UNIVERSITY OF TECHNOLOGY
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CHEMNITZ

Deep Reinforcement Learning

Function approximation

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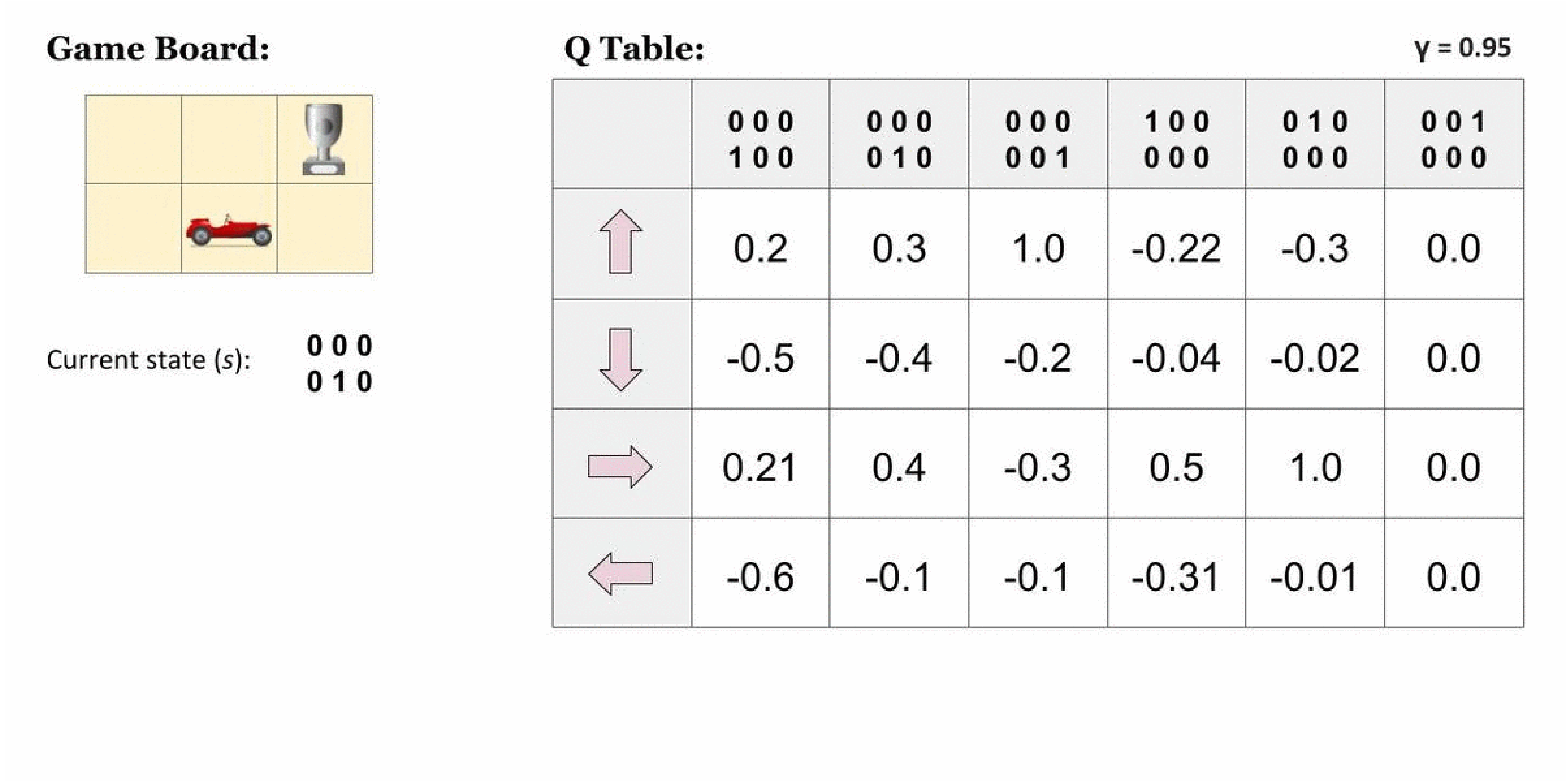
https://tu-chemnitz.de/informatik/KI/edu/deeprl

1 - Limits of tabular RL

Tabular reinforcement learning

- All the methods seen so far belong to **tabular RL**.
- Q-learning necessitates to store in a **Q-table** one Q-value per state-action pair (s, a).

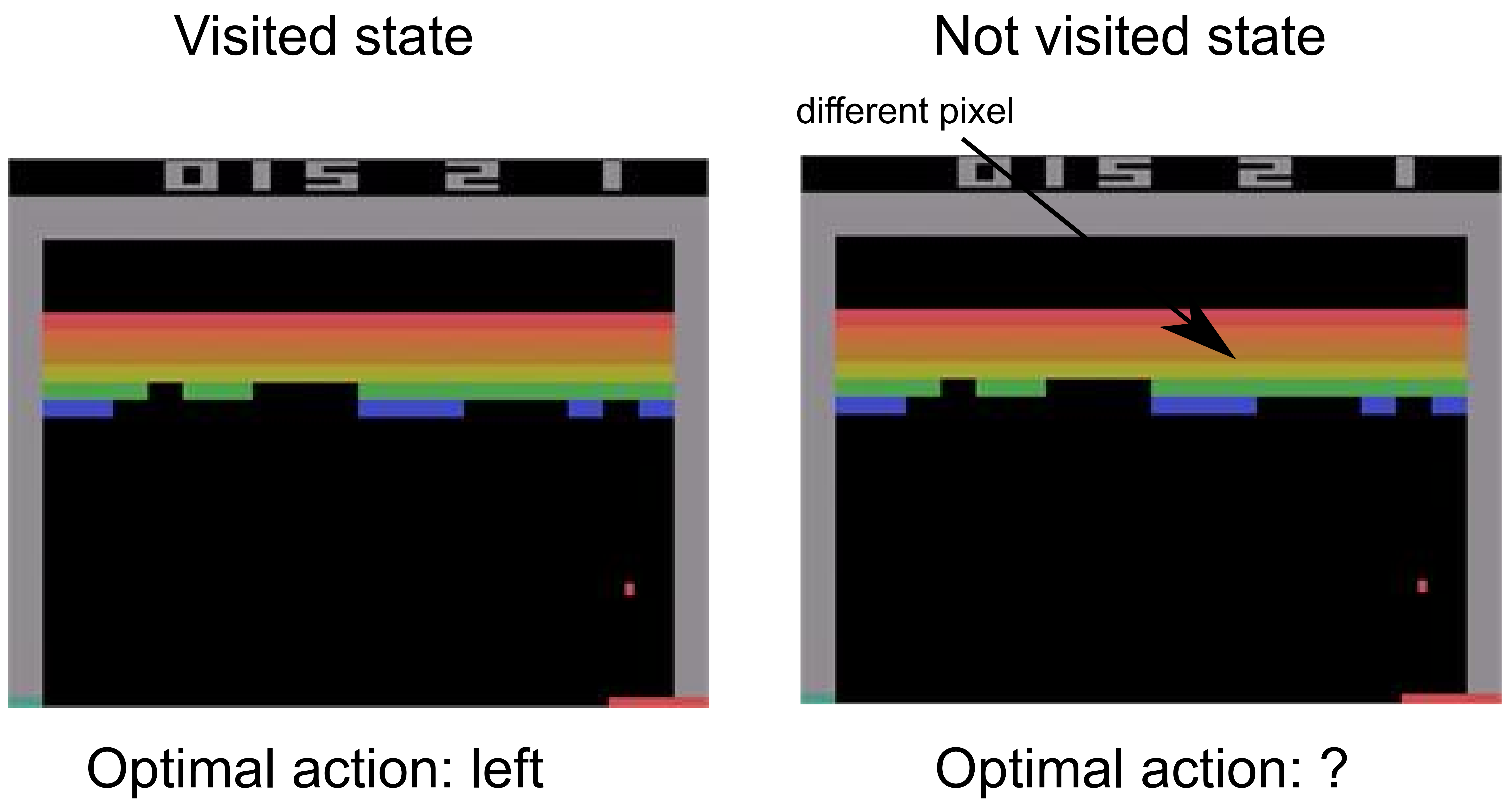


	000 100	000 010	000 001	100 000	010 000	001 000
↑	0.2	0.3	1.0	-0.22	-0.3	0.0
↓	-0.5	-0.4	-0.2	-0.04	-0.02	0.0
→	0.21	0.4	-0.3	0.5	1.0	0.0
←	-0.6	-0.1	-0.1	-0.31	-0.01	0.0

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

Tabular reinforcement learning

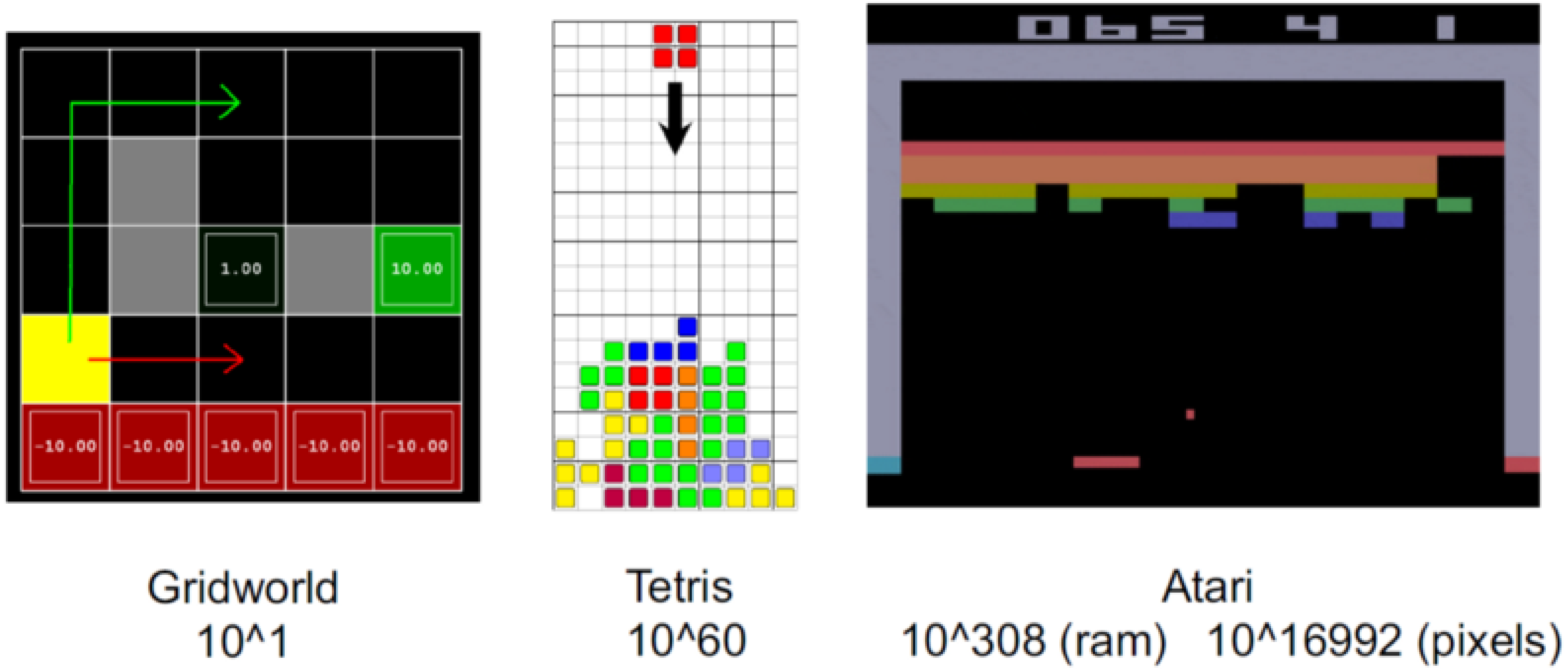
- If a state has never been visited during learning, the Q-values will still be at their initial value (0.0), no policy can be derived.



- Similar states likely have the same optimal action: we want to be able to **generalize** the policy between states.

Tabular reinforcement learning

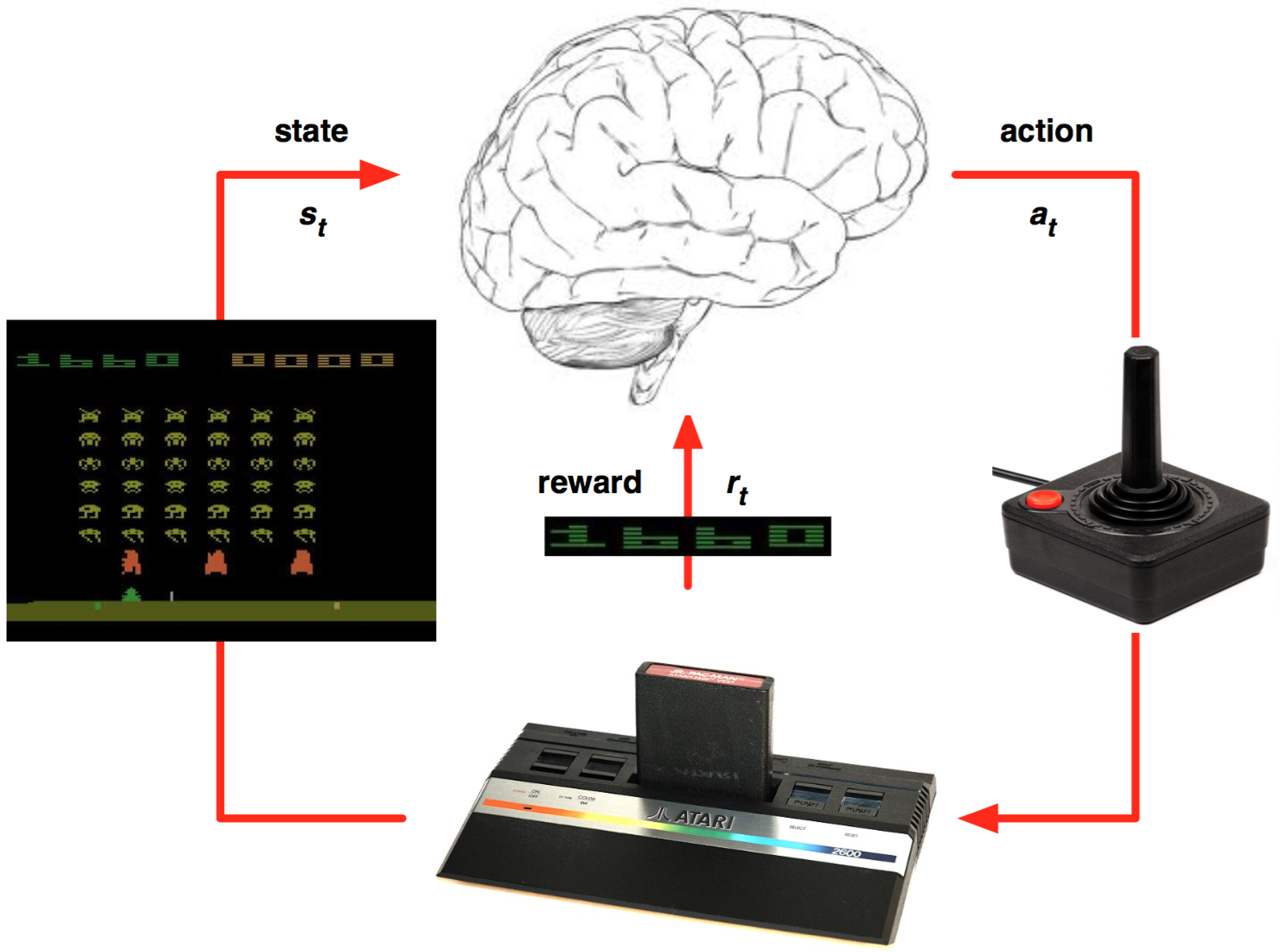
- For most realistic problems, the size of the Q-table becomes quickly untractable.



Source: https://medium.com/@twt446/a-summary-of-deep-reinforcement-learning-rl-bootcamp-lecture-2-c3a15db5934e

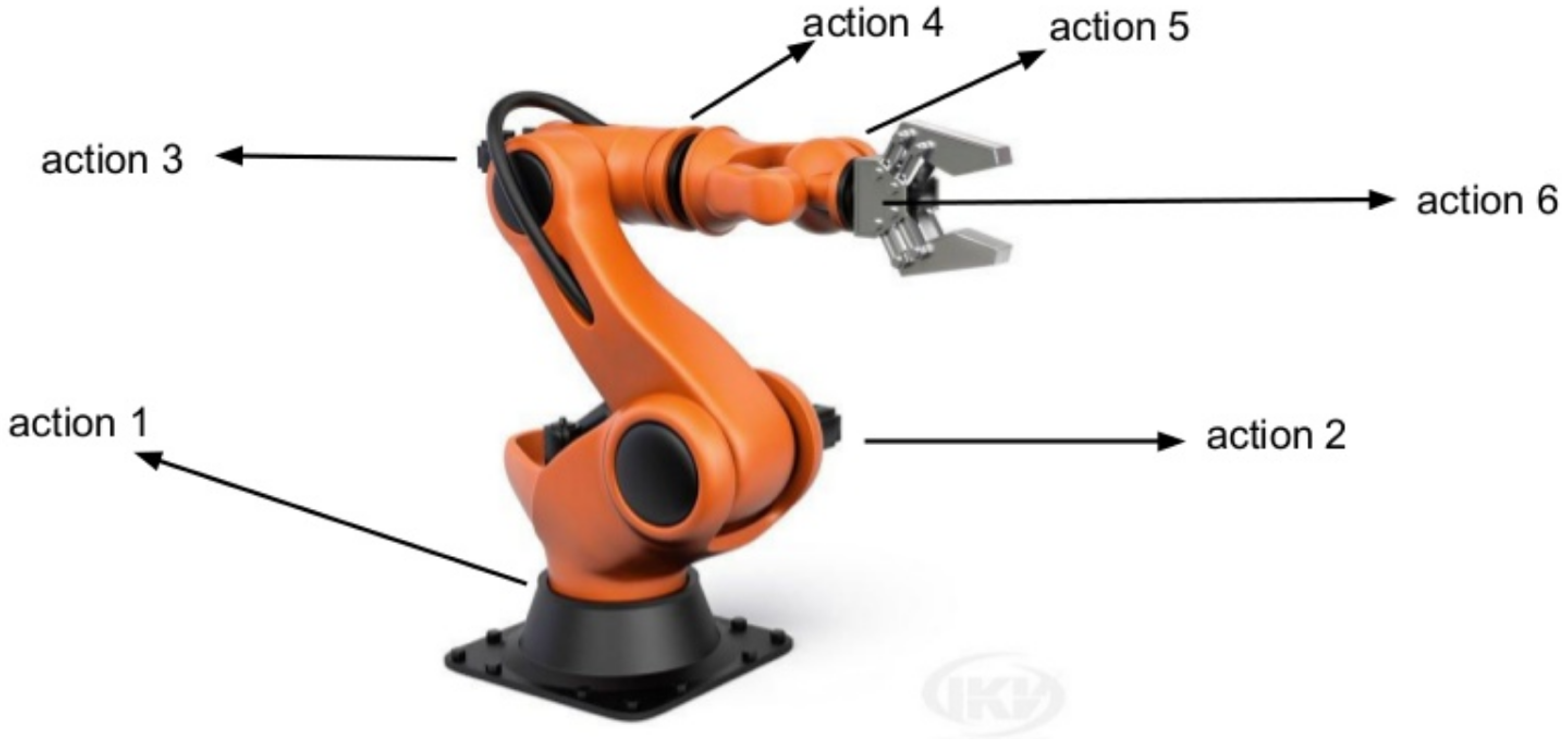
- If you use black-and-white 256x256 images as inputs, you have $2^{256 * 256} = 10^{19728}$ possible states!
- **Tabular RL** is limited to toy problems.

Tabular RL cannot learn to play video games



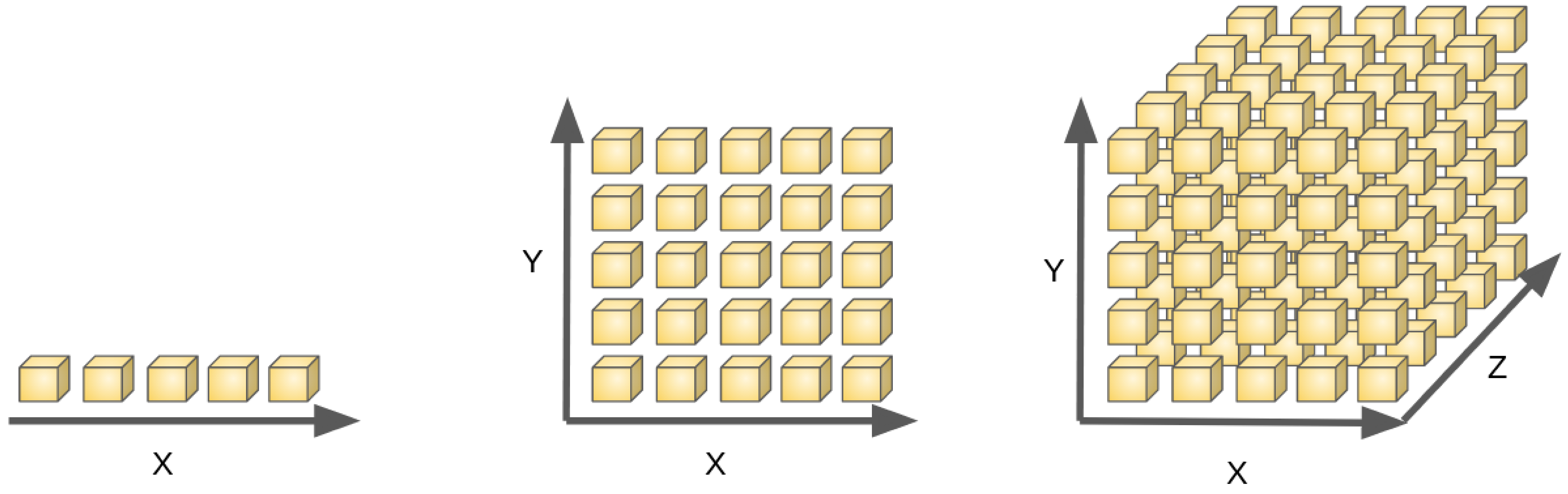
Continuous action spaces

- Tabular RL only works for small **discrete action spaces**.
- Robots have **continuous action spaces**, where the actions are changes in **joint angles** or **torques**.
- A joint angle could take any value in $[0, \pi]$.



Continuous action spaces

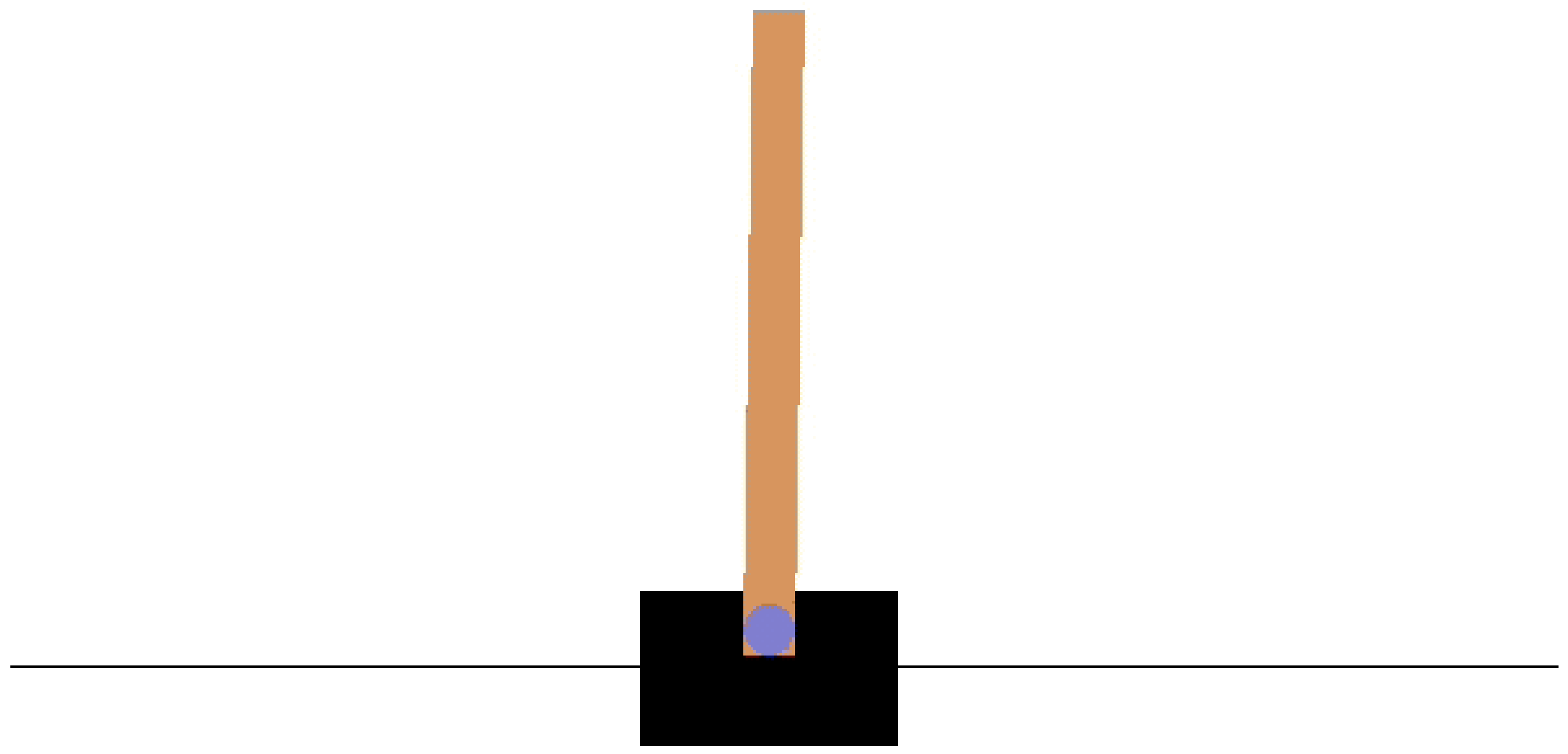
- A solution would be to **discretize** the action space (one action per degree), but we would fall into the **curse of dimensionality**.



- The more degrees of freedom, the more discrete actions, the more entries in the Q-table…
- Tabular RL cannot deal with continuous action spaces, unless we approximate the policy with an **actor-critic** architecture.

2 - Function approximation

Feature vectors



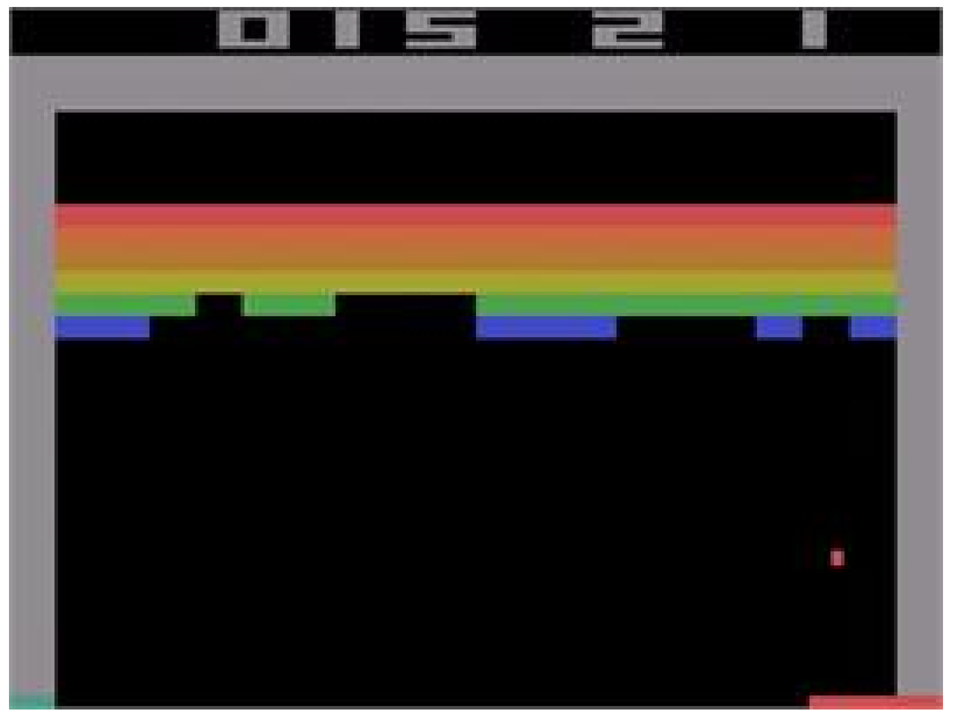
- Let's represent a state s by a vector of d **features** $\phi(s) = [\phi_1(s), \phi_2(s), \ldots, \phi_d(s)]^T$.
- For the cartpole, the feature vector would be:

$$\phi(s) = \begin{bmatrix} x \\ \dot{x} \\ \theta \\ \dot{\theta} \end{bmatrix}$$

- x is the position, θ the angle, $\dot{x}$ and $\dot{\theta}$ their derivatives.
- We are able to represent **any state** s using these four variables.

Feature vectors

- For more complex problems, the feature vector should include all the necessary information (Markov property).



$$\phi(s) = \begin{bmatrix} x \text{ position of the paddle} \\ x \text{ position of the ball} \\ y \text{ position of the ball} \\ x \text{ speed of the ball} \\ y \text{ speed of the position} \\ \text{presence of brick 1} \\ \text{presence of brick 2} \\ \vdots \end{bmatrix}$$

- In deep RL, we will **learn** these feature vectors, but let’s suppose for now that we have them.

Feature vectors

- Note that we can always fall back to the tabular case using **one-hot encoding** of the states:

$$\phi(s_1) = \begin{bmatrix} 1 \\ 0 \\ 0 \\ \ldots \\ 0 \end{bmatrix} \qquad \phi(s_2) = \begin{bmatrix} 0 \\ 1 \\ 0 \\ \ldots \\ 0 \end{bmatrix} \qquad \phi(s_3) = \begin{bmatrix} 0 \\ 0 \\ 1 \\ \ldots \\ 0 \end{bmatrix} \qquad \ldots$$

- But the idea is that we can represent states with much less values than the number of states:

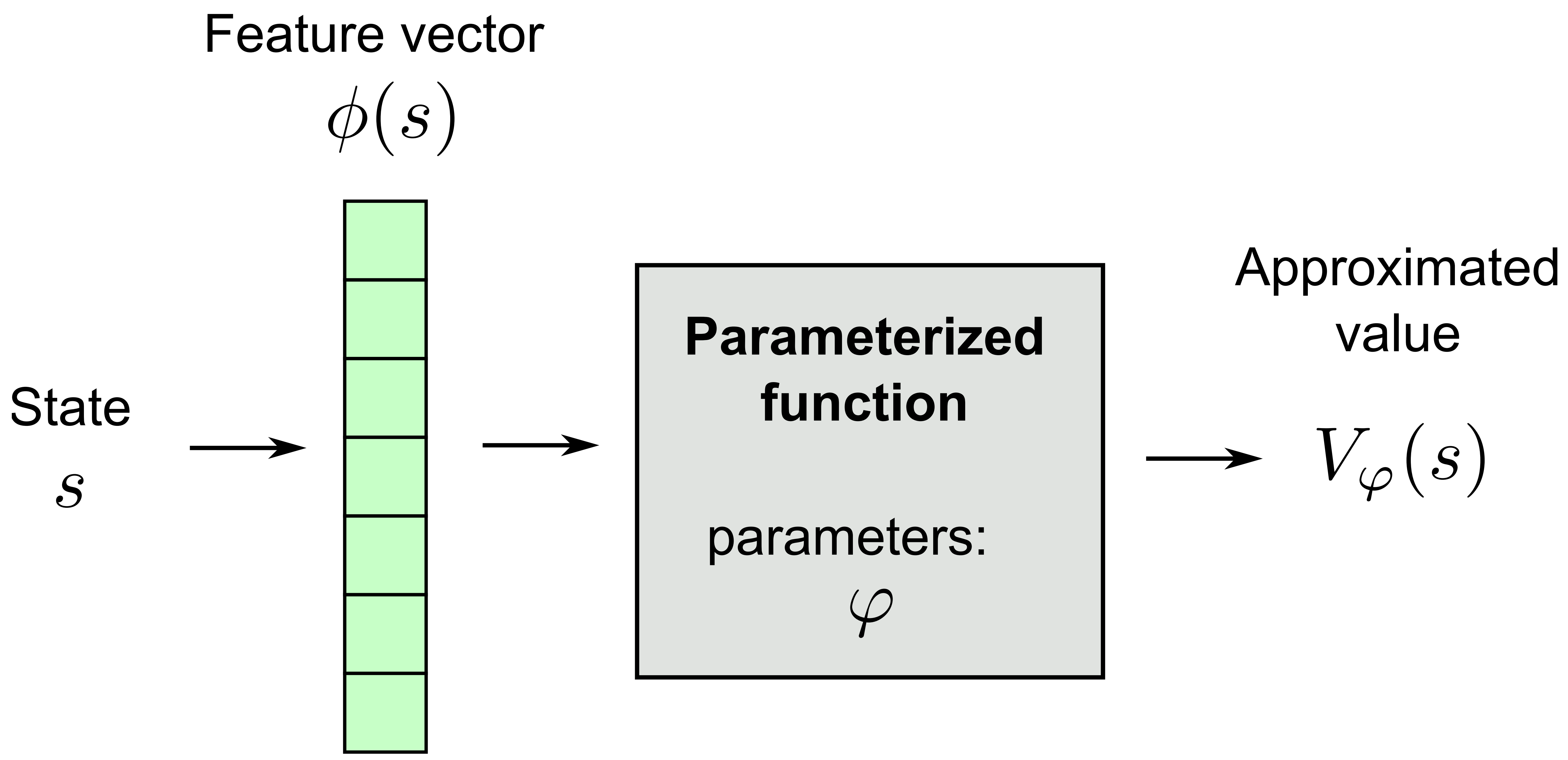
$$d \ll |\mathcal{S}|$$

- We can also represent **continuous state spaces** with feature vectors.

State value approximation

- In **state value approximation**, we want to approximate the state value function $V^\pi(s)$ with a **parameterized function** $V_\varphi(s)$:

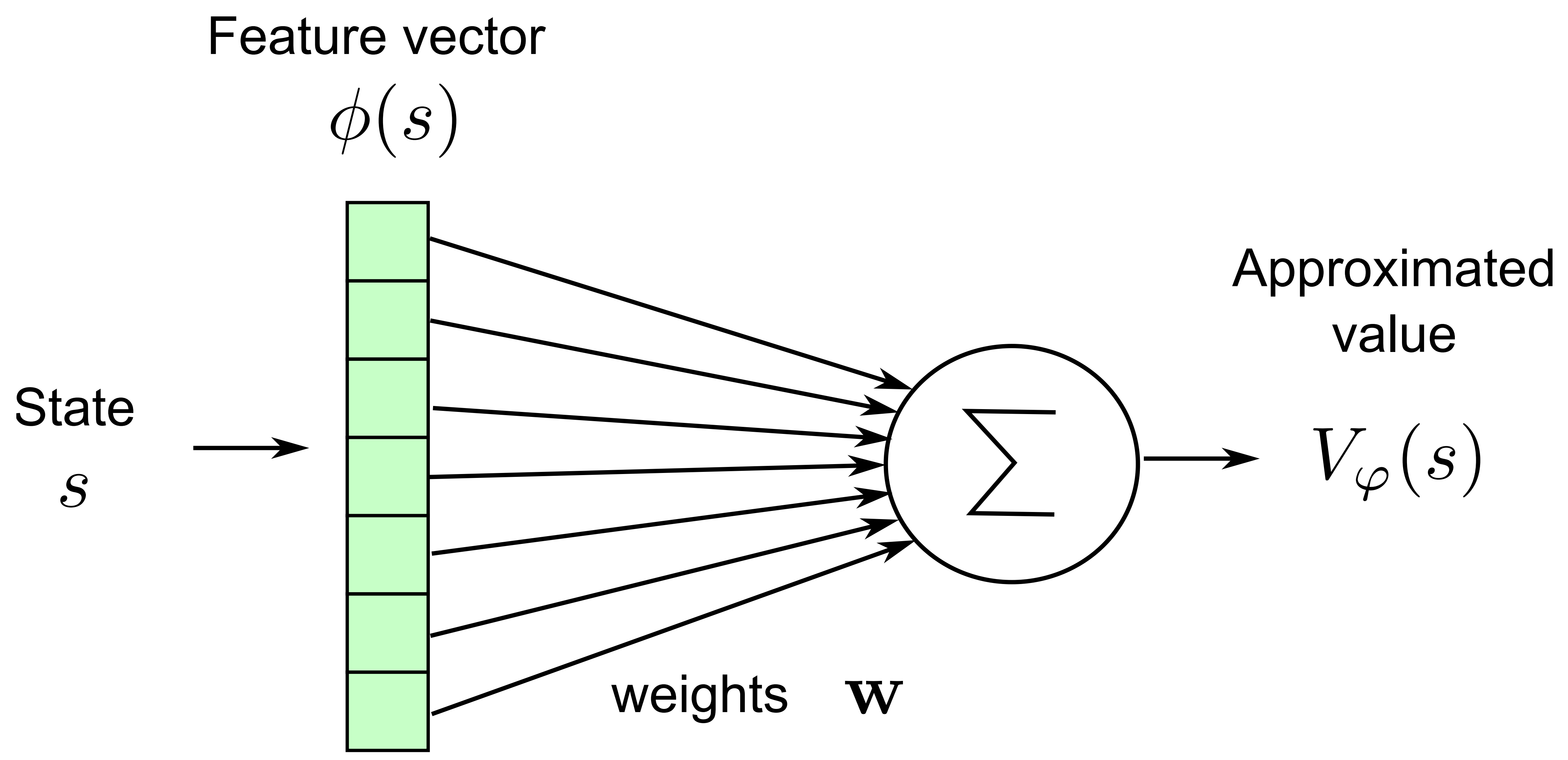
$$V_\varphi(s) \approx V^\pi(s)$$



- The parameterized function can have any form. Its has a set of parameters φ used to transform the feature vector $\phi(s)$ into an approximated value $V_\varphi(s)$.

Linear approximation of state value functions

- The simplest function approximator (FA) is the **linear approximator**.

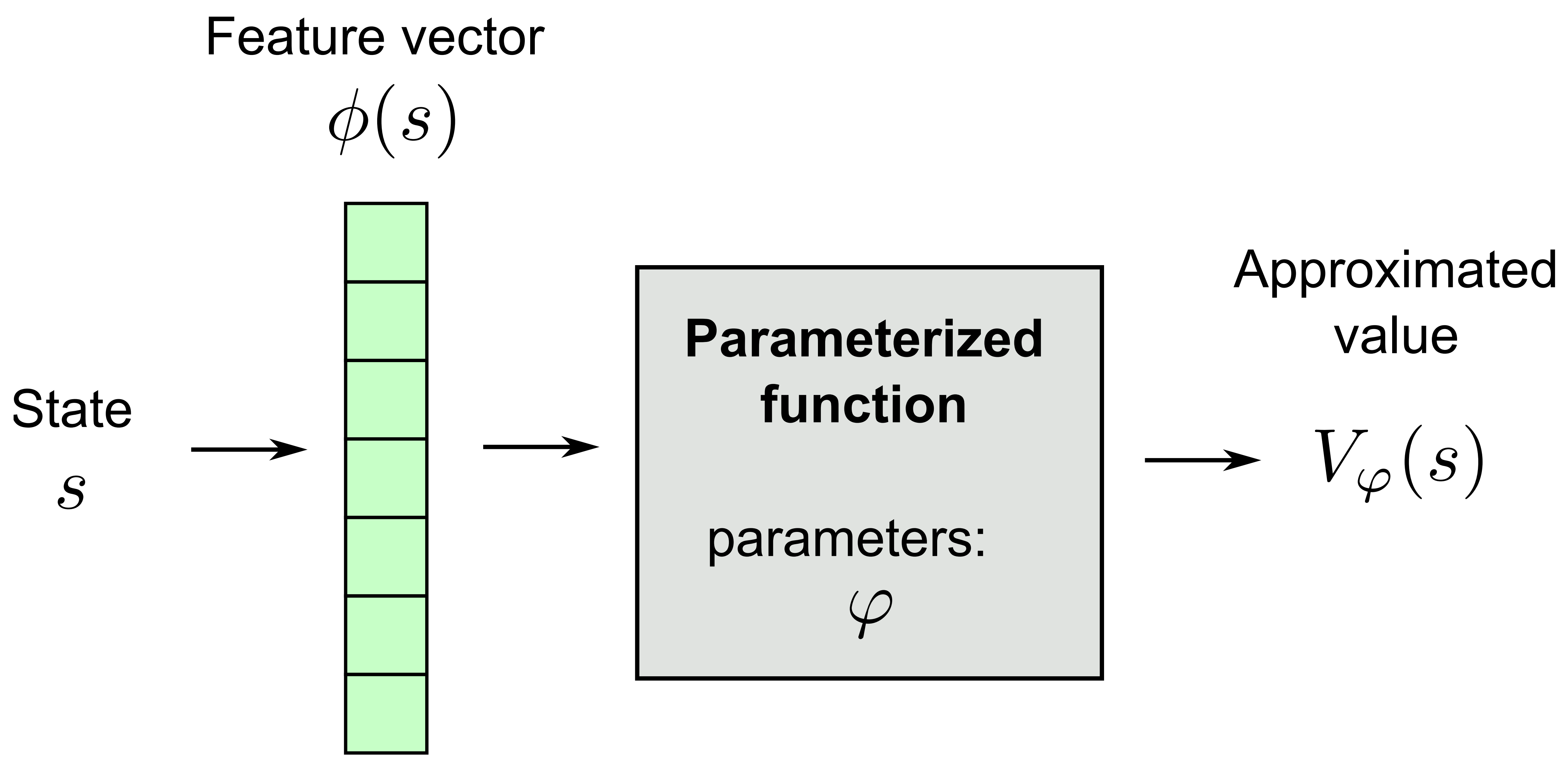


- The approximated value is a linear combination of the features:

$$V_\varphi(s) = \sum_{i=1}^d w_i \, \phi_i(s) = \mathbf{w}^T \times \phi(s)$$

- The **weight vector** $\mathbf{w} = [w_1, w_2, \ldots, w_d]^T$ is the set of parameters φ of the function.
- A linear approximator is a single **artificial neuron** (linear regression) without a bias.

Learning the state value approximation



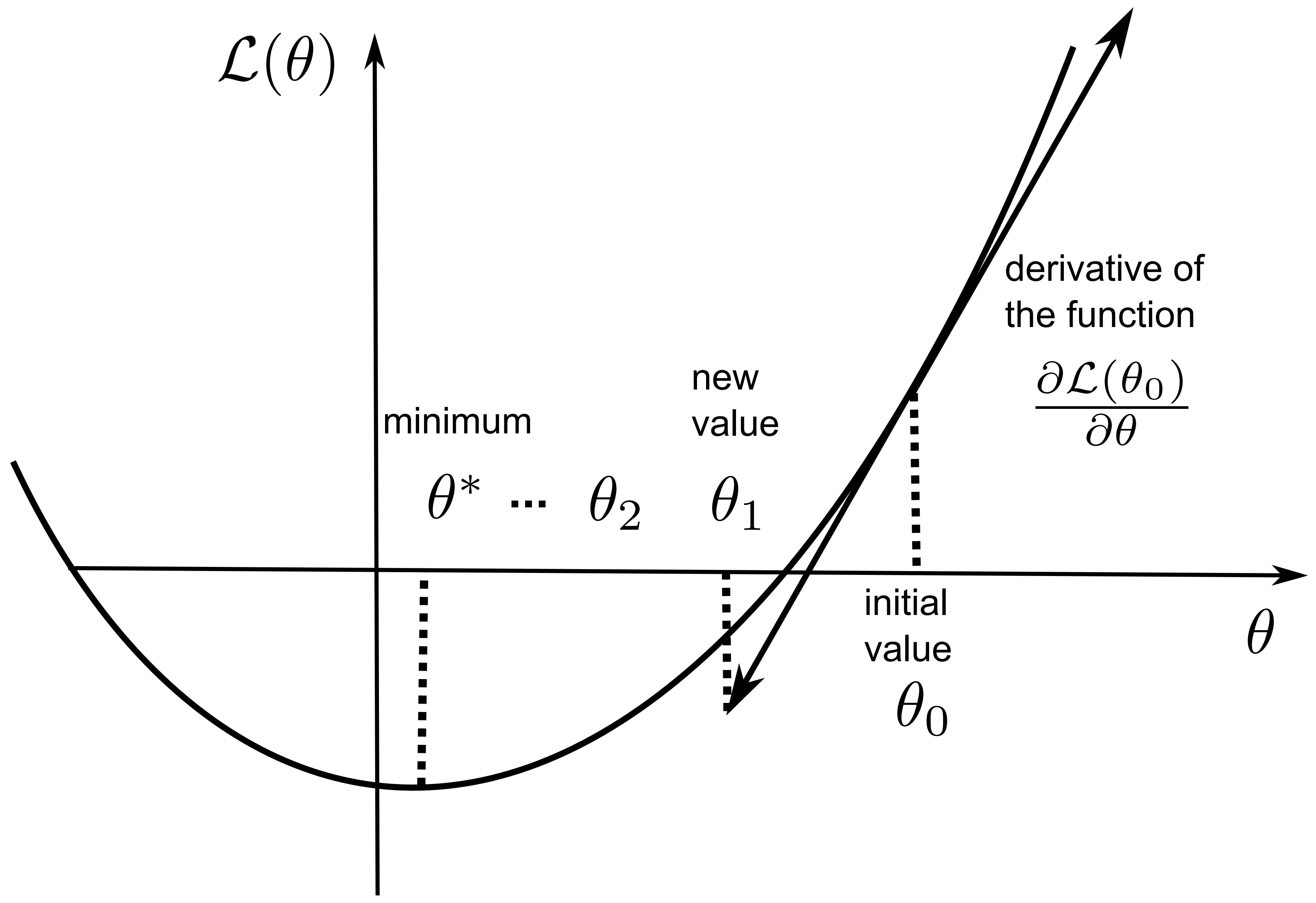
- Regardless the form of the function approximator, we want to find the parameters φ making the approximated values $V_\varphi(s)$ as close as possible from the true values $V^\pi(s)$ for all states s.
  - This is a **regression** problem.
- We want to minimize the **mean-square error** between the two quantities:

$$\min_\varphi \mathcal{L}(\varphi) = \mathbb{E}_{s \in \mathcal{S}}[(V^\pi(s) - V_\varphi(s))^2]$$

- The **loss function** $\mathcal{L}(\varphi)$ is minimal when the predicted values are close to the true ones on average.

Learning the state value approximation

- Let's suppose that we know the true state values $V^\pi(s)$ for all states and that the parametrized function is **differentiable**.



$\mathcal{L}(\theta)$
derivative of the function
$\frac{\partial \mathcal{L}(\theta_0)}{\partial \theta}$
minimum
new value
θ^* ... θ_2 θ_1
initial value
θ_0
θ

- We can find the minimum of the loss function by applying **gradient descent** (GD) iteratively:

$$\Delta \varphi = - \eta \, \nabla_\varphi \mathcal{L}(\varphi)$$

- $\nabla_\varphi \mathcal{L}(\varphi)$ is the gradient of the loss function w.r.t to the parameters φ.

$$\nabla_\varphi \mathcal{L}(\varphi) = \begin{bmatrix} \frac{\partial \mathcal{L}(\varphi)}{\partial \varphi_1} \\ \frac{\partial \mathcal{L}(\varphi)}{\partial \varphi_2} \\ \ldots \\ \frac{\partial \mathcal{L}(\varphi)}{\partial \varphi_K} \end{bmatrix}$$

- When applied repeatedly, GD converges to a local minimum of the loss function.

Learning the state value approximation

- To minimize the mean square error,

$$\min_\varphi \mathcal{L}(\varphi) = \mathbb{E}_{s \in \mathcal{S}}[(V^\pi(s) - V_\varphi(s))^2]$$

we will iteratively modify the parameters φ according to:

$$\begin{aligned}
\Delta \varphi = \varphi_{k+1} - \varphi_n & = -\eta \, \nabla_\varphi \mathcal{L}(\varphi) \\
& = -\eta \, \nabla_\varphi \mathbb{E}_{s \in \mathcal{S}}[(V^\pi(s) - V_\varphi(s))^2] \\
& = \mathbb{E}_{s \in \mathcal{S}}[-\eta \, \nabla_\varphi (V^\pi(s) - V_\varphi(s))^2] \\
& = \mathbb{E}_{s \in \mathcal{S}}[\eta \, (V^\pi(s) - V_\varphi(s)) \, \nabla_\varphi V_\varphi(s)]
\end{aligned}$$

- As it would be too slow to compute the expectation on the whole state space (**batch algorithm**), we will sample the quantity:

$$\delta_\varphi = \eta \, (V^\pi(s) - V_\varphi(s)) \, \nabla_\varphi V_\varphi(s)$$

and update the parameters with **stochastic gradient descent** (SGD).

Learning the state value approximation

- Gradient of the mse:

$$\Delta \varphi = \mathbb{E}_{s \in \mathcal{S}} [\eta \, (V^\pi (s) - V_\varphi(s)) \, \nabla_\varphi V_\varphi(s)]$$

- If we sample K states s_i from the state space:

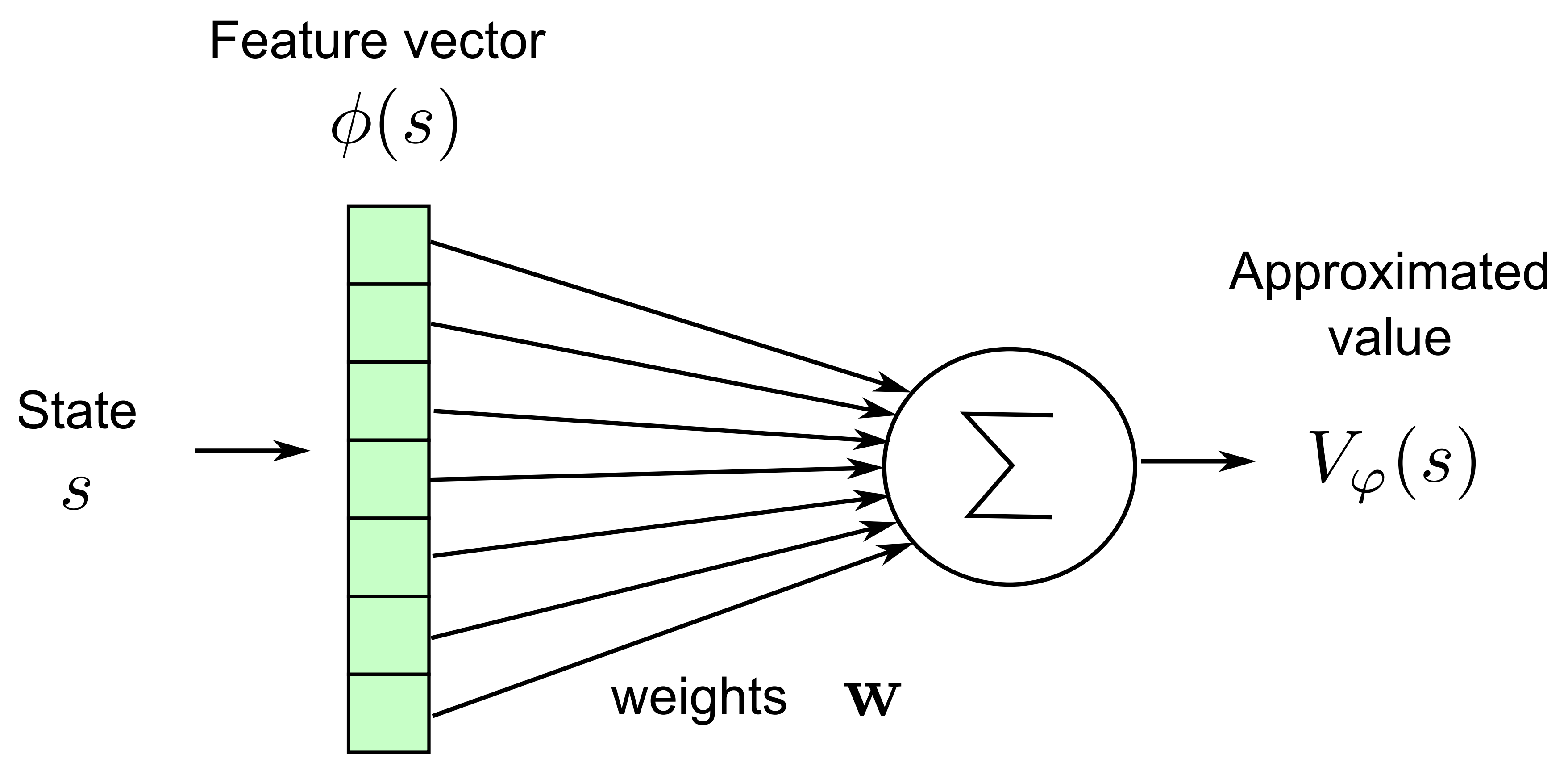
$$\Delta \varphi = \eta \, \frac{1}{K} \, \sum_{k=1}^K (V^\pi (s_k) - V_\varphi(s_k)) \, \nabla_\varphi V_\varphi(s_k)$$

- We can also sample a single state s (online algorithm):

$$\Delta \varphi = \eta \, (V^\pi (s) - V_\varphi(s)) \, \nabla_\varphi V_\varphi(s)$$

- Unless stated otherwise, we will sample single states in this section, but the parameter updates will be noisy (high variance).

Linear approximation



- The approximated value is a linear combination of the features:

$$V_\varphi(s) = \sum_{i=1}^d w_i \, \phi_i(s) = \mathbf{w}^T \times \phi(s)$$

- The weights are updated using stochastic gradient descent:

$$\Delta \mathbf{w} = \eta \, (V^\pi(s) - V_\varphi(s)) \, \phi(s)$$

- That is the **delta learning rule** of linear regression and classification, with $\phi(s)$ being the input vector and $V^\pi(s) - V_\varphi(s)$ the prediction error.

Function approximation with sampling

- The rule can be used with any function approximator, we only need to be able to differentiate it:

$$\Delta \varphi = \eta \, (V^\pi (s) - V_\varphi(s)) \, \nabla_\varphi V_\varphi(s)$$

- The problem is that we do not know $V^\pi (s)$, as it is what we are trying to estimate.
- We can replace $V^\pi (s)$ by a sampled estimate using Monte-Carlo or TD:
    - **Monte-Carlo** function approximation:

$$\Delta \varphi = \eta \, (R_t - V_\varphi(s)) \, \nabla_\varphi V_\varphi(s)$$

    - **Temporal Difference** function approximation:

$$\Delta \varphi = \eta \, (r_{t+1} + \gamma \, V_\varphi(s') - V_\varphi(s)) \, \nabla_\varphi V_\varphi(s)$$

- Note that for Temporal Difference, we actually want to minimize the TD reward-prediction error for all states, i.e. the surprise:

$$\mathcal{L}(\varphi) = \mathbb{E}_{s \in \mathcal{S}} [(r_{t+1} + \gamma \, V_\varphi(s') - V_\varphi(s))^2] = \mathbb{E}_{s \in \mathcal{S}} [\delta_t^2]$$

Gradient Monte Carlo Algorithm for value estimation

- Algorithm:
  - Initialize the parameter φ to 0 or randomly.
  - **while** not converged:
    1. Generate an episode according to the current policy π until a terminal state s_T is reached.

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

    2. For all encountered states $s_0, s_1, \ldots, s_{T-1}$:
        1. Compute the return $R_t = \sum_k \gamma^k r_{t+k+1}$.
        2. Update the parameters using function approximation:

$$\Delta\varphi = \eta \, (R_t - V_\varphi(s_t)) \, \nabla_\varphi V_\varphi(s_t)$$

- Gradient Monte-Carlo has no bias (real returns) but a high variance.

Semi-gradient Temporal Difference Algorithm for value estimation

- Algorithm:

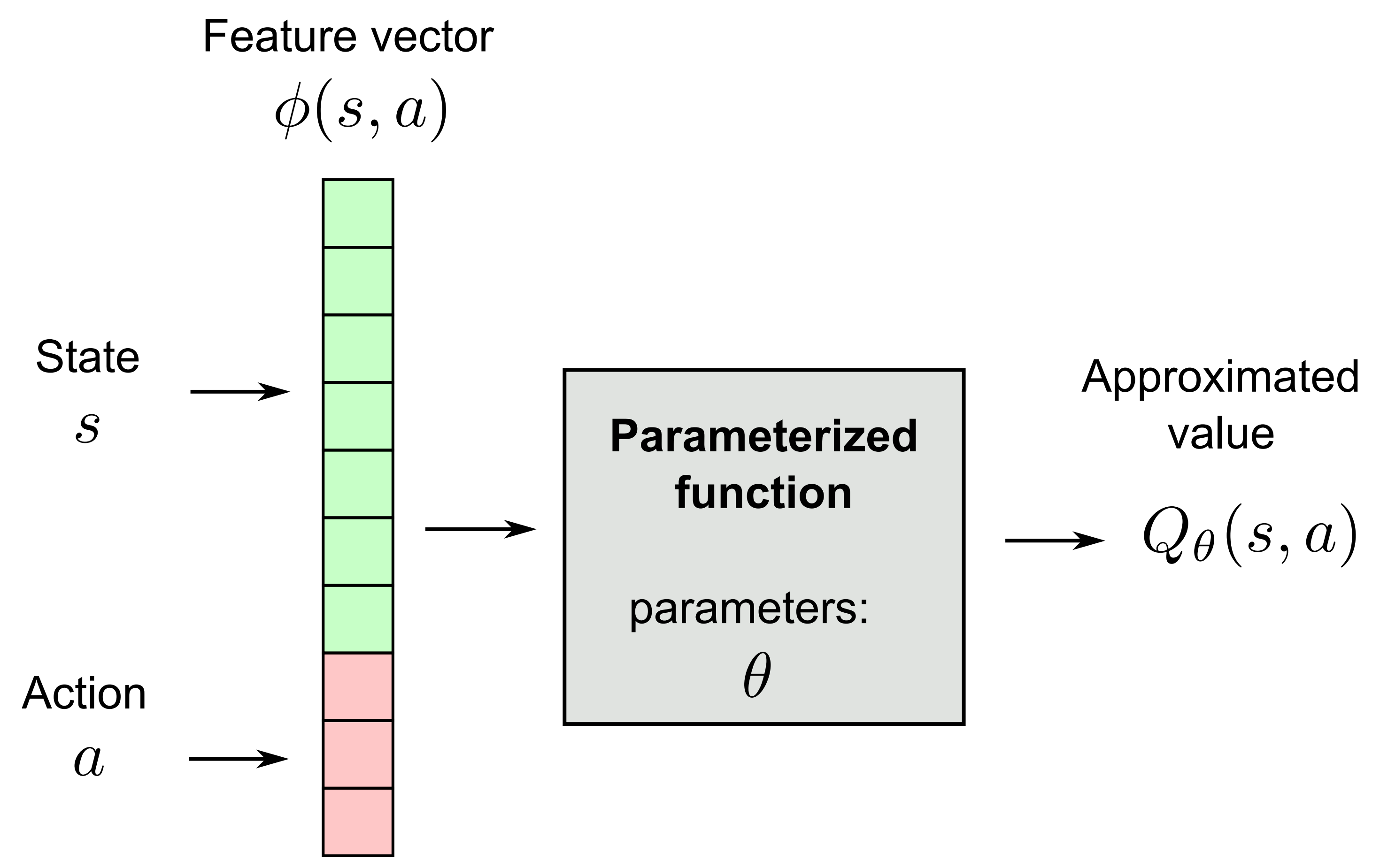
```
Initialize the parameter $\varphi$ to 0 or randomly.
while not converged:
    Start from an initial state $s_0$.
    foreach step $t$ of the episode:
        Select $a_t$ using the current policy $\pi$ in state $s_t$.
        Observe $r_{t+1}$ and $s_{t+1}$.
        Update the parameters using function approximation:
            $\Delta \varphi = \eta \, (r_{t+1} + \gamma \, V_\varphi(s_{t+1}) - V_\varphi(s_t)) \, \nabla_\varphi V_\varphi(s_t)$
        if $s_{t+1}$ is terminal: break
```

- Semi-gradient TD has less variance, but a significant bias as $V_\varphi(s_{t+1})$ is initially wrong. You can never trust these estimates completely.

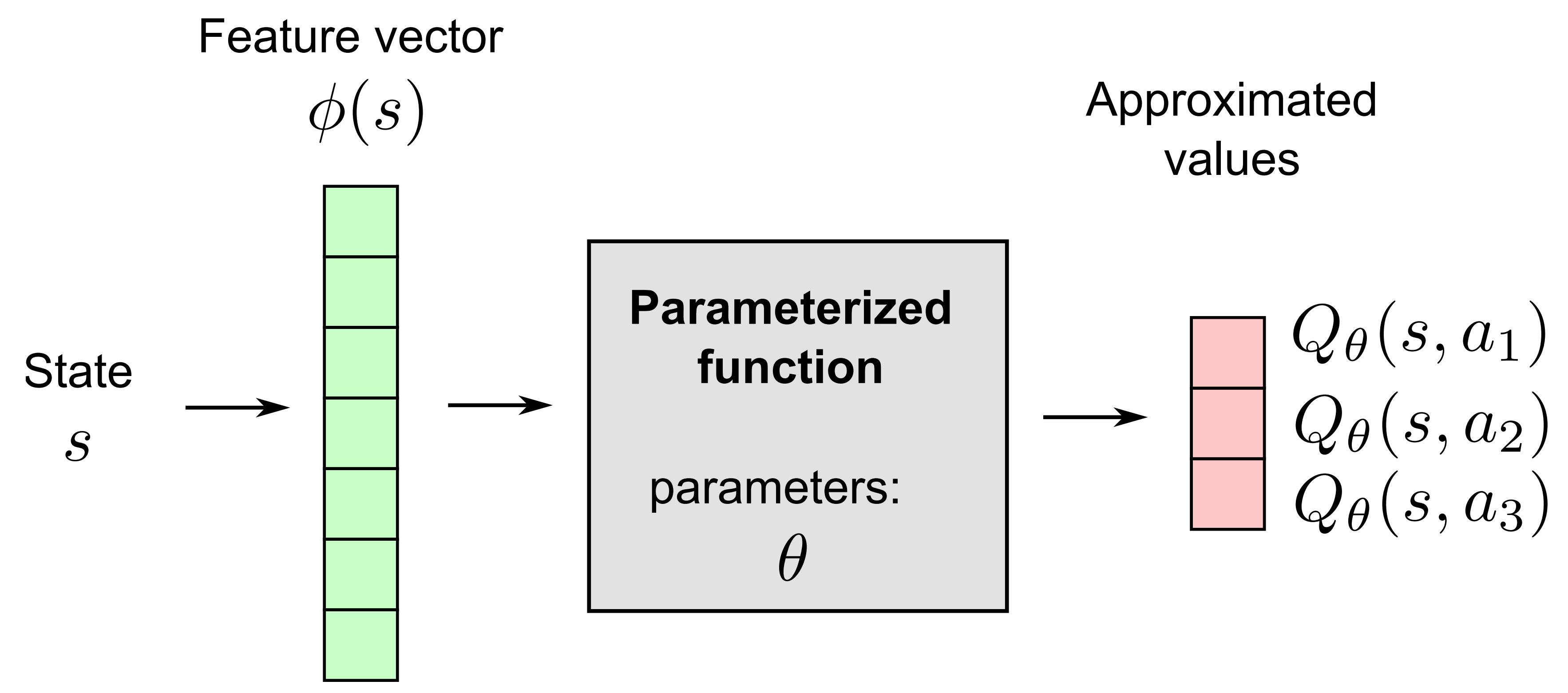
Function approximation for Q-values

- Q-values can be approximated by a parameterized function $Q_\theta(s, a)$ in the same manner.
- There are basically two options for the structure of the function approximator:

- The FA takes a feature vector for both the state s and the action a (which can be continuous) as inputs, and outputs a single Q-value $Q_\theta(s, a)$.



- The FA takes a feature vector for the state s as input, and outputs one Q-value $Q_\theta(s, a)$ per possible action (the action space must be discrete).



- In both cases, we minimize the mse between the true value $Q^\pi(s, a)$ and the approximated value $Q_\theta(s, a)$.

Q-learning with function approximation

- Initialize the parameters θ.
- **while** True:
    - Start from an initial state s_0.
    - **foreach** step t of the episode:
        - Select a_t using the behavior policy b (e.g. derived from π).
        - Take a_t, observe r_{t+1} and s_{t+1}.
        - Update the parameters θ:

$$\Delta\theta = \eta \, (r_{t+1} + \gamma \, \max_a Q_\theta(s_{t+1}, a) - Q_\theta(s_t, a_t)) \, \nabla_\theta Q_\theta(s_t, a_t)$$

        - Improve greedily the learned policy:

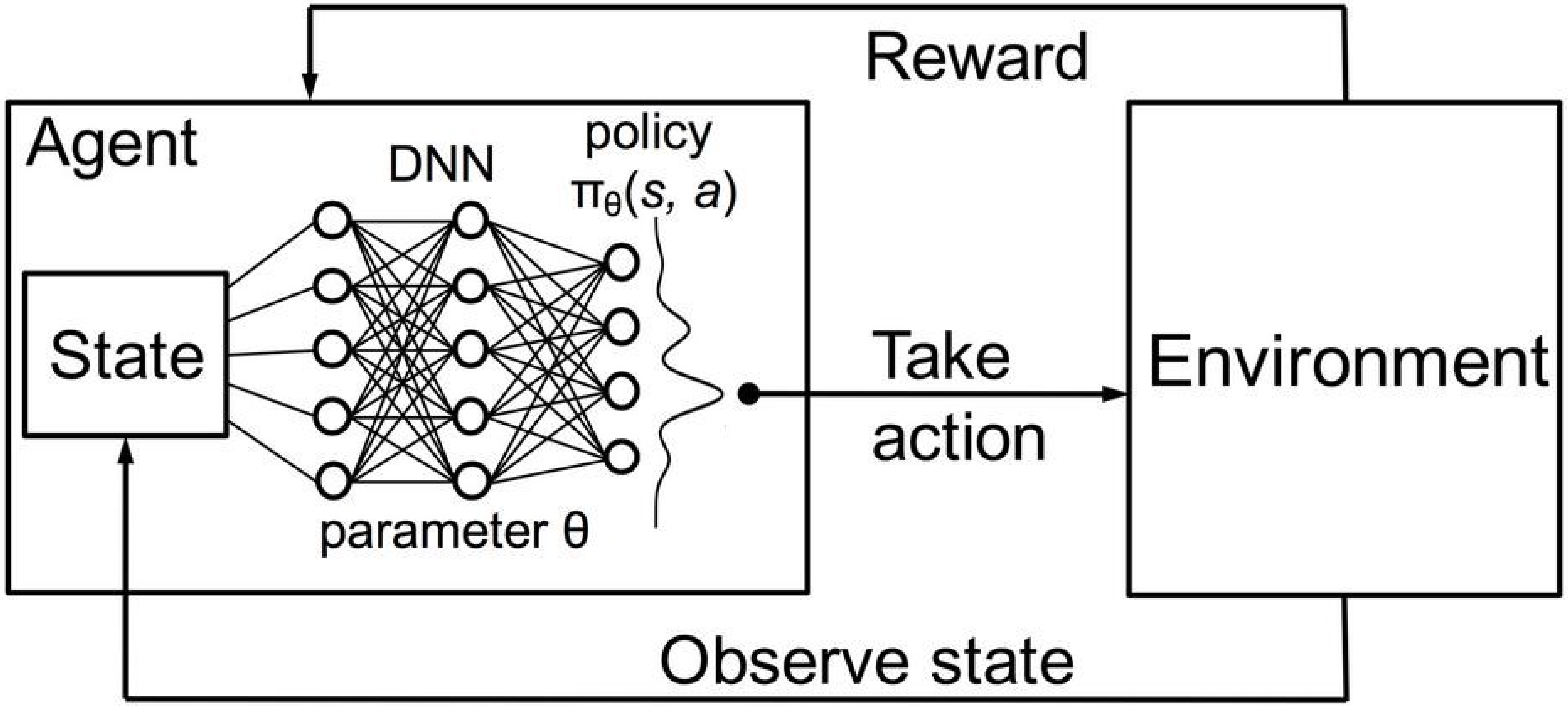
$$\pi(s_t, a) = \text{Greedy}(Q_\theta(s_t, a))$$

        - **if** s_{t+1} is terminal: **break**

3 - Feature construction

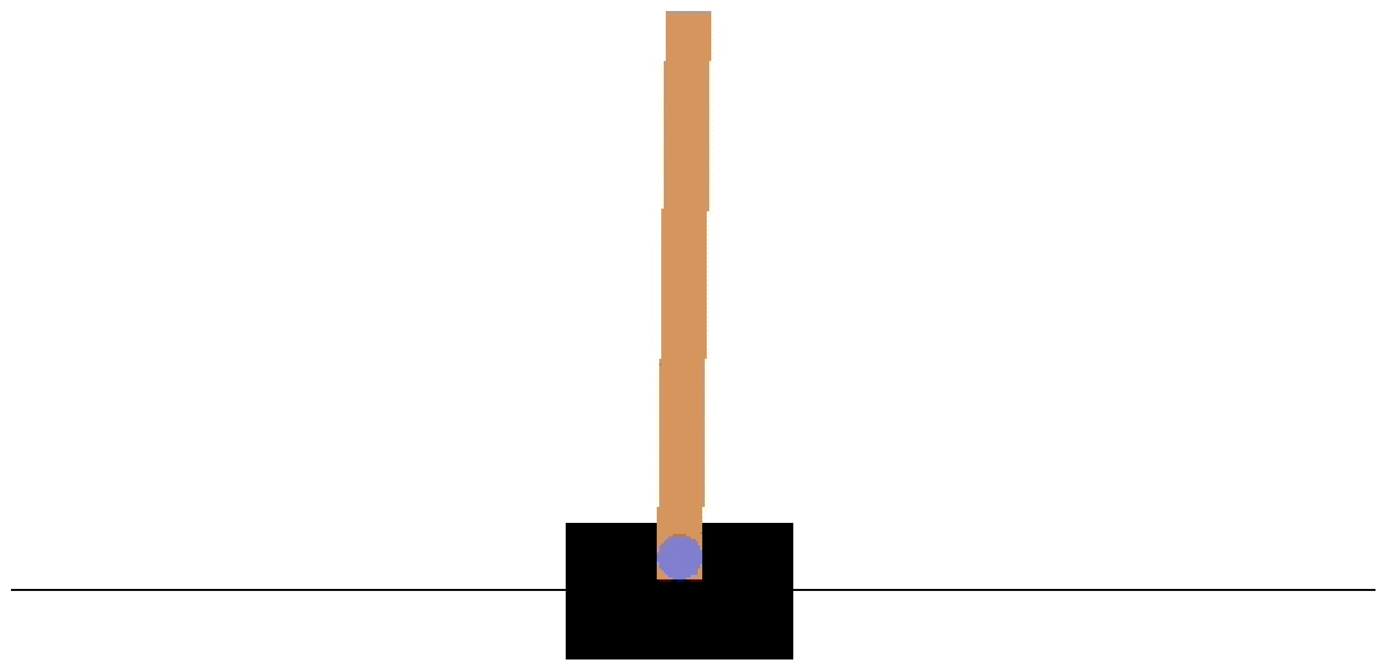
Feature construction

- Before we dive into deep RL (i.e. RL with non-linear FA), let's see how we can design good **feature vectors** for linear function approximation.



- The problem with deep NN is that they need a lot of samples to converge, what worsens the fundamental problem of RL: **sample efficiency**.
- By engineering the right features, we could use linear approximators, which converge much faster.
- The convergence of linear FA is **guaranteed**, not (always) non-linear ones.

Why do we need to choose features?



- For the cartpole, the feature vector $\phi(s)$ could be:

$$\phi(s) = \begin{bmatrix} x \\ \dot{x} \\ \theta \\ \dot{\theta} \end{bmatrix}$$

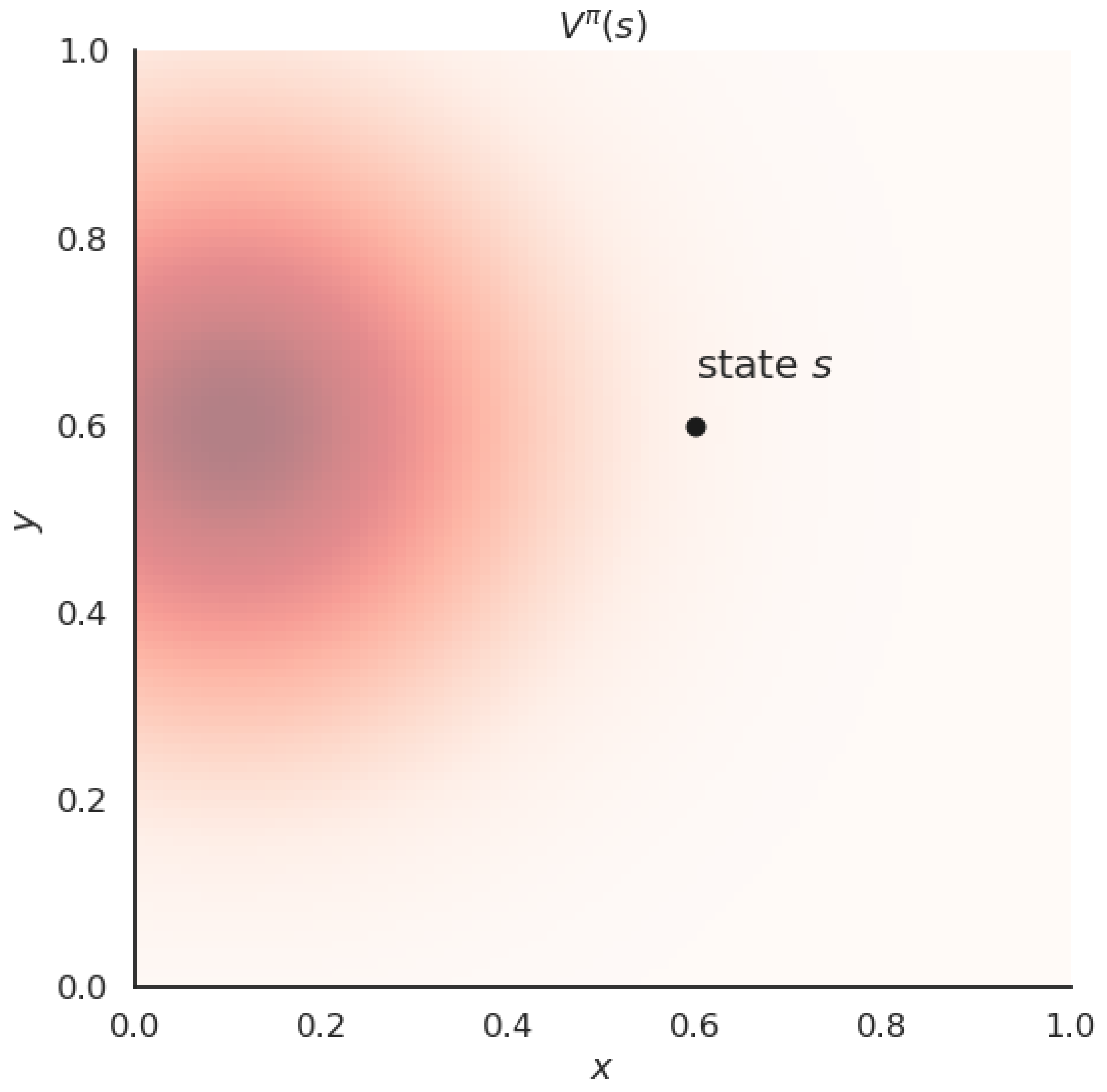
- x is the position, θ the angle, $\dot{x}$ and $\dot{\theta}$ their derivatives.
- Can we predict the value of a state **linearly**?

$$V_\varphi(s) = \sum_{i=1}^d w_i \, \phi_i(s) = \mathbf{w}^T \times \phi(s)$$

- No, a high angular velocity $\dot{\theta}$ is good when the pole is horizontal (going up) but bad if the pole is vertical (will not stop).
- The value would depends linearly on something like $\dot{\theta} \, \sin \theta$, which is a non-linear combination of features.

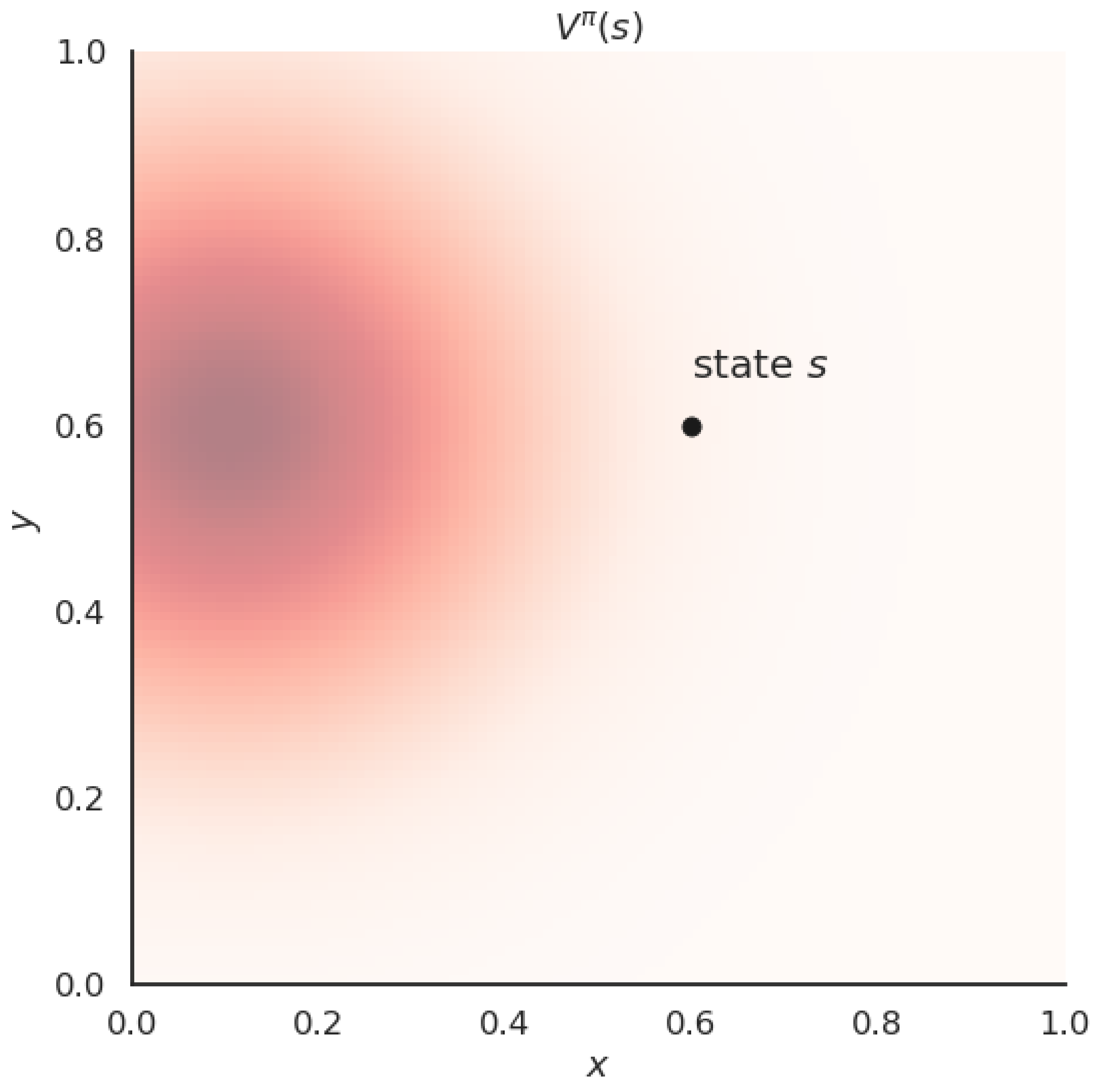
Feature coding

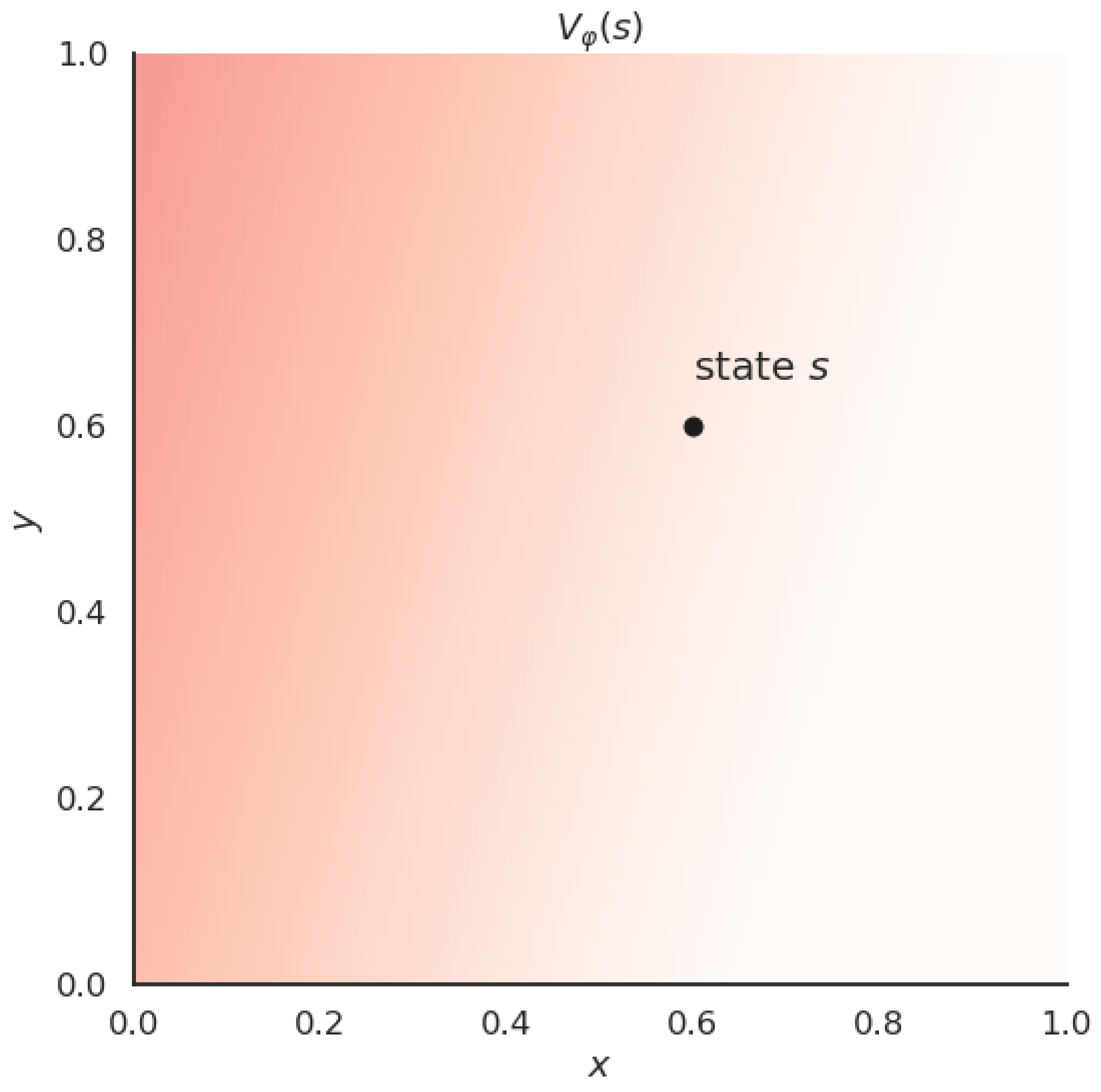
- Let's suppose we have a simple problem where the state s is represented by two continuous variables x and y.
- The true value function $V^{\pi}(s)$ is a non-linear function of x and y.



Linear approximation

- If we apply linear FA directly on the feature vector $[x, y]$, we catch the tendency of $V^\pi(s)$ but we make a lot of bad predictions:
    - **high bias** (underfitting).





Polynomials

- To introduce non-linear relationships between continuous variables, a simple method is to construct the feature with **polynomials** of the variables.
- Example with polynomials of order 2:

$$\phi(s) = \begin{bmatrix}1 & x & y & x\,y & x^2 & y^2 \end{bmatrix}^T$$

- We transform the two input variables x and y into a vector with 6 elements. The 1 (order 0) is there to learn the offset.
- Example with polynomials of order 3:

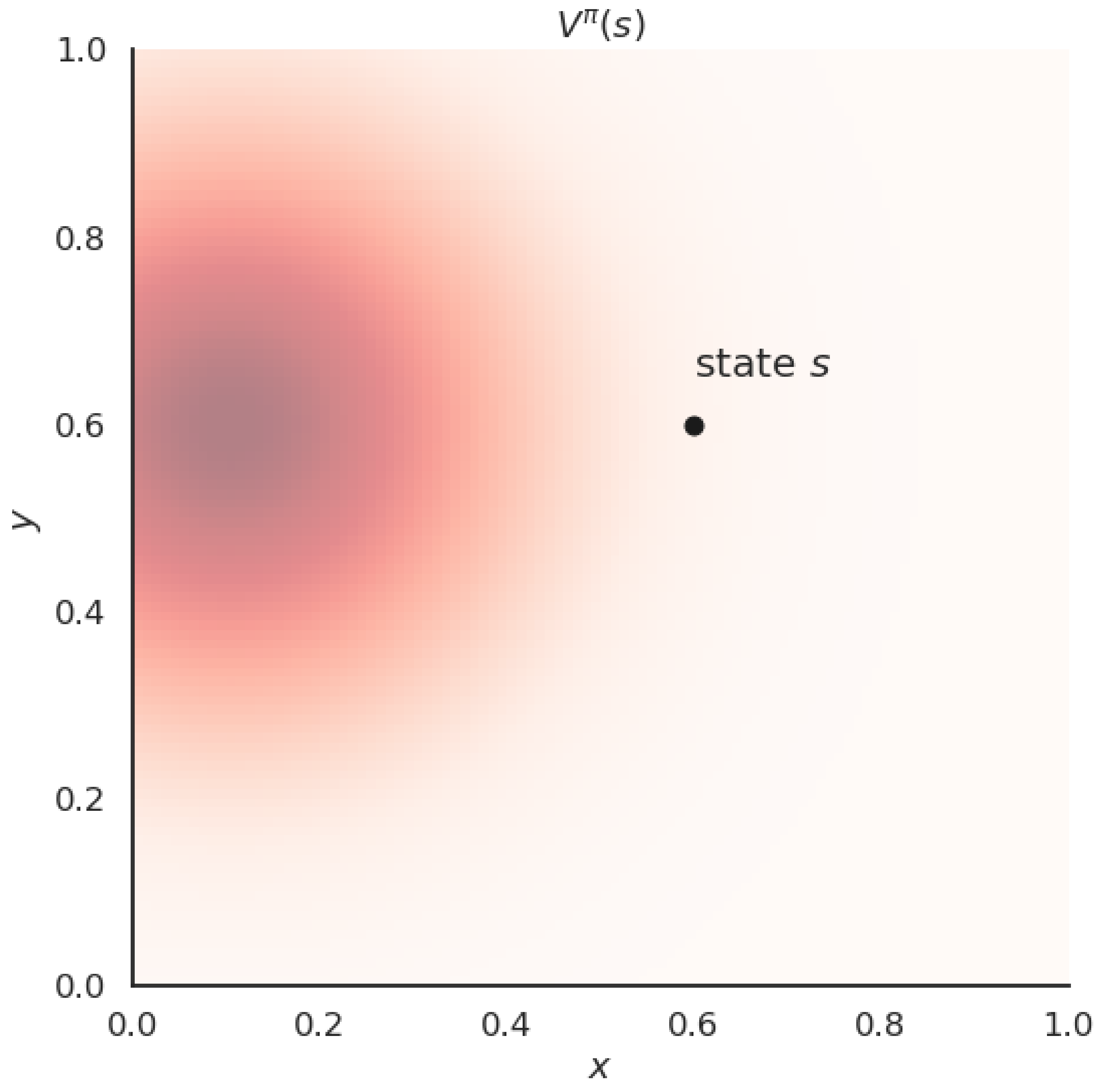
$$\phi(s) = \begin{bmatrix}1 & x & y & x\,y & x^2 & y^2 & x^2\,y & x\,y^2 & x^3 & y^3 \end{bmatrix}^T$$

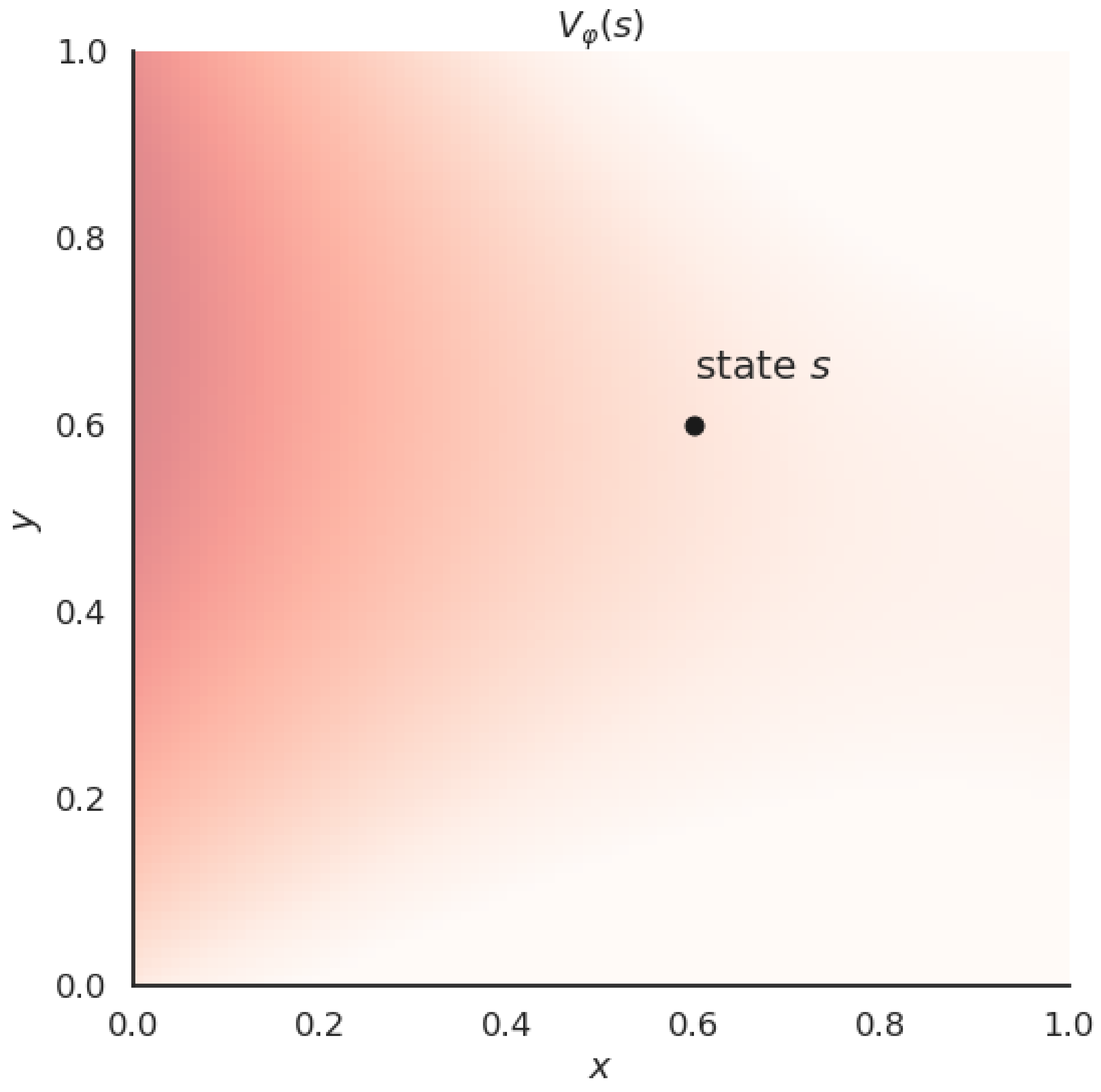
- And so on. We then just need to apply linear FA on these feature vectors (**polynomial regression**).

$$V_\varphi(s) = w_0 + w_1\,x + w_2\,y + w_3\,x\,y + w_4\,x^2 + w_5\,y^2 + \ldots$$

Polynomials

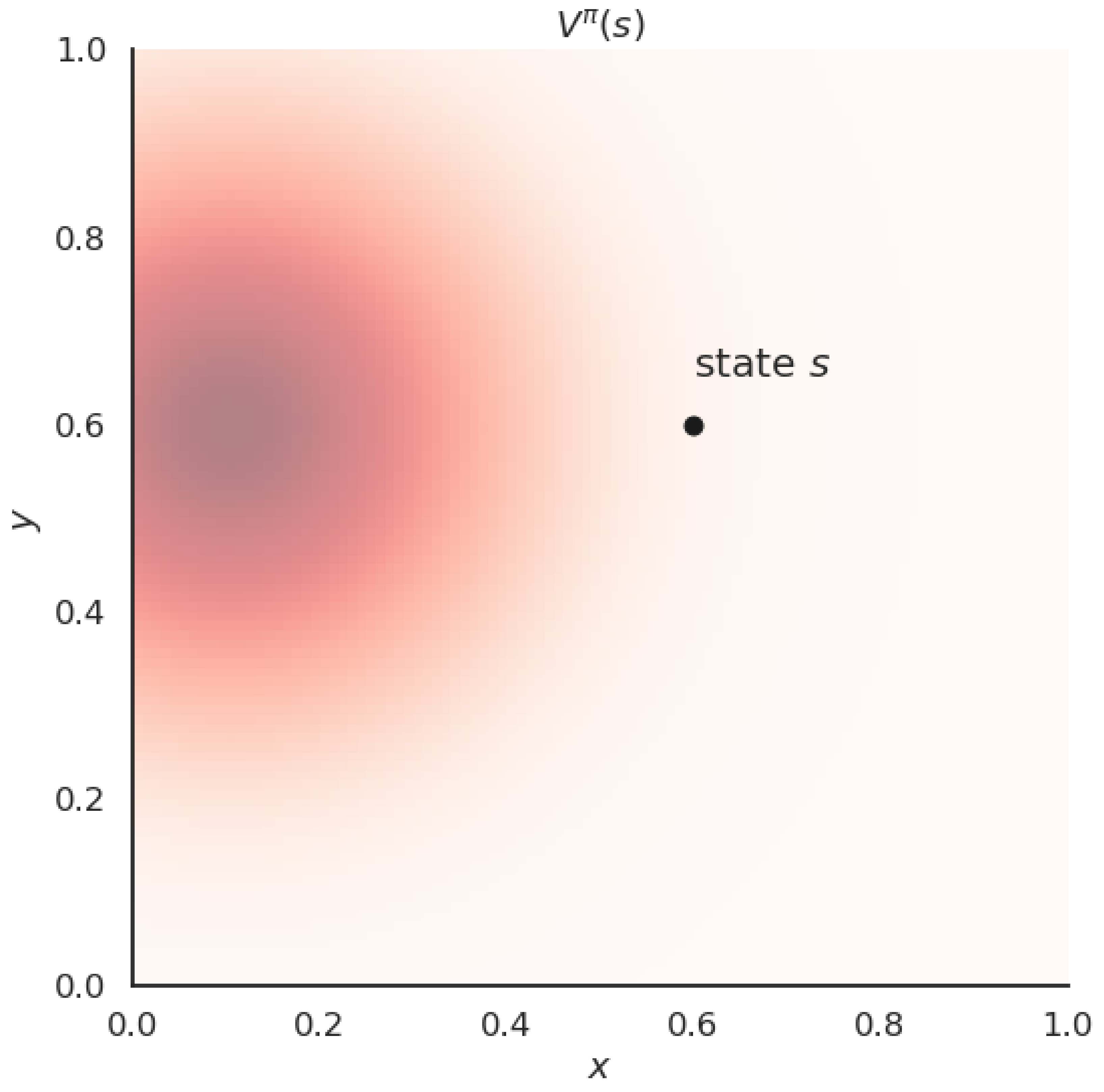
- Polynomials of order 2 already allow to get a better approximation.

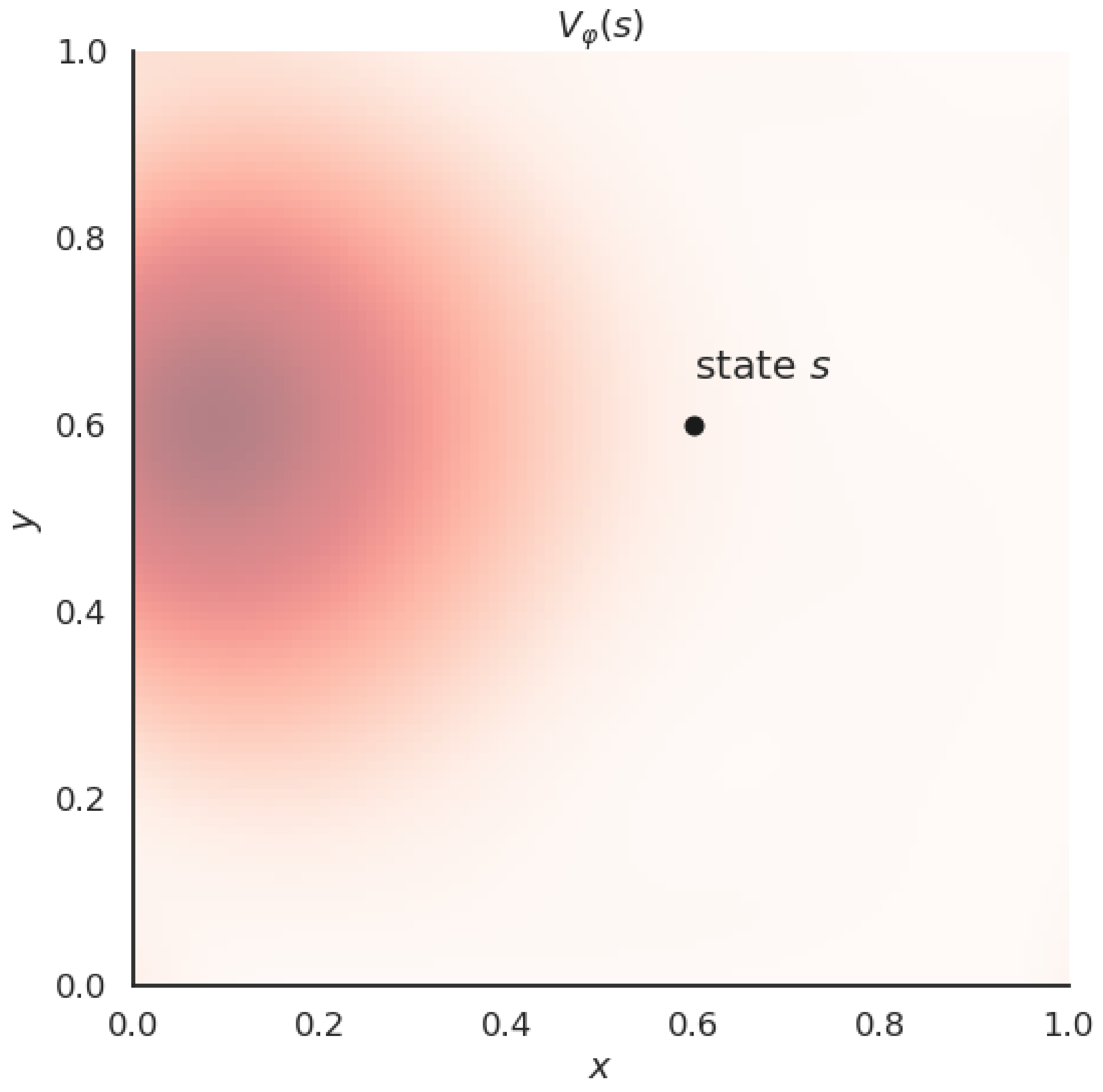




Polynomials

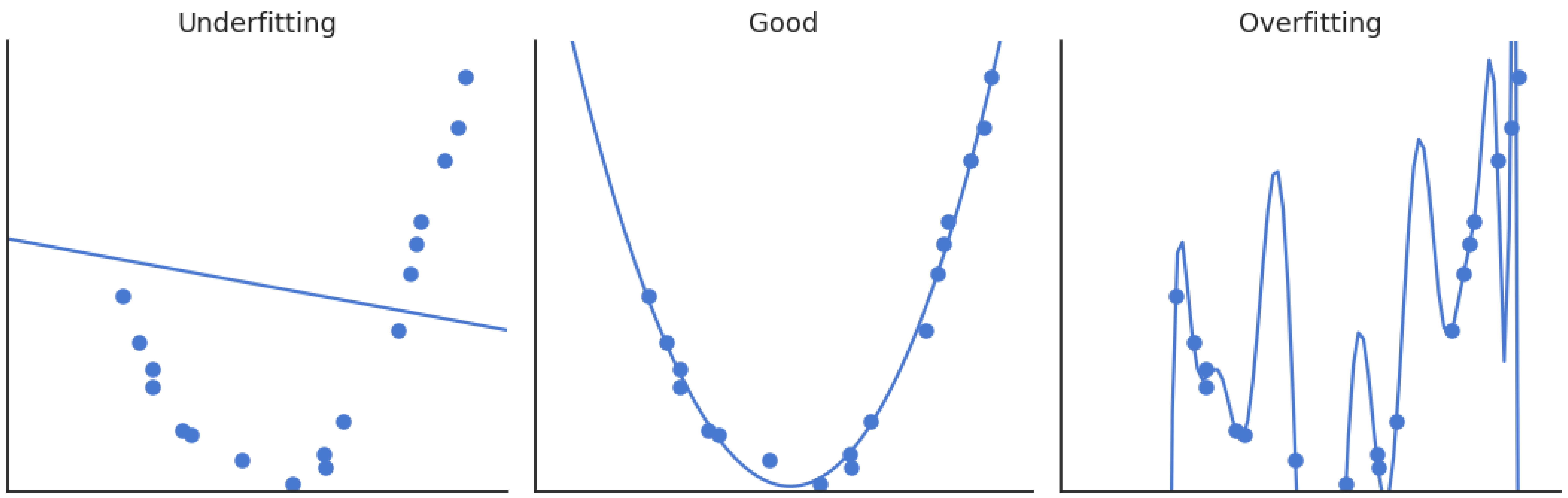
- Polynomials of order 6 are an even better fit for our problem.





Polynomials

- The higher the degree of the polynomial, the better the fit, but the number of features grows exponentially.
    - Computational complexity.
    - **Overfitting**: if we only sample some states, high-order polynomials will not interpolate correctly.



Fourier transforms

- Instead of approximating a state variable x by a polynomial:

$$V_\varphi(s) = w_0 + w_1 \, x + w_2 \, x^2 + w_3 \, x^3 + \ldots$$

- we could also use its **Fourier decomposition** (here DCT, discrete cosine transform):

$$V_\varphi(s) = w_0 + w_1 \, \cos(\pi \, x) + w_2 \, \cos(2 \, \pi \, x) + w_3 \, \cos(3 \, \pi \, x) + \ldots$$

- Fourier tells us that, if we take enough frequencies, we can reconstruct the signal $V_\varphi(s)$ perfectly.

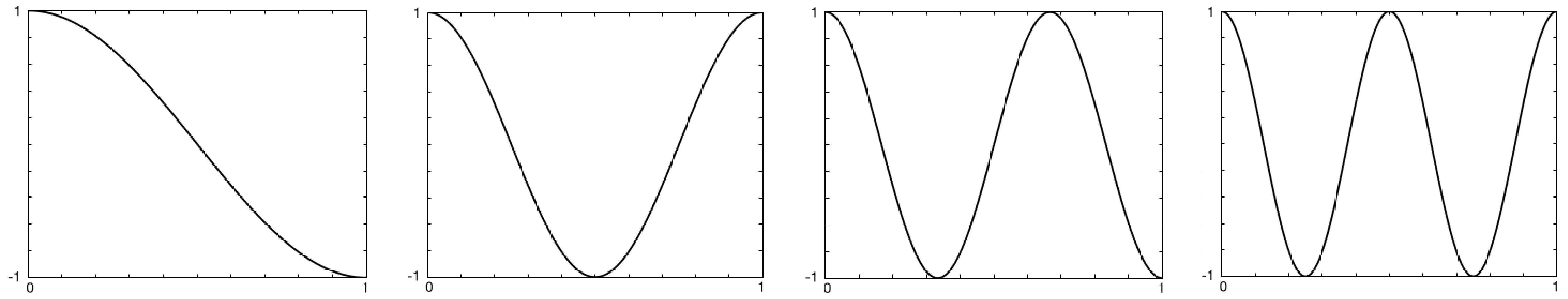


Figure 9.3: One-dimensional Fourier cosine-basis features x_i, $i = 1, 2, 3, 4$, for approximating functions over the interval $[0, 1]$. After Konidaris et al. (2011).

- It is just a change of basis, the problem stays a linear regression to find w_0, w_1, w_2, etc.

Fourier transforms

- Fourier transforms can be applied on multivariate functions as well.

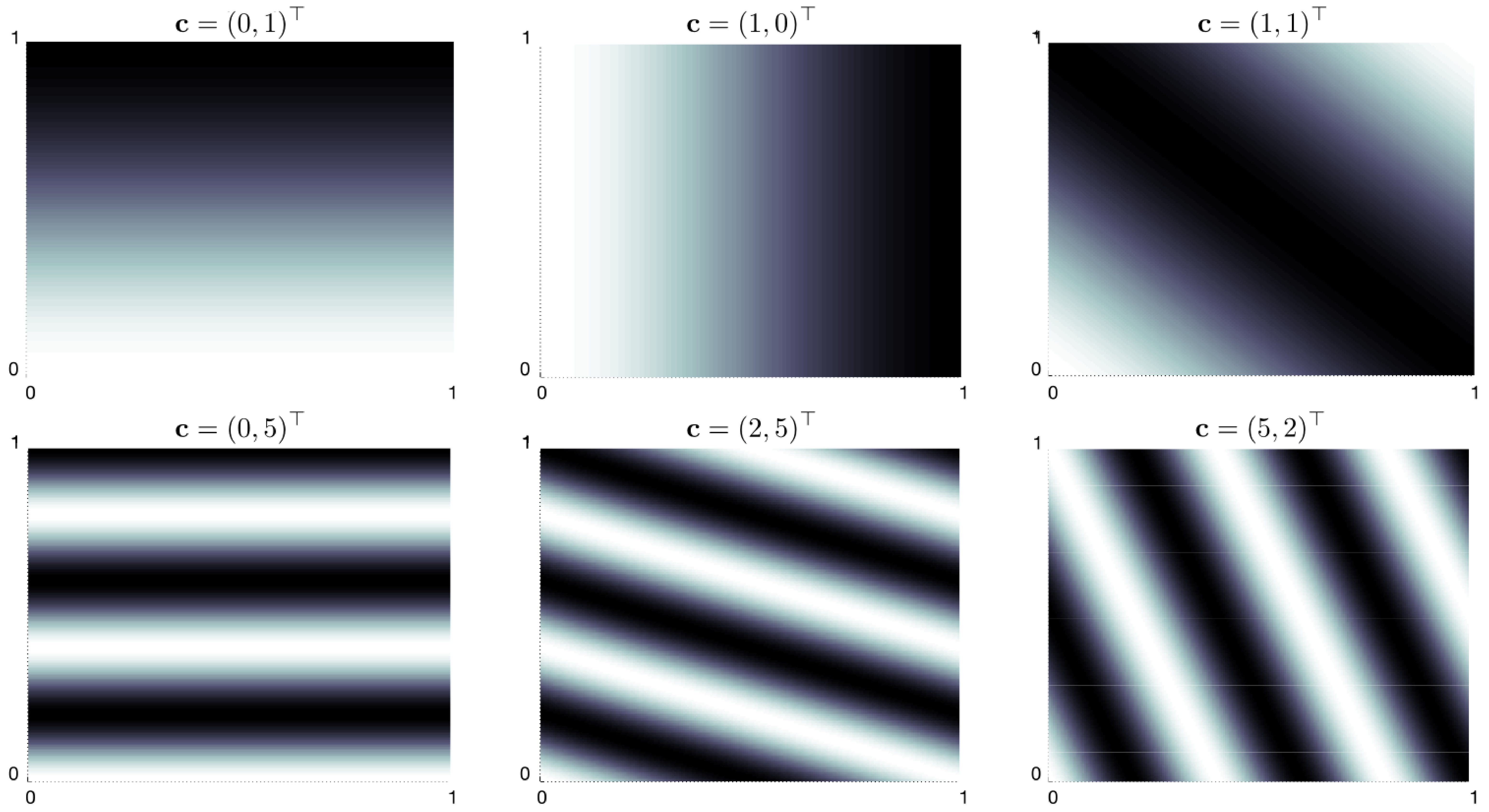


Figure 9.4: A selection of six two-dimensional Fourier cosine features, each labeled by the vector $\mathbf{c}^i$ that defines it (s_1 is the horizontal axis, and $\mathbf{c}^i$ is shown with the index i omitted). After Konidaris et al. (2011).

Polynomial vs. Fourier basis

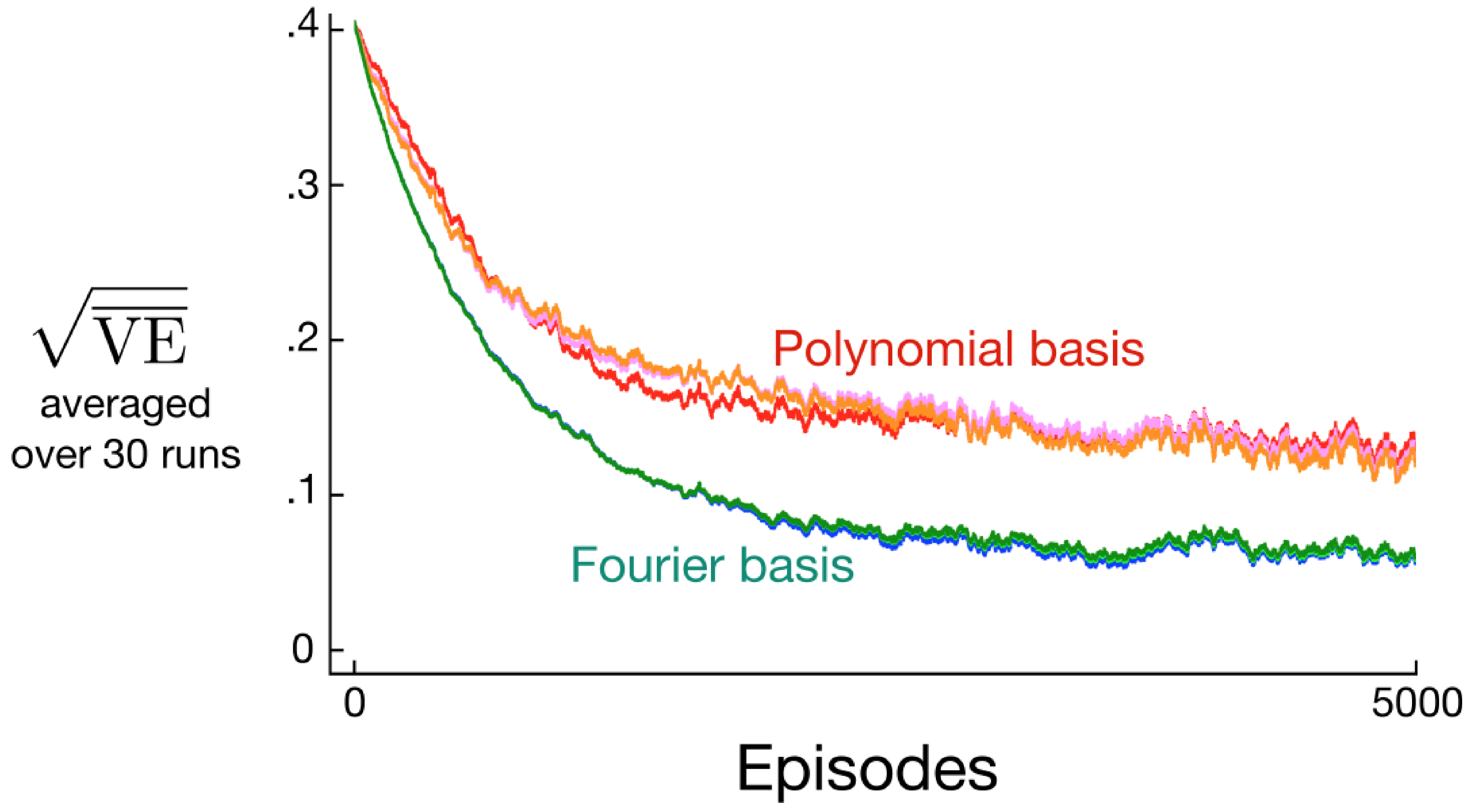
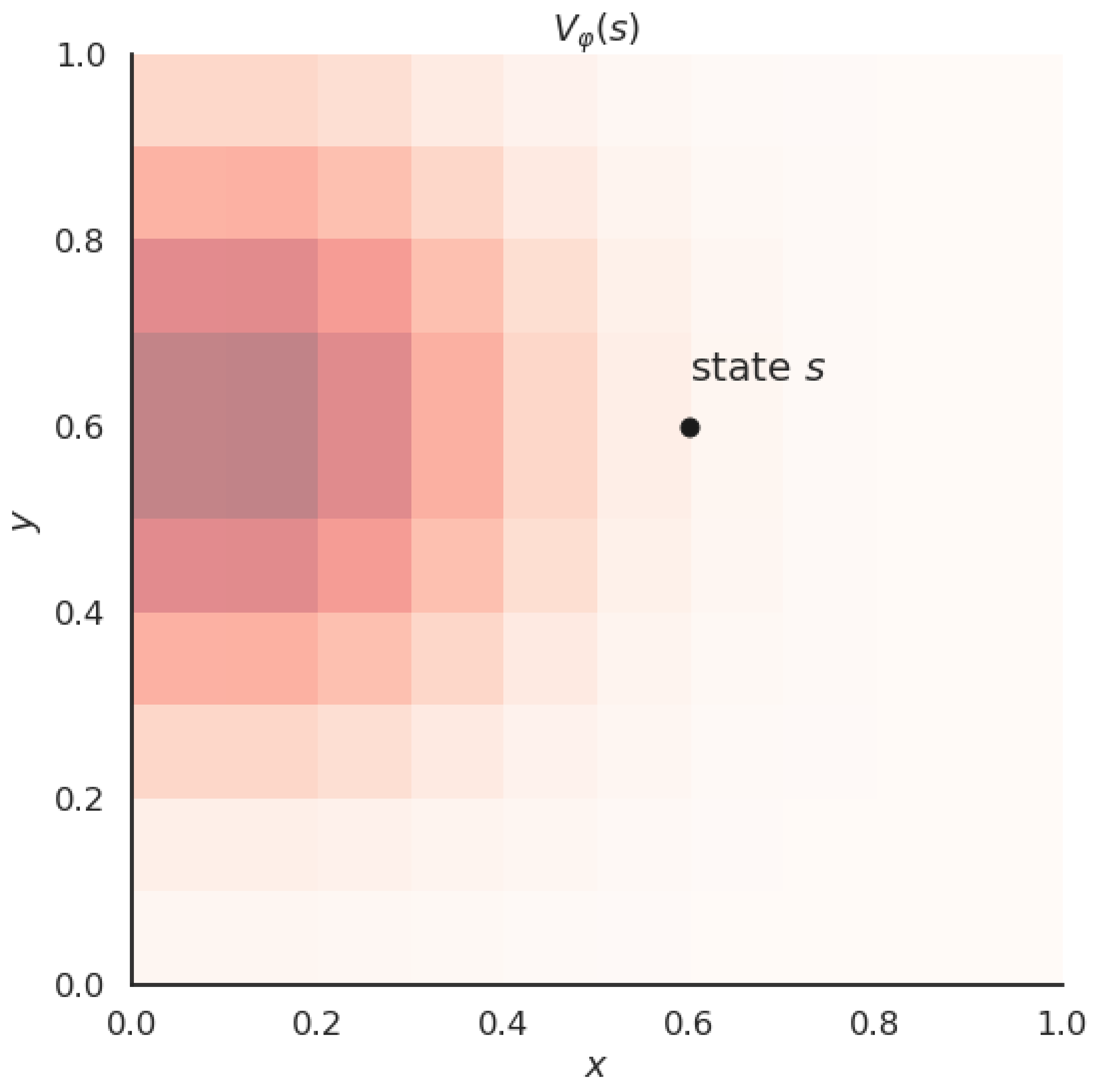


Figure 9.5: Fourier basis vs polynomials on the 1000-state random walk. Shown are learning curves for the gradient Monte Carlo method with Fourier and polynomial bases of order 5, 10, and 20. The step-size parameters were roughly optimized for each case: $\alpha = 0.0001$ for the polynomial basis and $\alpha = 0.00005$ for the Fourier basis. The performance measure (y-axis) is the root mean squared value error (9.1).

- A Fourier basis tends to work better than a polynomial basis.
- The main problem is that the number of features increases very fast with:
  - the number of input dimensions.
  - the desired precision (higher-order polynomials, more frequencies).

Discrete coding

- An obvious solution for continuous state variables is to **discretize** the input space.
- The input space is divided into a grid of non-overlapping **tiles**.

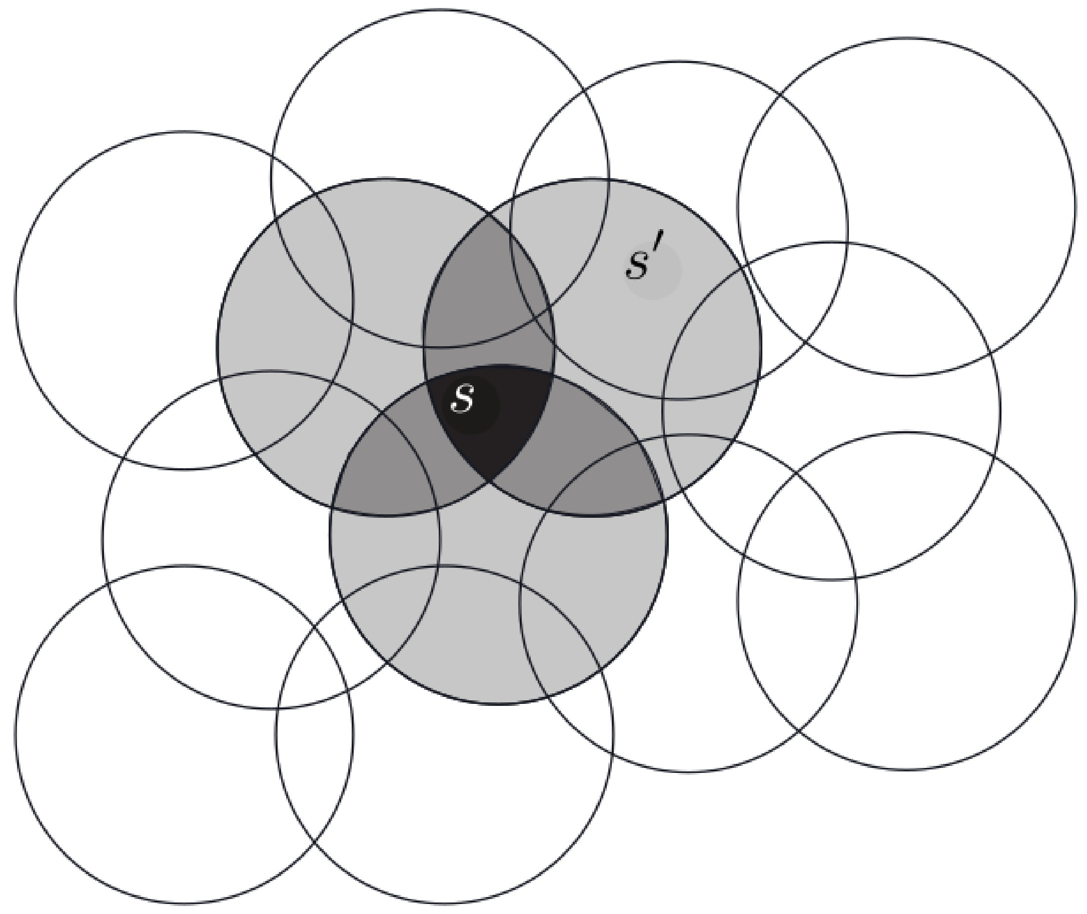


- The feature vector is a **binary** vector with a 1 when the input is inside a tile, 0 otherwise.

$$\phi(s) = \begin{bmatrix} 0 & 0 & \ldots & 0 & 1 & 0 & \ldots & 0 \end{bmatrix}^T$$

- This ensures **generalization** inside a tile: you only need a couple of samples inside a tile to know the mean value of all the states.
- Drawbacks:
  - the value function is step-like (discontinuous).
  - what is the correct size of a tile?
  - curse of dimensionality.

Coarse coding

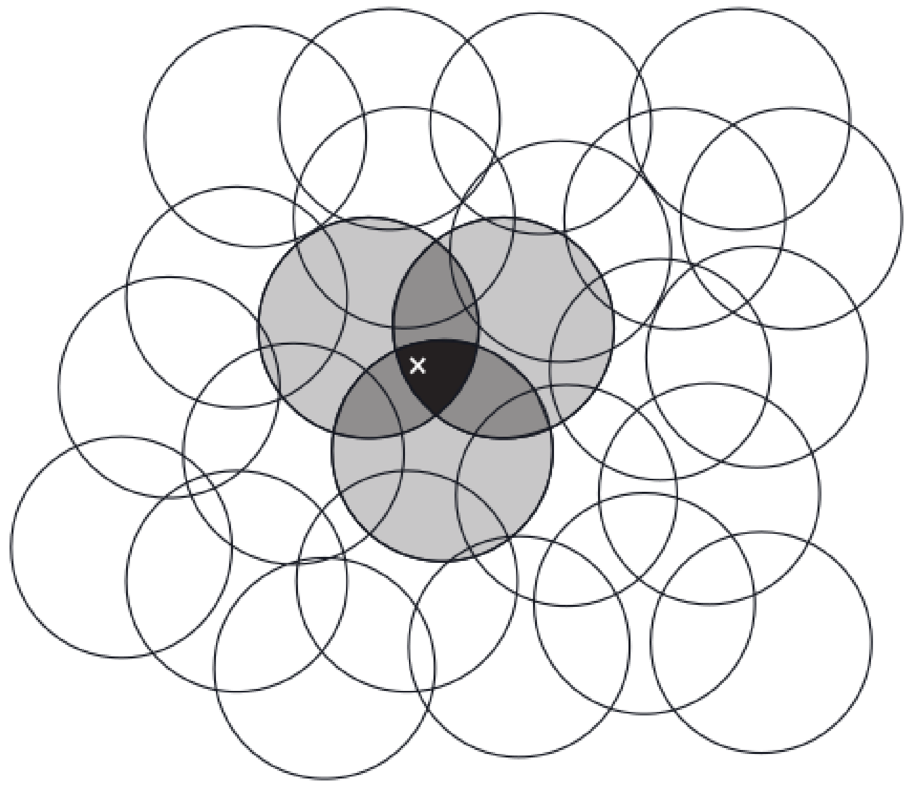


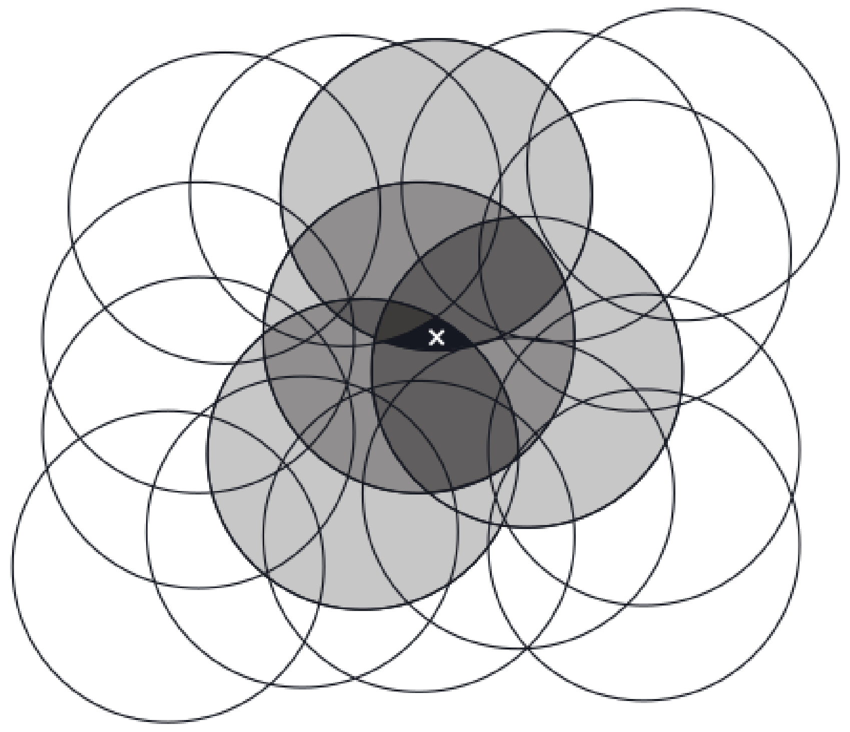
- A more efficient solution is **coarse coding**.
- The tiles (rectangles, circles, or what you need) need to **overlap**.
- A state s is encoded by a **binary vector**, but with several 1, for each tile it belongs.

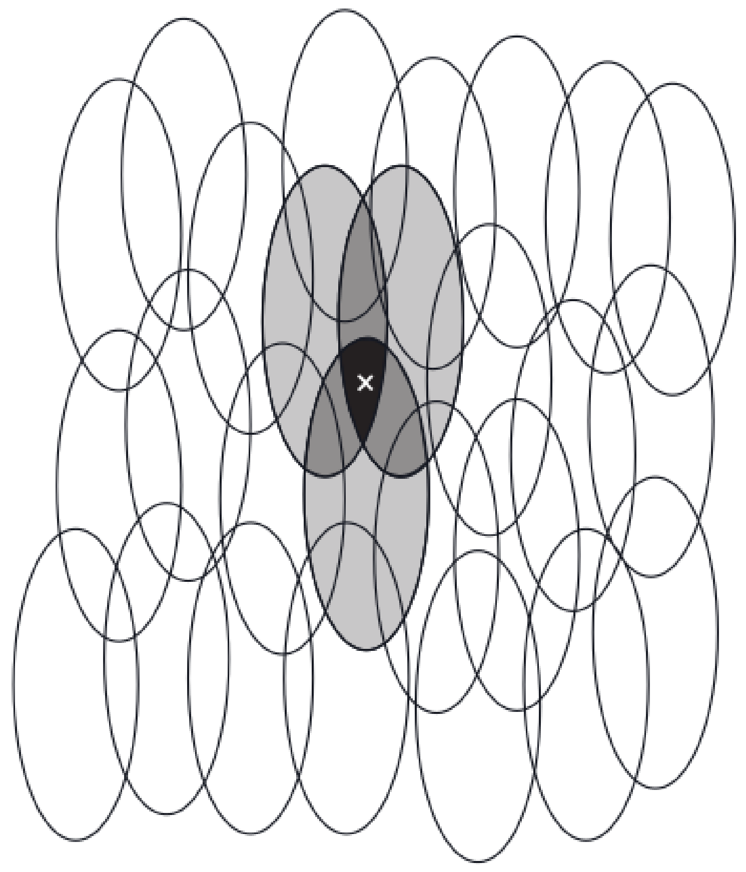
$$\phi(s) = \begin{bmatrix} 0 & 1 & 0 & \ldots & 1 & 1 & 0 & \ldots & 0 \end{bmatrix}^T$$

- This allows generalization inside a tile, but also **across tiles**.

- The size and shape of the **"receptive field"** influences the generalization properties.


Narrow generalization


Broad generalization


Asymmetric generalization

Tile coding

- A simple way to ensure that tiles overlap is to use several regular grids with an **offset**.
- Each tiling will be **coarse**, but the location of a state will be quite precise as it may belong to many tiles.

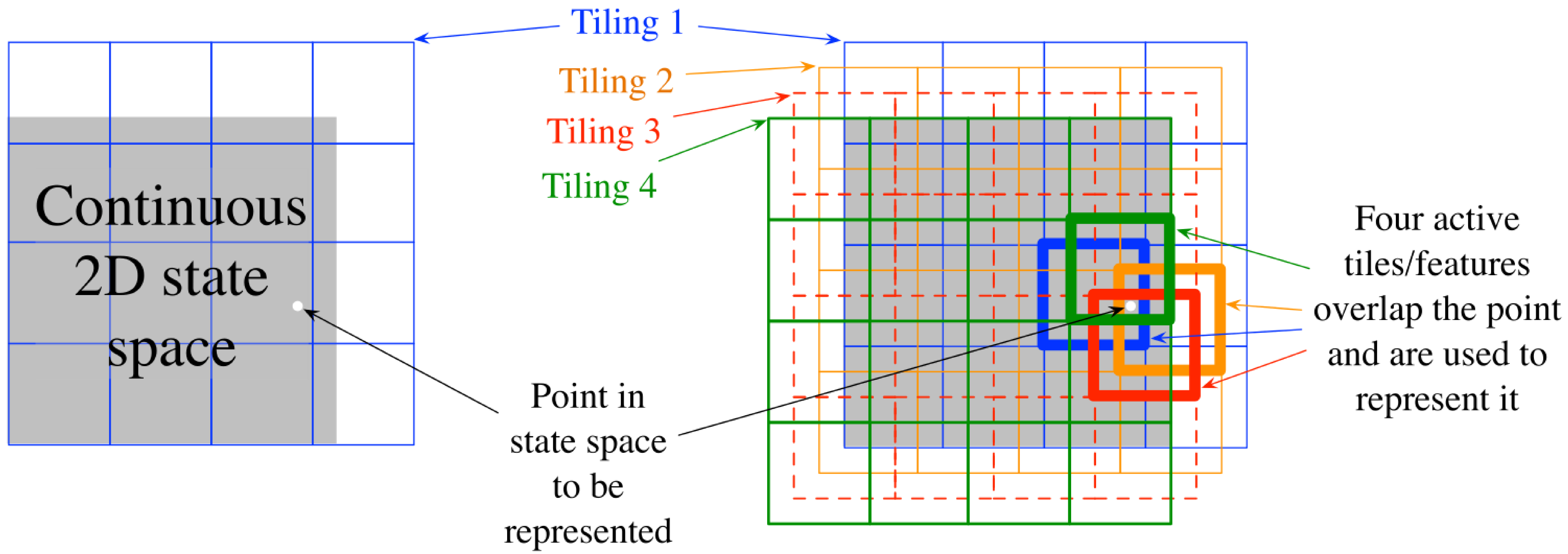
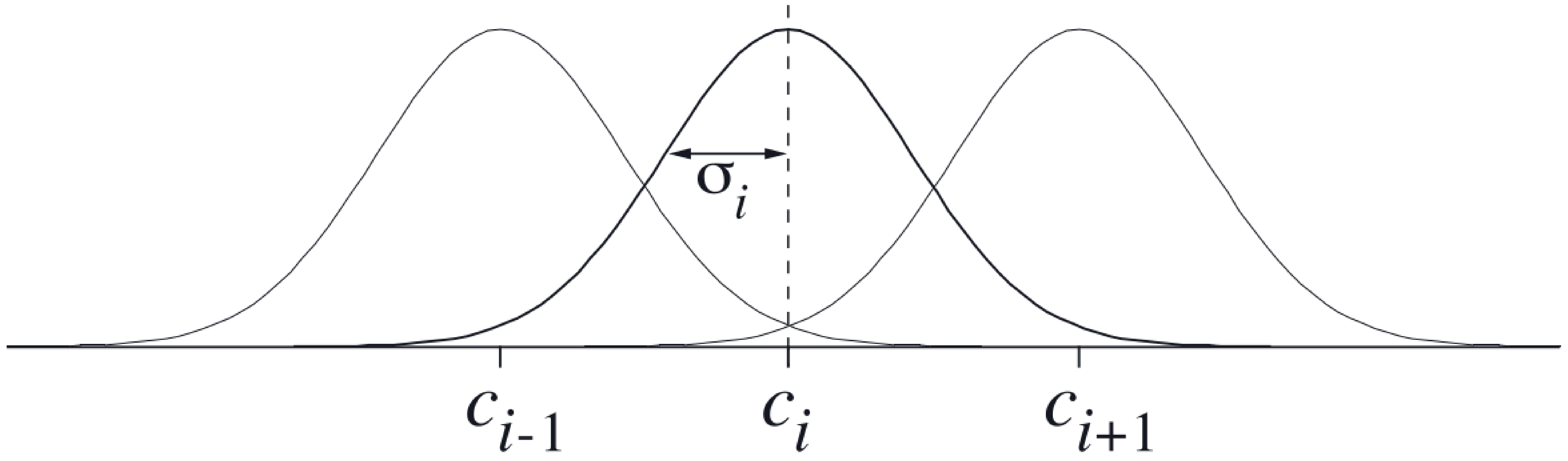

Tiling 1
Tiling 2
Tiling 3
Tiling 4
Continuous 2D state space
Point in state space to be represented
Four active tiles/features overlap the point and are used to represent it

Figure 9.9: Multiple, overlapping grid-tilings on a limited two-dimensional space. These tilings are offset from one another by a uniform amount in each dimension.

- This helps against the curse of dimensionality: high precision, but the number of tiles does not grow exponentially.

Radial-basis functions (RBF)

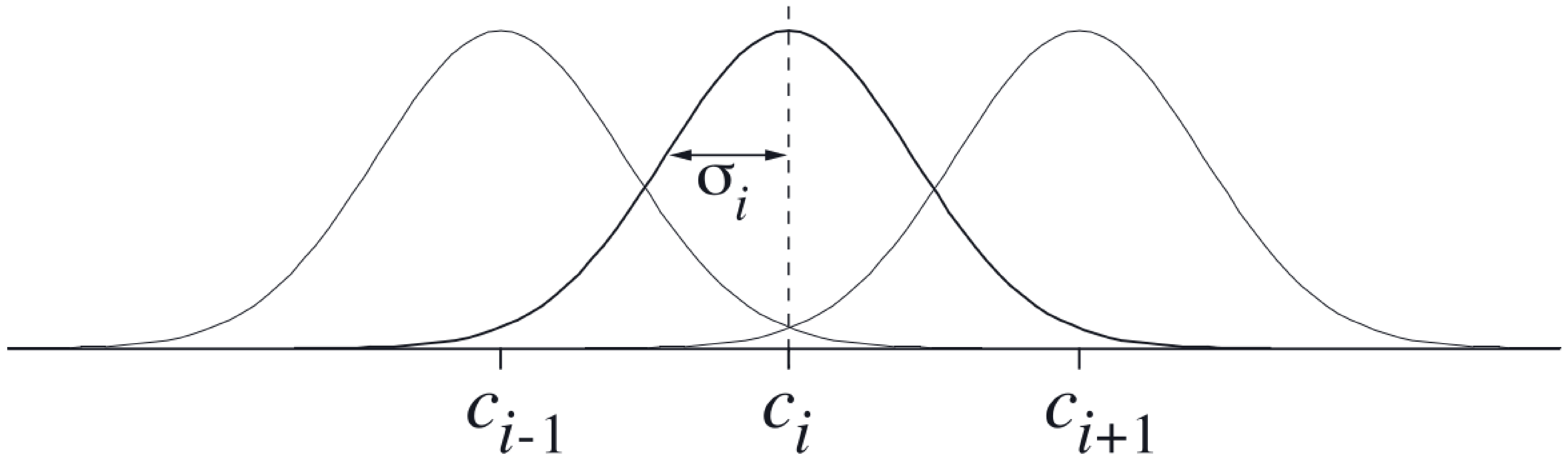
- The feature vector in tile coding is a binary vector: there will be **discontinuous jumps** in the approximated value function when moving between tiles.
- We can use **radial-basis functions** (RBF) such as Gaussians to map the state space.



- We set a set of centers $\{c_i\}_{i=1}^K$ in the input space on a regular grid (or randomly).
- Each element of the feature vector will be a Gaussian function of the distance between the state s and one center:

$$\phi_i(s) = \exp \frac{-(s - c_i)^2}{2\, \sigma_i^2}$$

Radial-basis functions (RBF)



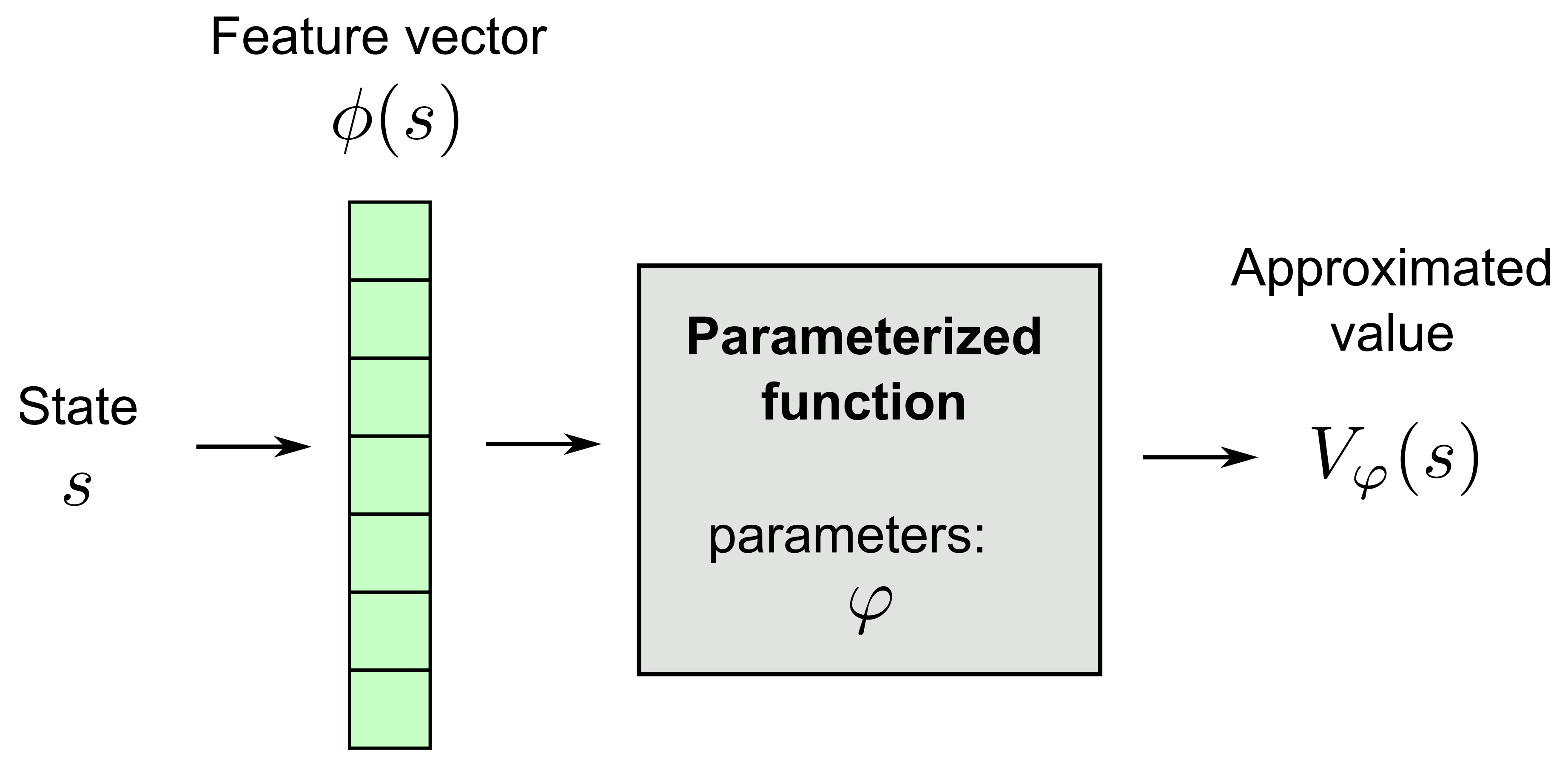
- The approximated value function now represents **continuously** the states:

$$V_\varphi(s) = \sum_{i=1}^d w_i \, \phi_i(s) = \sum_{i=1}^d w_i \, \exp \frac{-(s - c_i)^2}{2\, \sigma_i^2}$$

- If you have enough centers and they overlap sufficiently, you can even **decode** the original state perfectly:

$$\hat{s} = \sum_{i=1}^d \phi_i(s) \, c_i$$

Summary of function approximation



- In FA, we project the state information into a **feature space** to get a better representation.
- We then apply a linear approximation algorithm to estimate the value function:

$$V_\varphi(s) = \mathbf{w}^T \, \phi(s)$$

- The linear FA is trained using some variant of gradient decent:

$$\Delta \mathbf{w} = \eta \, (V^\pi(s) - V_\varphi(s)) \, \phi(s)$$

- **Deep neural networks** are the most powerful function approximators in supervised learning.
- Do they also work with RL?