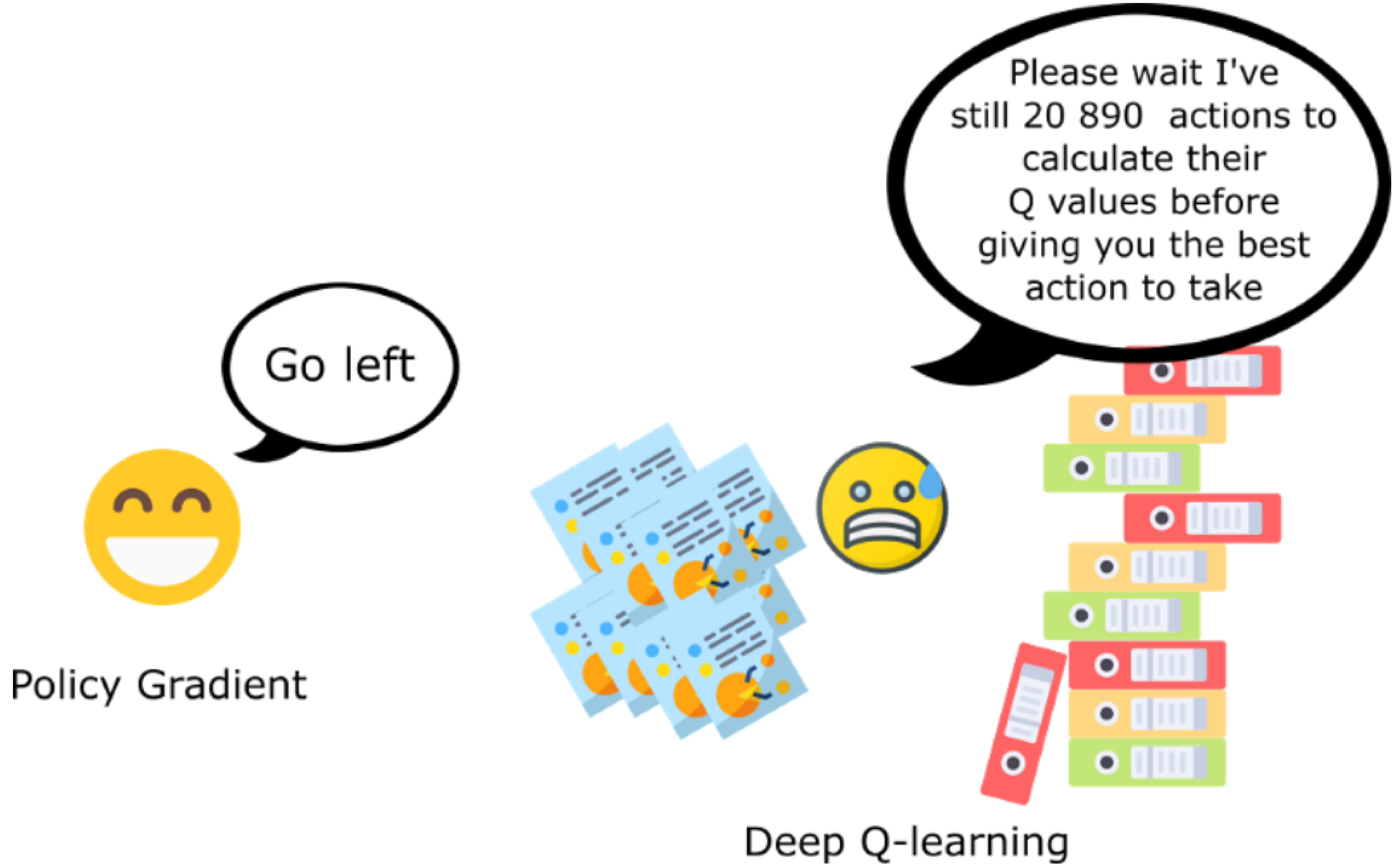
Policy search



- Instead of learning the Q-values, one could approximate directly the policy $\pi_\theta(s, a)$ with a neural network.
- $\pi_\theta(s, a)$ is called a **parameterized policy**: it depends directly on the parameters θ of the NN.
- For discrete action spaces, the output of the NN can be a **softmax** layer, directly giving the probability of selecting an action.
- For continuous action spaces, the output layer can directly control the effector (joint angles).

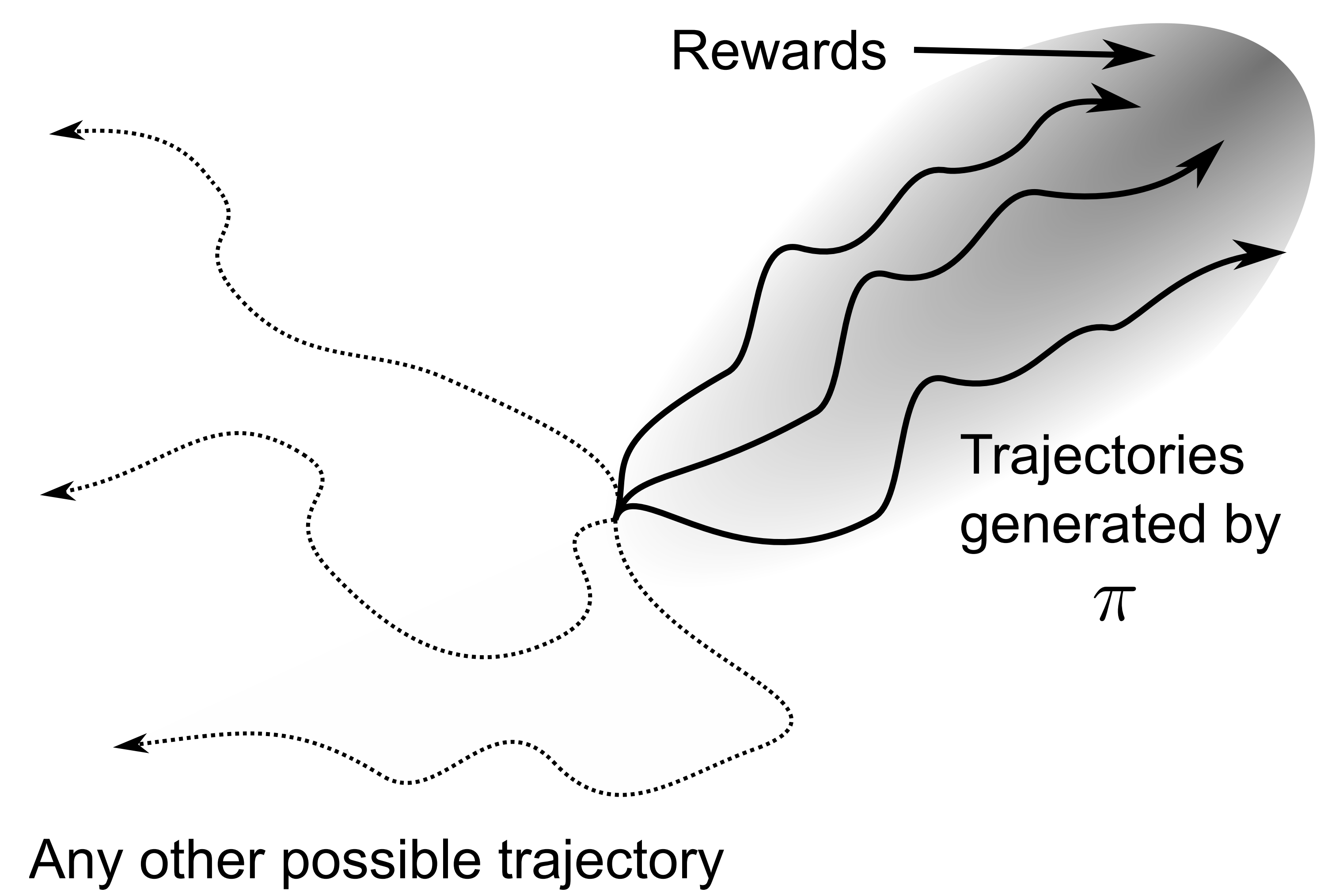
Policy search

- Parameterized policies can represent continuous policies and avoid the curse of dimensionality.



Source: https://www.freecodecamp.org/news/an-introduction-to-policy-gradients-with-cartpole-and-doom-495b5ef2207f/

Policy search



- **Policy search** methods aim at maximizing directly the expected return over all possible trajectories (episodes) $\tau = (s_0, a_0, \dots, s_T, a_T)$

$$\mathcal{J}(\theta) = \mathbb{E}_{\tau \sim \rho_\theta}[R(\tau)] = \int_\tau \rho_\theta(\tau)\; R(\tau)\; d\tau$$

- All trajectories τ selected by the policy π_θ should be associated with a high expected return $R(\tau)$ in order to maximize this objective function.
- $\rho_\theta(\tau)$ is the **likelihood** of the trajectory τ under the policy π_θ.
- This means that the optimal policy should only select actions that maximizes the expected return: exactly what we want.

Policy search

- Objective function to be maximized:

$$\mathcal{J}(\theta) = \mathbb{E}_{\tau \sim \rho_\theta}[R(\tau)] = \int_\tau \rho_\theta(\tau) \; R(\tau) \; d\tau$$

- The objective function is however not **model-free**, as the likelihood of a trajectory does depend on the environments dynamics:

$$\rho_\theta(\tau) = p_\theta(s_0, a_0, \ldots, s_T, a_T) = p_0(s_0) \; \prod_{t=0}^T \pi_\theta(s_t, a_t) \, p(s_{t+1} | s_t, a_t)$$

- The objective function is furthermore **not computable**:
  - An **infinity** of possible trajectories to integrate if the action space is continuous.
  - Even if we sample trajectories, we would need a huge number of them to correctly estimate the objective function (**sample complexity**) because of the huge **variance** of the returns.

$$\mathcal{J}(\theta) = \mathbb{E}_{\tau \sim \rho_\theta}[R(\tau)] \approx \frac{1}{M} \; \sum_{i=1}^M R(\tau_i)$$

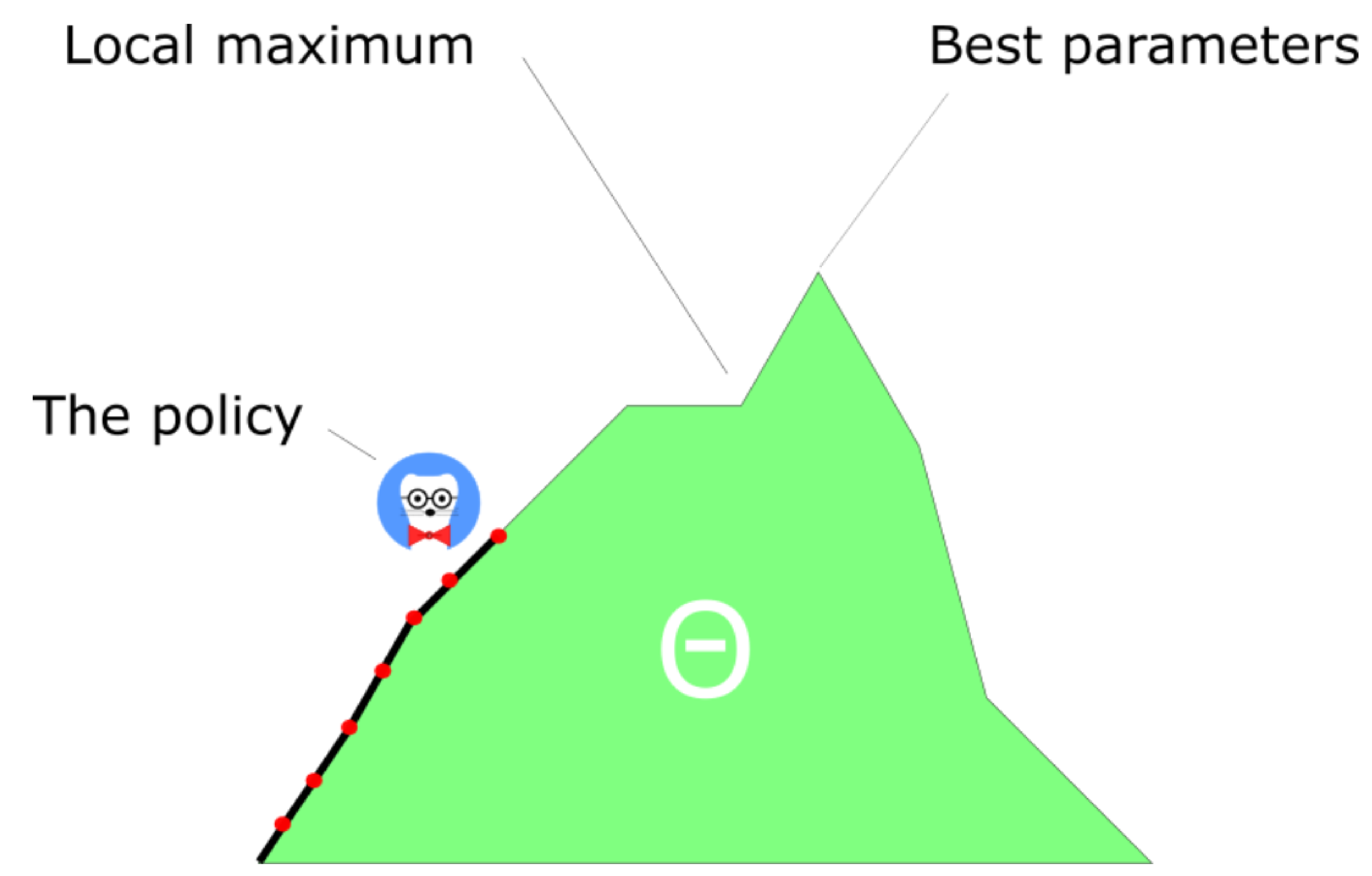
Policy gradient

- All we need to find is a computable gradient $\nabla_\theta \mathcal{J}(\theta)$ to apply gradient ascent and backpropagation.

$$\Delta \theta = \eta \, \nabla_\theta \mathcal{J}(\theta)$$

- **Policy Gradient** (PG) methods only try to estimate this gradient, but do not care about the objective function itself...

$$g = \nabla_\theta \mathcal{J}(\theta)$$



Source: https://www.freecodecamp.org/news/an-introduction-to-policy-gradients-with-cartpole-and-doom-495b5ef2207f/

- In particular, any function $\mathcal{J}'(\theta)$ whose gradient is locally the same (or has the same direction) will do:

$$\mathcal{J}'(\theta) = \alpha \, \mathcal{J}(\theta) + \beta \;\Rightarrow\; \nabla_\theta \mathcal{J}'(\theta) \propto \nabla_\theta \mathcal{J}(\theta) \;\Rightarrow\; \Delta \theta = \eta \, \nabla_\theta \mathcal{J}'(\theta)$$

- This is called **surrogate optimization**: we actually want to maximize $\mathcal{J}(\theta)$ but we cannot compute it.
- We instead create a surrogate objective $\mathcal{J}'(\theta)$ which is locally the same as $\mathcal{J}(\theta)$ and tractable.

2 - REINFORCE

Simple Statistical Gradient-Following Algorithms for Connectionist Reinforcement Learning

Ronald J. Williams
College of Computer Science
Northeastern University
Boston, MA 02115

Appears in *Machine Learning, 8*, pp. 229-256, 1992.

REINFORCE

- The **REINFORCE** algorithm (Williams, 1992) proposes an unbiased estimate of the policy gradient:

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

by noting that the return of a trajectory does not depend on the weights θ (the agent only controls its actions, not the environment).

- We now use the **log-trick**, a simple identity based on the fact that:

$$\frac{d \log f(x)}{dx} = \frac{f'(x)}{f(x)}$$

or:

$$f'(x) = f(x) \times \frac{d \log f(x)}{dx}$$

to rewrite the gradient of the likelihood of a single trajectory:

$$\nabla_\theta \, \rho_\theta (\tau) = \rho_\theta (\tau) \times \nabla_\theta \log \rho_\theta (\tau)$$

REINFORCE

- The policy gradient becomes:

$$\nabla_\theta \mathcal{J}(\theta) = \int_\tau (\nabla_\theta \rho_\theta(\tau)) R(\tau) \, d\tau = \int_\tau \rho_\theta(\tau) \nabla_\theta \log \rho_\theta(\tau) R(\tau) \, d\tau$$

which now has the form of a mathematical expectation:

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

- The policy gradient is, in expectation, the gradient of the **log-likelihood** of a trajectory multiplied by its return.

REINFORCE

- The advantage of REINFORCE is that it is **model-free**:

$$\rho_\theta(\tau) = p_\theta(s_0, a_0, \dots, s_T, a_T) = p_0(s_0) \prod_{t=0}^{T} \pi_\theta(s_t, a_t) p(s_{t+1} | s_t, a_t)$$

$$\log \rho_\theta(\tau) = \log p_0(s_0) + \sum_{t=0}^{T} \log \pi_\theta(s_t, a_t) + \sum_{t=0}^{T} \log p(s_{t+1} | s_t, a_t)$$

$$\nabla_\theta \log \rho_\theta(\tau) = \sum_{t=0}^{T} \nabla_\theta \log \pi_\theta(s_t, a_t)$$

- The transition dynamics $p(s_{t+1} | s_t, a_t)$ disappear from the gradient.
- The **Policy Gradient** does not depend on the dynamics of the environment:

$$\nabla_\theta \mathcal{J}(\theta) = \mathbb{E}_{\tau \sim \rho_\theta}[\sum_{t=0}^{T} \nabla_\theta \log \pi_\theta(s_t, a_t) \, R(\tau)]$$

REINFORCE algorithm

The REINFORCE algorithm is a policy-based variant of Monte-Carlo control:

- **while** not converged:
  - Sample M trajectories $\{\tau_i\}$ using the current policy π_θ and observe the returns $\{R(\tau_i)\}$.
  - Estimate the policy gradient as an average over the trajectories:

$$\nabla_\theta \mathcal{J}(\theta) \approx \frac{1}{M} \sum_{i=1}^M \sum_{t=0}^T \nabla_\theta \log \pi_\theta(s_t, a_t) \, R(\tau_i)$$

  - Update the policy using gradient ascent:

$$\theta \leftarrow \theta + \eta \, \nabla_\theta \mathcal{J}(\theta)$$

Williams, R. J. (1992). Simple statistical gradient-following algorithms for connectionist reinforcement learning. Machine Learning 8, 229–256.

REINFORCE

$$\nabla_\theta \mathcal{J}(\theta) = \mathbb{E}_{\tau \sim \rho_\theta}[\sum_{t=0}^T \nabla_\theta \log \pi_\theta(s_t, a_t) \, R(\tau)]$$

Advantages

- The policy gradient is **model-free**.
- Works with **partially observable** problems (POMDP): as the return is computed over complete trajectories, it does not matter whether the states are Markov or not.

Inconvenients

- Only for **episodic tasks**.
- The gradient has a **high variance**: returns may change a lot during learning.
- It has therefore a high **sample complexity**: we need to sample many episodes to correctly estimate the policy gradient.
- Strictly **on-policy**: trajectories must be frequently sampled and immediately used to update the policy.

REINFORCE with baseline

- To reduce the variance of the estimated gradient, a baseline is often subtracted from the return:

$$\nabla_\theta \mathcal{J}(\theta) = \mathbb{E}_{\tau \sim \rho_\theta}[\sum_{t=0}^T \nabla_\theta \log \pi_\theta(s_t, a_t) \, (R(\tau) - b)]$$

- As long as the baseline b is independent from θ, it does not introduce a bias:

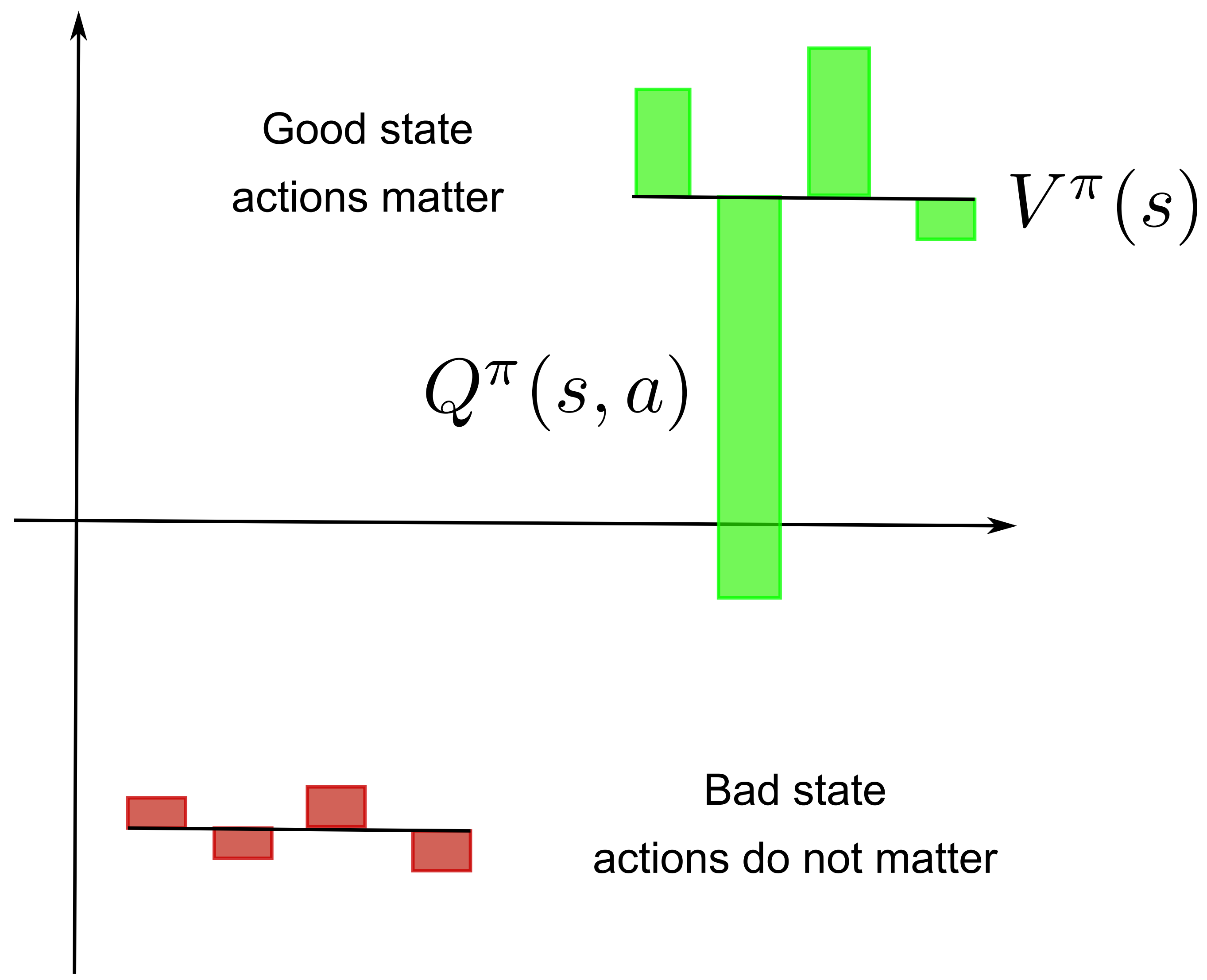
$$\begin{aligned}
\mathbb{E}_{\tau \sim \rho_\theta}[\nabla_\theta \log \rho_\theta(\tau) \, b] &= \int_\tau \rho_\theta(\tau) \nabla_\theta \log \rho_\theta(\tau) \, b \, d\tau \\
&= \int_\tau \nabla_\theta \rho_\theta(\tau) \, b \, d\tau \\
&= b \, \nabla_\theta \int_\tau \rho_\theta(\tau) \, d\tau \\
&= b \, \nabla_\theta 1 \\
&= 0
\end{aligned}$$

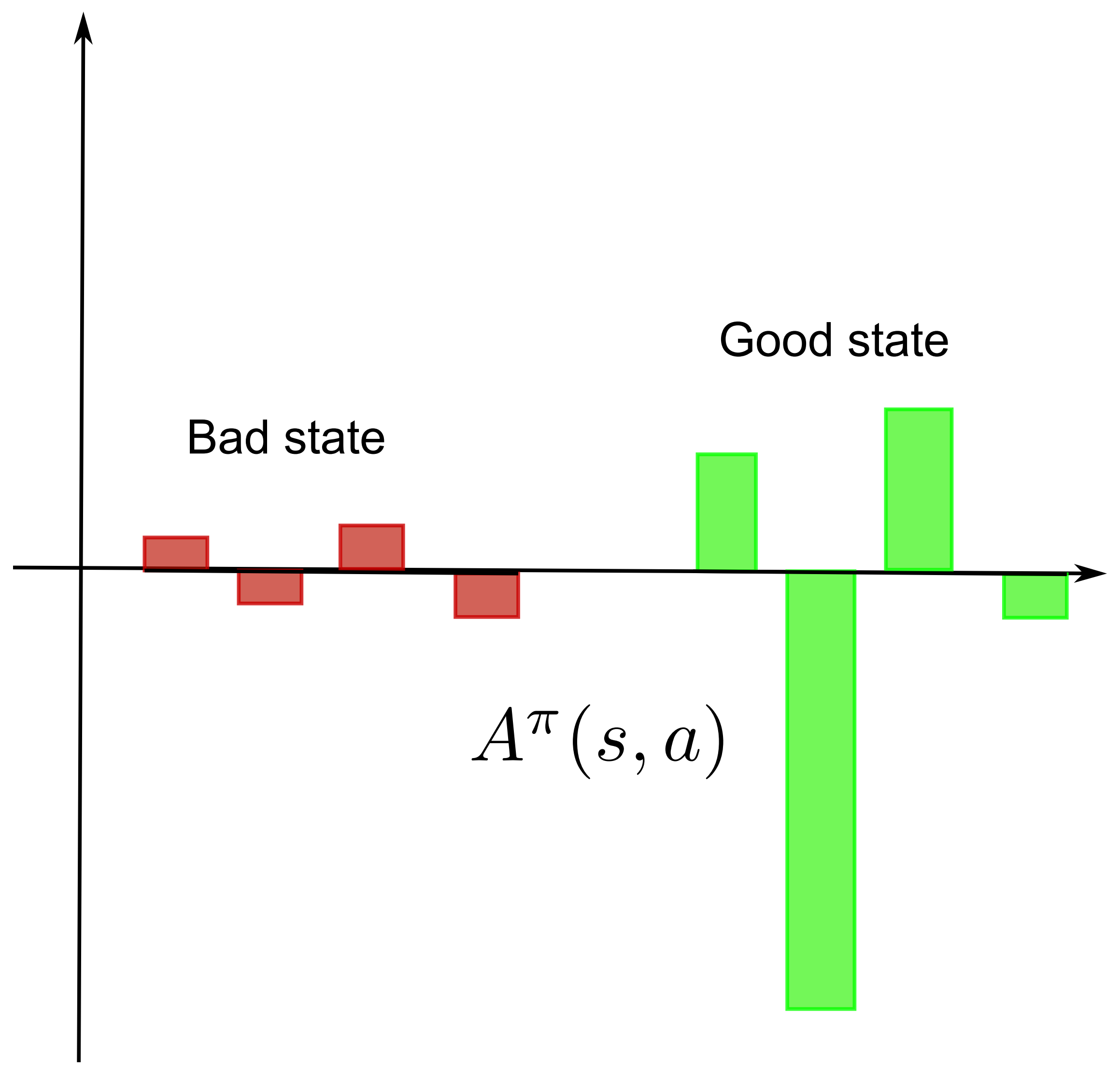
REINFORCE with baseline

- In practice, a baseline that works well is the value of the encountered states:

$$\nabla_\theta \mathcal{J}(\theta) = \mathbb{E}_{\tau \sim \rho_\theta}[\sum_{t=0}^T \nabla_\theta \log \pi_\theta(s_t, a_t) \, (R(\tau) - V^\pi(s_t))]$$

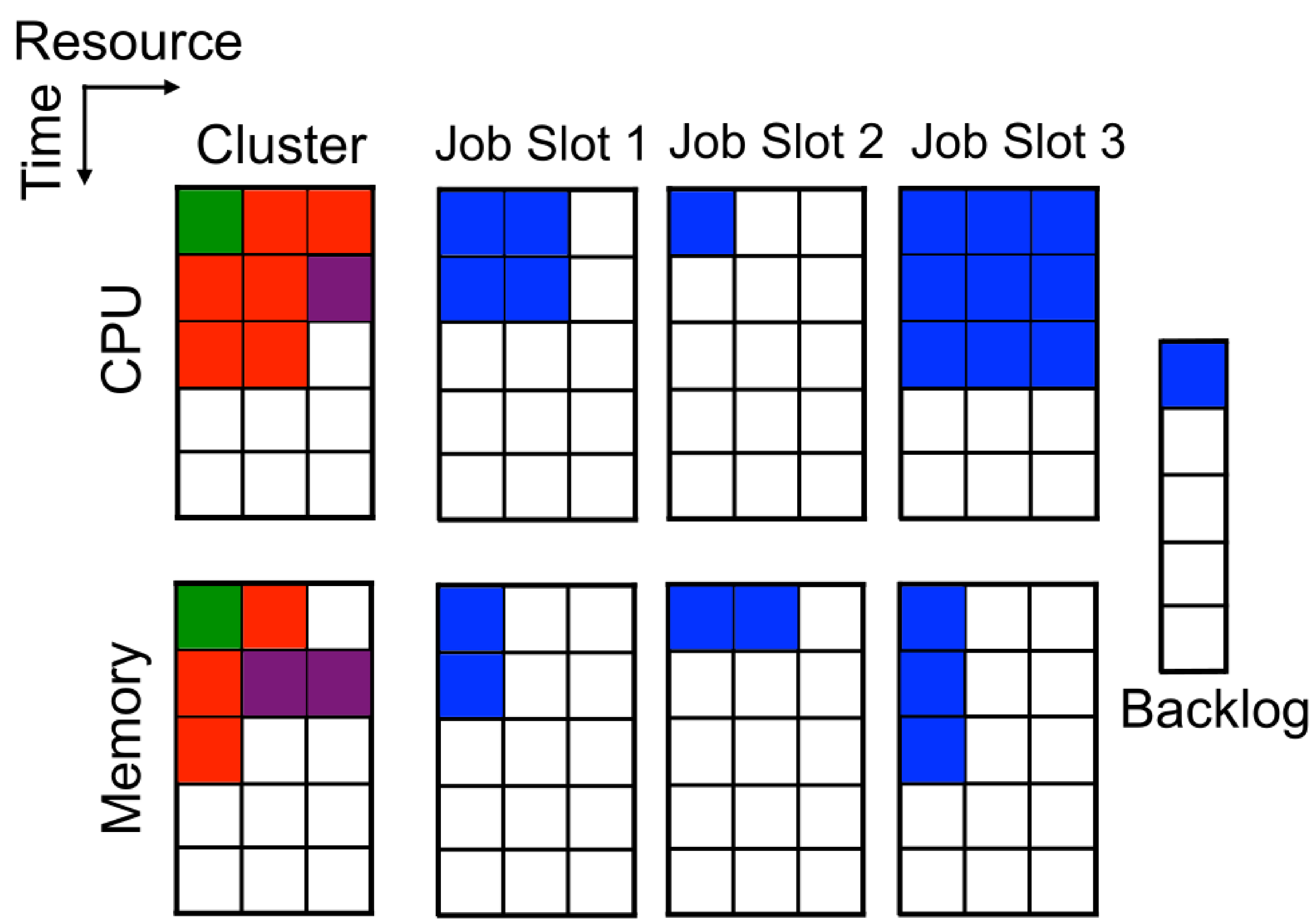
- $R(\tau) - V^\pi(s_t)$ becomes the **advantage** of the action a_t in s_t: how much return does it provide compared to what can be expected in s_t generally:





- As in **dueling networks**, it reduces the variance of the returns.
- Problem: the value of each state has to be learned separately (see actor-critic architectures).

Application of REINFORCE to resource management



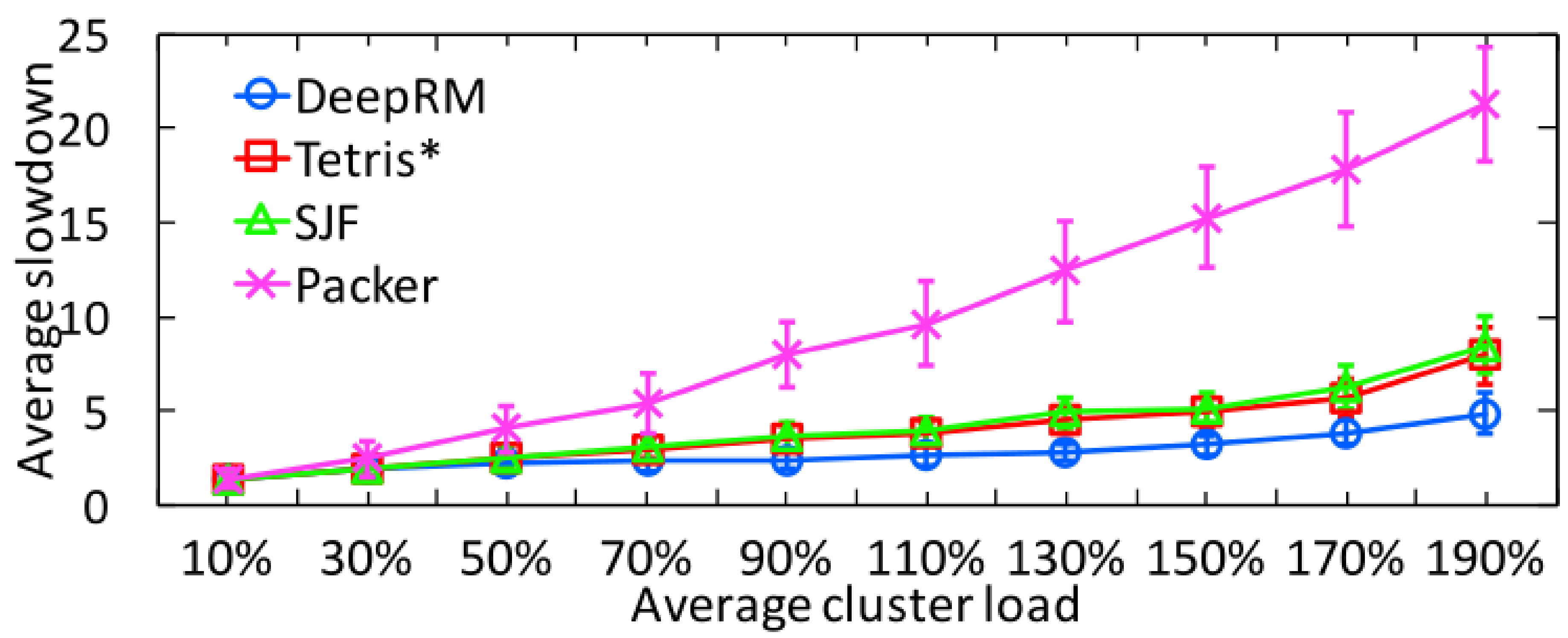


Figure 4: Job slowdown at different levels of load.

- REINFORCE with baseline can be used to allocate resources (CPU cores, memory, etc) when scheduling jobs on a cloud of compute servers.
- The policy is approximated by a shallow NN (one hidden layer with 20 neurons).
- The state space is the current occupancy of the cluster as well as the job waiting list.
- The action space is sending a job to a particular resource.
- The reward is the negative **job slowdown**: how much longer the job needs to complete compared to the optimal case.
- DeepRM outperforms all alternative job schedulers.

Mao, H., Alizadeh, M., Menache, I., and Kandula, S. (2016). Resource Management with Deep Reinforcement Learning. HotNets '16 doi:10.1145/3005745.3005750.

3 - Policy Gradient Theorem

Policy Gradient Methods for Reinforcement Learning with Function Approximation

Richard S. Sutton, David McAllester, Satinder Singh, Yishay Mansour
AT&T Labs – Research, 180 Park Avenue, Florham Park, NJ 07932

Sutton, R. S., McAllester, D., Singh, S., and Mansour, Y. (1999). Policy gradient methods for reinforcement learning with function approximation. NIPS.

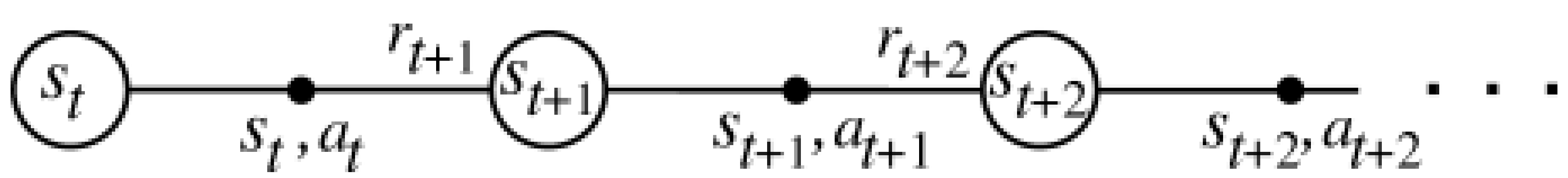
Policy Gradient

- The REINFORCE gradient estimate is the following:

$$\nabla_\theta \mathcal{J}(\theta) = \mathbb{E}_{\tau \sim \rho_\theta}[\sum_{t=0}^T \nabla_\theta \log \pi_\theta(s_t, a_t) \, R(\tau)] = \mathbb{E}_{\tau \sim \rho_\theta}[\sum_{t=0}^T (\nabla_\theta \log \pi_\theta(s_t, a_t)) \, (\sum_{t'=0}^T \gamma^{t'} \, r_{t'+1})]$$

- For each state-action pair (s_t, a_t) encountered during the episode, the gradient of the log-policy is multiplied by the complete return of the episode:

$$R(\tau) = \sum_{t'=0}^T \gamma^{t'} \, r_{t'+1}$$



- The **causality principle** states that rewards obtained before time t are not caused by that action.
- The policy gradient can be rewritten as:

$$\nabla_\theta \mathcal{J}(\theta) = \mathbb{E}_{\tau \sim \rho_\theta}[\sum_{t=0}^T \nabla_\theta \log \pi_\theta(s_t, a_t) \, (\sum_{t'=t}^T \gamma^{t'-t} \, r_{t'+1})] = \mathbb{E}_{\tau \sim \rho_\theta}[\sum_{t=0}^T \nabla_\theta \log \pi_\theta(s_t, a_t) \, R_t]$$

Sutton, R. S., McAllester, D., Singh, S., and Mansour, Y. (1999). Policy gradient methods for reinforcement learning with function approximation. NIPS.

Policy Gradient

- The return at time t (**reward-to-go**) multiplies the gradient of the log-likelihood of the policy (the **score**) for each transition in the episode:

$$\nabla_\theta \mathcal{J}(\theta) = \mathbb{E}_{\tau \sim \rho_\theta}[\sum_{t=0}^T \nabla_\theta \log \pi_\theta(s_t, a_t) \, R_t]$$

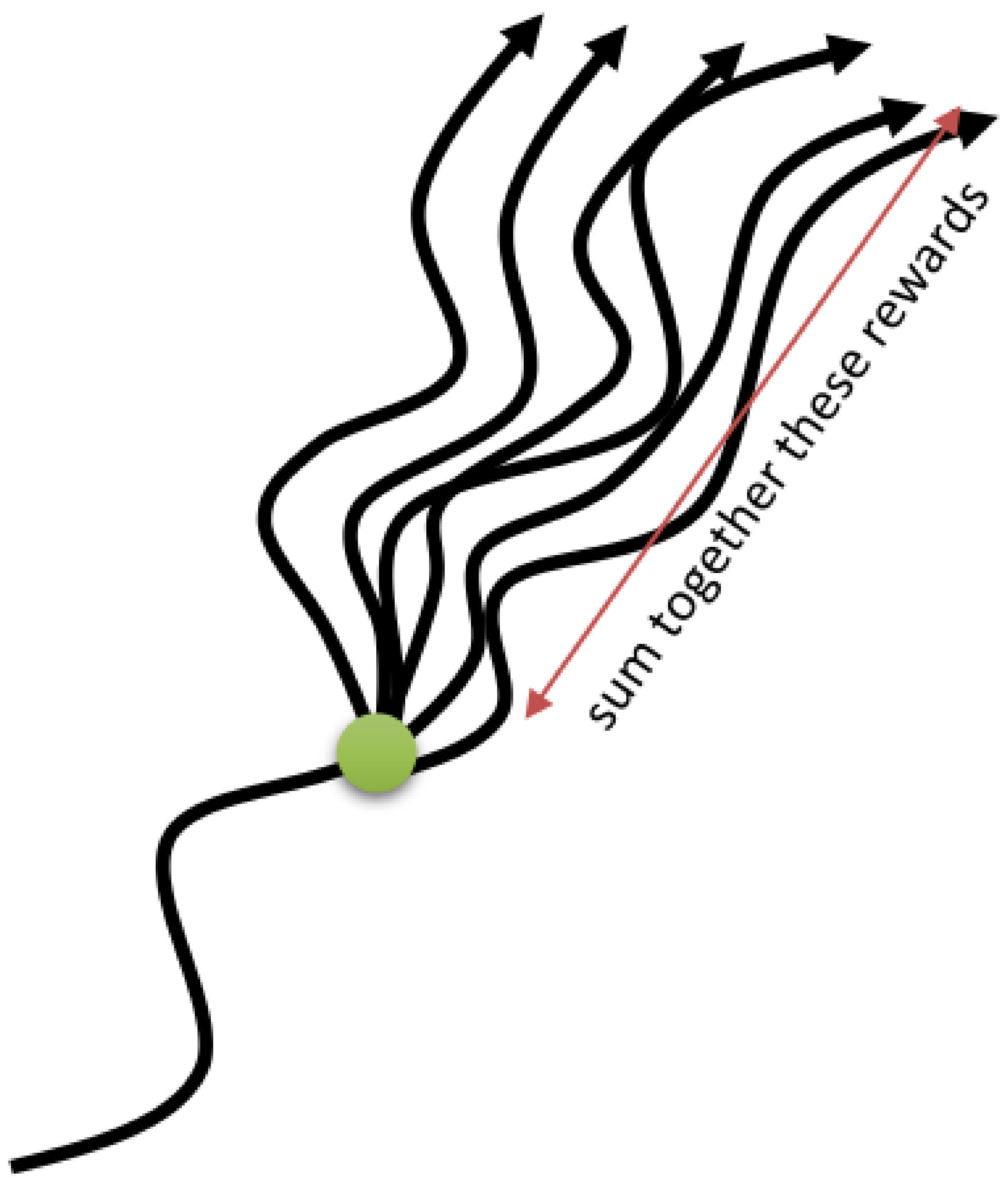
- As we have:

$$Q^\pi(s, a) = \mathbb{E}_\pi[R_t | s_t = s; a_t = a]$$

we can replace R_t with $Q^{\pi_\theta}(s_t, a_t)$ without introducing any bias:

$$\nabla_\theta \mathcal{J}(\theta) = \mathbb{E}_{\tau \sim \rho_\theta}[\sum_{t=0}^T \nabla_\theta \log \pi_\theta(s_t, a_t) \, Q^{\pi_\theta}(s_t, a_t)]$$

- This is true on average (no bias if the Q-value estimates are correct) and has a much lower variance!



Sutton, R. S., McAllester, D., Singh, S., and Mansour, Y. (1999). Policy gradient methods for reinforcement learning with function approximation. NIPS.

Policy Gradient

- The policy gradient is defined over complete trajectories:

$$\nabla_\theta \mathcal{J}(\theta) = \mathbb{E}_{\tau \sim \rho_\theta}[\sum_{t=0}^T \nabla_\theta \log \pi_\theta(s_t, a_t) \, Q^{\pi_\theta}(s_t, a_t)]$$

- However, $\nabla_\theta \log \pi_\theta(s_t, a_t) \, Q^{\pi_\theta}(s_t, a_t)$ now only depends on (s_t, a_t), not the future nor the past.
- Each step of the episode is now independent from each other (if we have the Markov property).
- We can then **sample single transitions** instead of complete episodes:

$$\nabla_\theta \mathcal{J}(\theta) \propto \mathbb{E}_{s \sim \rho_\theta, a \sim \pi_\theta}[\nabla_\theta \log \pi_\theta(s, a) \, Q^{\pi_\theta}(s, a)]$$

- Note that this is not directly the gradient of $\mathcal{J}(\theta)$, as the value of $\mathcal{J}(\theta)$ changes (computed over single transitions instead of complete episodes, so it is smaller), but the gradients both go in the same direction!

Sutton, R. S., McAllester, D., Singh, S., and Mansour, Y. (1999). Policy gradient methods for reinforcement learning with function approximation. NIPS.

Policy Gradient Theorem

> For any MDP, the policy gradient is:

$$g = \nabla_\theta \mathcal{J}(\theta) = \mathbb{E}_{s\sim\rho_\theta, a\sim\pi_\theta}\left[\nabla_\theta \log \pi_\theta(s,a)\, Q^{\pi_\theta}(s,a)\right]$$

Sutton, R. S., McAllester, D., Singh, S., and Mansour, Y. (1999). Policy gradient methods for reinforcement learning with function approximation. NIPS.

Policy Gradient Theorem with function approximation

- Better yet, (Sutton et al. 1999) showed that we can replace the true Q-value $Q^{\pi_\theta}(s, a)$ by an estimate $Q_\varphi(s, a)$ as long as this one is unbiased:

$$\nabla_\theta \mathcal{J}(\theta) = \mathbb{E}_{s \sim \rho_\theta, a \sim \pi_\theta}[\nabla_\theta \log \pi_\theta(s, a) \, Q_\varphi(s, a)]$$

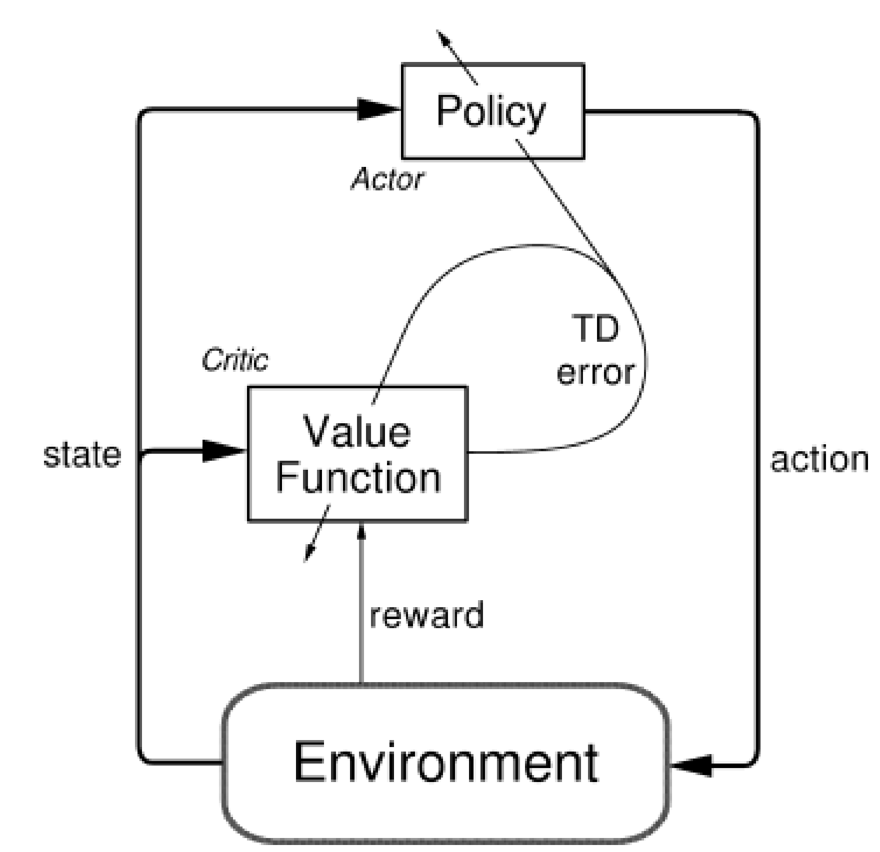
- We only need to have:

$$Q_\varphi(s, a) \approx Q^{\pi_\theta}(s, a) \; \forall s, a$$

- The approximated Q-values can for example minimize the **mean square error** with the true Q-values:

$$\mathcal{L}(\varphi) = \mathbb{E}_{s \sim \rho_\theta, a \sim \pi_\theta}[(Q^{\pi_\theta}(s, a) - Q_\varphi(s, a))^2]$$

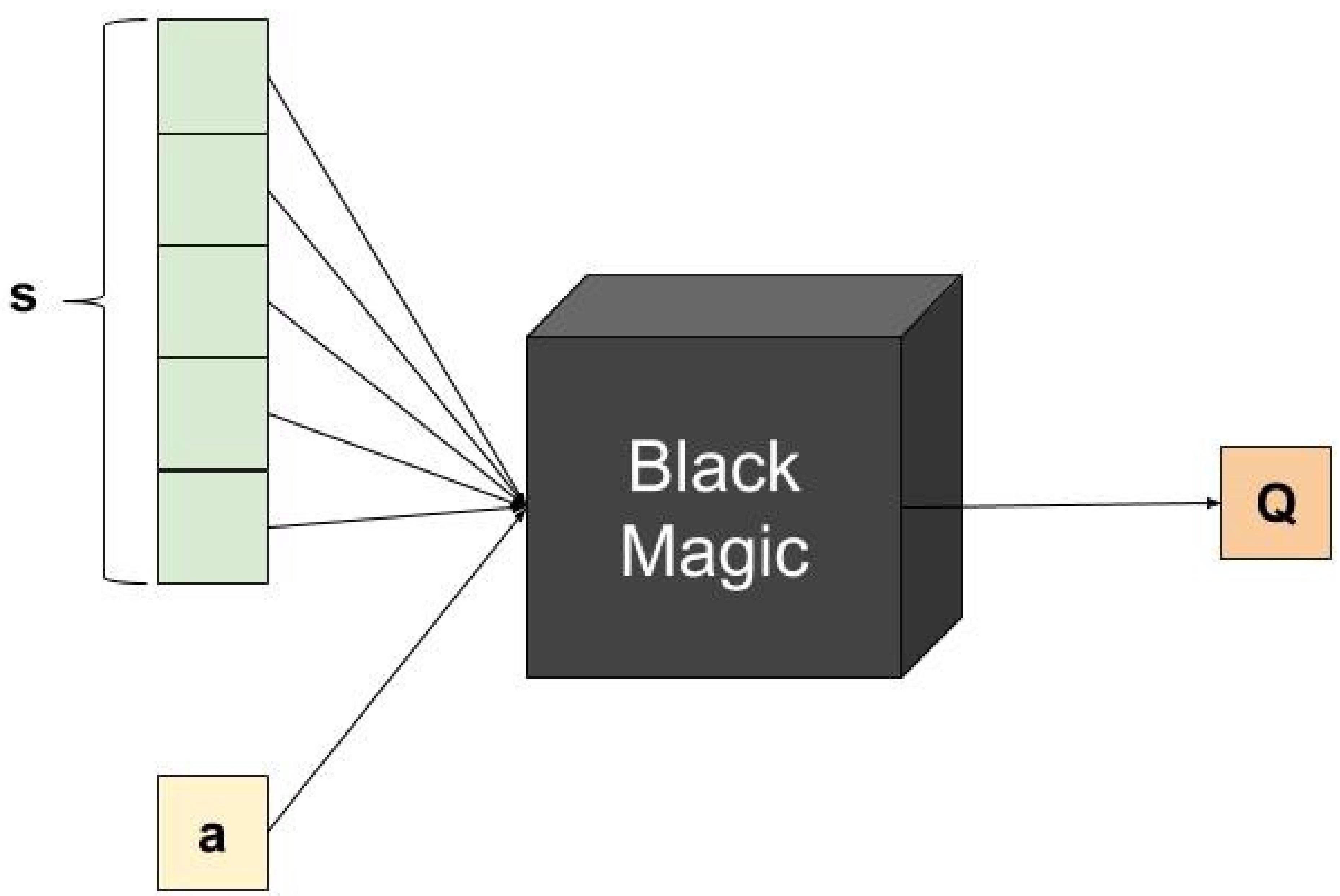
- We obtain an **actor-critic** architecture:
  - the **actor** $\pi_\theta(s, a)$ implements the policy and selects an action a in a state s.
  - the **critic** $Q_\varphi(s, a)$ estimates the value of that action and drives learning in the actor.



Function approximators to learn the Q-values

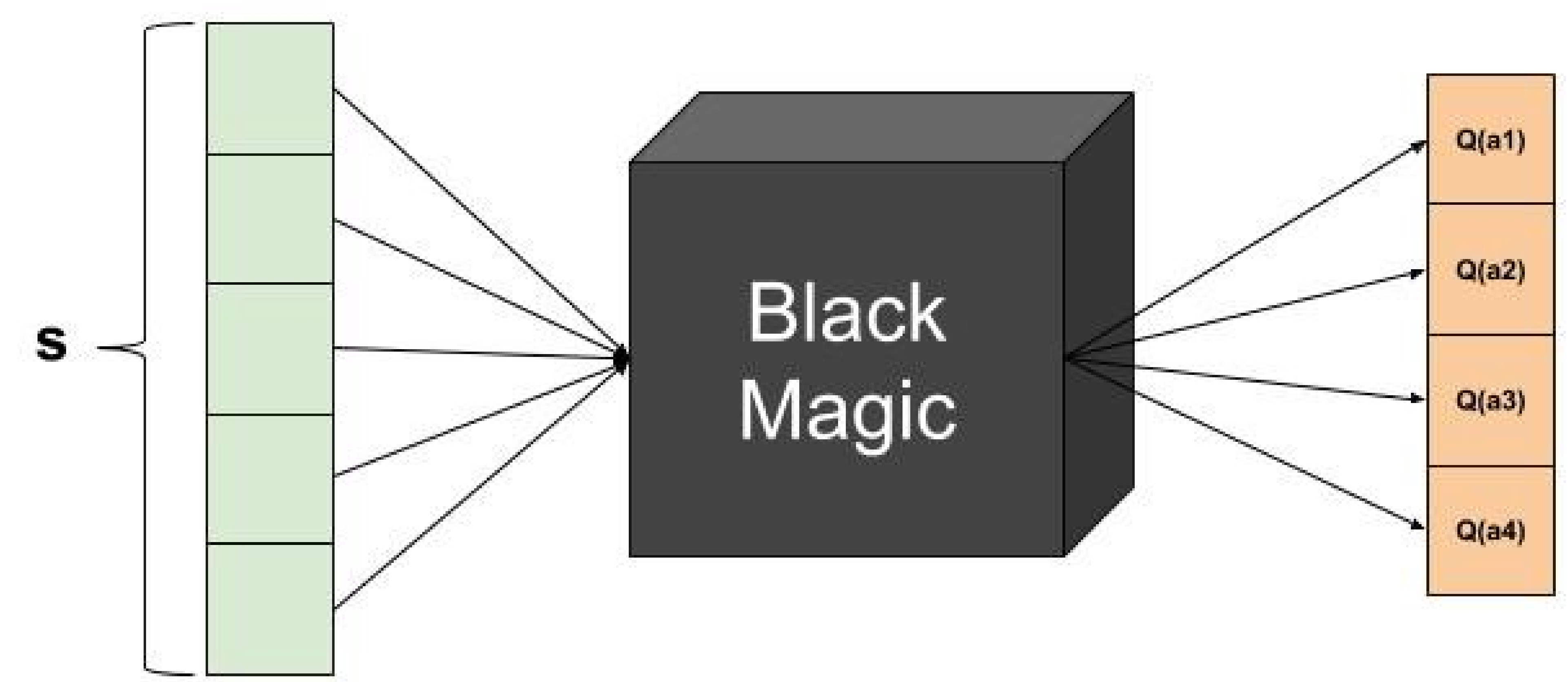
There are two possibilities to approximate Q-values $Q_\theta(s, a)$:

- The DNN approximates the Q-value of a single (s, a) pair.



- The action space can be continuous.

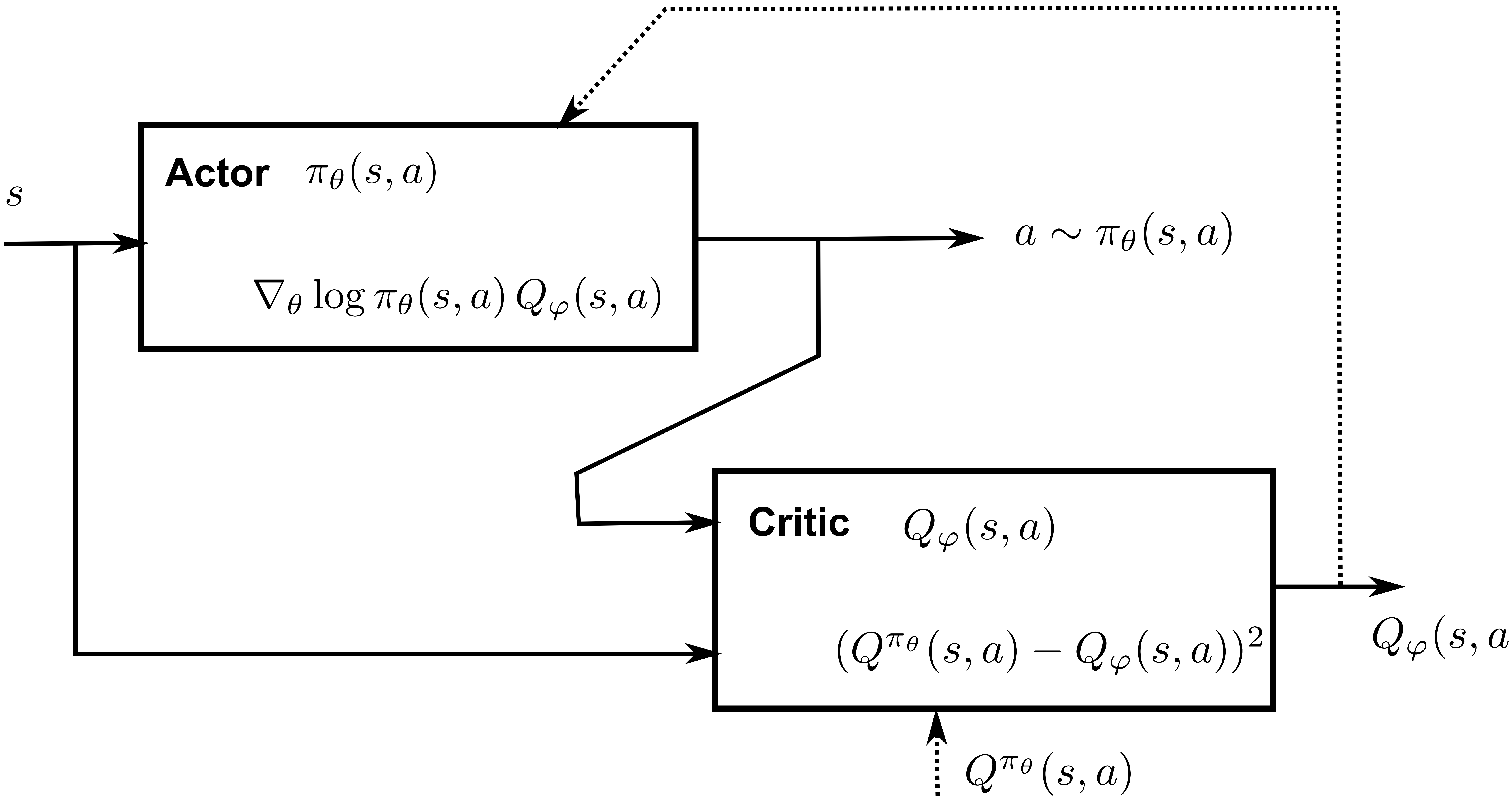
- The DNN approximates the Q-value of all actions a in a state s.



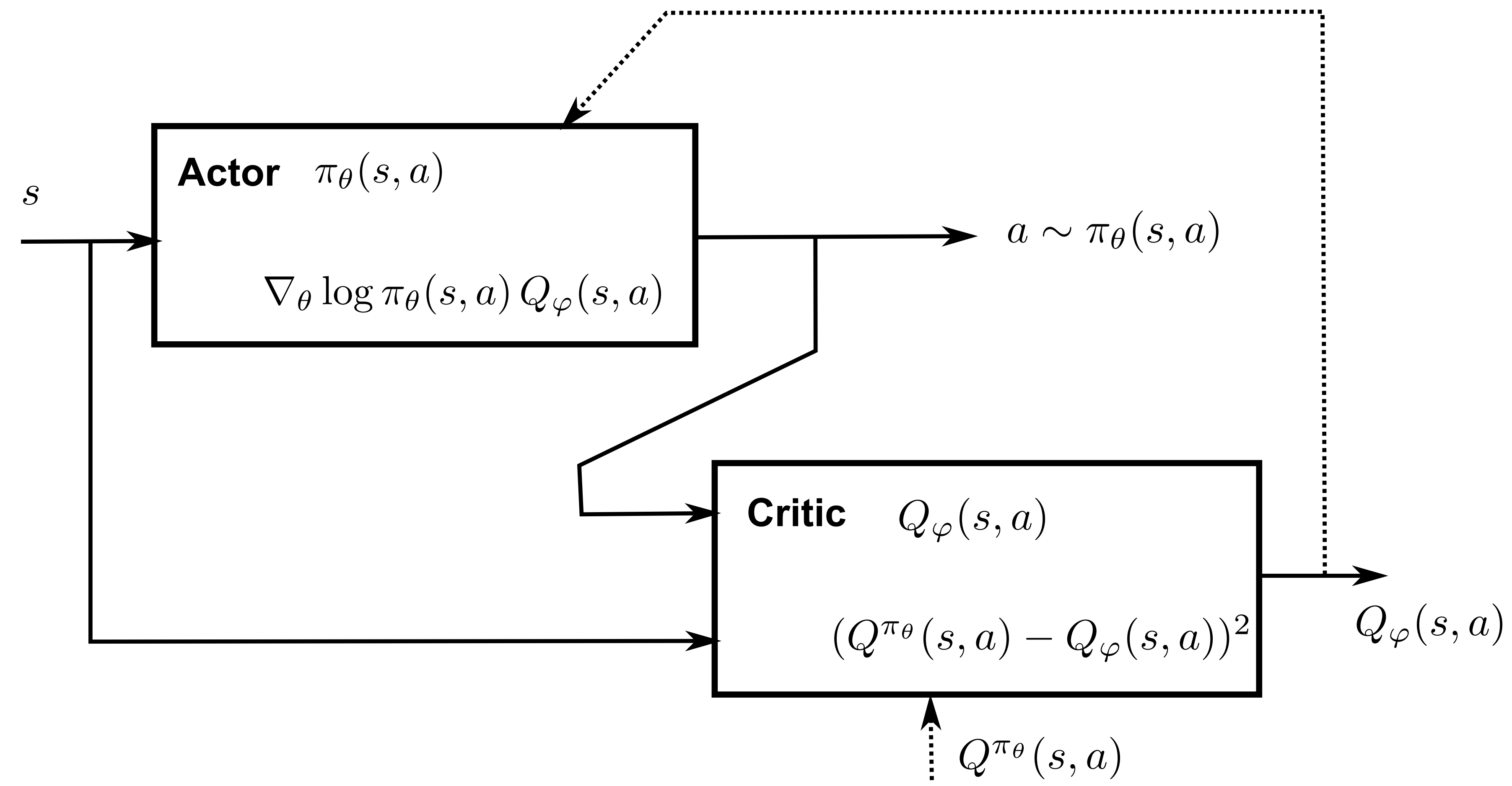
- The action space must be discrete (one neuron per action).

Source: https://towardsdatascience.com/qrash-course-deep-q-networks-from-the-ground-up-1bbda41d3677

Policy Gradient : Actor-critic



Policy Gradient : Actor-critic



- But how to train the critic? We do not know $Q^{\pi_\theta}(s, a)$. As always, we can estimate it through **sampling**:
  - **Monte-Carlo** critic: sampling the complete episode.

$$\mathcal{L}(\varphi) = \mathbb{E}_{s \sim \rho_\theta, a \sim \pi_\theta}[(R(s, a) - Q_\varphi(s, a))^2]$$

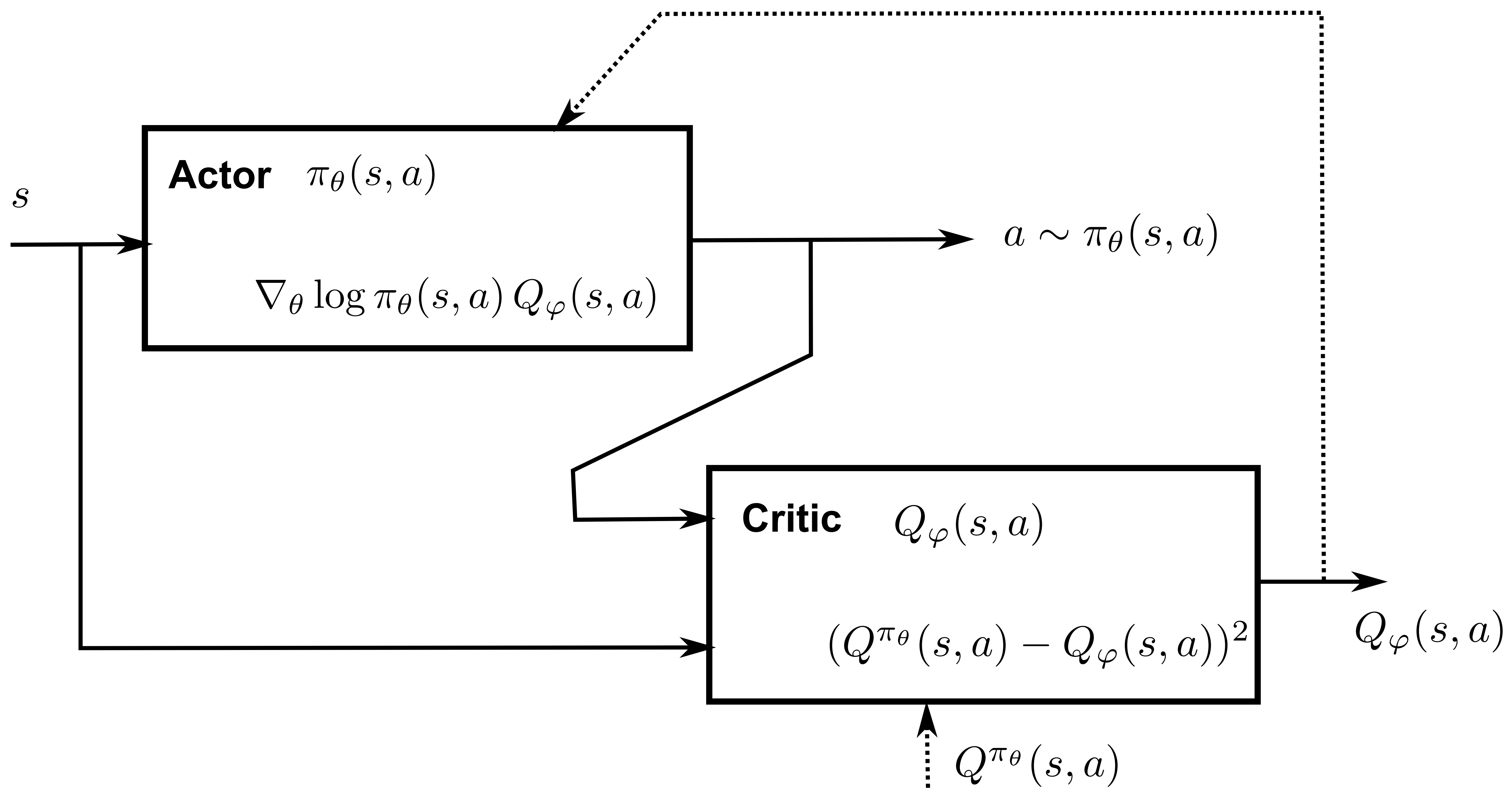
  - **SARSA** critic: sampling (s, a, r, s', a') transitions.

$$\mathcal{L}(\varphi) = \mathbb{E}_{s, s' \sim \rho_\theta, a, a' \sim \pi_\theta}[(r + \gamma\, Q_\varphi(s', a') - Q_\varphi(s, a))^2]$$

  - **Q-learning** critic: sampling (s, a, r, s') transitions.

$$\mathcal{L}(\varphi) = \mathbb{E}_{s, s' \sim \rho_\theta, a \sim \pi_\theta}[(r + \gamma\, \max_{a'} Q_\varphi(s', a') - Q_\varphi(s, a))^2]$$

Policy Gradient : Actor-critic



- The policy gradient (PG) theorem implies an **actor-critic** architecture.
- The **actor** learns using the PG theorem:

$$\nabla_\theta \mathcal{J}(\theta) = \mathbb{E}_{s \sim \rho_\theta, a \sim \pi_\theta}[\nabla_\theta \log \pi_\theta(s, a)\, Q_\varphi(s, a)]$$

- The **critic** learns using Q-learning:

$$\mathcal{L}(\varphi) = \mathbb{E}_{s, s' \sim \rho_\theta, a \sim \pi_\theta}[(r + \gamma \, \max_{a'} Q_\varphi(s', a') - Q_\varphi(s, a))^2]$$

Policy Gradient : reducing the variance

- As with REINFORCE, the PG actor suffers from the **high variance** of the Q-values.
- It is possible to use a **baseline** in the PG without introducing a bias:

$$\nabla_\theta \mathcal{J}(\theta) = \mathbb{E}_{s \sim \rho_\theta, a \sim \pi_\theta}[\nabla_\theta \log \pi_\theta(s, a) \, (Q^{\pi_\theta}(s, a) - b)]$$

- In particular, the **advantage actor-critic** uses the value of a state as the baseline:

$$\nabla_\theta \mathcal{J}(\theta) = \mathbb{E}_{s \sim \rho_\theta, a \sim \pi_\theta}[\nabla_\theta \log \pi_\theta(s, a) \, (Q^{\pi_\theta}(s, a) - V^{\pi_\theta}(s))]$$

$$= \mathbb{E}_{s \sim \rho_\theta, a \sim \pi_\theta}[\nabla_\theta \log \pi_\theta(s, a) \, A^{\pi_\theta}(s, a)]$$

- The critic can either:
  - learn to approximate both $Q^{\pi_\theta}(s, a)$ and $V^{\pi_\theta}(s)$ with two different NN (SAC).
  - replace one of them with a sampling estimate (A3C, DDPG)
  - learn the advantage $A^{\pi_\theta}(s, a)$ directly (GAE, PPO)

Many variants of the Policy Gradient

- **Policy Gradient methods** can take many forms :

$$\nabla_\theta J(\theta) = \mathbb{E}_{s_t \sim \rho_\theta, a_t \sim \pi_\theta}[\nabla_\theta \log \pi_\theta (s_t, a_t) \, \psi_t]$$

where:

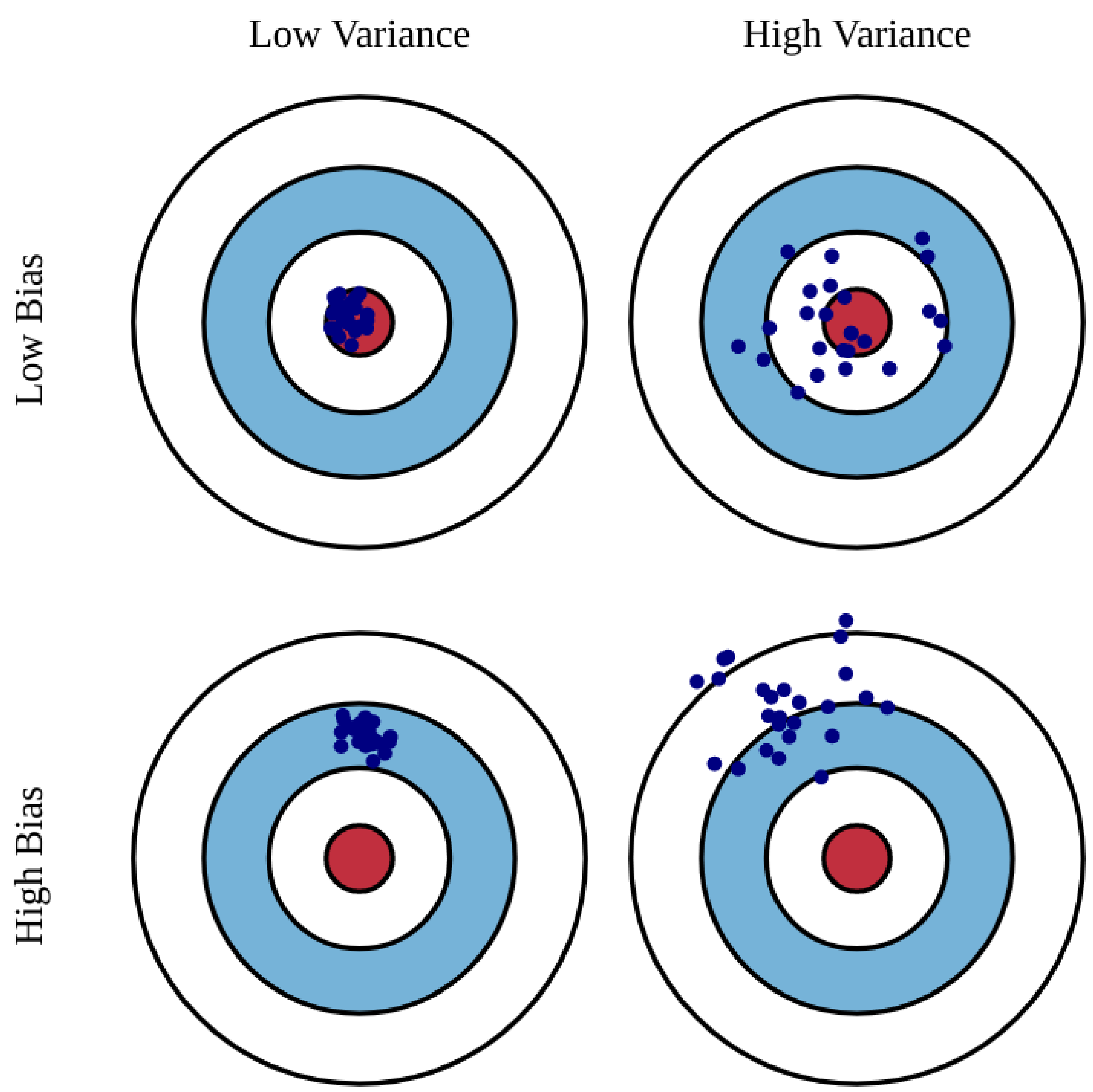
- $\psi_t = R_t$ is the *REINFORCE* algorithm (MC sampling).
- $\psi_t = R_t - b$ is the *REINFORCE with baseline* algorithm.
- $\psi_t = Q^\pi(s_t, a_t)$ is the *policy gradient theorem*.
- $\psi_t = A^\pi(s_t, a_t) = Q^\pi(s_t, a_t) - V^\pi(s_t)$ is the *advantage actor-critic*.
- $\psi_t = r_{t+1} + \gamma \, V^\pi(s_{t+1}) - V^\pi(s_t)$ is the *TD actor-critic*.
- $\psi_t = \displaystyle\sum_{k=0}^{n-1} \gamma^k \, r_{t+k+1} + \gamma^n \, V^\pi(s_{t+n}) - V^\pi(s_t)$ is the *n-step advantage*.

and many others…

Bias and variance of Policy Gradient methods

- The different variants of PG deal with the bias/variance trade-off.

$$\nabla_\theta J(\theta) = \mathbb{E}_{s_t \sim \rho_\theta, a_t \sim \pi_\theta}[\nabla_\theta \log \pi_\theta (s_t, a_t) \, \psi_t]$$



1. the more ψ_t relies on **sampled rewards** (e.g. R_t), the more the gradient will be correct on average (small bias), but the more it will vary (high variance).
    - This increases the sample complexity: we need to average more samples to correctly estimate the gradient.
2. the more ψ_t relies on **estimations** (e.g. the TD error), the more stable the gradient (small variance), but the more incorrect it is (high bias).
    - This can lead to suboptimal policies, i.e. local optima of the objective function.

- All the methods we will see in the rest of the course are attempts at finding the best trade-off.