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Deep Reinforcement Learning

Successor representations

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

1 - Model-based vs. Model-free

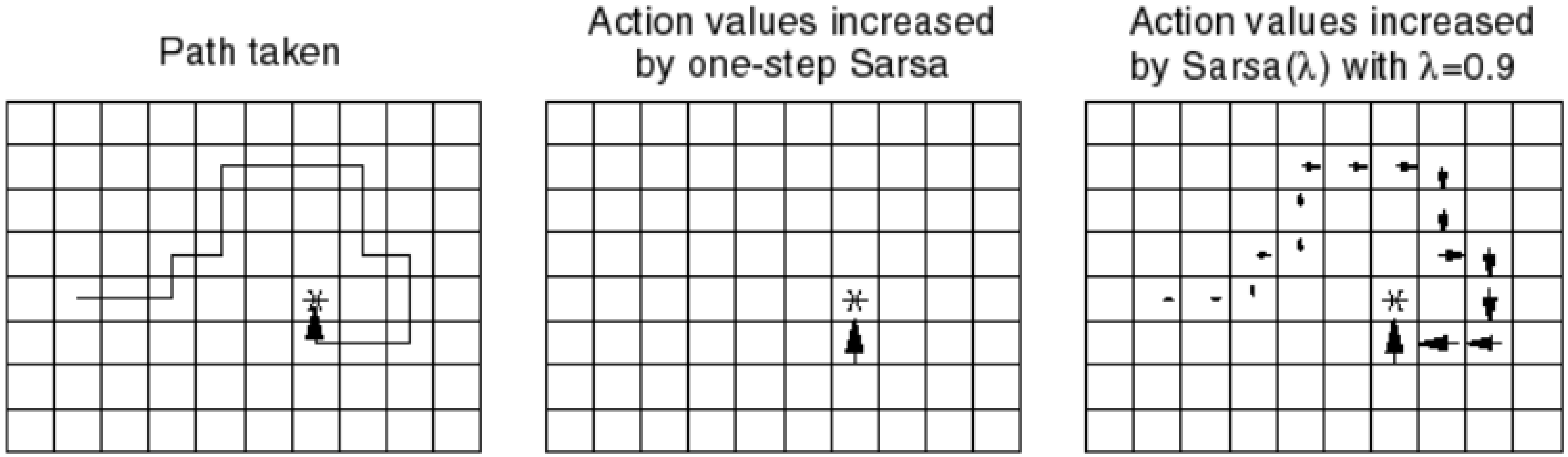
Model-based vs. Model-free

- Model-free methods use the **reward prediction error** (RPE) to update values:

$$\delta_t = r_{t+1} + \gamma \, V^\pi(s_{t+1}) - V^\pi(s_t)$$

$$\Delta V^\pi(s_t) = \alpha \, \delta_t$$

Encountered rewards propagate very slowly to all states and actions.


Path taken
Action values increased by one-step Sarsa
Action values increased by Sarsa(λ) with λ=0.9

- If the environment changes (transition probabilities, rewards), they have to relearn everything.
- After training, selecting an action is very fast.

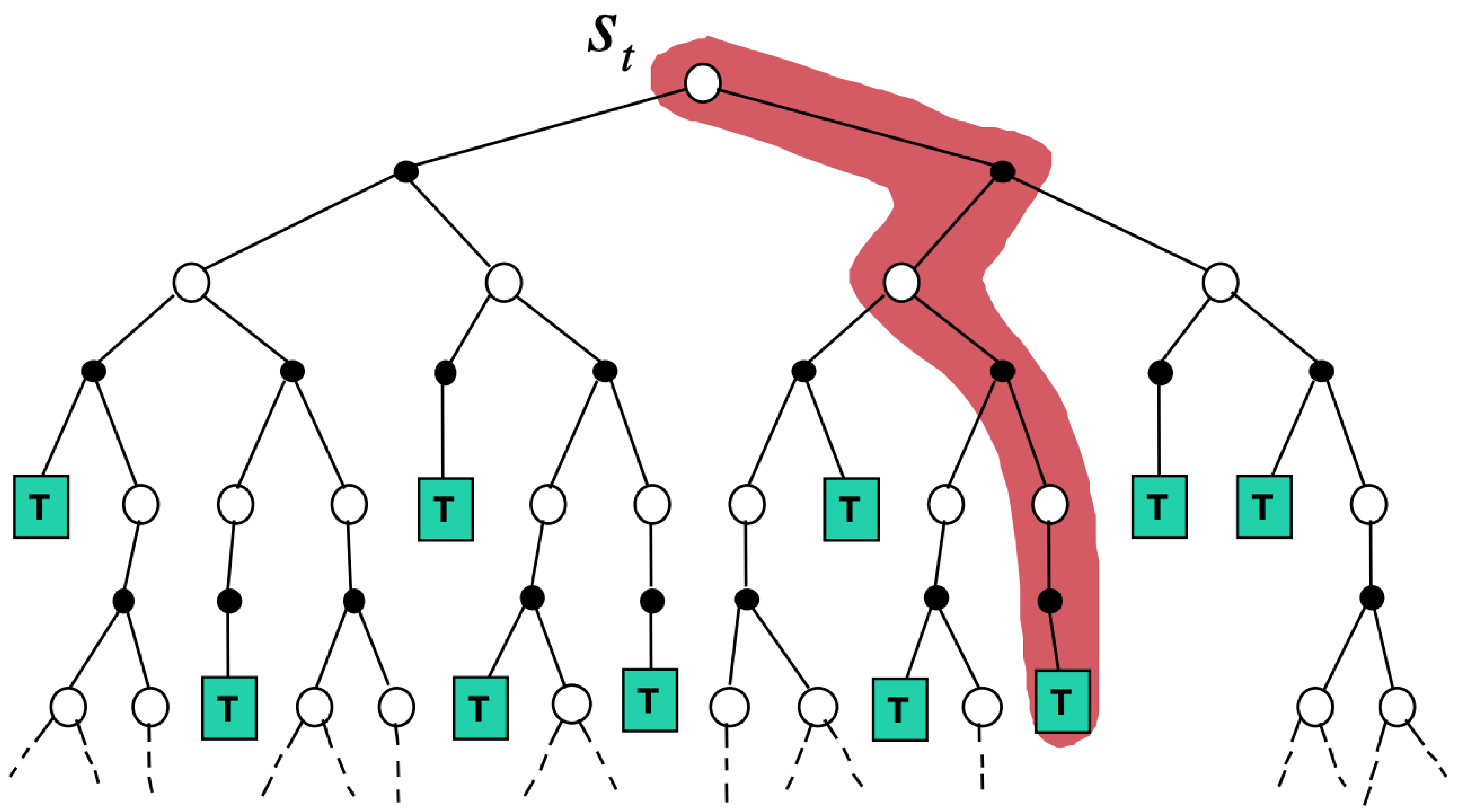
Model-based vs. Model-free

- Model-based RL can learn very fast changes in the transition or reward distributions:

$$\Delta r(s_t, a_t, s_{t+1}) = \alpha \, (r_{t+1} - r(s_t, a_t, s_{t+1}))$$

$$\Delta p(s' | s_t, a_t) = \alpha \, (\mathbb{I}(s_{t+1} = s') - p(s' | s_t, a_t))$$

- But selecting an action requires planning in the tree of possibilities (slow).



Model-based vs. Model-free

- Relative advantages of MF and MB methods:

	Inference speed	**Sample complexity**	**Optimality**	**Flexibility**
Model-free	fast	high	yes	no
Model-based	slow	low	as good as the model	yes

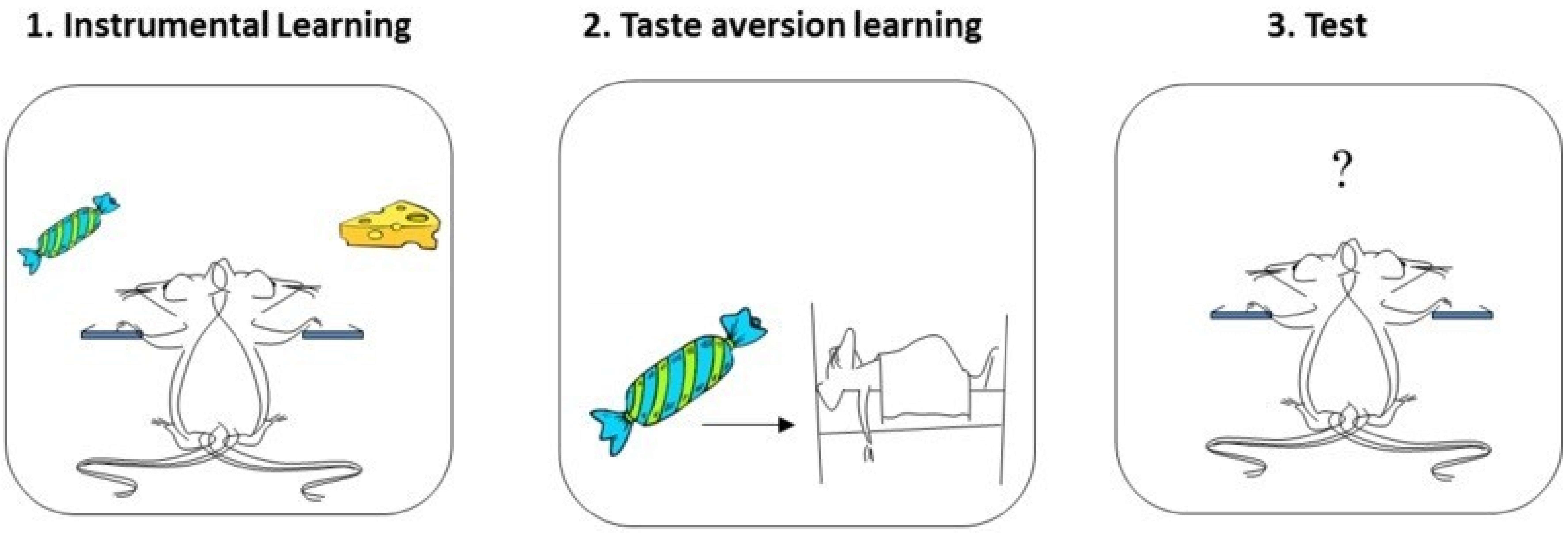
- A trade-off would be nice… Most MB models in the deep RL literature are hybrid MB/MF models anyway.

Outcome devaluation

- Two forms of behavior are observed in the animal psychology literature:

1. **Goal-directed** behavior learns Stimulus $\rightarrow$ Response $\rightarrow$ Outcome associations.
2. **Habits** are developed by overtraining Stimulus $\rightarrow$ Response associations.

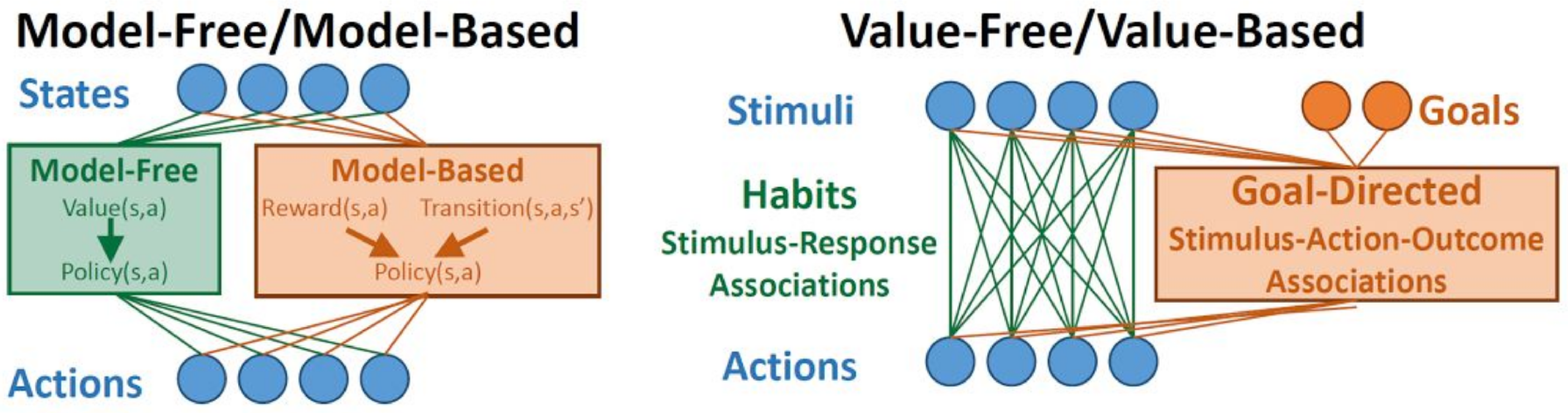
- The main difference is that habits are not influenced by **outcome devaluation**, i.e. when rewards lose their value.



Source: Bernard W. Balleine

Goal-directed / habits = MB / MF ?

- The classical theory assigns MF to habits and MB to goal-directed, mostly because their sensitivity to outcome devaluation.



- The open question is the arbitration mechanism between these two segregated process: who takes control?
- Recent work suggests both systems are largely overlapping.

References

Doll, B. B., Simon, D. A., and Daw, N. D. (2012). The ubiquity of model-based reinforcement learning. Current Opinion in Neurobiology 22, 1075–1081. doi:10.1016/j.conb.2012.08.003.

Miller, K., Ludvig, E. A., Pezzulo, G., and Shenhav, A. (2018). "Re-aligning models of habitual and goal-directed decision-making," in Goal-Directed Decision Making : Computations and Neural Circuits, eds. A. Bornstein, R. W. Morris, and A. Shenhav (Academic Press)

2 - Successor representations

Successor Representations (SR)

- Successor representations (SR) have been introduced to combine MF and MB properties. Let's split the definition of the value of a state:

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

$$\tag{2}$$

$$= \mathbb{E}_\pi[\begin{bmatrix} 1 \\ \gamma \\ \gamma^2 \\ \dots \\ \gamma^\infty \end{bmatrix} \times \begin{bmatrix} \mathbb{I}(s_t) \\ \mathbb{I}(s_{t+1}) \\ \mathbb{I}(s_{t+2}) \\ \dots \\ \mathbb{I}(s_\infty) \end{bmatrix} \times \begin{bmatrix} r_{t+1} \\ r_{t+2} \\ r_{t+3} \\ \dots \\ r_{t+\infty} \end{bmatrix} | s_t = s] \tag{3}$$

where $\mathbb{I}(s_t)$ is 1 when the agent is in s_t at time t, 0 otherwise.

- The left part corresponds to the **transition dynamics**: which states will be visited by the policy, discounted by γ.
- The right part corresponds to the **immediate reward** in each visited state.
- Couldn't we learn the transition dynamics and the reward distribution separately in a model-free manner?

Successor Representations (SR)

- SR rewrites the value of a state into an **expected discounted future state occupancy** $M^\pi(s, s')$ and an **expected immediate reward** $r(s')$ by summing over all possible states s' of the MDP:

$$V^\pi(s) = \mathbb{E}_\pi[\sum_{k=0}^{\infty} \gamma^k \, r_{t+k+1} | s_t = s] \tag{4}$$

$$\tag{5}$$

$$= \sum_{s' \in \mathcal{S}} \mathbb{E}_\pi[\sum_{k=0}^{\infty} \gamma^k \, \mathbb{I}(s_{t+k} = s') \times r_{t+k+1} | s_t = s] \tag{6}$$

$$\tag{7}$$

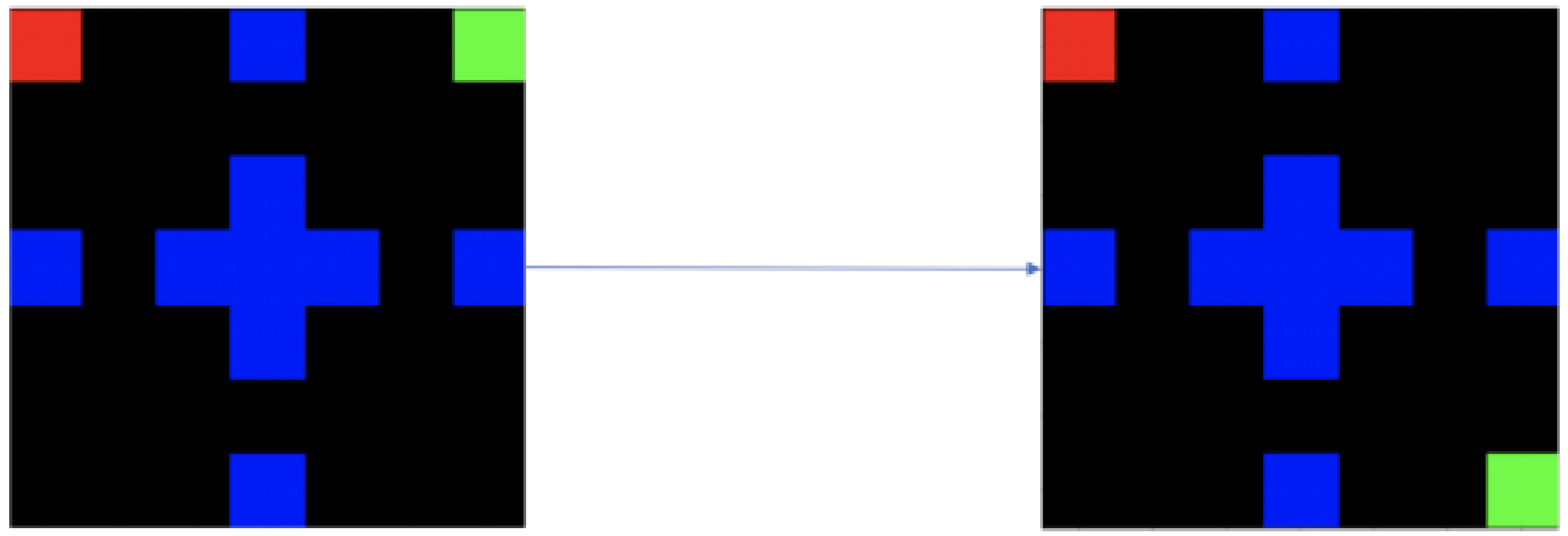
$$\approx \sum_{s' \in \mathcal{S}} \mathbb{E}_\pi[\sum_{k=0}^{\infty} \gamma^k \, \mathbb{I}(s_{t+k} = s') | s_t = s] \times \mathbb{E}[r_{t+1} | s_t = s'] \tag{8}$$

$$\tag{9}$$

$$\approx \sum_{s' \in \mathcal{S}} M^\pi(s, s') \times r(s') \tag{10}$$

Successor Representations (SR)

- The underlying assumption is that the world dynamics are independent from the reward function (which does not depend on the policy).
- This allows to re-use knowledge about world dynamics in other contexts (e.g. a new reward function in the same environment): **transfer learning**.



Source: https://awjuliani.medium.com/the-present-in-terms-of-the-future-successor-representations-in-reinforcement-learning-316b78c5fa3

- What matters is the states that you will visit and how interesting they are, not the order in which you visit them.
- Knowing that being in the mensa will eventually get you some food is enough to know that being in the mensa is a good state: you do not need to remember which exact sequence of transitions will put food in your mouth.

Successor Representations (SR)

- SR algorithms must estimate two quantities:
   1. The **expected immediate reward** received after each state:

$$r(s) = \mathbb{E}[r_{t+1} | s_t = s]$$

   2. The **expected discounted future state occupancy** (the **SR** itself):

$$M^\pi(s, s') = \mathbb{E}_{\pi} [\sum_{k=0}^\infty \gamma^k \, \mathbb{I}(s_{t+k} = s') | s_t = s]$$

- The value of a state s is then computed with:

$$V^\pi(s) = \sum_{s' \in \mathcal{S}} M(s, s') \times r(s')$$

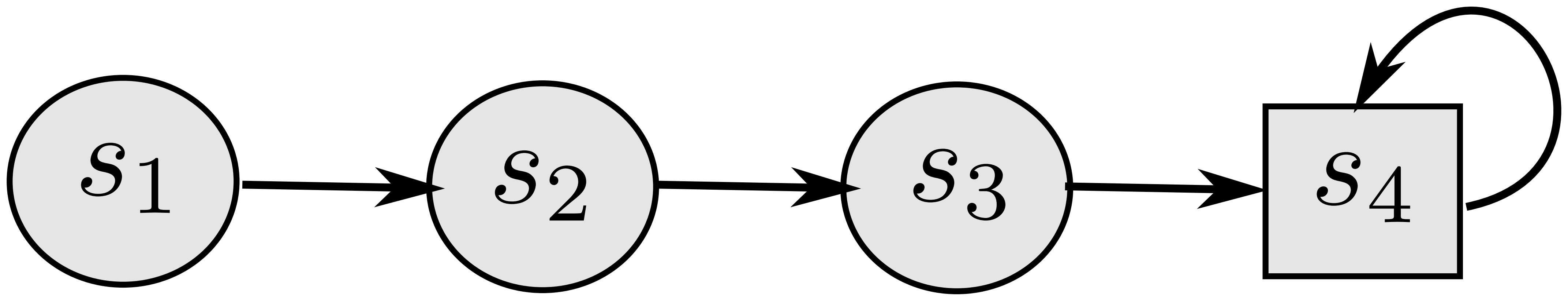
what allows to infer the policy (e.g. using an actor-critic architecture).

- The immediate reward for a state can be estimated very quickly and flexibly after receiving each reward:

$$\Delta \, r(s_t) = \alpha \, (r_{t+1} - r(s_t))$$

SR and transition matrix

- Imagine a very simple MDP with 4 states and a single deterministic action:


$$\begin{tikzcd} s_1 \arrow[r] & s_2 \arrow[r] & s_3 \arrow[r] & \boxed{s_4} \arrow[loop right] \end{tikzcd}$$

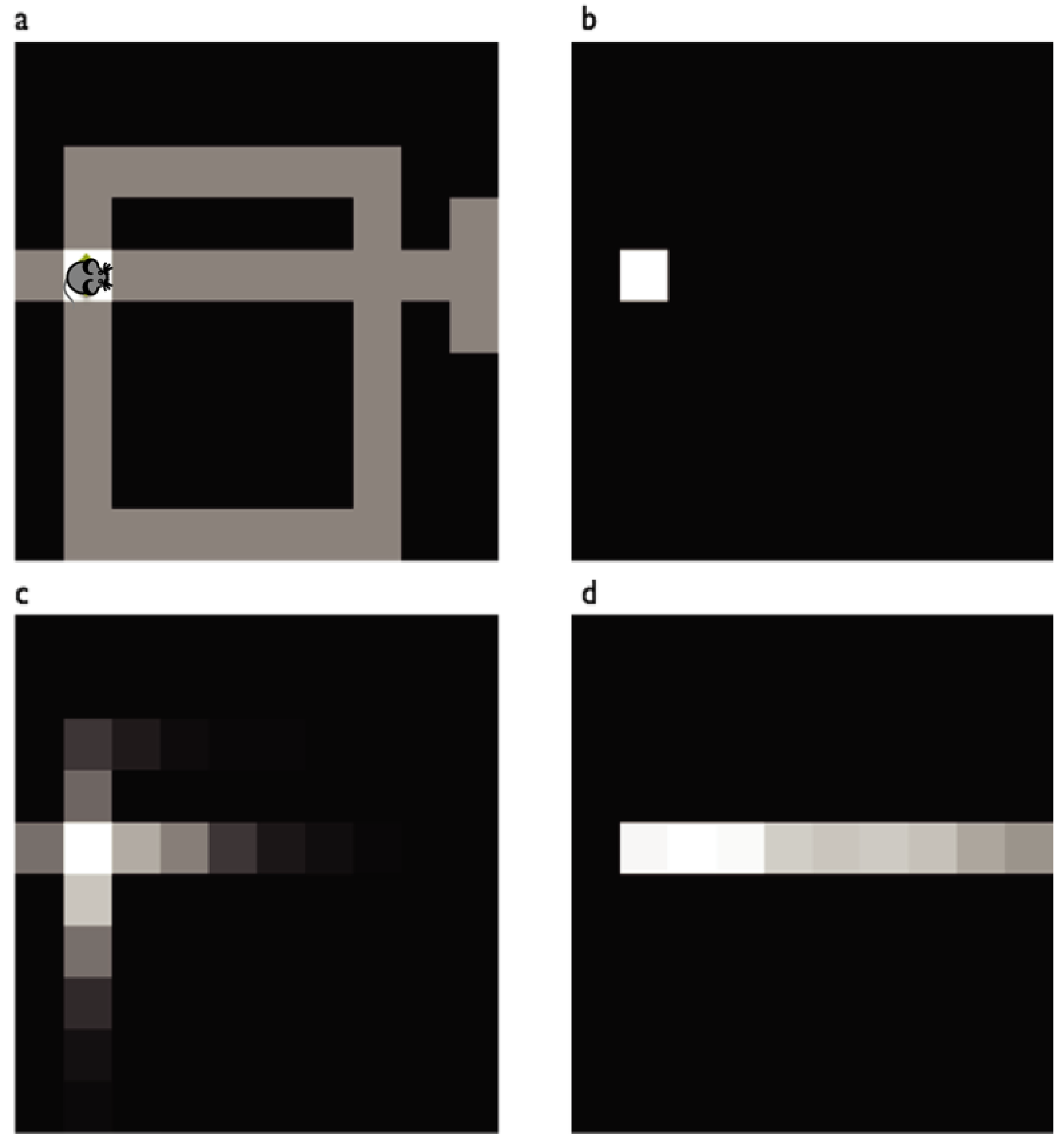
- The transition matrix $\mathcal{P}^\pi$ depicts the possible (s, s') transitions:

$$\mathcal{P}^\pi = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

- The SR matrix M also represents the future transitions discounted by γ:

$$M = \begin{bmatrix} 1 & \gamma & \gamma^2 & \gamma^3 \\ 0 & 1 & \gamma & \gamma^2 \\ 0 & 0 & 1 & \gamma \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

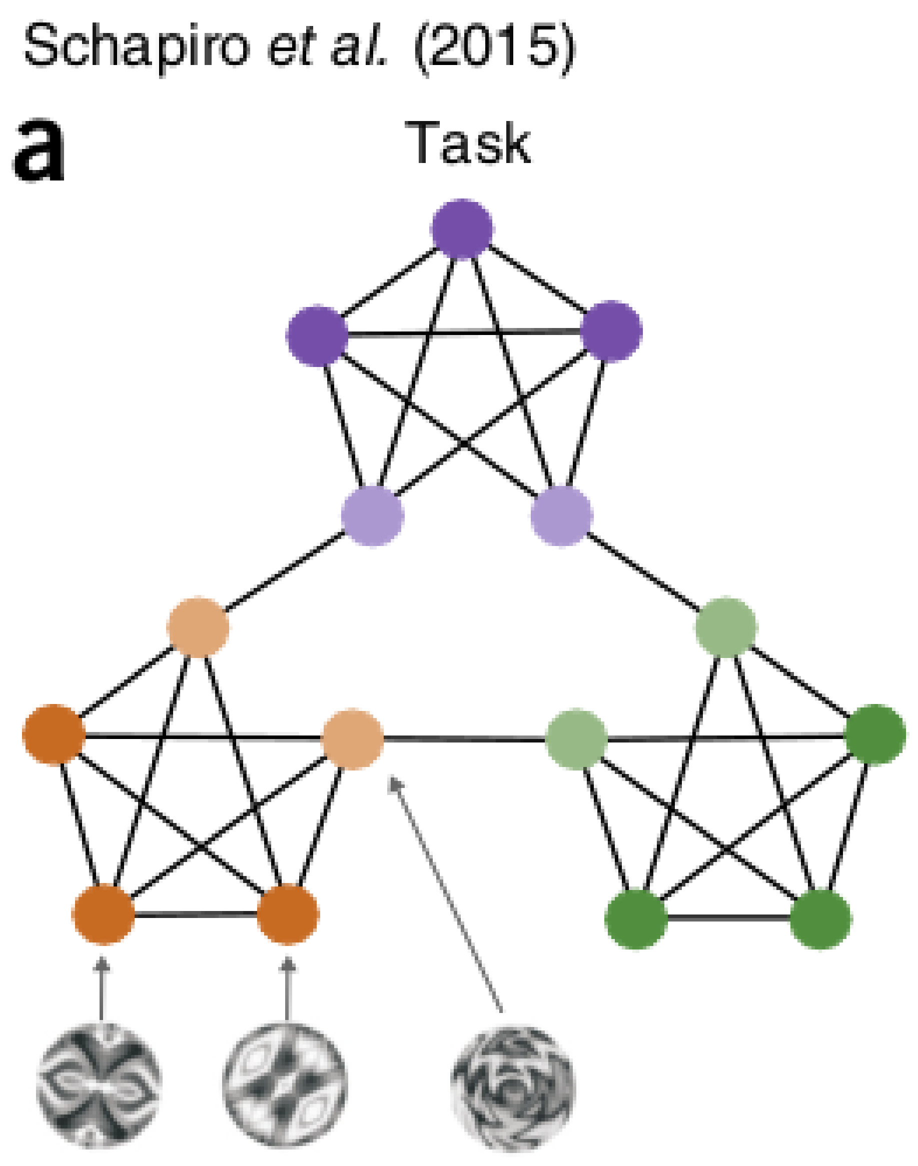
SR matrix in a Tolman's maze

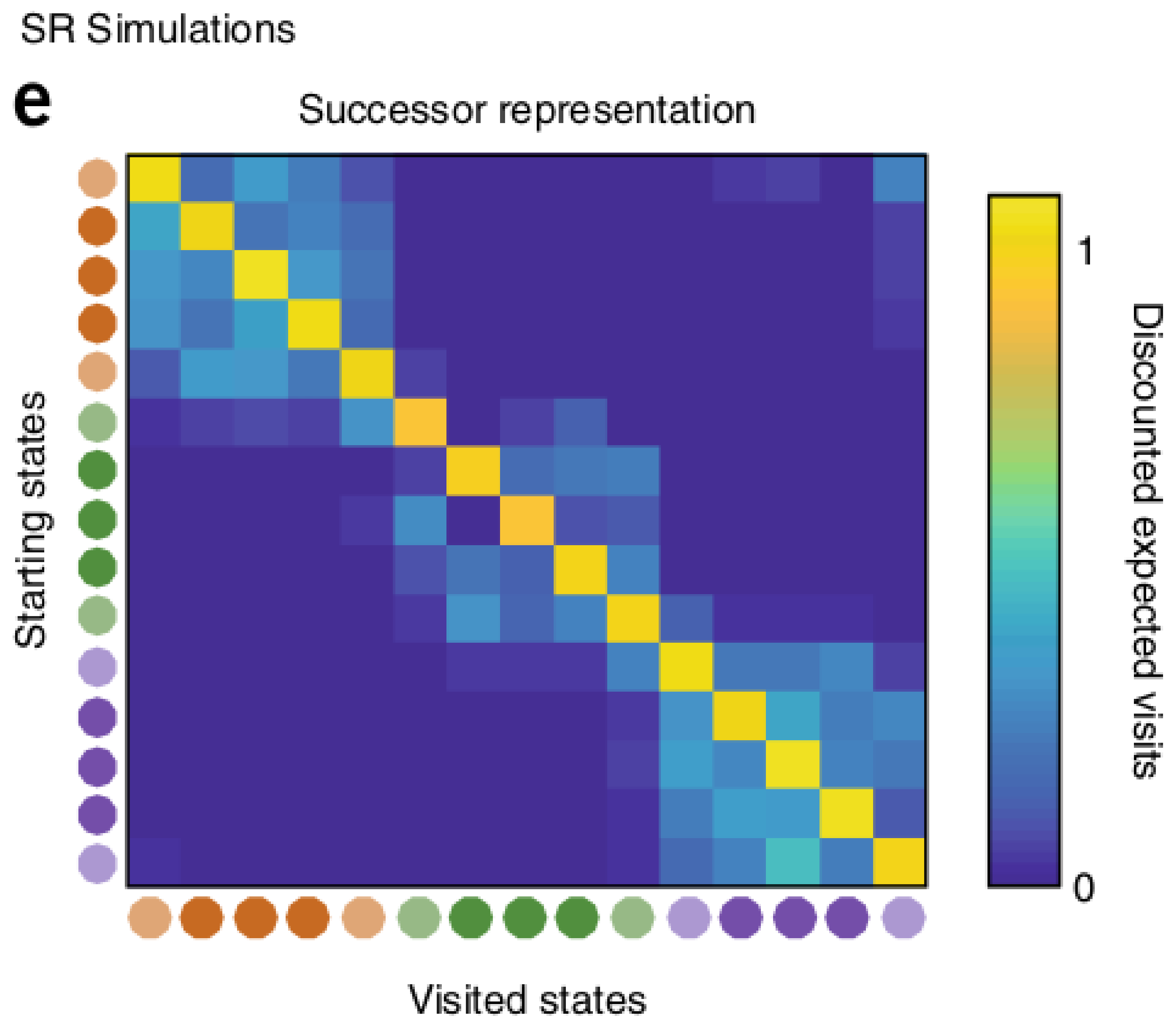


- The SR represents whether a state can be reached soon from the current state (b) using the current policy.
- The SR depends on the policy:
    - A random agent will map the local neighborhood (c).
    - A goal-directed agent will have SR representations that follow the optimal path (d).
- It is therefore different from the transition matrix, as it depends on behavior and rewards.
- The exact dynamics are lost compared to MB: it only represents whether a state is reachable, not how.

Example of a SR matrix

- The SR matrix reflects the proximity between states depending on the transitions and the policy. it does not have to be a spatial relationship.





Learning the SR

- How can we learn the SR matrix for all pairs of states?

$$M^\pi(s, s') = \mathbb{E}_\pi [\sum_{k=0}^\infty \gamma^k \, \mathbb{I}(s_{t+k} = s') | s_t = s]$$

- We first notice that the SR obeys a recursive Bellman-like equation:

$$\begin{aligned}
M^\pi(s, s') &= \mathbb{I}(s_t = s') + \mathbb{E}_\pi [\sum_{k=1}^\infty \gamma^k \, \mathbb{I}(s_{t+k} = s') | s_t = s] \\
&= \mathbb{I}(s_t = s') + \gamma \, \mathbb{E}_\pi [\sum_{k=0}^\infty \gamma^k \, \mathbb{I}(s_{t+k+1} = s') | s_t = s] \\
&= \mathbb{I}(s_t = s') + \gamma \, \mathbb{E}_{s_{t+1} \sim \mathcal{P}^\pi(s'|s)} [\mathbb{E}_\pi [\sum_{k=0}^\infty \gamma^k \, \mathbb{I}(s_{t+k} = s') | s_{t+1} = s]] \\
&= \mathbb{I}(s_t = s') + \gamma \, \mathbb{E}_{s_{t+1} \sim \mathcal{P}^\pi(s'|s)} [M^\pi(s_{t+1}, s')]
\end{aligned}$$

- This is reminiscent of TDM: the remaining distance to the goal is 0 if I am already at the goal, or gamma the distance from the next state to the goal.

Model-based SR

- Bellman-like SR:

$$M^\pi(s, s') = \mathbb{I}(s_t = s') + \gamma \, \mathbb{E}_{s_{t+1} \sim \mathcal{P}^\pi(s'|s)} [M^\pi(s_{t+1}, s')]$$

- If we know the transition matrix for a fixed policy π:

$$\mathcal{P}^\pi(s, s') = \sum_a \pi(s, a) \, p(s'|s, a)$$

we can obtain the SR directly with matrix inversion as we did in **dynamic programming**:

$$M^\pi = I + \gamma \, \mathcal{P}^\pi \times M^\pi$$

so that:

$$M^\pi = (I - \gamma \, \mathcal{P}^\pi)^{-1}$$

- This DP approach is called **model-based SR** (MB-SR) as it necessitates to know the environment dynamics.

Model-free SR

- If we do not know the transition probabilities, we simply sample a single s_t, s_{t+1} transition:

$$M^\pi(s_t, s') \approx \mathbb{I}(s_t = s') + \gamma \, M^\pi(s_{t+1}, s')$$

- We can define a **sensory prediction error** (SPE):

$$\delta_t^{\text{SR}} = \mathbb{I}(s_t = s') + \gamma \, M^\pi(s_{t+1}, s') - M(s_t, s')$$

that is used to update an estimate of the SR:

$$\Delta M^\pi(s_t, s') = \alpha \, \delta_t^{\text{SR}}$$

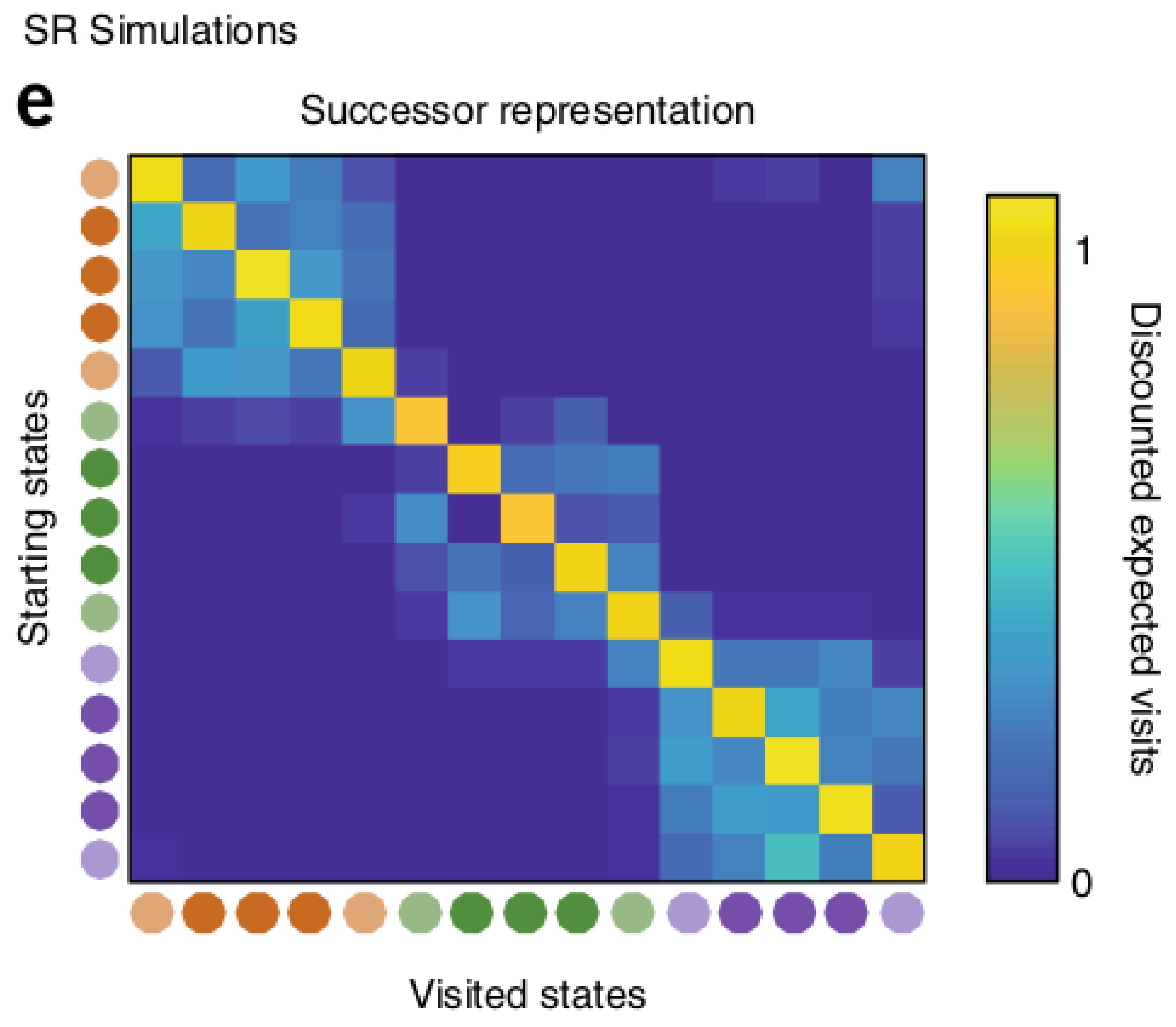
- This is **SR-TD**, using a SPE instead of RPE, which learns only from transitions but ignores rewards.

The sensory prediction error - SPE

- The SPE has to be applied on ALL successor states s' after a transition (s_t, s_{t+1}):

$$M^\pi(s_t, \mathbf{s'}) = M^\pi(s_t, \mathbf{s'}) + \alpha \, (\mathbb{I}(s_t = \mathbf{s'}) + \gamma \, M^\pi(s_{t+1}, \mathbf{s'}) - M(s_t, \mathbf{s'}))$$

- Contrary to the RPE, the SPE is a **vector** of prediction errors, used to update one row of the SR matrix.
- The SPE tells how **surprising** a transition $s_t \rightarrow s_{t+1}$ is for the SR.



Successor representations

- The SR matrix represents the **expected discounted future state occupancy**:

$$M^\pi(s, s') = \mathbb{E}_\pi [\sum_{k=0}^\infty \gamma^k \, \mathbb{I}(s_{t+k} = s') | s_t = s]$$

- It can be learned using a TD-like SPE from single transitions:

$$M^\pi(s_t, \mathbf{s'}) = M^\pi(s_t, \mathbf{s'}) + \alpha \, (\mathbb{I}(s_t = \mathbf{s'}) + \gamma \, M^\pi(s_{t+1}, \mathbf{s'}) - M(s_t, \mathbf{s'}))$$

- The immediate reward in each state can be learned **independently from the policy**:

$$\Delta \, r(s_t) = \alpha \, (r_{t+1} - r(s_t))$$

- The value $V^\pi(s)$ of a state is obtained by summing of all successor states:

$$V^\pi(s) = \sum_{s' \in \mathcal{S}} M(s, s') \times r(s')$$

- This critic can be used to train an **actor** π_θ using regular TD learning (e.g. A3C).

Successor representation of actions

- Note that it is straightforward to extend the idea of SR to state-action pairs:

$$M^\pi(s, a, s') = \mathbb{E}_\pi [\sum_{k=0}^\infty \gamma^k \, \mathbb{I}(s_{t+k} = s') | s_t = s, a_t = a]$$

allowing to estimate Q-values:

$$Q^\pi(s, a) = \sum_{s' \in \mathcal{S}} M(s, a, s') \times r(s')$$

using SARSA or Q-learning-like SPEs:

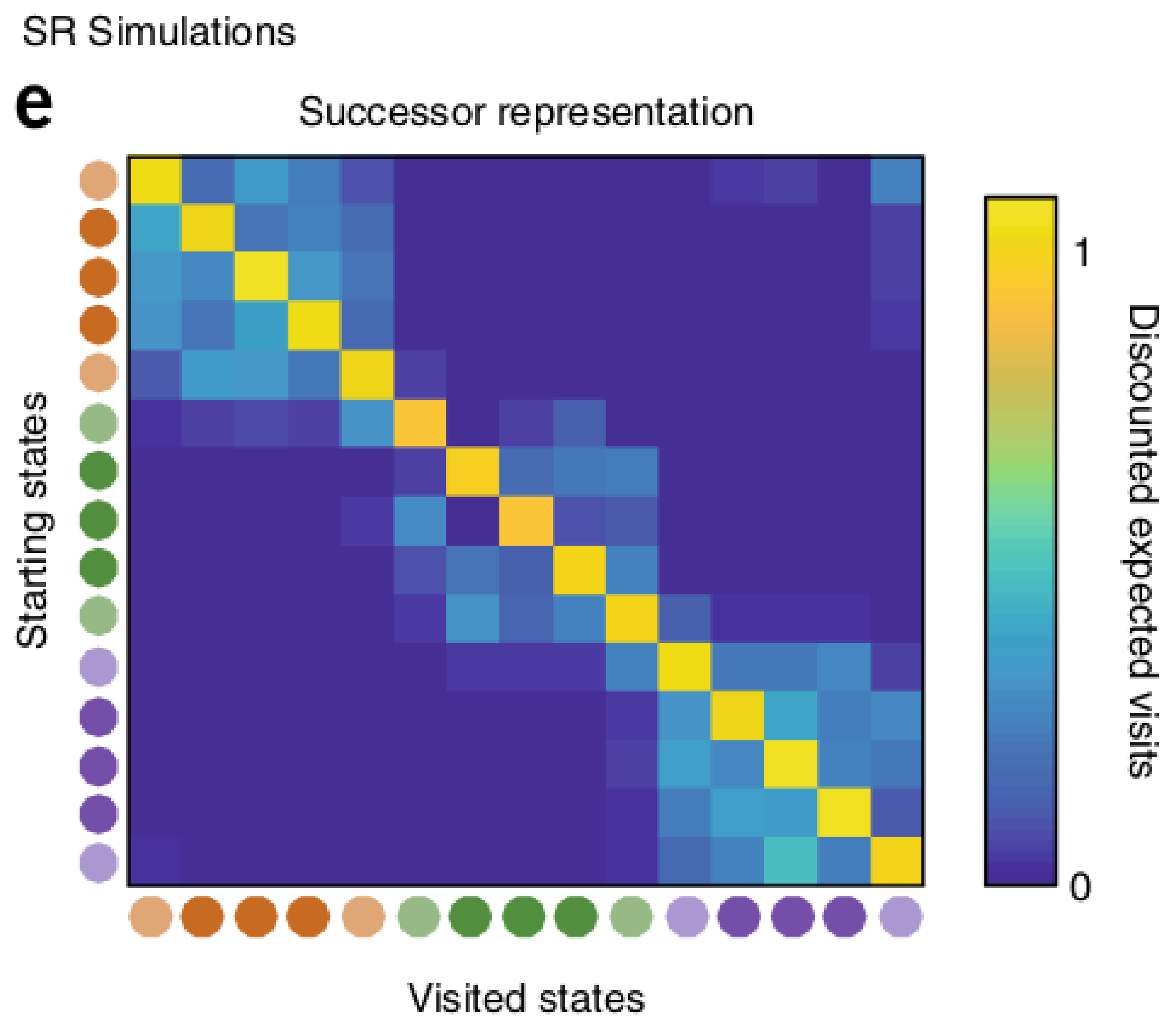
$$\delta^\text{SR}_t = \mathbb{I}(s_t = s') + \gamma \, M^\pi(s_{t+1}, a_{t+1}, s') - M(s_t, a_t, s')$$

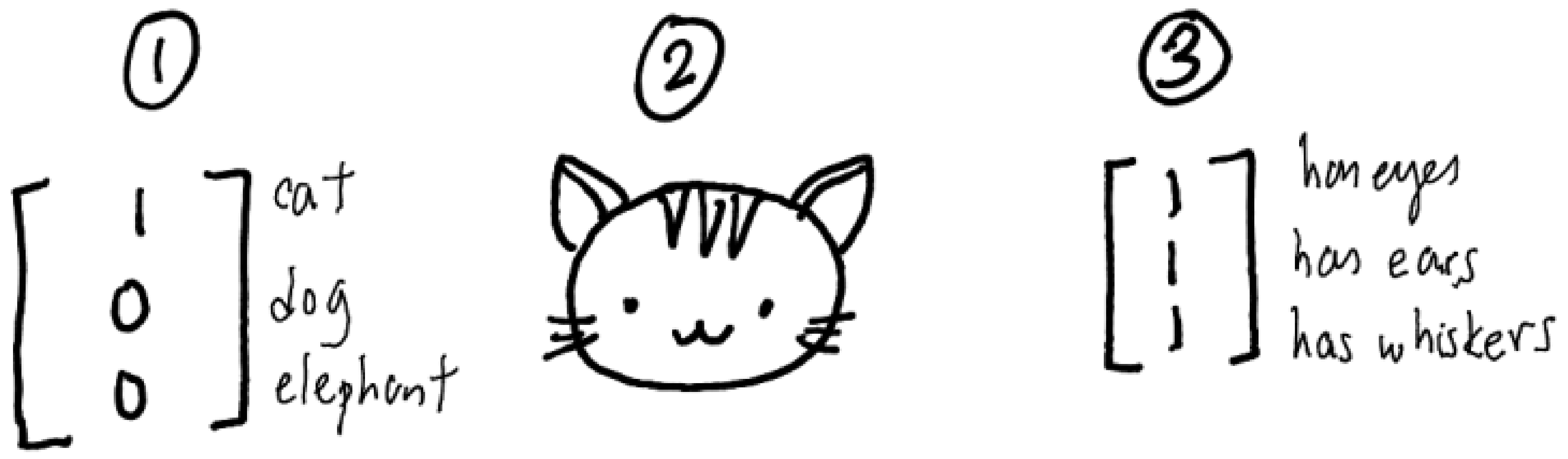
depending on the choice of the next action a_{t+1} (on- or off-policy).

3 - Successor features

Successor features

- The SR matrix associates each state to all others ($N \times N$ matrix):
    - curse of dimensionality.
    - only possible for discrete state spaces.
- A better idea is to describe each state s by a feature vector $\phi(s) = [\phi_i(s)]_{i=1}^d$ with less dimensions than the number of states.
- This feature vector can be constructed (see the lecture on function approximation) or learned by an autoencoder (latent representation).

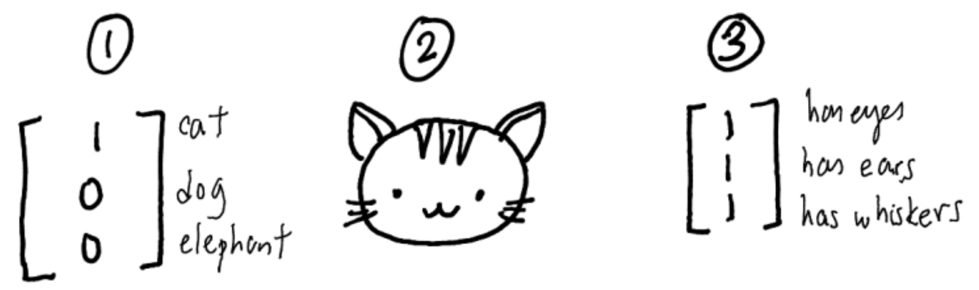




Source: http://www.jessicayung.com/the-successor-representation-1-generalising-between-states/

Successor features

- The **successor feature representation** (SFR) represents the discounted probability of observing a feature ϕ_j after being in s.



Source: http://www.jessicayung.com/the-successor-representation-1-generalising-between-states/

- Instead of predicting when the agent will see a cat after being in the current state s, the SFR predicts when it will see eyes, ears or whiskers independently:

$$M^\pi_j(s) = M^\pi(s, \phi_j) = \mathbb{E}_\pi [\sum_{k=0}^\infty \gamma^k \, \mathbb{I}(\phi_j(s_{t+k})) | s_t = s, a_t = a]$$

- Linear SFR (Gehring, 2015) supposes that it can be linearly approximated from the features of the current state:

$$M^\pi_j(s) = M^\pi(s, \phi_j) = \sum_{i=1}^d m_{i,j} \, \phi_i(s)$$

Successor features

- The value of a state is now defined as the sum over successor features of their immediate reward discounted by the SFR:

$$V^\pi(s) = \sum_{j=1}^d M_j^\pi(s) \, r(\phi_j) = \sum_{j=1}^d r(\phi_j) \, \sum_{i=1}^d m_{i,j} \, \phi_i(s)$$

- The SFR matrix $M^\pi = [m_{i,j}]_{i,j}$ associates each feature ϕ_i of the current state to all successor features ϕ_j.
    - Knowing that I see a kitchen door in the current state, how likely will I see a food outcome in the near future?
- Each successor feature ϕ_j is associated to an expected immediate reward $r(\phi_j)$.
    - A good state is a state where food features (high $r(\phi_j)$) are likely to happen soon (high $m_{i,j}$).
- In matrix-vector form:

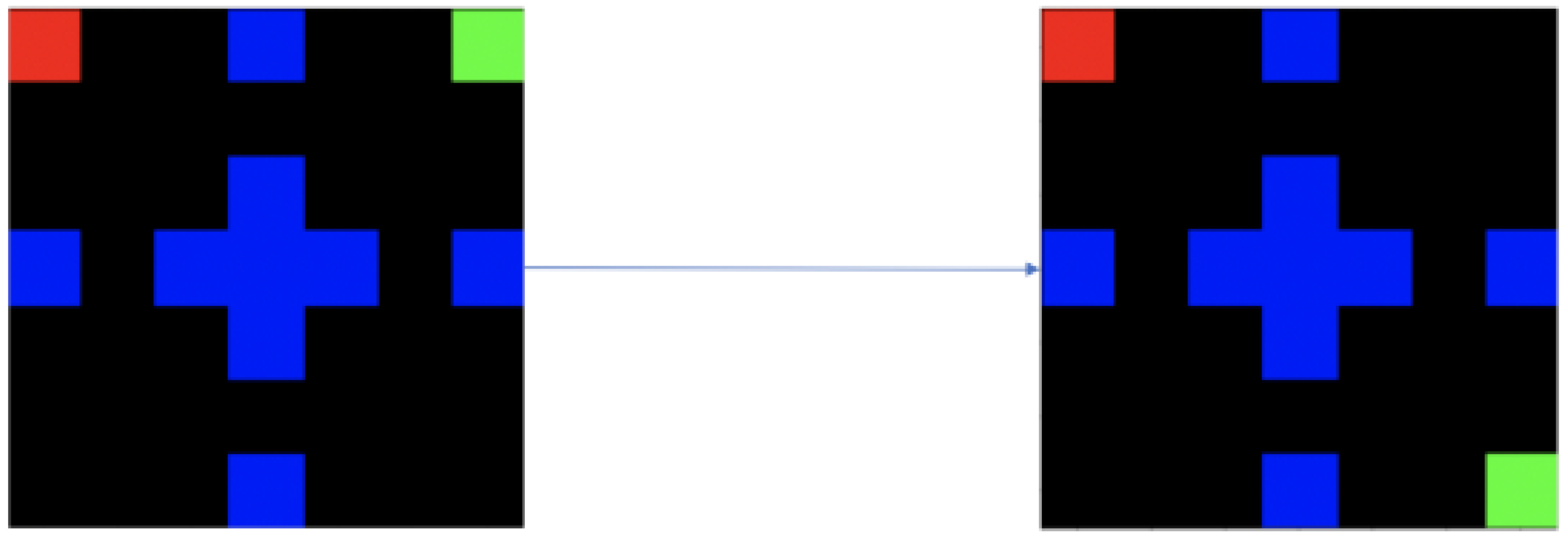
$$V^\pi(s) = \mathbf{r}^T \times M^\pi \times \phi(s)$$

Successor features

- Value of a state:

$$V^\pi(s) = \mathbf{r}^T \times M^\pi \times \phi(s)$$

- The reward vector $\mathbf{r}$ only depends on the features and can be learned independently from the policy, but can be made context-dependent:
    - Food features can be made more important when the agent is hungry, less when thirsty.
- **Transfer learning** becomes possible in the same environment:
    - Different goals (searching for food or water, going to place A or B) only require different reward vectors.
    - The dynamics of the environment are stored in the SFR.



Source: https://awjuliani.medium.com/the-present-in-terms-of-the-future-successor-representations-in-reinforcement-learning-316b78c5fa3

Successor features

- How can we learn the SFR matrix M^π?

$$V^\pi(s) = \mathbf{r}^T \times M^\pi \times \phi(s)$$

- We only need to use the sensory prediction error for a transition between the feature vectors $\phi(s_t)$ and $\phi(s_{t+1})$:

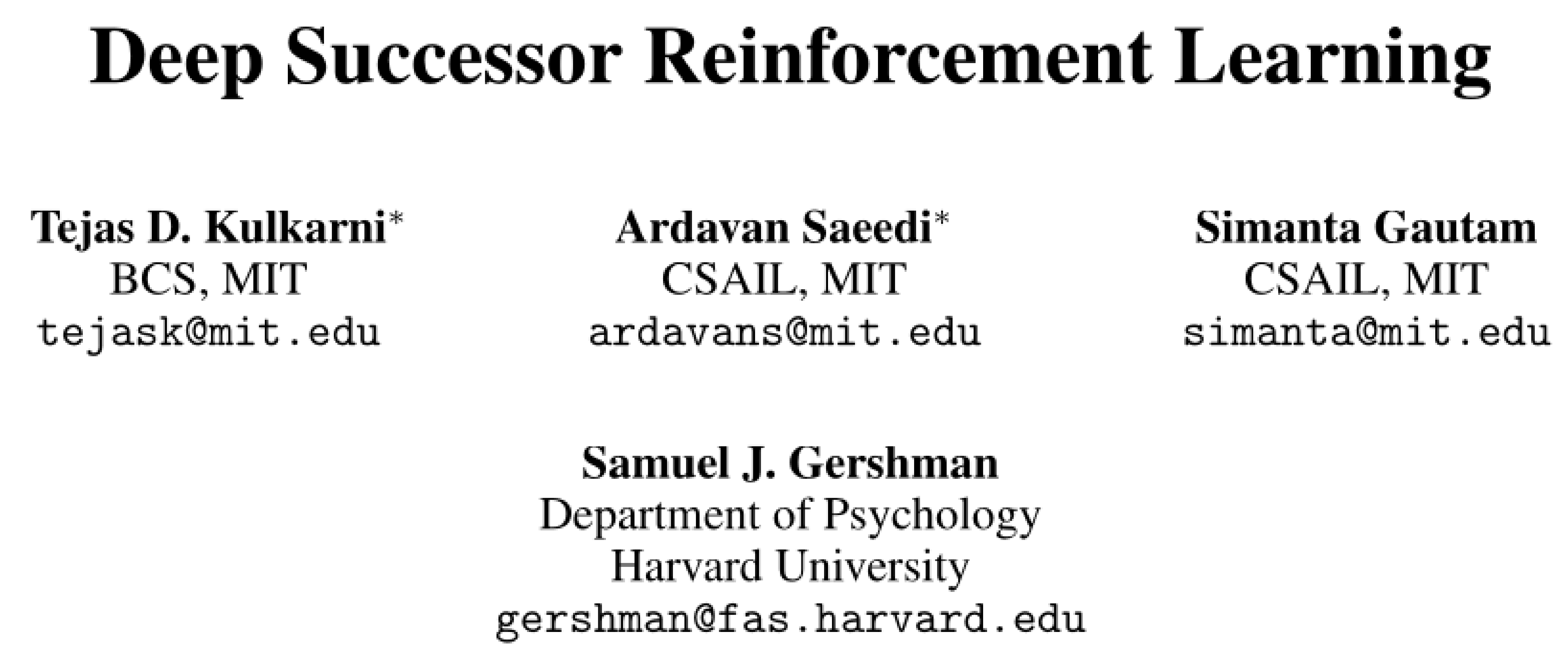
$$\delta_t^{\text{SFR}} = \phi(s_t) + \gamma \, M^\pi \times \phi(s_{t+1}) - M^\pi \times \phi(s_t)$$

and use it to update the whole matrix:

$$\Delta M^\pi = \delta_t^{\text{SFR}} \times \phi(s_t)^T$$

- However, this linear approximation scheme only works for **fixed** feature representation $\phi(s)$. We need to go deeper…

4 - Deep Successor Reinforcement Learning



Deep Successor Reinforcement Learning

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Deep Successor Reinforcement Learning

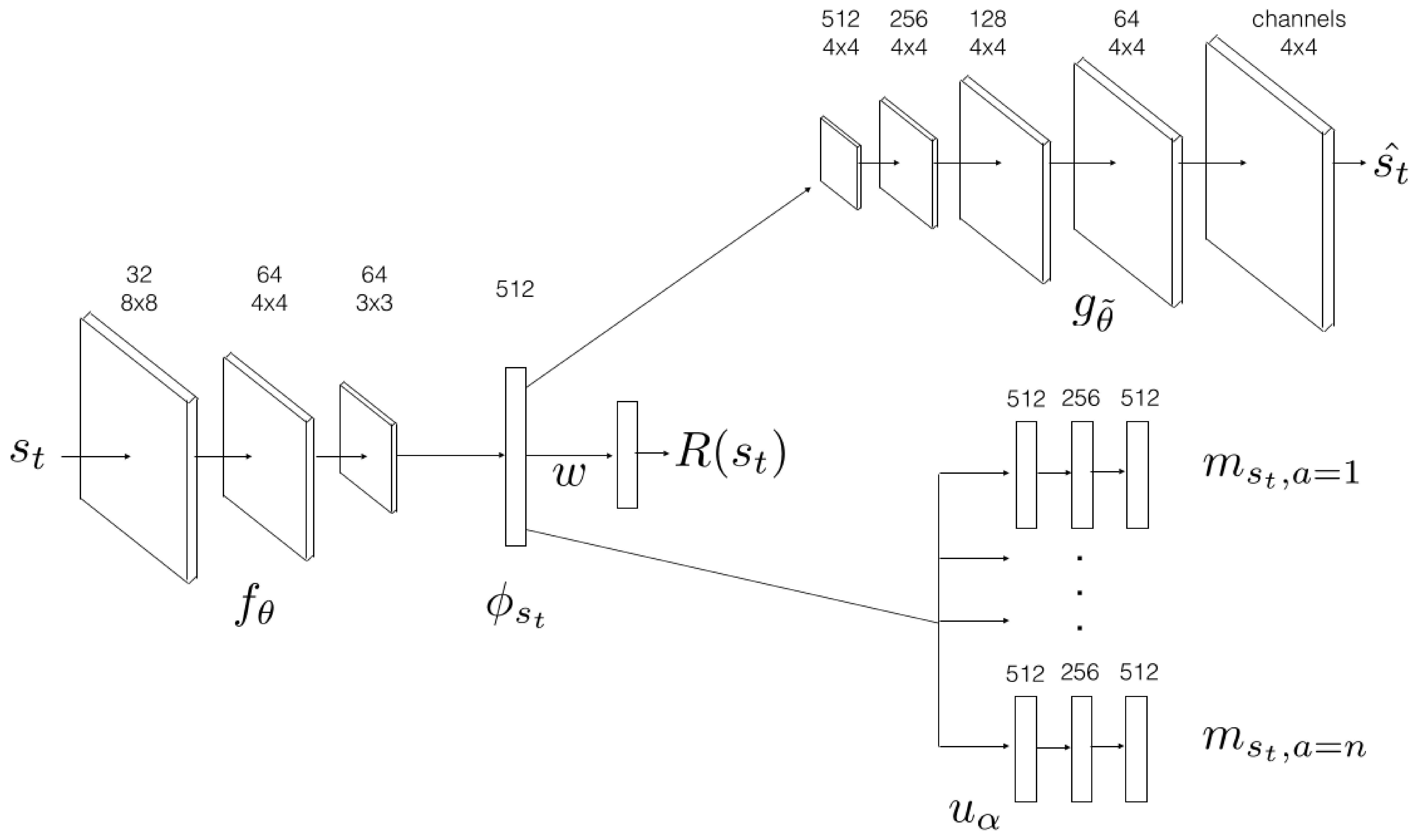

Figure 1: **Model Architecture:** DSR consists of: (1) feature branch f_θ (CNN) which takes in raw images and computes the features ϕ_{s_t}, (2) successor branch u_α which computes the SR $m_{s_t,a}$ for each possible action $a \in \mathcal{A}$, (3) a deep convolutional decoder which produces the input reconstruction $\hat{s}_t$ and (4) a linear regressor to predict instantaneous rewards at s_t. The Q-value function can be estimated by taking the inner-product of the SR with reward weights: $Q^\pi(s,a) \approx m_{sa} \cdot \mathbf{w}$.

Deep Successor Reinforcement Learning

- Each state s_t is represented by a D-dimensional (D=512) vector $\phi(s_t) = f_\theta(s_t)$ which is the output of an encoder.
- A decoder $g_{\hat{\theta}}$ is used to provide a reconstruction loss, so $\phi(s_t)$ is a latent representation of an autoencoder:

$$\mathcal{L}_\text{reconstruction}(\theta, \hat{\theta}) = \mathbb{E}[(g_{\hat{\theta}}(\phi(s_t)) - s_t)^2]$$

- The immediate reward $R(s_t)$ is linearly predicted from the feature vector $\phi(s_t)$ using a reward vector $\mathbf{w}$.

$$R(s_t) = \phi(s_t)^T \times \mathbf{w}$$

$$\mathcal{L}_\text{reward}(\mathbf{w}, \theta) = \mathbb{E}[(r_{t+1} - \phi(s_t)^T \times \mathbf{w})^2]$$

- The reconstruction loss is important, otherwise the latent representation $\phi(s_t)$ would be too reward-oriented and would not generalize.
- The reward function is learned on a single task, but it can fine-tuned on another task, with all other weights frozen.

Deep Successor Reinforcement Learning

- For each action a, a NN u_α predicts the future feature occupancy $M(s, s', a)$ for the current state:

$$m_{s_t a} = u_\alpha(s_t, a)$$

- The Q-value of an action is simply the dot product between the SR of an action and the reward vector $\mathbf{w}$:

$$Q(s_t, a) = \mathbf{w}^T \times m_{s_t a}$$

- The selected action is ϵ-greedily selected around the greedy action:

$$a_t = \arg\max_a Q(s_t, a)$$

- The SR of each action is learned using the Q-learning-like SPE (with fixed θ and a target network $u_{\alpha'}$):

$$\mathcal{L}^{\text{SPE}}(\alpha) = \mathbb{E}[\sum_a (\phi(s_t) + \gamma \max_{a'} u_{\alpha'}(s_{t+1}, a') - u_\alpha(s_t, a))^2]$$

- The compound loss is used to train the complete network end-to-end **off-policy** using a replay buffer (DQN-like).

$$\mathcal{L}(\theta, \hat{\theta}, \mathbf{w}, \alpha) = \mathcal{L}_\text{reconstruction}(\theta, \hat{\theta}) + \mathcal{L}_\text{reward}(\mathbf{w}, \theta) + \mathcal{L}^{\text{SPE}}(\alpha)$$

Kulkarni, T. D., Saeedi, A., Gautam, S., and Gershman, S. J. (2016). Deep Successor Reinforcement Learning. arXiv:1606.02396

Deep Successor Reinforcement Learning

Algorithm 1 Learning algorithm for DSR

```
 1: Initialize experience replay memory $\mathcal{D}$, parameters $\{\theta, \alpha, \mathbf{w}, \tilde{\theta}\}$ and exploration probability
    $\epsilon = 1$.
 2: for $i = 1 : \#episodes$ do
 3:     Initialize game and get start state description $s$
 4:     while  not terminal do
 5:         $\phi_s = f_\theta(s)$
 6:         With probability $\epsilon$, sample a random action $a$, otherwise choose $\text{argmax}_a u_\alpha(\phi_s, a) \cdot \mathbf{w}$
 7:         Execute $a$ and obtain next state $s'$ and reward $R(s')$ from environment
 8:         Store transition $(s, a, R(s'), s')$ in $\mathcal{D}$
 9:         Randomly sample mini-batches from $\mathcal{D}$
10:         Perform gradient descent on the loss $L^r(\mathbf{w}, \theta) + L^a(\tilde{\theta}, \theta)$ with respect to $\mathbf{w}$, $\theta$ and $\tilde{\theta}$.
11:         Fix $(\theta, \tilde{\theta}, \mathbf{w})$ and perform gradient descent on $L^m(\alpha, \theta)$ with respect to $\alpha$.
12:         $s \leftarrow s'$
13:     end while
14:     Anneal exploration variable $\epsilon$
15: end for
```

Deep Successor Reinforcement Learning

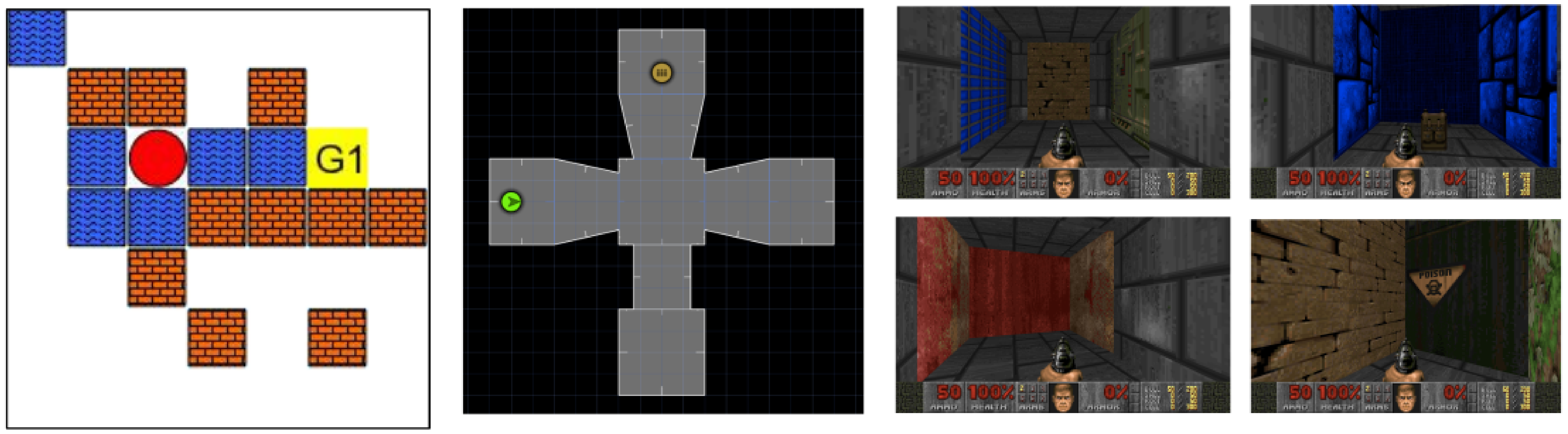

Figure 2: **Environments**: **(left)** MazeBase [37] map where the agent starts at an arbitrary location and needs to get to the goal state. The agent gets a penalty of -0.5 per-step, -1 to step on the water-block (blue) and +1 for reaching the goal state. The model observes raw pixel images during learning. **(center)** A *Doom* map using the VizDoom engine [13] where the agent starts in a room and has to get to another room to collect ammo (per-step penalty = -0.01, reward for reaching goal = +1). **(right)** Sample screen-shots of the agent exploring the 3D maze.

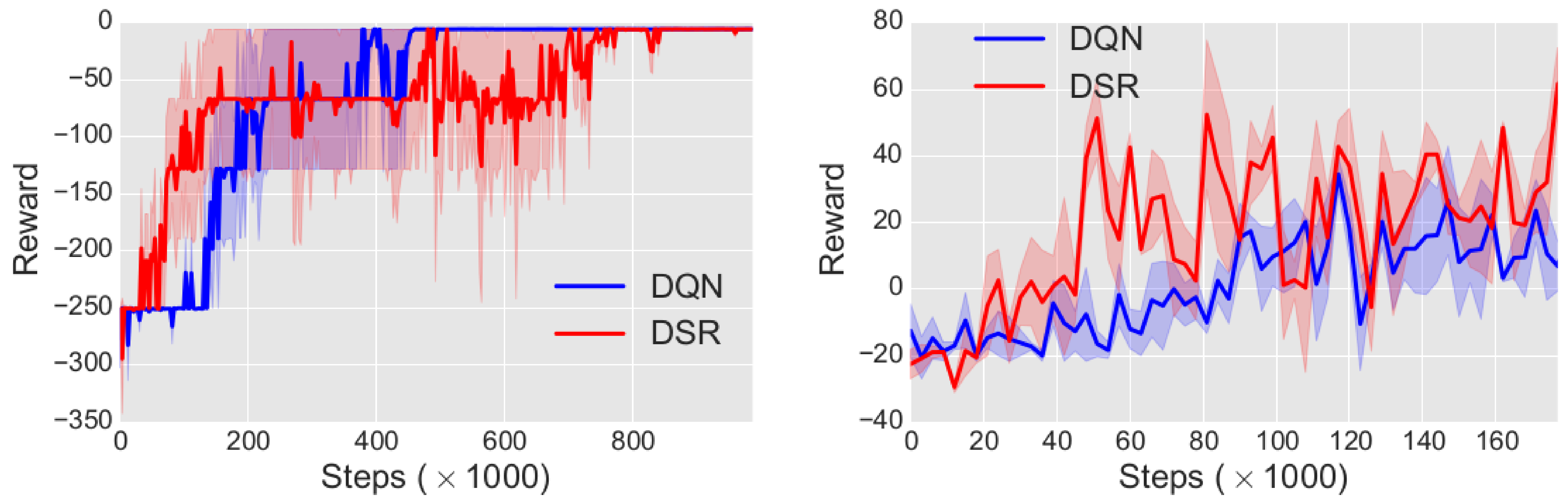

Figure 3: Average trajectory of the reward **(left)** over 100k steps for the grid-world maze. **(right)** over 180k steps for the Doom map over multiple runs.

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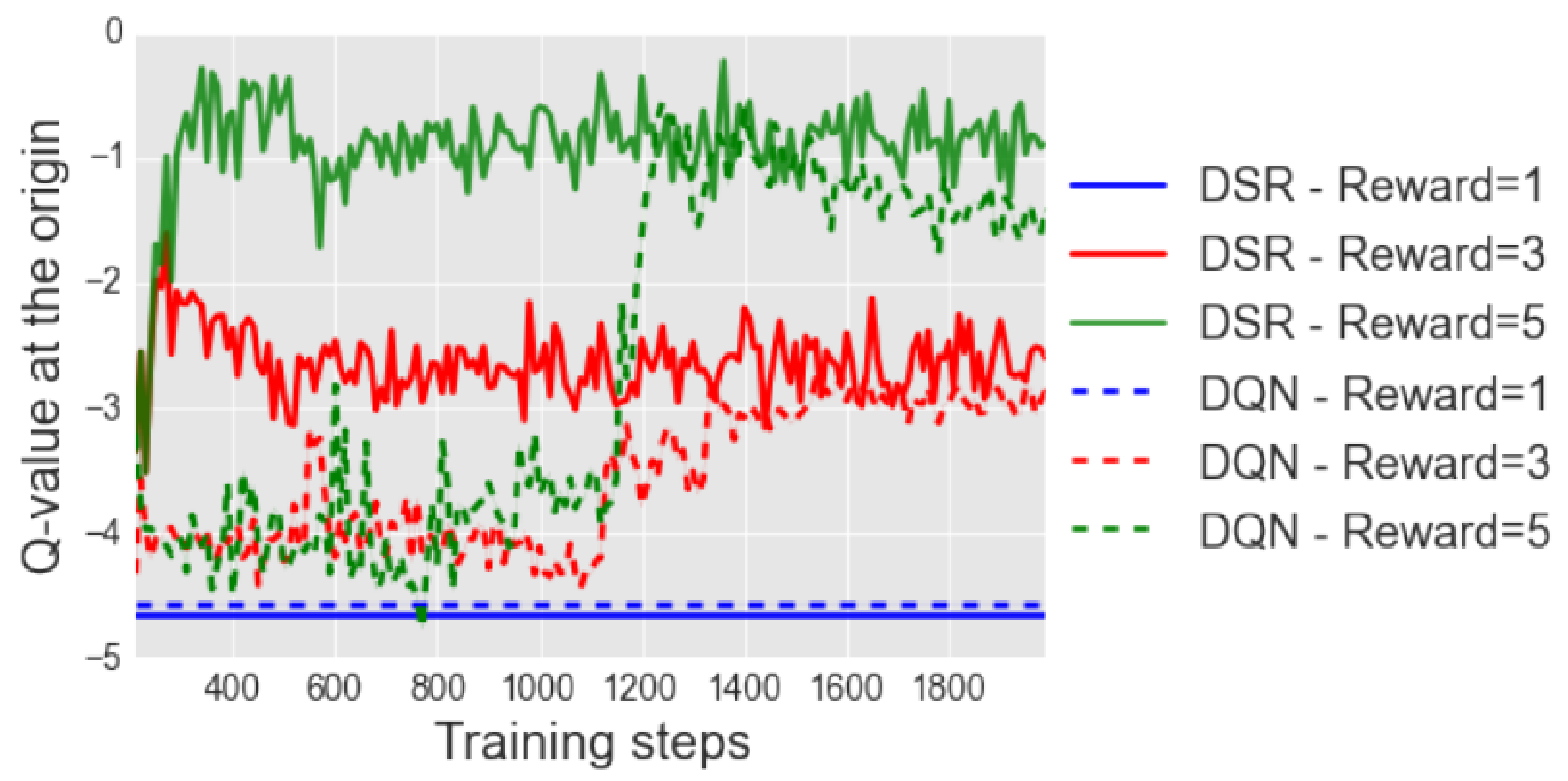
- The interesting property is that you do not need rewards to learn:
  - A random agent can be used to learn the encoder and the SR, but $\mathbf{w}$ can be left untouched.
  - When rewards are introduced (or changed), only $\mathbf{w}$ has to be adapted, while DQN would have to re-learn all Q-values.



- This is the principle of **latent learning** in animal psychology: fooling around in an environment without a goal allows to learn the structure of the world, what can speed up learning when a task is introduced.
- The SR is a **cognitive map** of the environment: learning task-unspecific relationships.

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- Note: the same idea was published by three different groups at the same time (preprint in 2016, conference in 2017):
    - Barreto A, Dabney W, Munos R, Hunt JJ, Schaul T, van Hasselt H, Silver D. (2016). Successor Features for Transfer in Reinforcement Learning. arXiv:160605312.
    - Kulkarni, T. D., Saeedi, A., Gautam, S., and Gershman, S. J. (2016). Deep Successor Reinforcement Learning. arXiv:1606.02396.
    - Zhang J, Springenberg JT, Boedecker J, Burgard W. (2016). Deep Reinforcement Learning with Successor Features for Navigation across Similar Environments. arXiv:161205533.
- The (Barreto et al., 2016) is from Deepmind, so it tends to be cited more…

Visual Semantic Planning using Deep Successor Representations