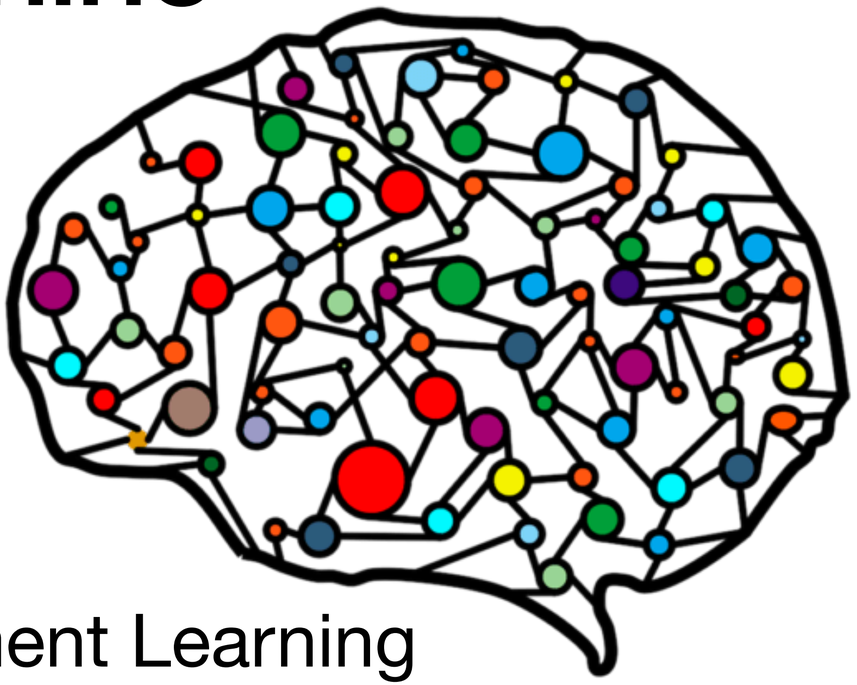
General Principles of Human and Machine Learning



Lecture 5: Advances in Reinforcement Learning

Dr. Charley Wu

https://hmc-lab.com/GPHML.html

Schedule

Week 6:	Guest lecturer: Alexandra Witt	Nov 19: Social learning	Nov 20	Alex	Witt et al., (2024)
Week 7:	Guest lecturer: Dr. David Nagy	Nov 26: Compression and resource constraints	Nov 27	David	Nagy et al,. (under review)
Week 8:		Dec 3: Concepts and Categories	Dec 4	Hanqi	Murphy (2023)
Week 9:		Dec 10: Supervised and Unsupervised learning	Dec 11	Hanqi	Bishop (Ch. 4)
	Holiday break				
Week 10:		Jan 14: Function learning	Jan 15	Alex	Wu, Meder, & Schulz (2024)
Week 11:		Jan 21: No Lecture	Jan 22: No Tutorial		
Week 12:		Jan 28: Language and semantics	Jan 29	TBD	Kamath et al., (2024)
Week 13:		Feb 4: General Principles	Feb 5	Charley	Gershman (2023)

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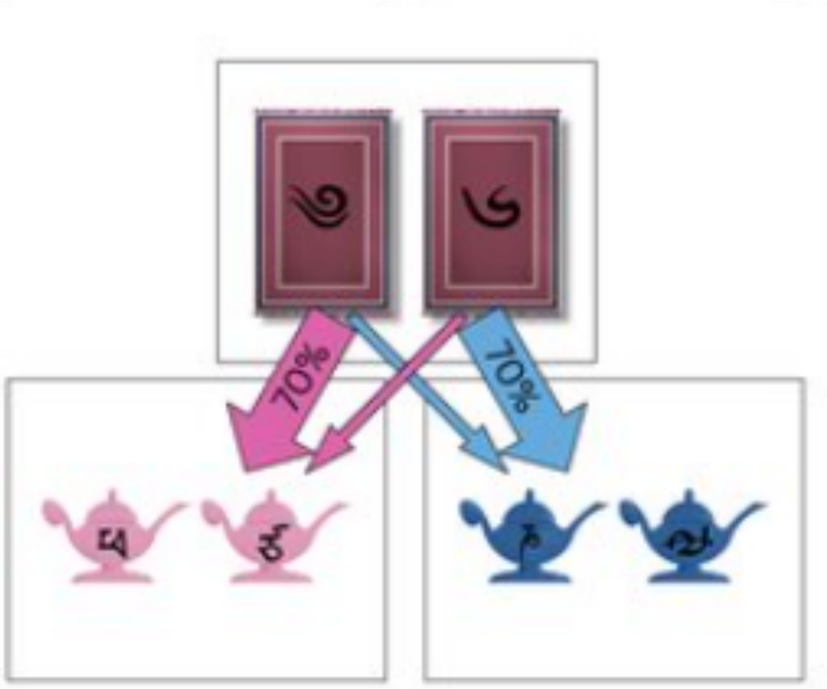
Swapped

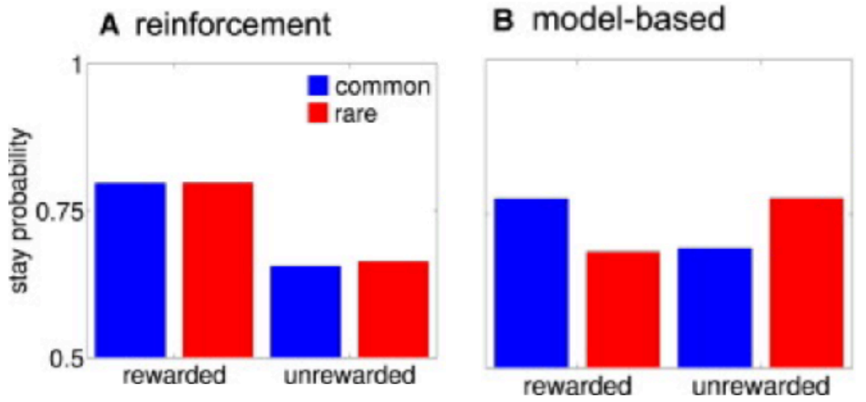
Exam times

Exam 1	13:00-15:00 21.02.2025 Hörsaal 1 F119 (SAND)
Exam 2	12:00-14:00 11.04.2025 (to be confirmed)

Clarification

- Two-step tasks
  - Transitions are a property of the environment and the participants choice
  - The participant chooses  or 
    - But then probabilistically (common=70% vs. rare = 30%), transitions to either pink or blue on the 2nd step
- The key takeaway is that MF vs MB have different responses to the same outcome
  - MF: If rewarded —> stay
    if not rewarded —> go
  - MB: depends on whether reward followed a common or rare transition… *you shouldn't expect a rare transition to occur again*
    if (common & reward | rare & no reward) —> stay
    if (common & no reward| rare & reward) —> stay



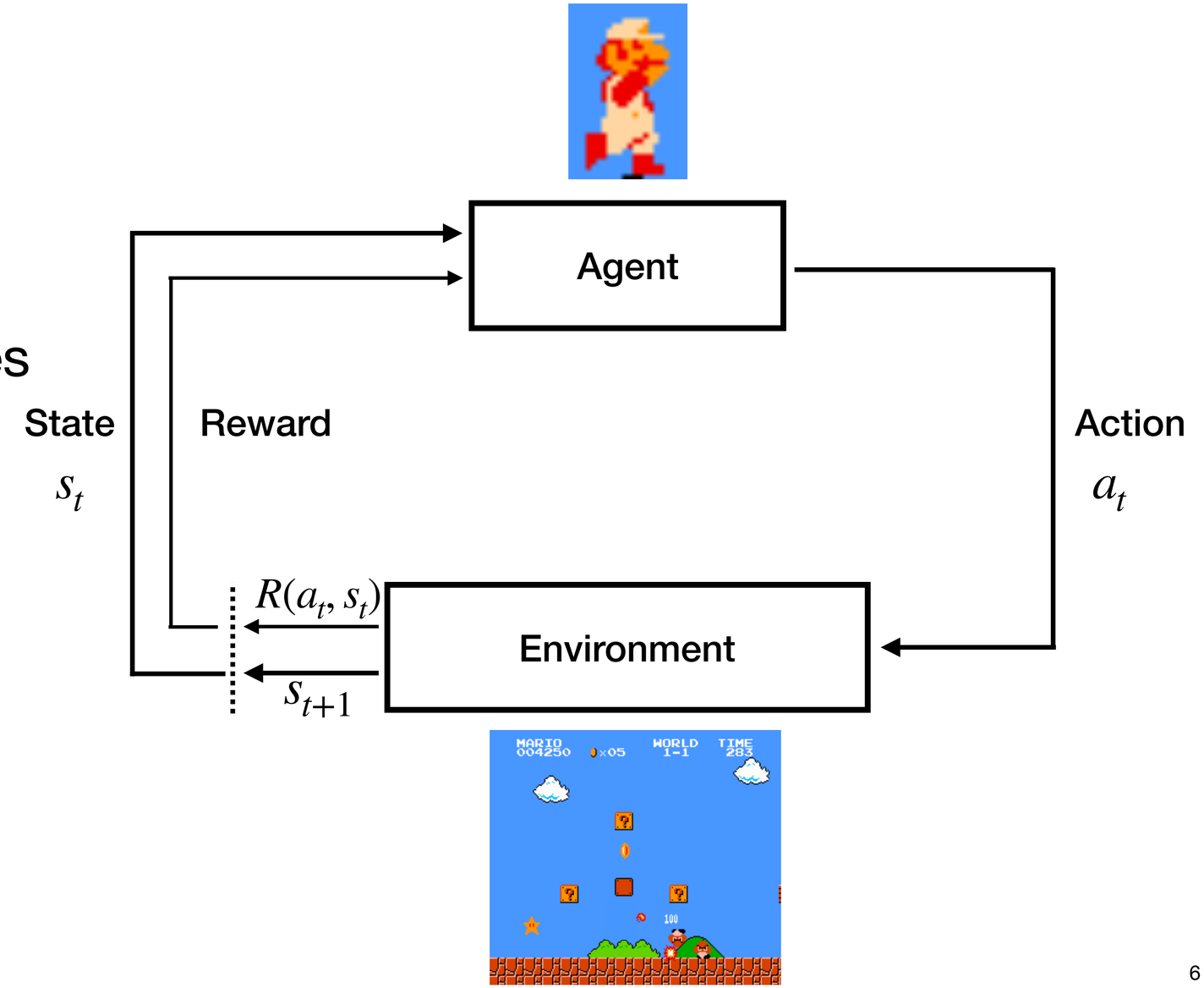


Last week…

Reinforcement Learning

The Agent:

- Selects actions a_t
- Receives feedback from the environment in terms of new states s_{t+1} and rewards $R(a_t, s_t)$



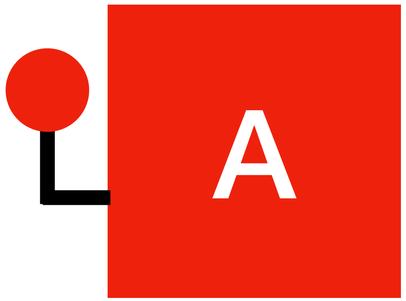
The Environment:

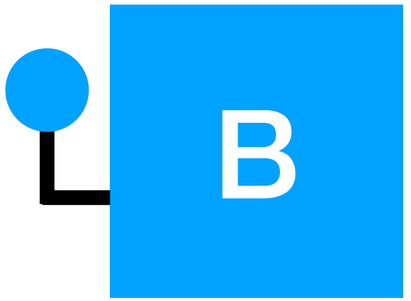
- Governs the transition between states $s_t \rightarrow s_{t+1}$
- Provides rewards $R(a_t, s_t)$

Q-Learning in a bandit task

Value learning

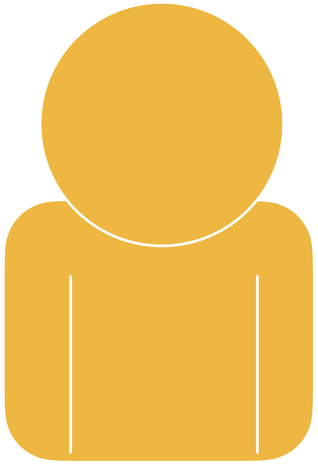
$$Q_t(a) \leftarrow Q_t(a) + \eta \left[r - Q_t(a) \right]$$





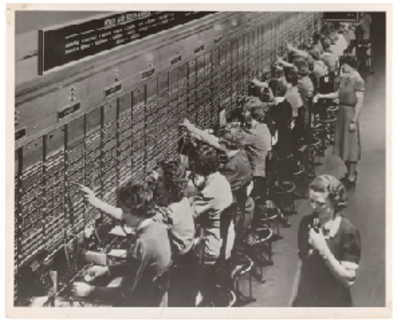
Policy

$$P(a) \propto \exp(Q_t(a)/\tau)$$



Model-free RL ⟷ **Model-based RL**

- Habit
- Cheap
- $Q(s, a)$
- Myopically selecting actions that have been associated with reward



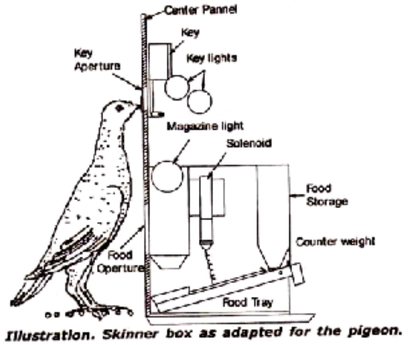
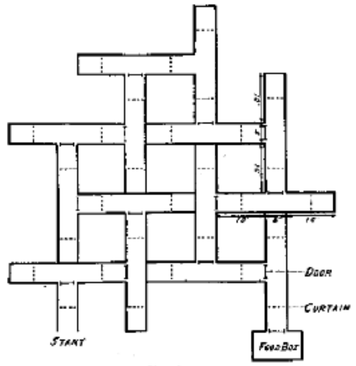


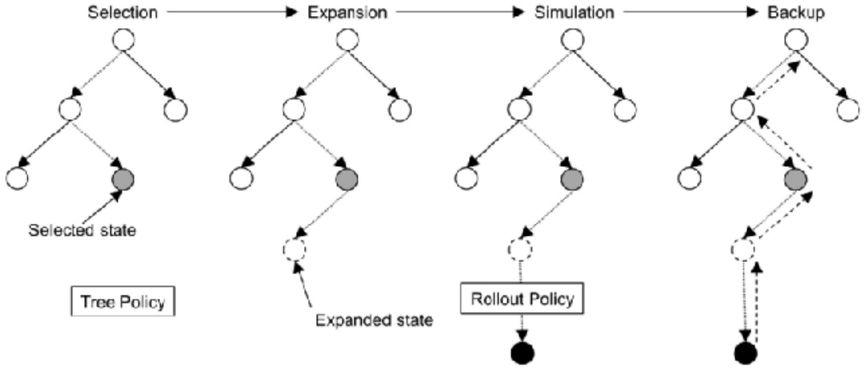
Illustration. Skinner box as adapted for the pigeon.

- Goal-directed
- Computationally costly
- $P(s', r \mid s, a)$
- Planning and seeking of long term outcomes



Plan of maze
14 Unit T-Alley Maze
FIG. 1
(From M. H. Elliott, The effect of change of reward on the maze performance of rats. *Univ. Calif. Publ. Psychol.*, 1928, 4, p. 20.)

Monte carlo tree search

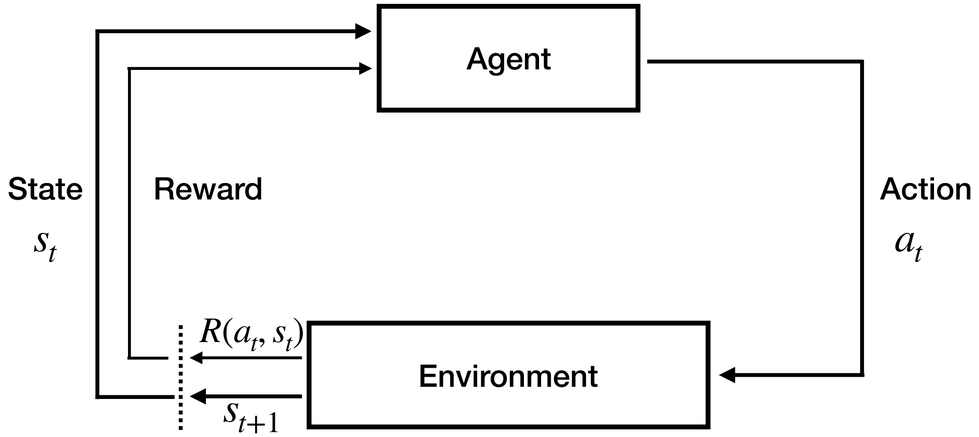


Duarte et al,. (2020)

Today's agenda

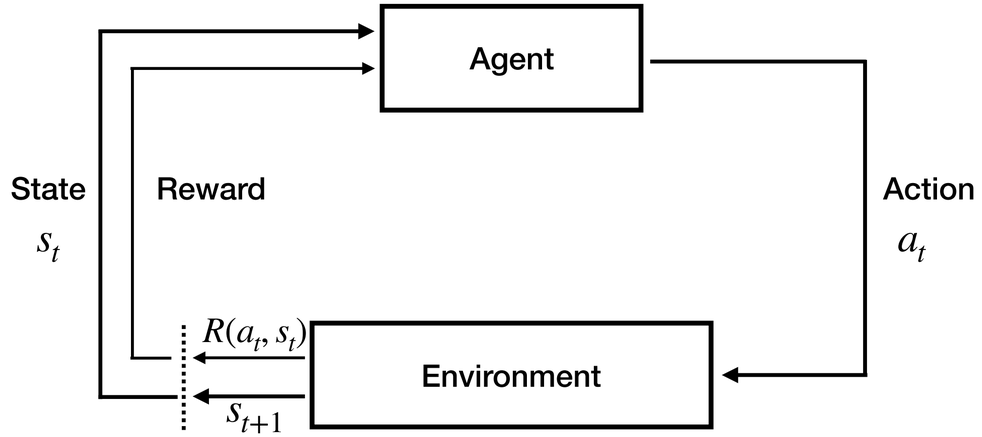
- Advances in …
  - **Model-free methods**
    - Deep Q-learning, policy gradient & Actor-Critic
  - **Model-based methods**
    - DYNA, World models, & Dreamer
  - **Something in between**
    - Successor representation

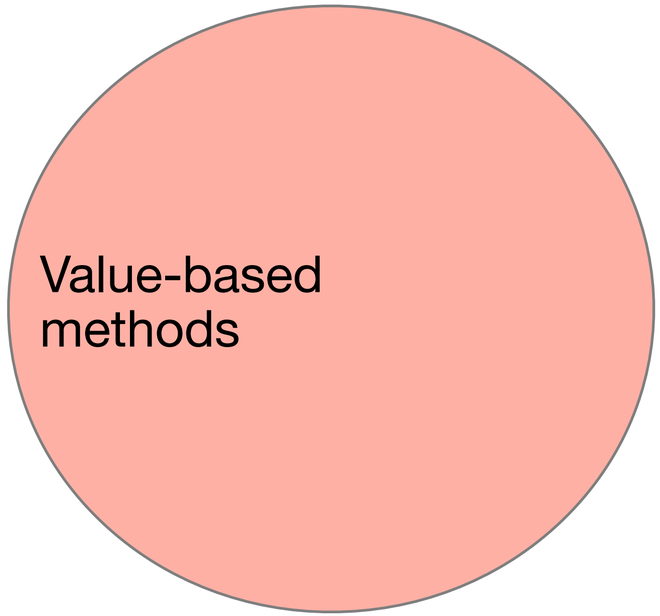
Advances in Model-free RL



Advances in Model-free RL

- **Value-based methods**
  - Last week: Value iteration, Q-Learning & TD-learning
    - Problem: what if the state-space is too large to visit?
  - *Deep Q-Learning* for function approximation





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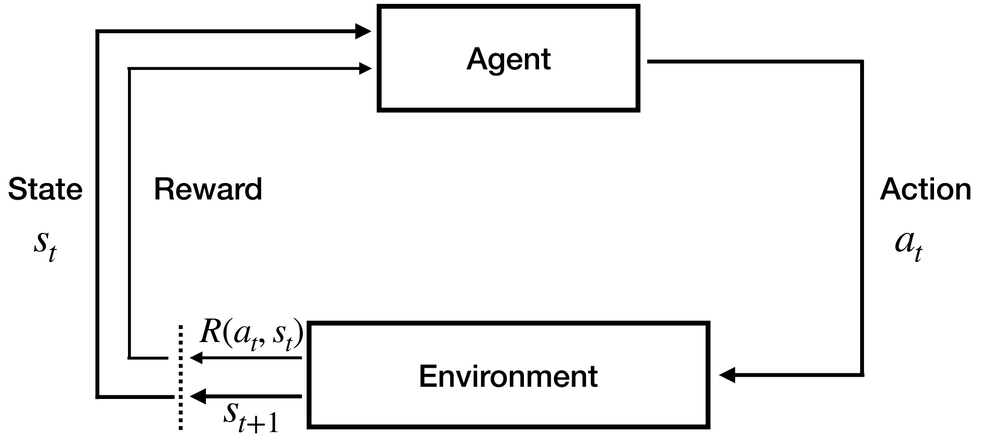
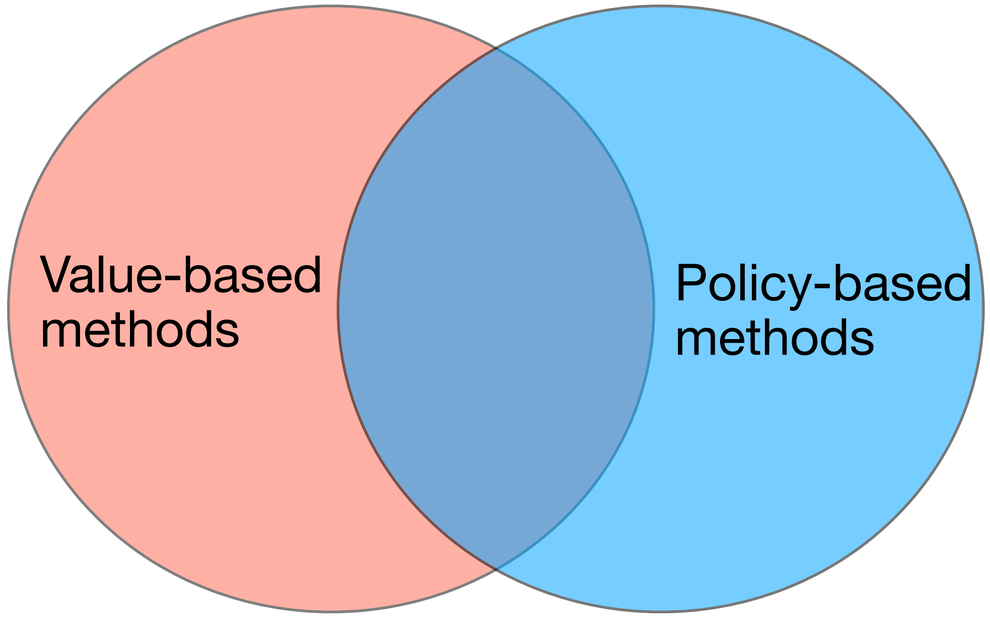
  - Policy-gradient for directly optimizing a policy





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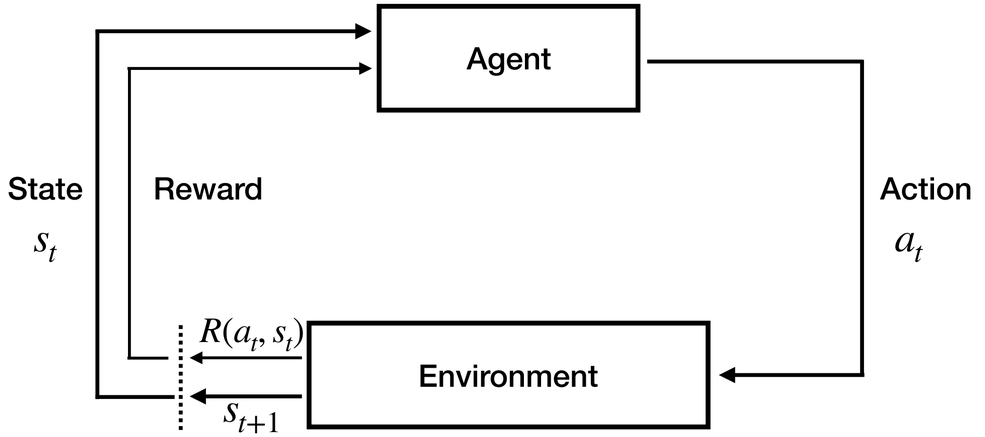
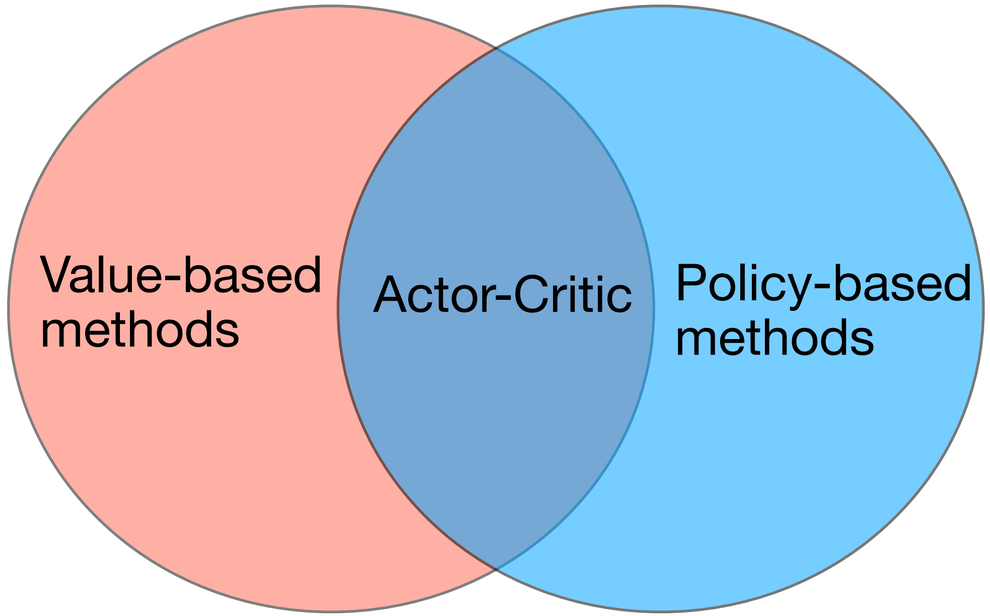
  - Policy-gradient for directly optimizing a policy
- **Actor-Critic**
  - Modern version of Policy-iteration: Value ⟷ Policy

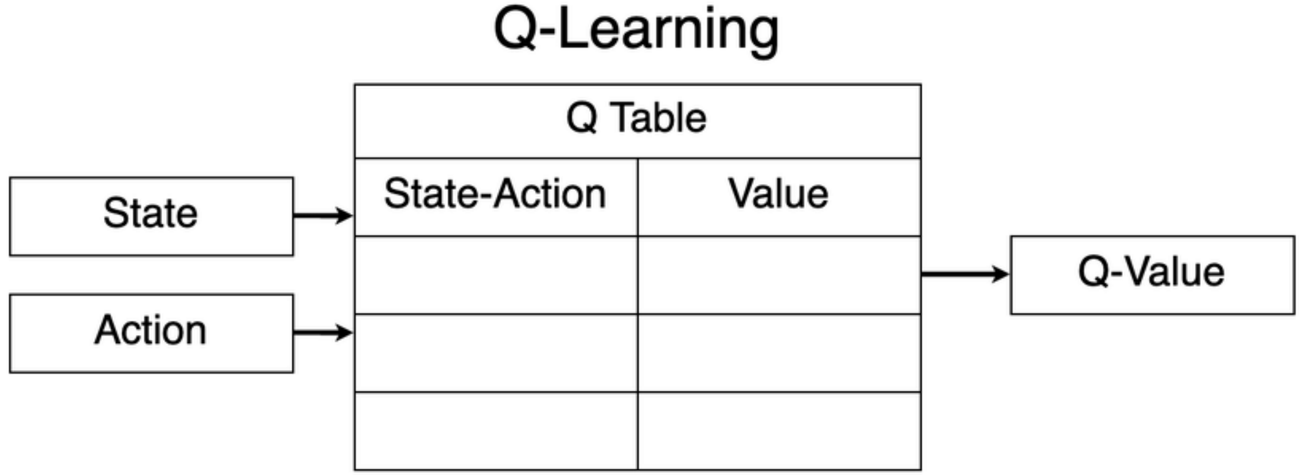




Deep Q-learning

Tabular methods:

- Q-Learning: learn Q-values by updating a look-up table



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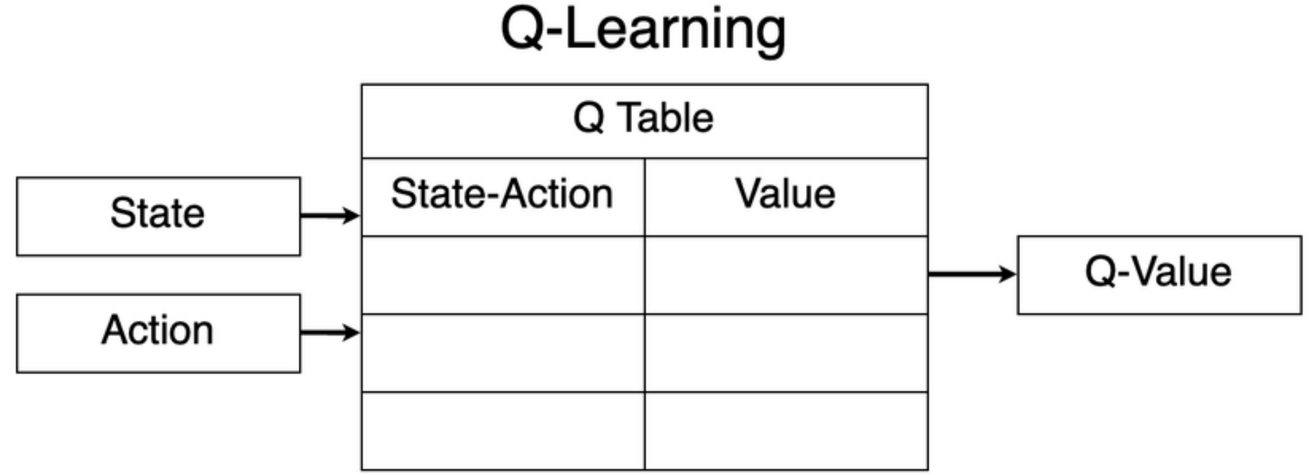

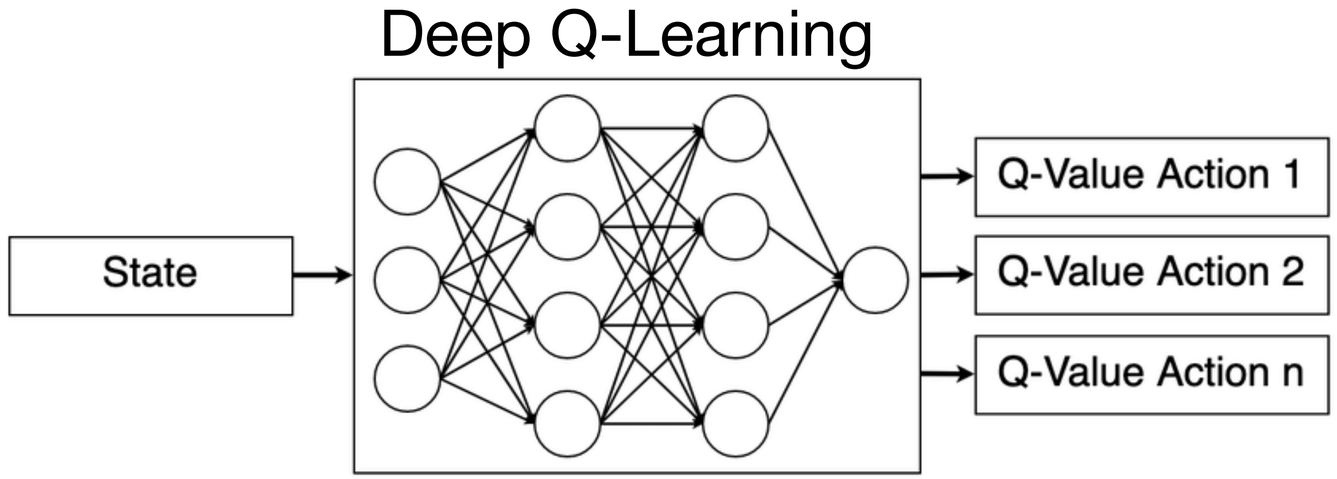

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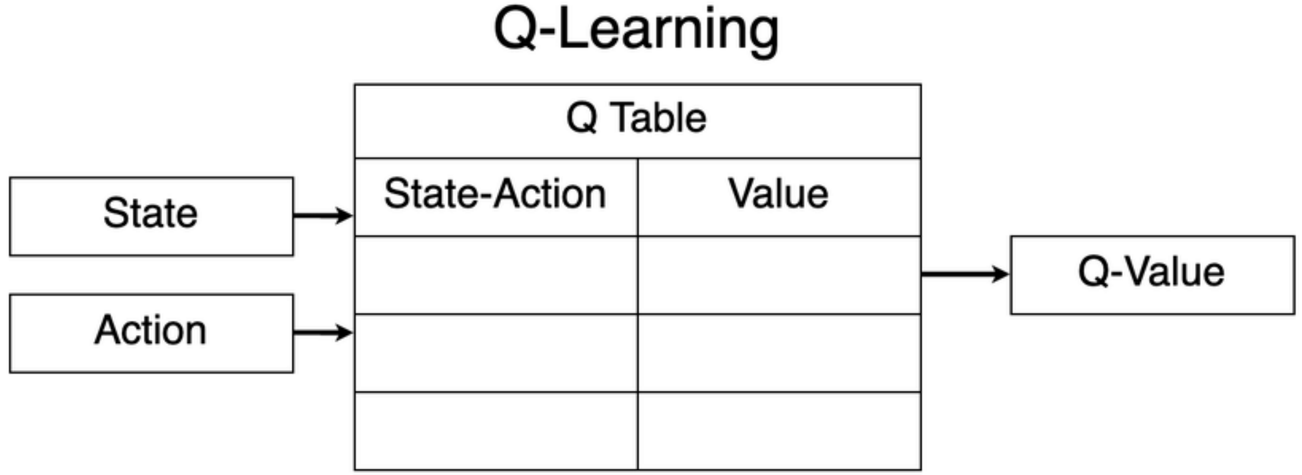

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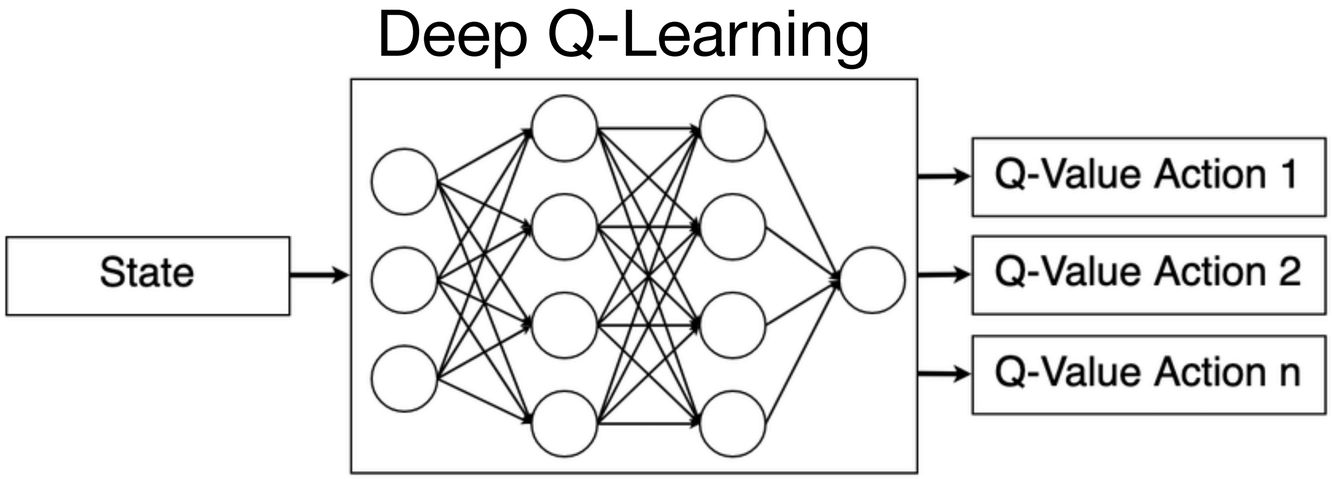

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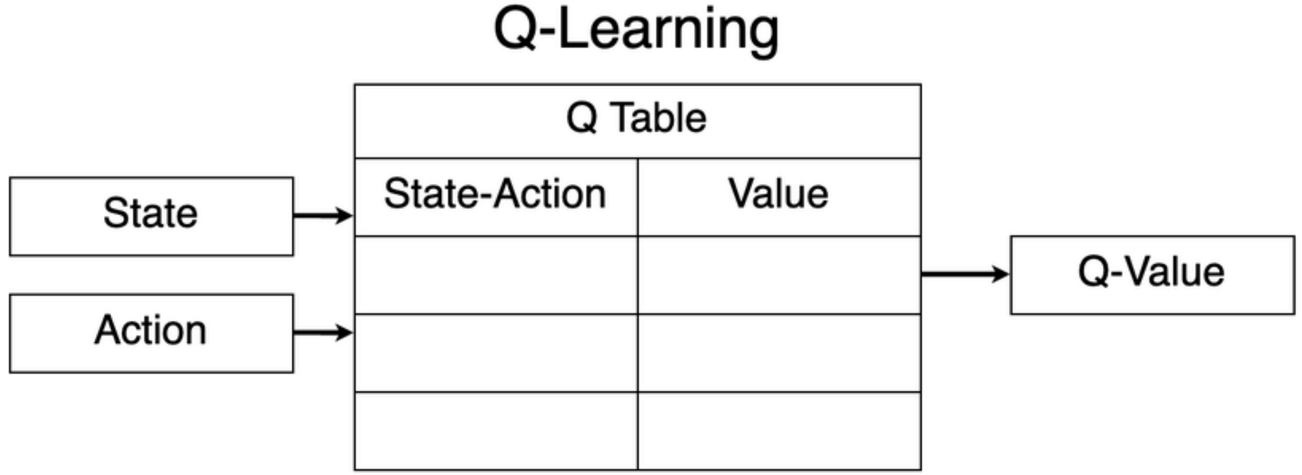

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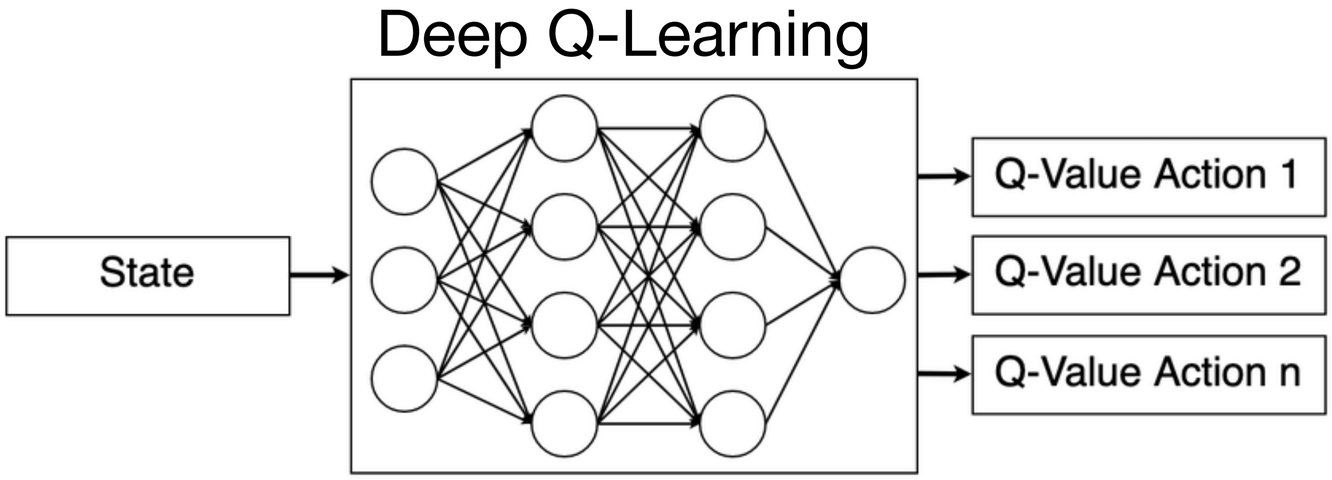

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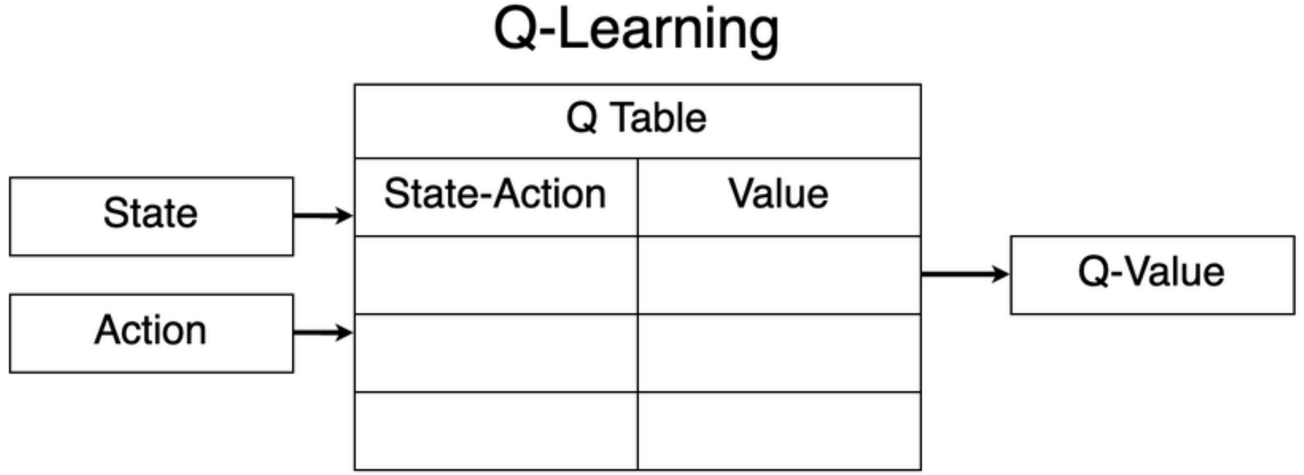

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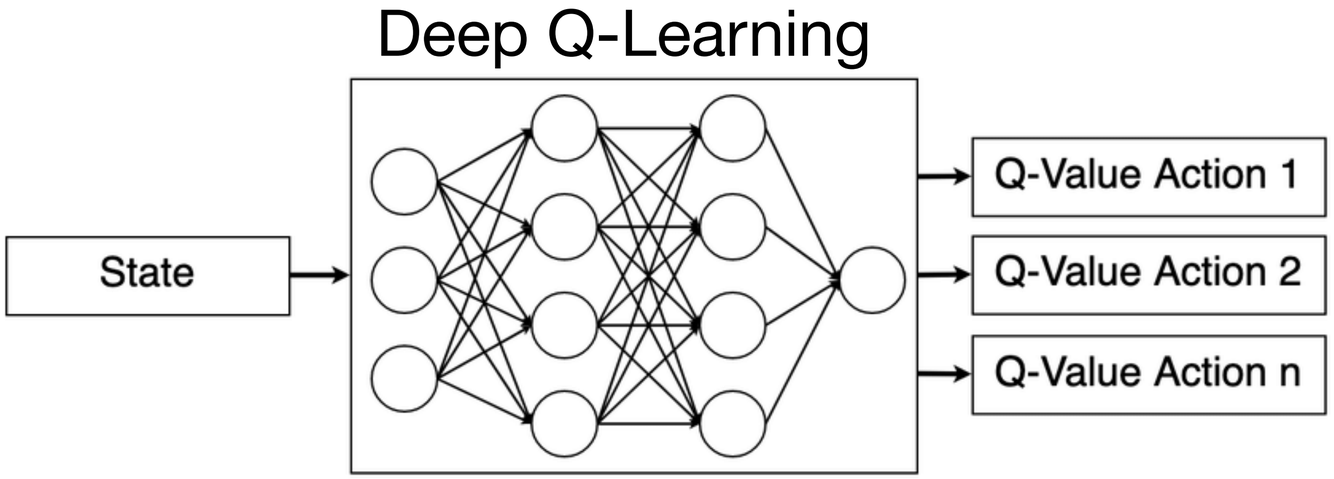
- **TD prediction error**

$$\delta = r + \gamma \max_{a'} Q_{\mathbf{w}}(s', a') - Q_{\mathbf{w}}(s, a)$$



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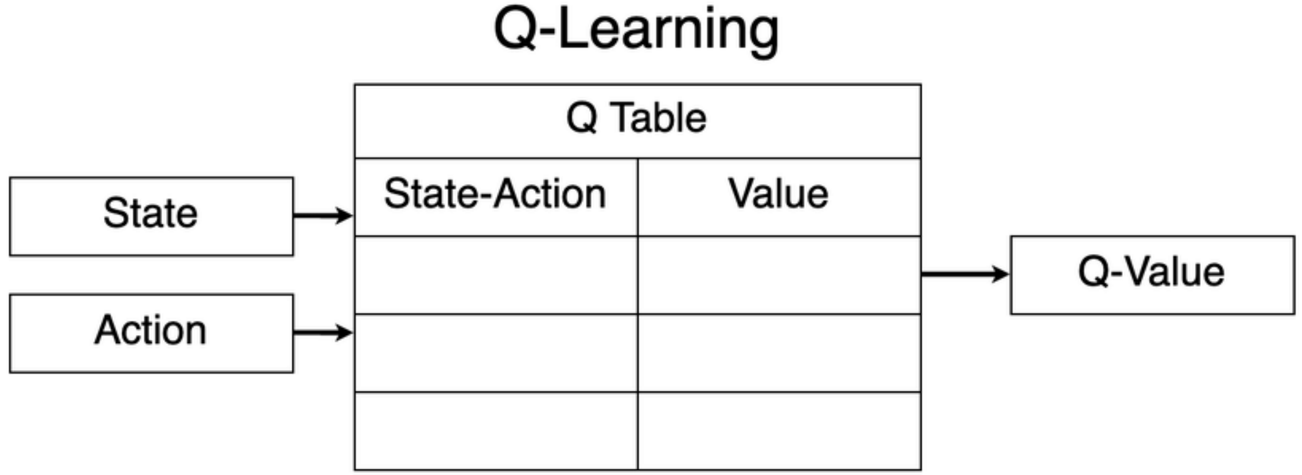

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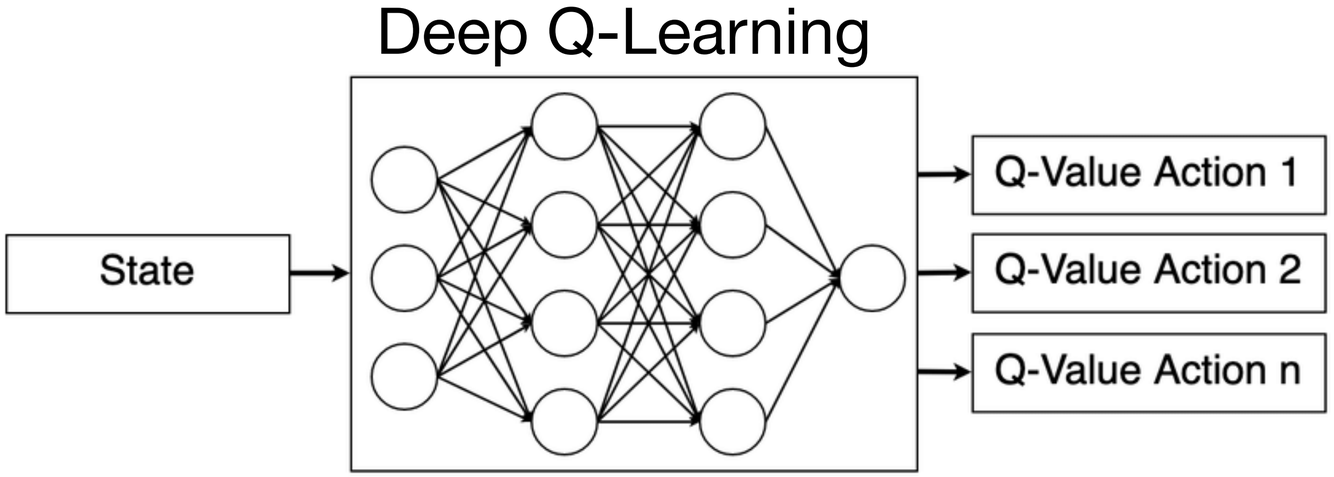

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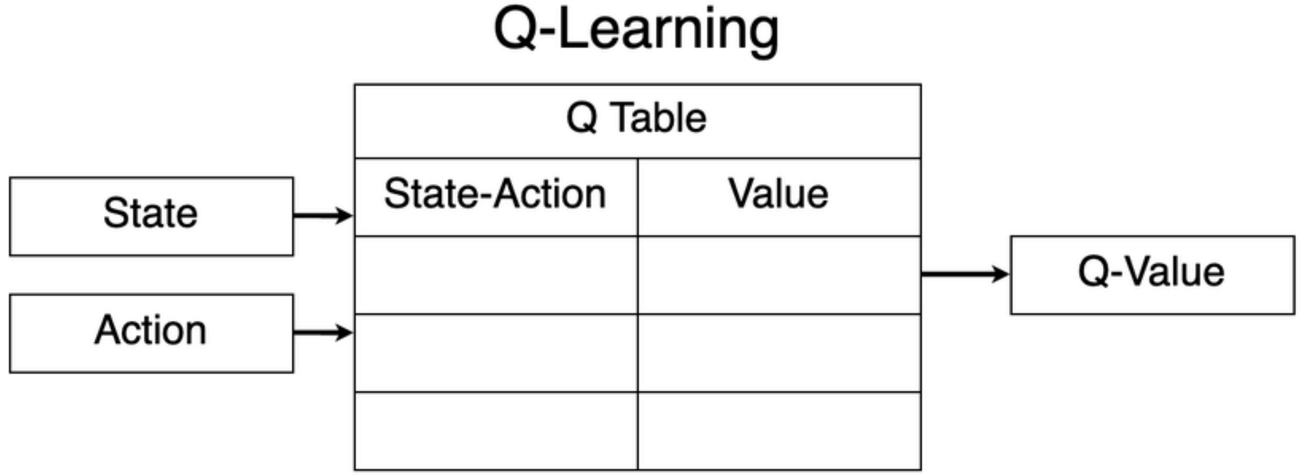

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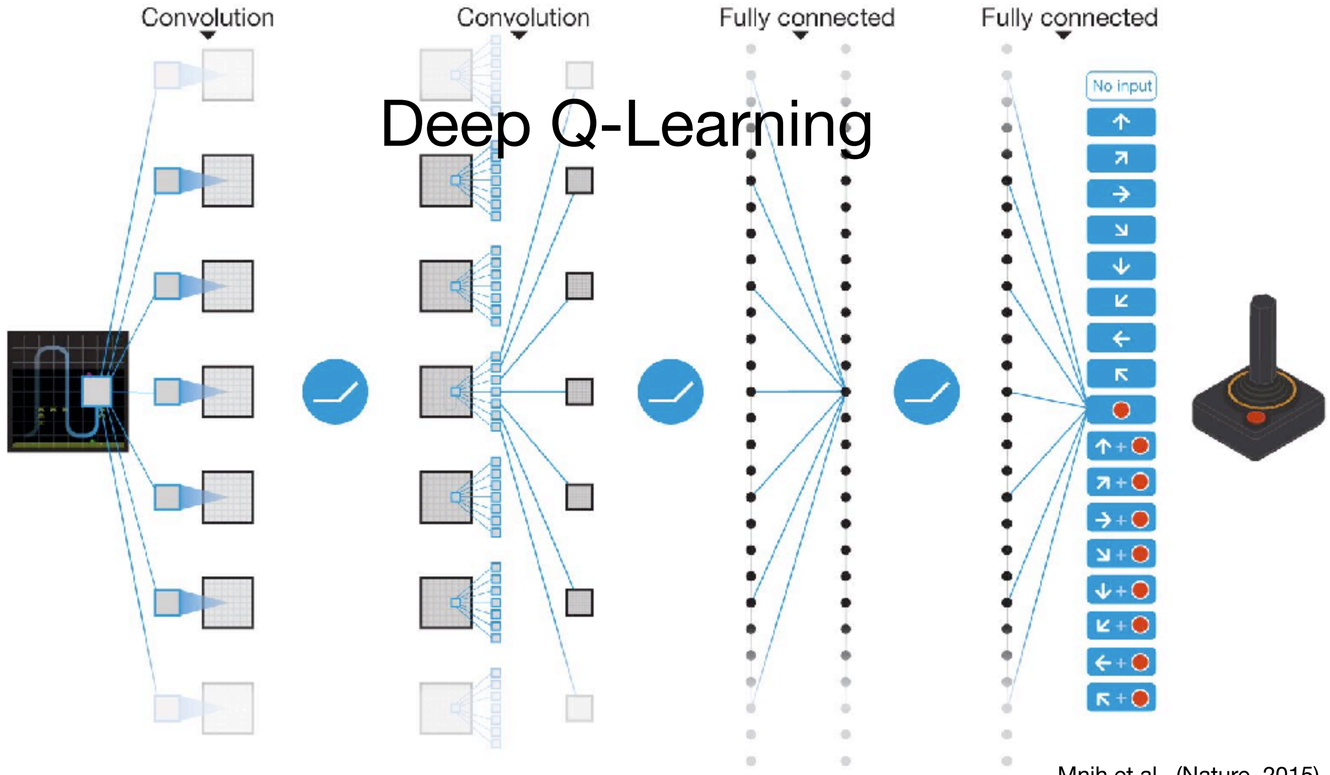
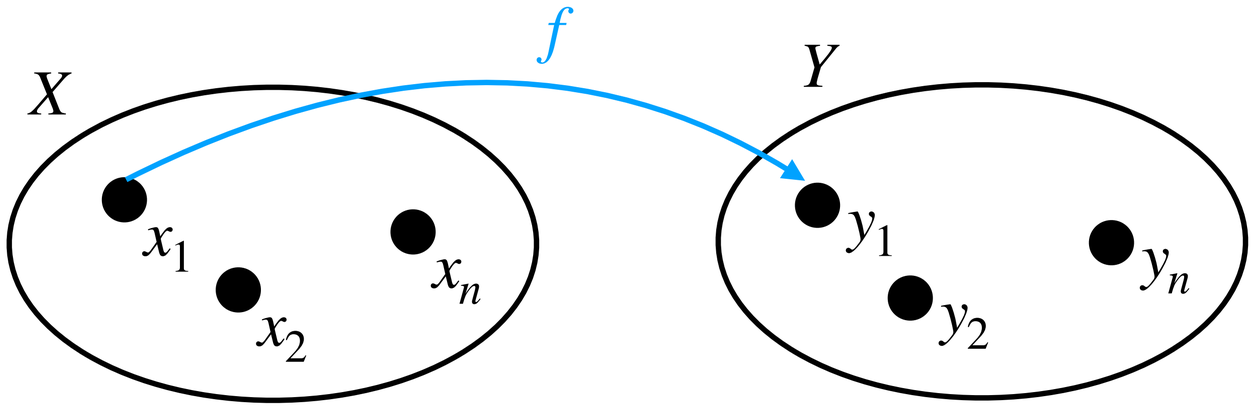


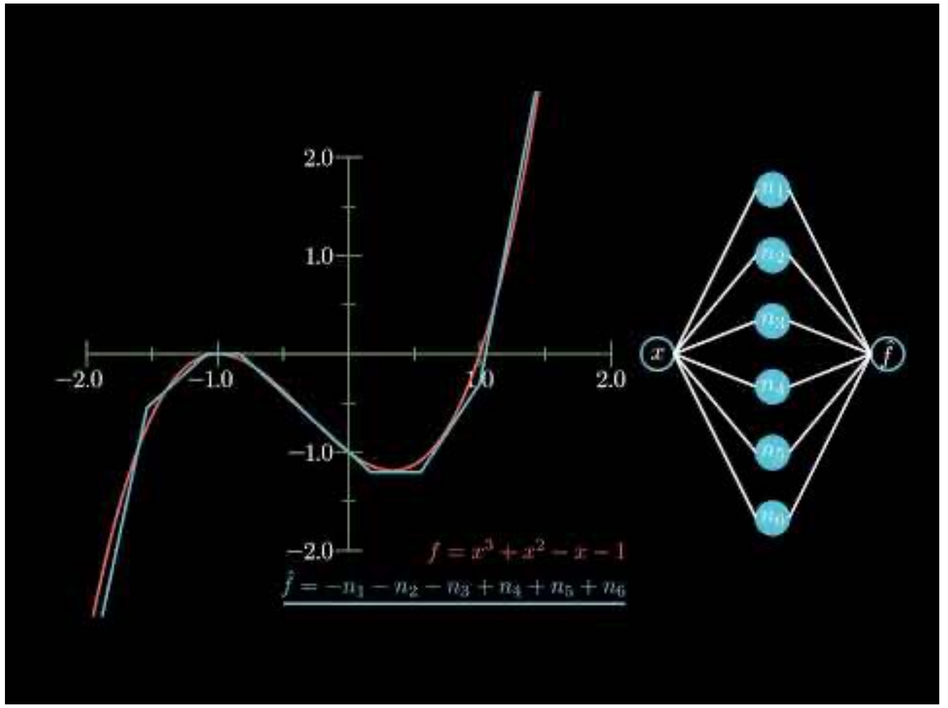
Mnih et al,. (Nature, 2015)

Universal Approximation Theorem

Cybenko (1989)

- What is a function?
  - $y = f(x)$
  - $f : X \rightarrow Y$
- ANNs are also functions
  - $g_{\mathbf{w}}(x) = \sigma(x)$ where $\mathbf{w}$ are the connection weights
- *At least one neural network exists that can approximate any continuous function with arbitrary precision*
  - $|\, g_{\mathbf{w}}(x) - f(x)\,| < \epsilon$





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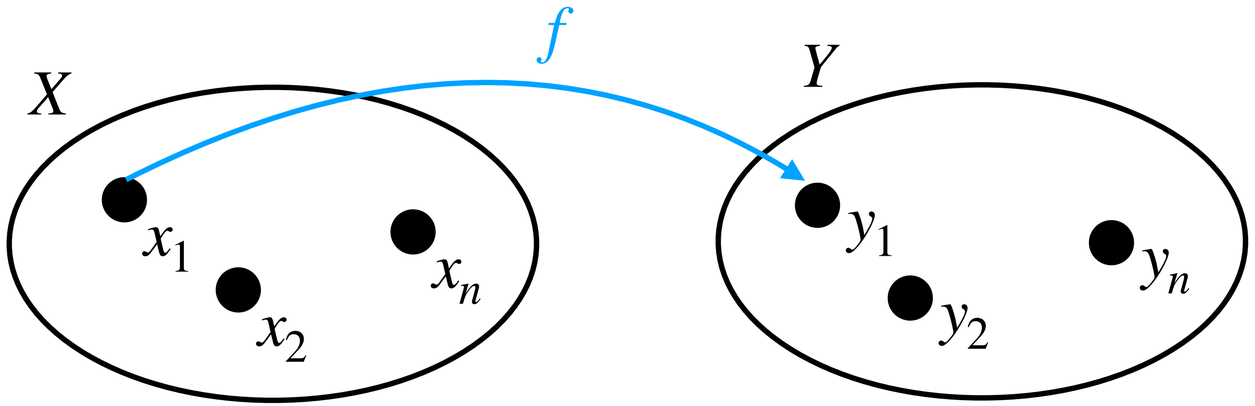
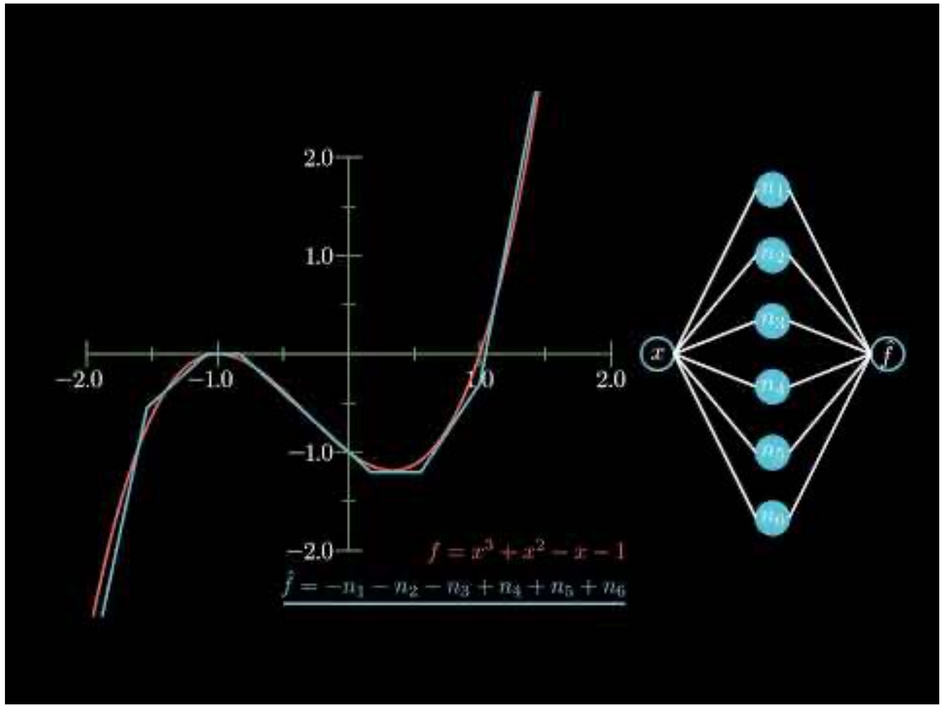
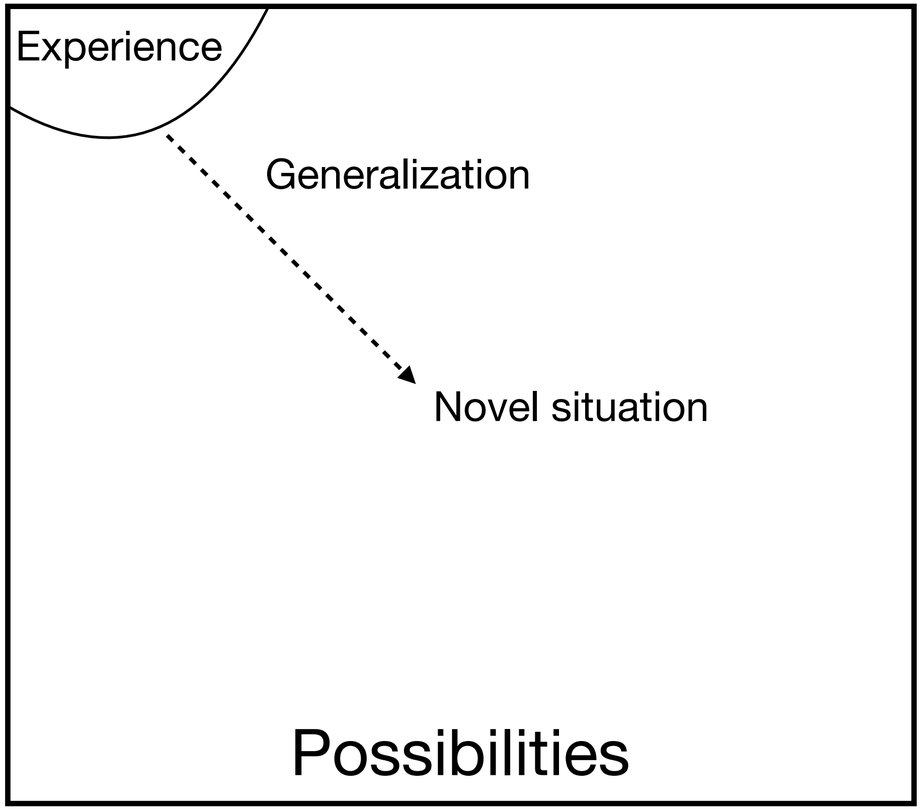




Caveat: Approximation does not guarantee generalization



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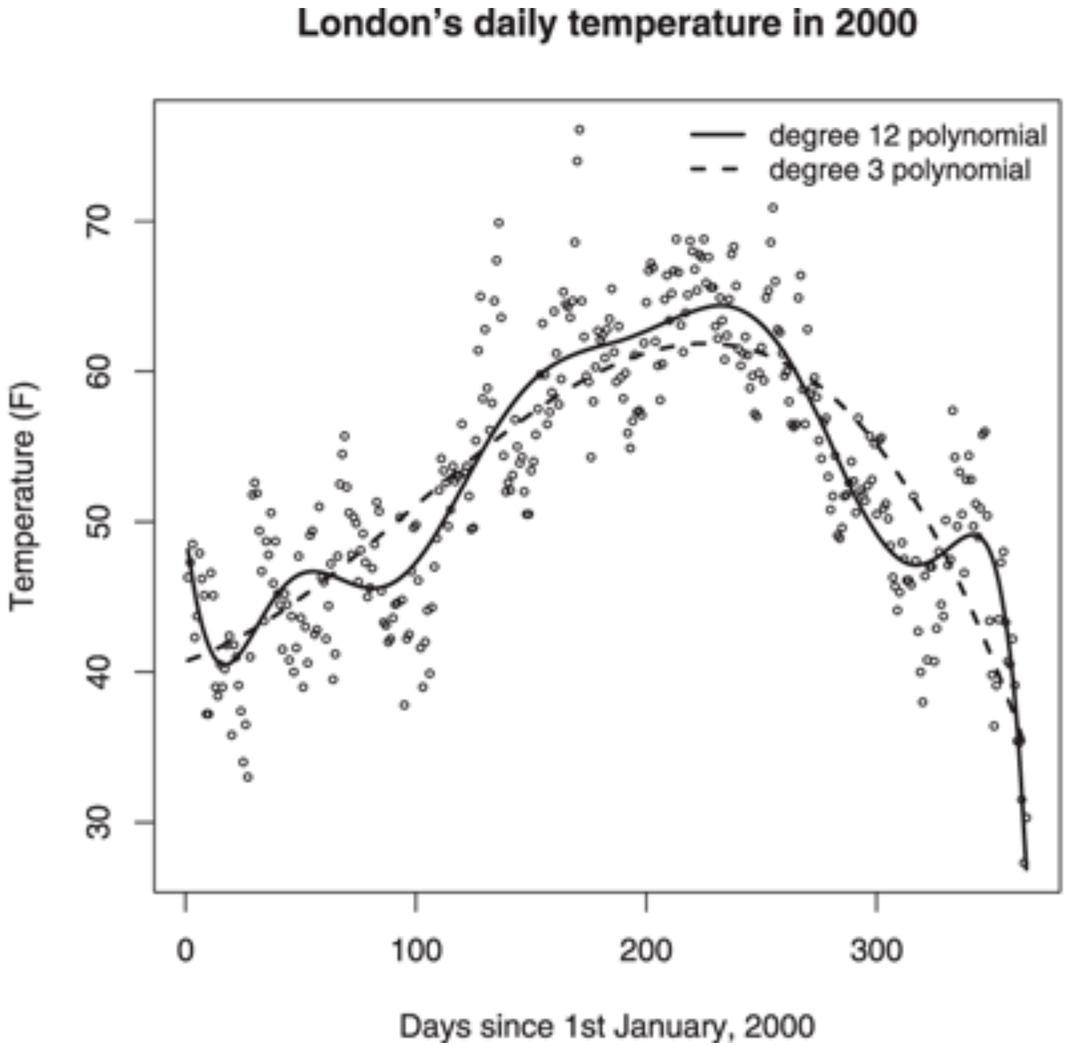

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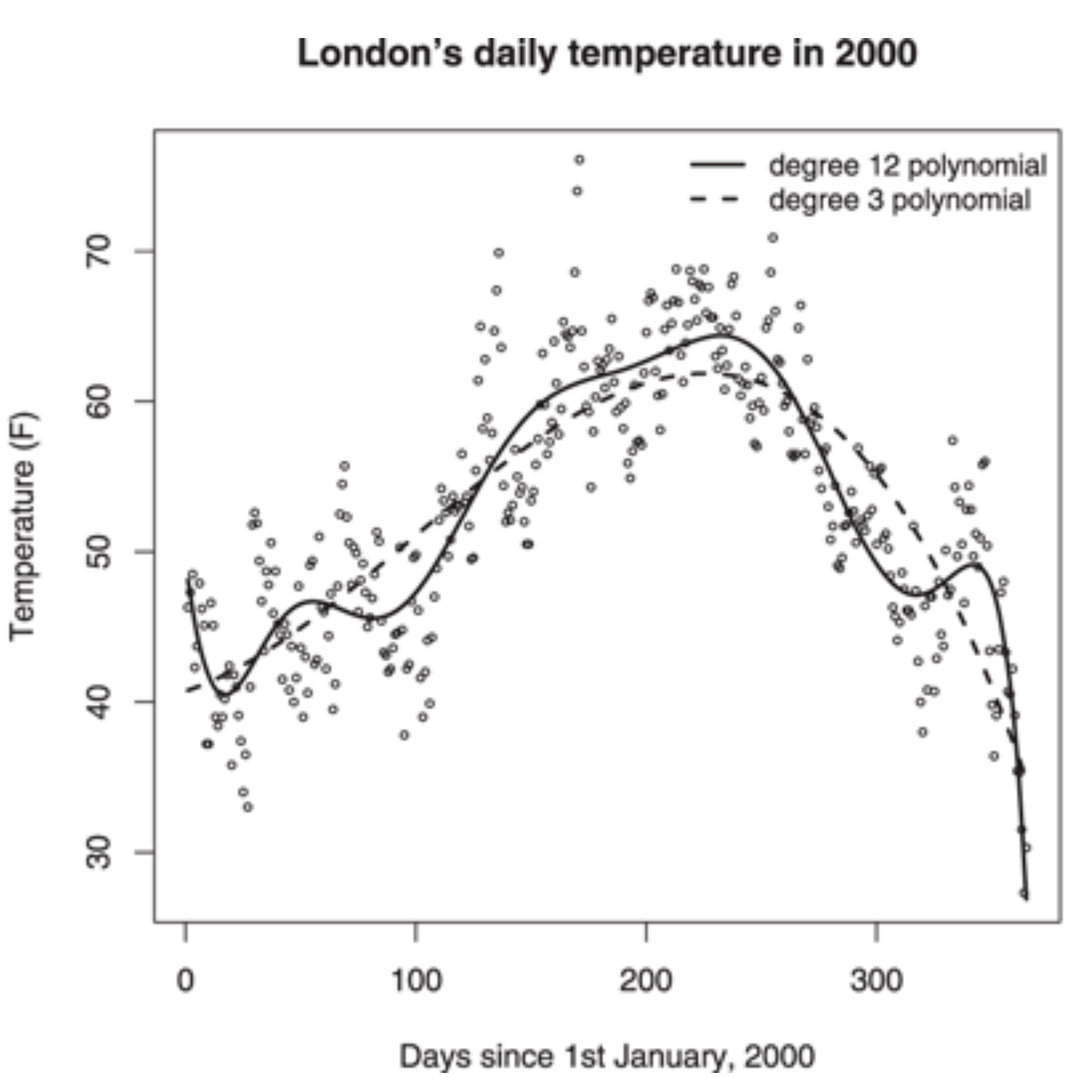
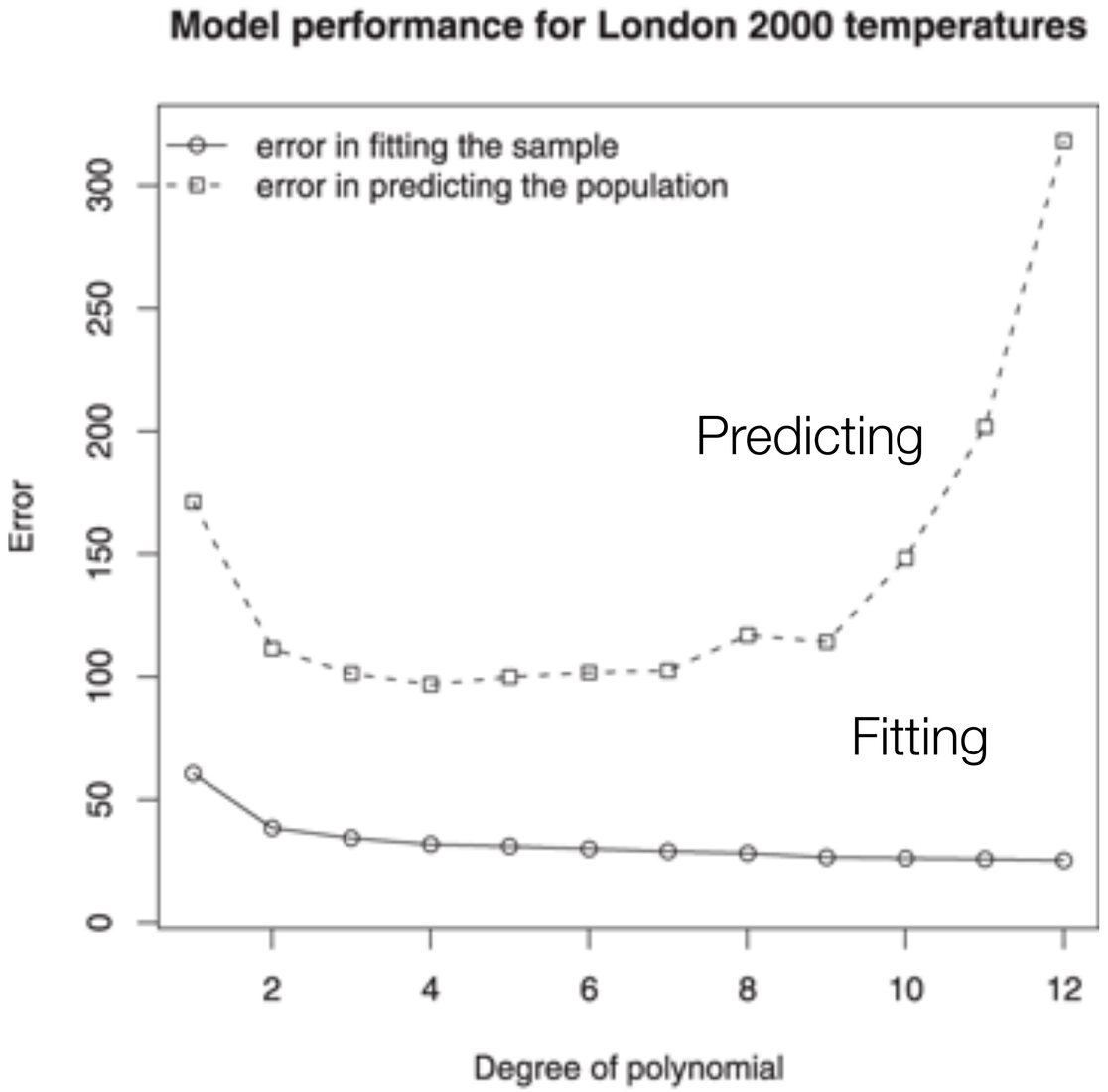


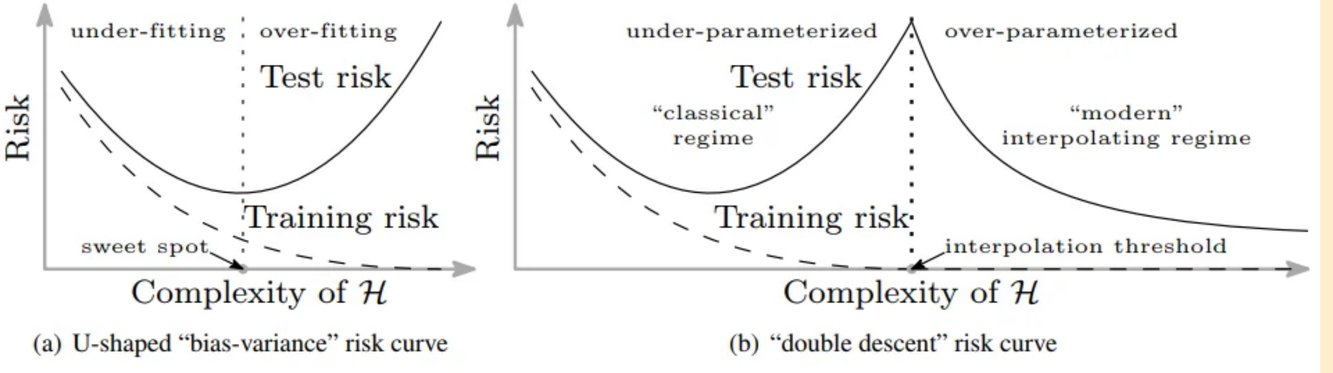


Yet why do large ANNs work so well?

Not on the exam but very cool

- Double descent phenomena
  - left: standard story
  - right: over-parameterized models start to reduce prediction error

Belkin et al., (2019)



(a) U-shaped "bias-variance" risk curve

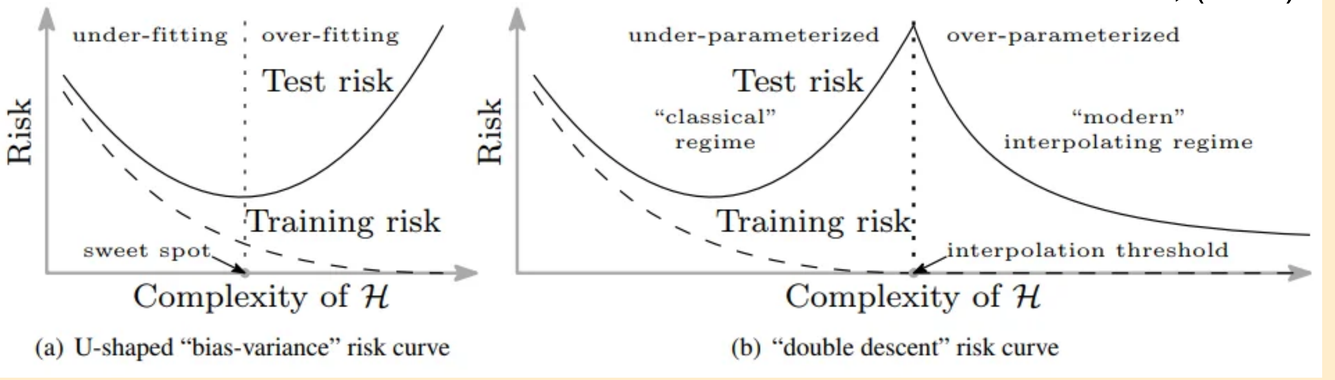
(b) "double descent" risk curve

Yet why do large ANNs work so well?

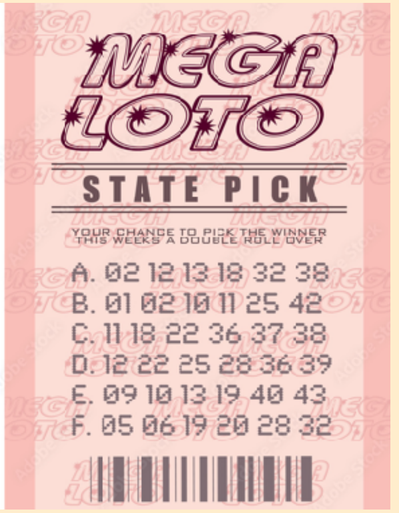
Not on the exam but very cool

- Double descent phenomena
  - left: standard story
  - right: over-parameterized models start to reduce prediction error
- Lottery Ticket conjecture
  - *if you buy enough lottery tickets, one is bound to be a winner**
  - Large "over-parameterized" ANNs have a bunch of different **subnetworks** that are randomly initialized (i.e., lottery tickets)
  - SGD focuses on training winning subnetworks
  - Pruning connections not part of the winning ticket can improve efficiency and even performance
  - The *effective* complexity $\neq |\theta|$

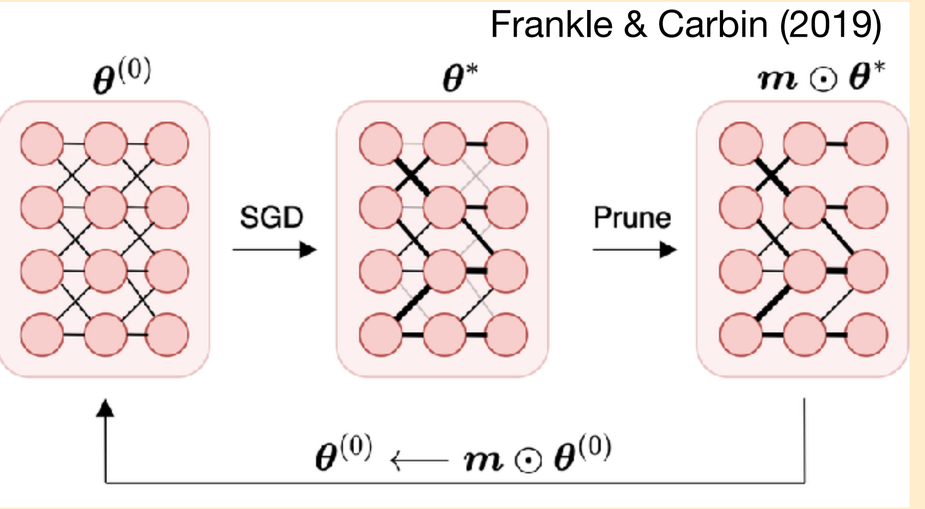
Belkin et al., (2019)



(a) U-shaped "bias-variance" risk curve (b) "double descent" risk curve



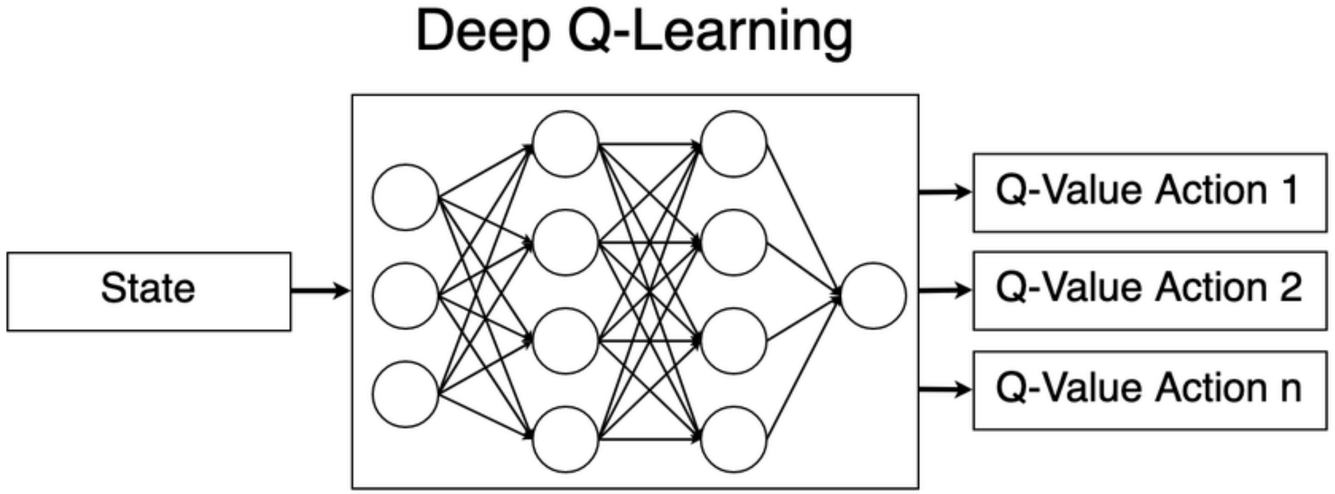
Frankle & Carbin (2019)



*not actually good financial advice

Policy Gradient

- **Deep Q-learning** uses an ANN to approximate the value function
  - the policy is implicit (e.g., a softmax over Q-values)



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- **Policy gradient** uses a function to approximate the optimal policy
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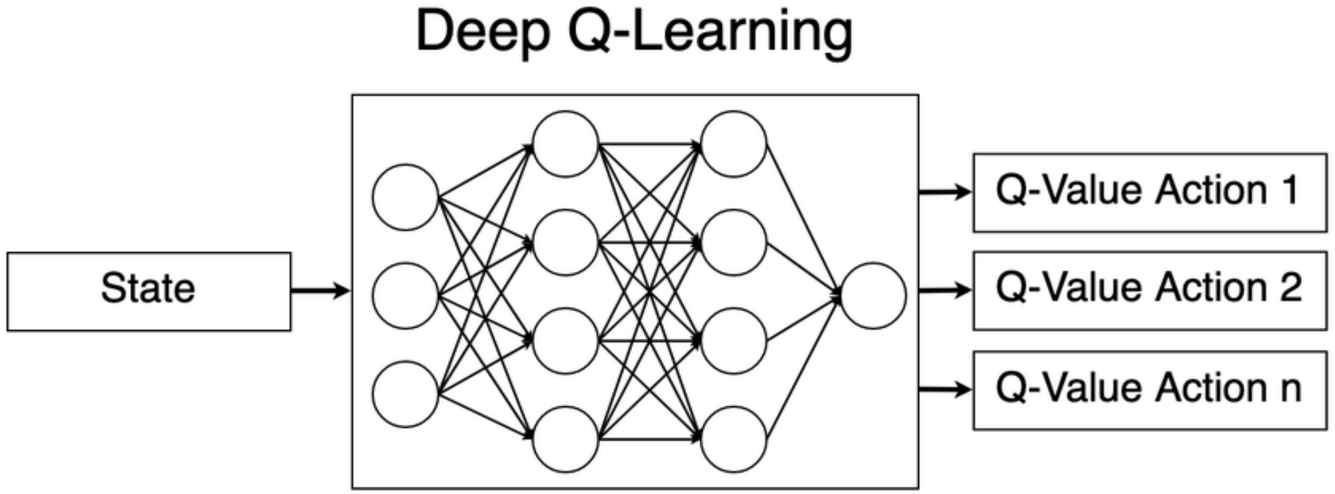

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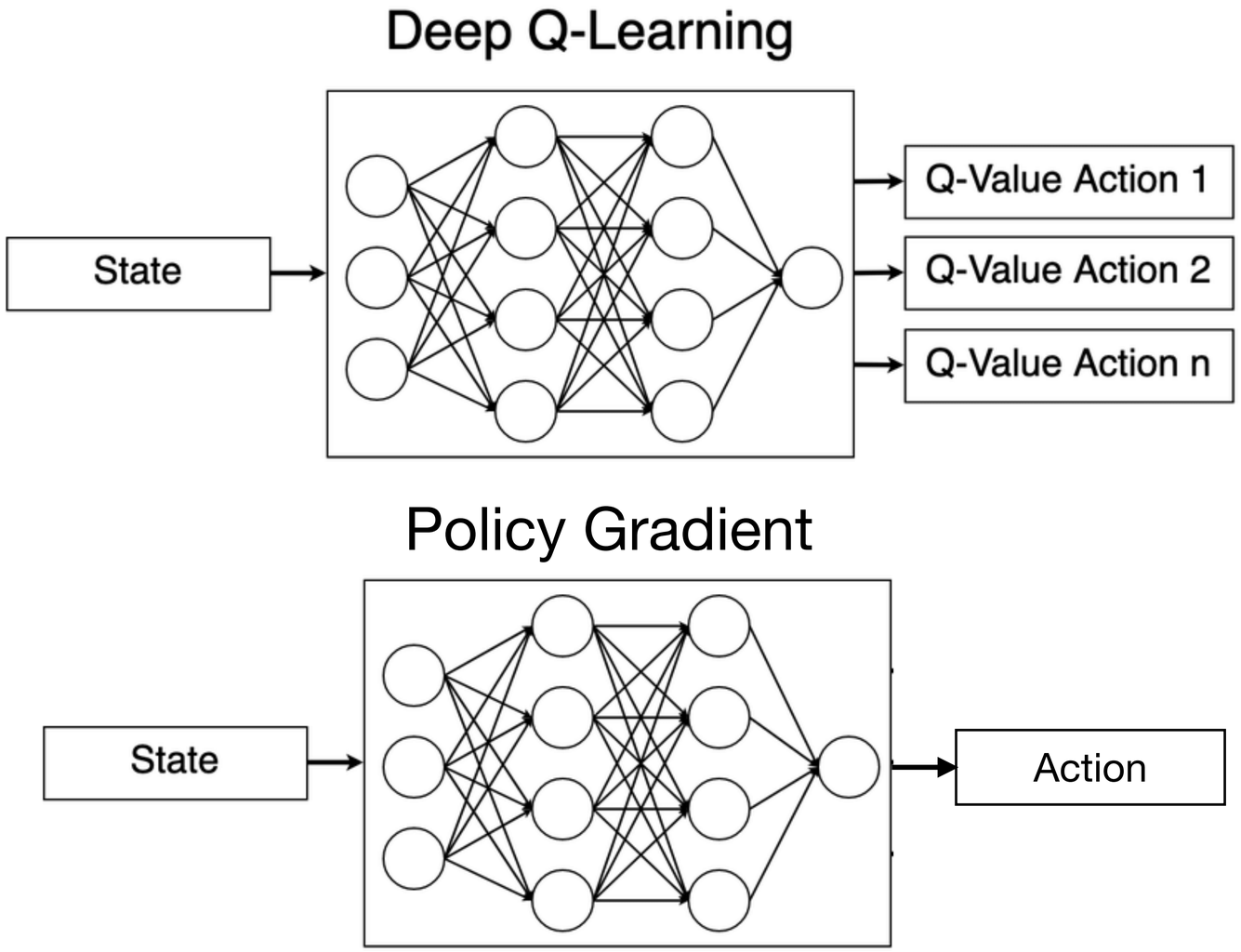

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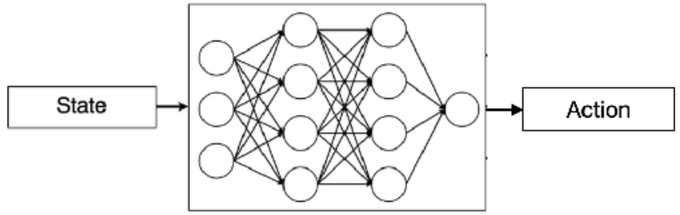
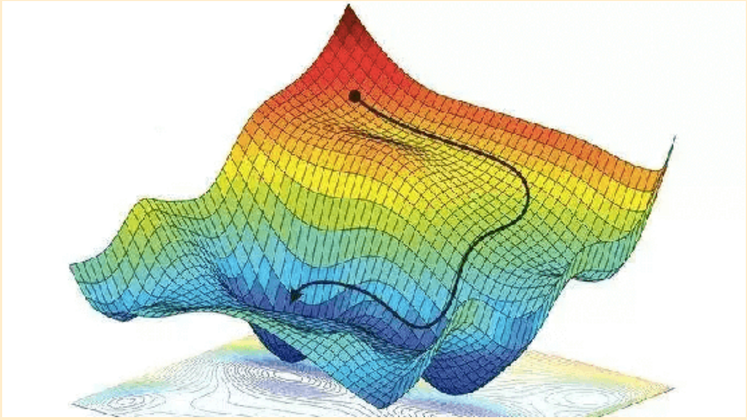


Formulas not on exam, but you should understand the general concept!

- Use a neural network to parameterize a policy $\pi_\theta(a \mid s)$
- Objective: Maximize expected reward following a parameterized policy: $J(\theta) = \mathbb{E}_{\tau \sim \pi_\theta}[r(\tau)]$
- Method: using gradient ascent $\theta_{t+1} = \theta_t + \beta \nabla_\theta J(\theta_t)$

  learning rate
- Using the Markov principle, we can write the gradient as:

$$\nabla J(\theta_t) = \mathbb{E}_{\pi_\theta}\left[\sum_{t \in \tau}^{|\tau|} \nabla \log \pi_\theta(a_t \mid s_t) Q(a_t, s_t)\right]$$

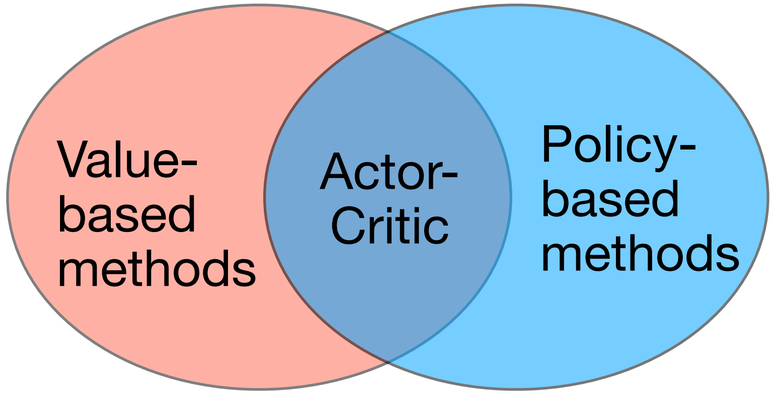


- Updates to θ follow the **gradient** to increase the probabability of highly rewarding actions:

$$\theta_{t+1} = \theta_t + \alpha \nabla_\theta \log \pi_\theta(a_t \mid s_t) Q(a_t, s_t)$$

- Here, $Q(a_t, s_t)$ is usually estimated through Monte Carlo sampling

Actor-Critic



- Actor-critic combines **value-based** and **policy-based** methods and is a generalization of policy iteration
  - **Actor** provides the policy $\pi_\theta(a \mid s)$ parameterized by θ
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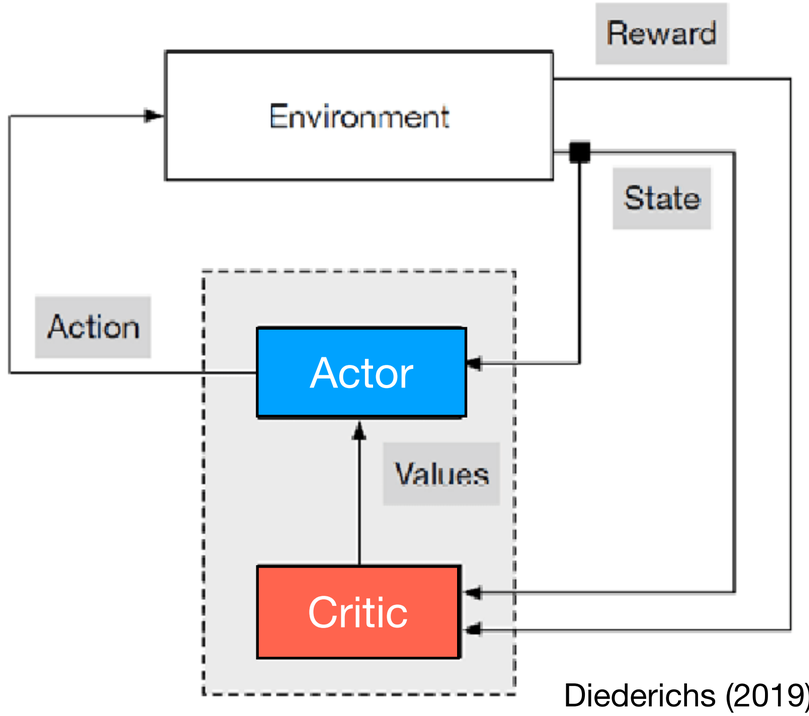

Diederichs (2019)

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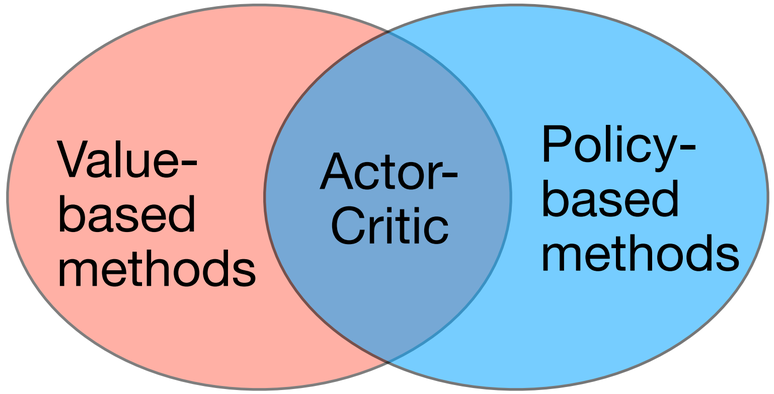

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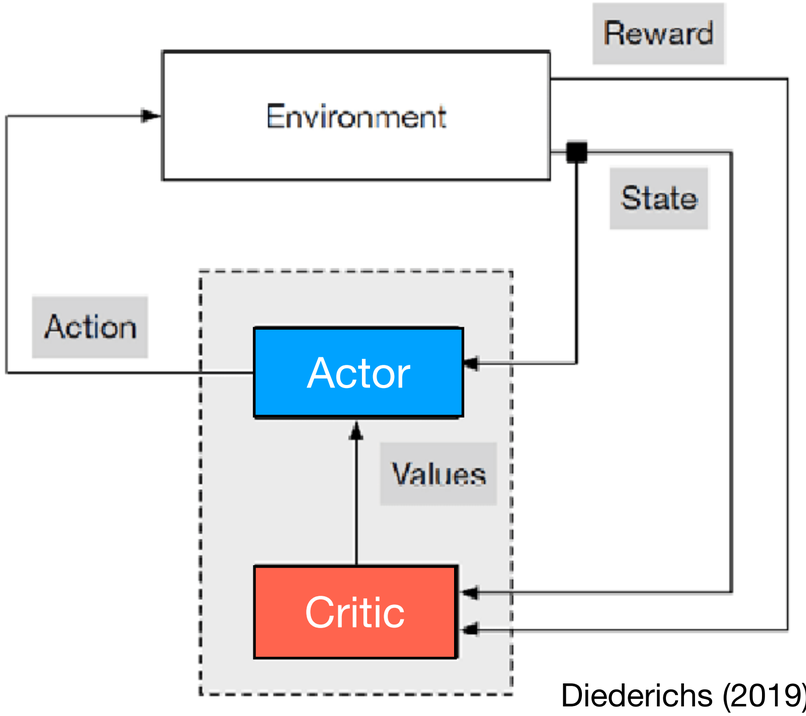
$$\delta = r + \gamma \max_{a'} Q_{\mathbf{w}}(s', a') - Q_{\mathbf{w}}(s, a)$$



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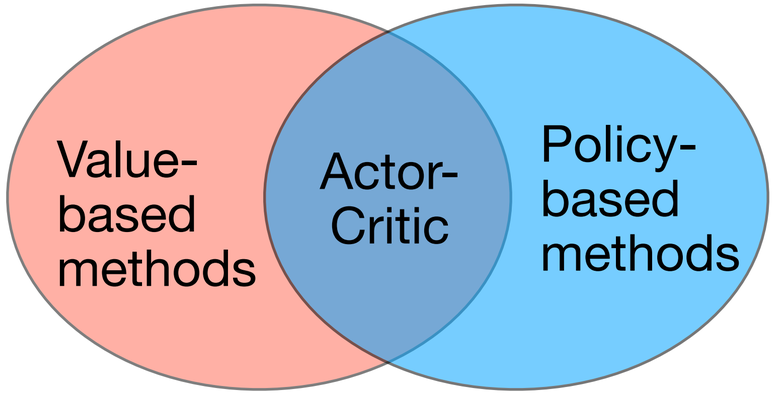

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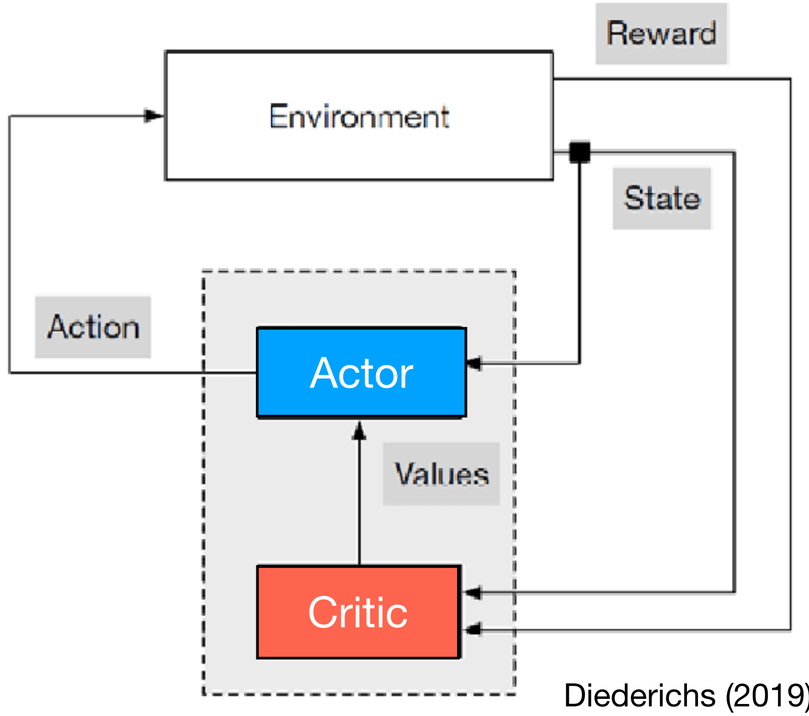

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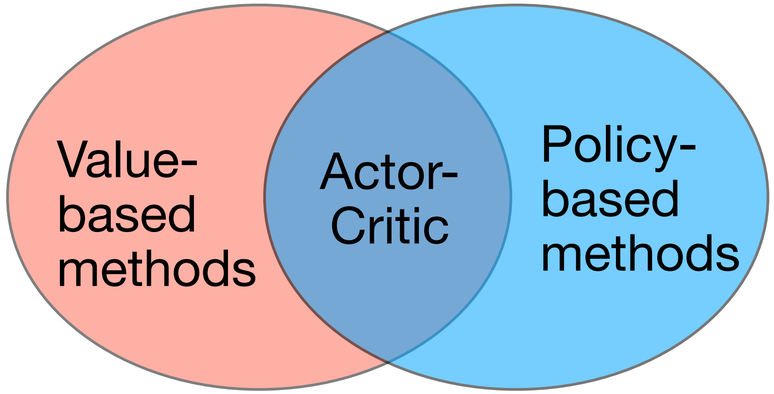

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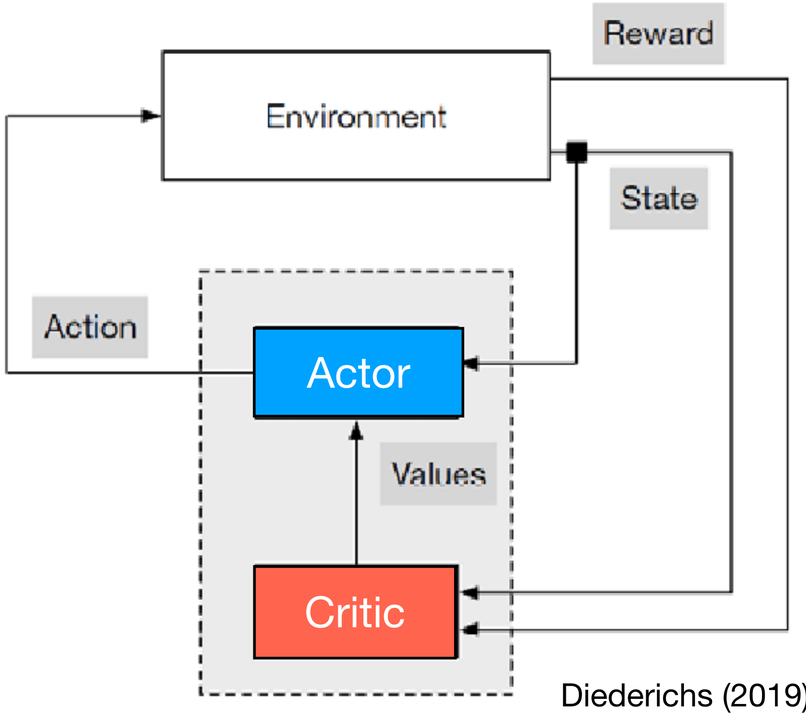

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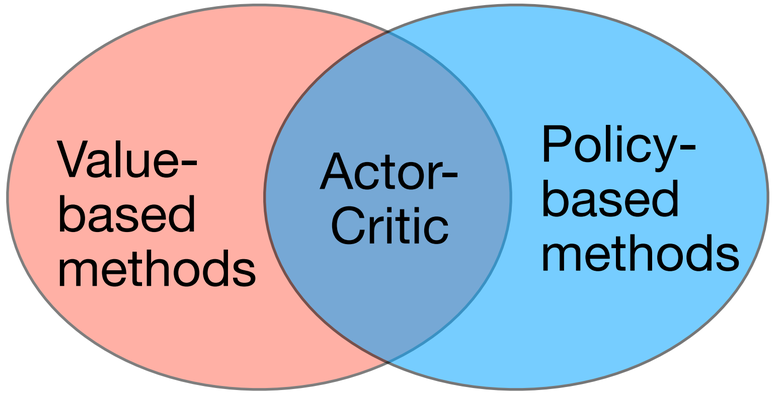

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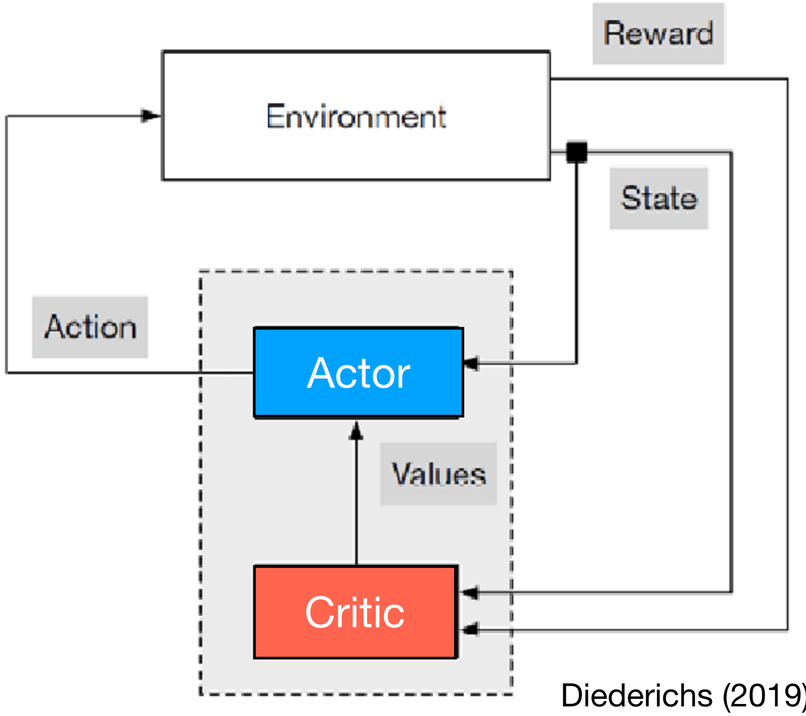
    increase probability of highly rewarding actions



Diederichs (2019)

Model-free methods summary

- *Just put ANNs everywhere!*
- **Value-based** methods
  - Deep Q Learning
- **Policy-based** methods
  - Policy Gradient
- **Actor**-**Critic**
  - Integration of both value-based and policy-based methods

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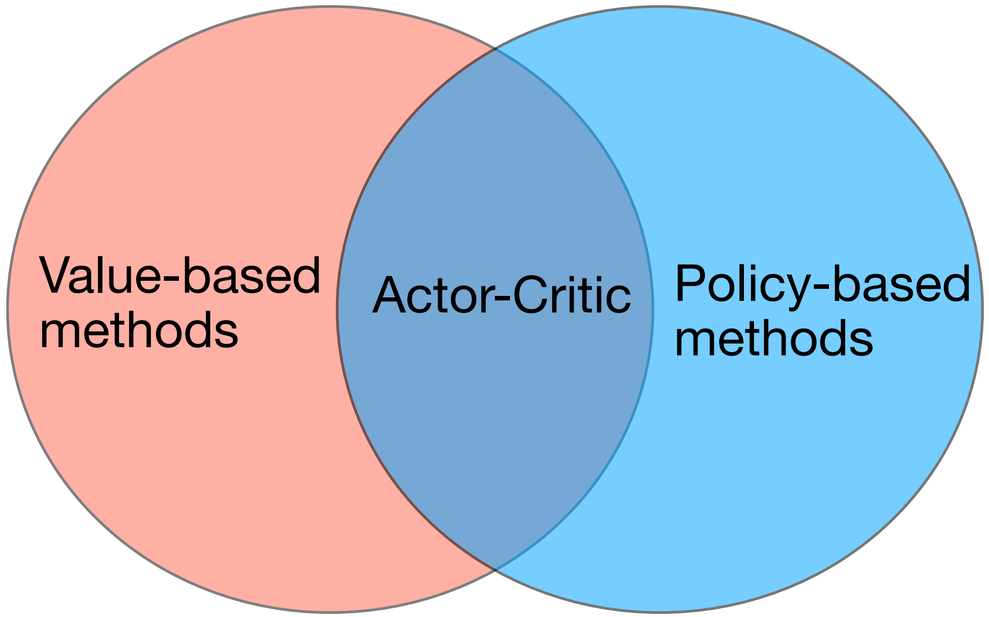
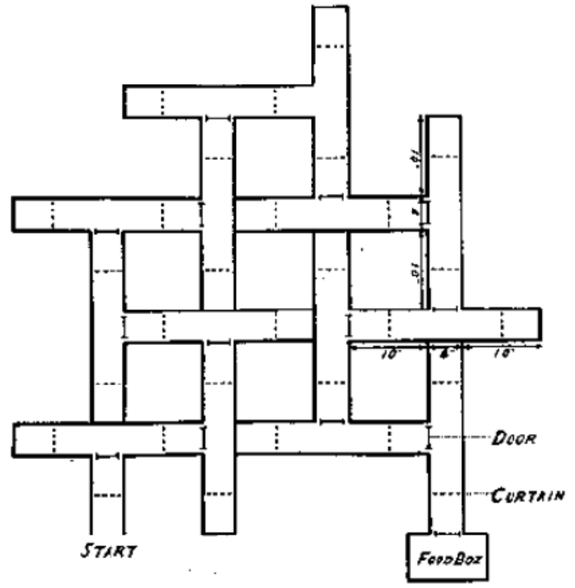


Model-based methods

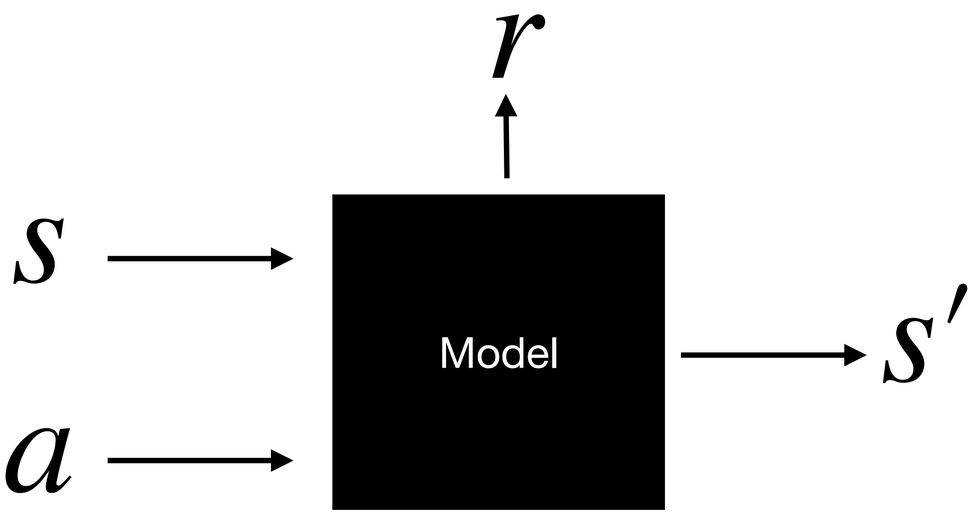
- Learning a “field map of the environment” helps with planning and generalization
- But how is the model learned?
- And how is it used to in RL?
- We will discuss
  - Learning transitions via Delta-Rule
  - DYNA for simulating experiences
  - World Models
  - Dreamer V3



Plan of maze
14-Unit T-Alley Maze

FIG. 1

(From M. H. Elliott, The effect of change of reward on the maze performance of rats. *Univ. Calif. Publ. Psychol.*, 1928, 4, p. 20.)



Learning the model through experience

- Follow whatever policy (e.g., random) and update the transition matrix using delta-rule

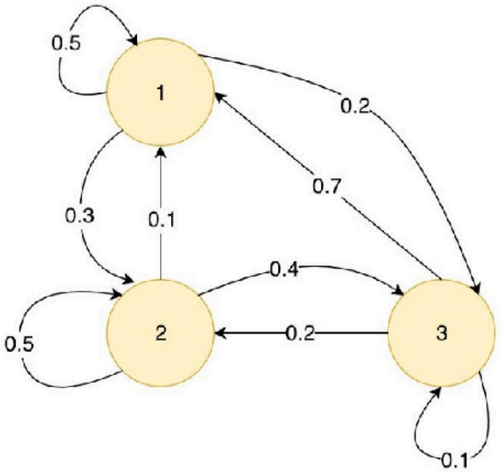
$$T_{t+1}(s' \mid s, a) \leftarrow T_t(s' \mid s, a) + \alpha \left(\delta(s', s) - T_t(s' \mid s, a)\right)$$

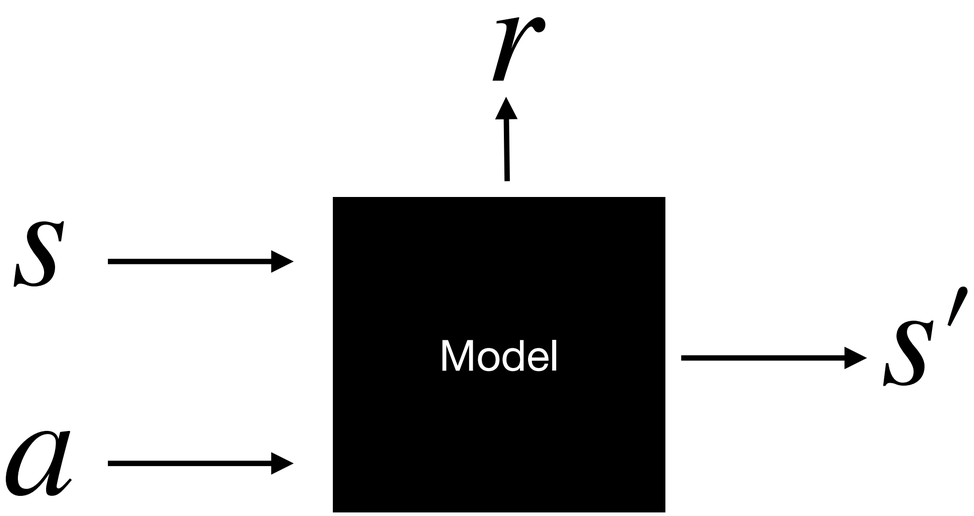
  - Kronecker delta $\delta(s', s') = 1$ when the transition occurs (i.e., $s \rightarrow s'$)
- $Model(s, a) \rightarrow [s', r]$ provided by learned transition matrix $T(s' \mid s, a)$ and value function $Q(s, a)$ or $V(s)$

Transition Matrix

	S_1	S_2	S_3
S_1	0.5	0.1	0.7
S_2	0.3	0.5	0.2
S_3	0.2	0.4	0.1

MDP





Simulating experiences with DYNA

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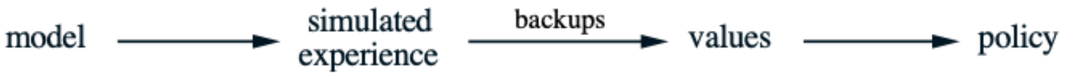
- DYNA uses simulated experiences to update policy/value functions, just like real experiences



Sutton (1990)

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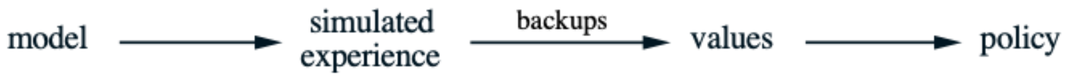

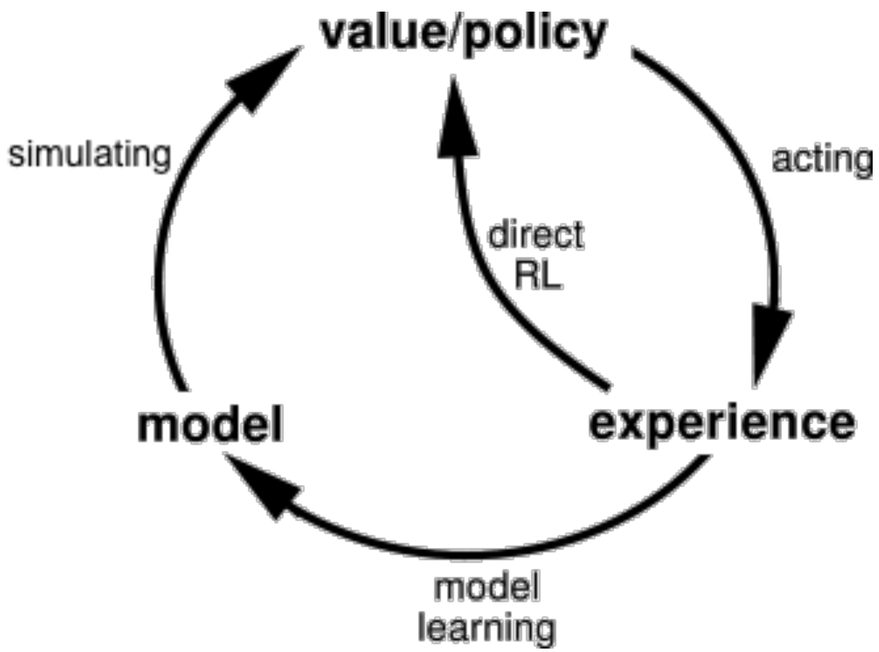

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1. **Direct RL**: Execute real actions and update value function

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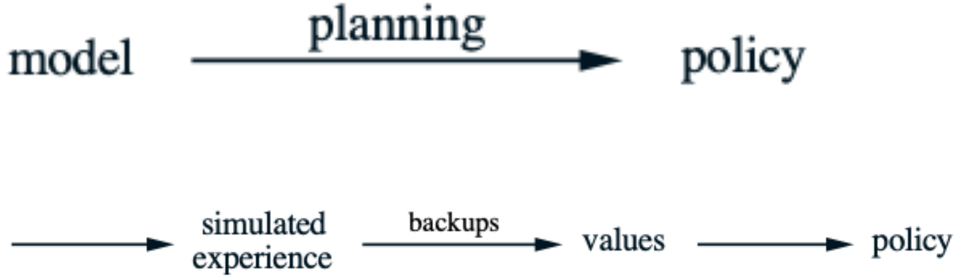

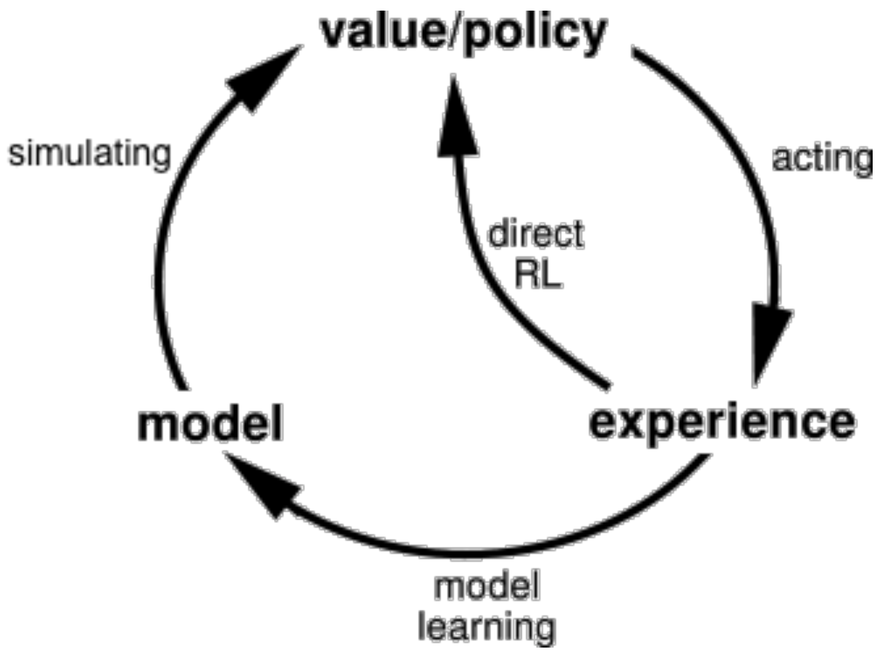

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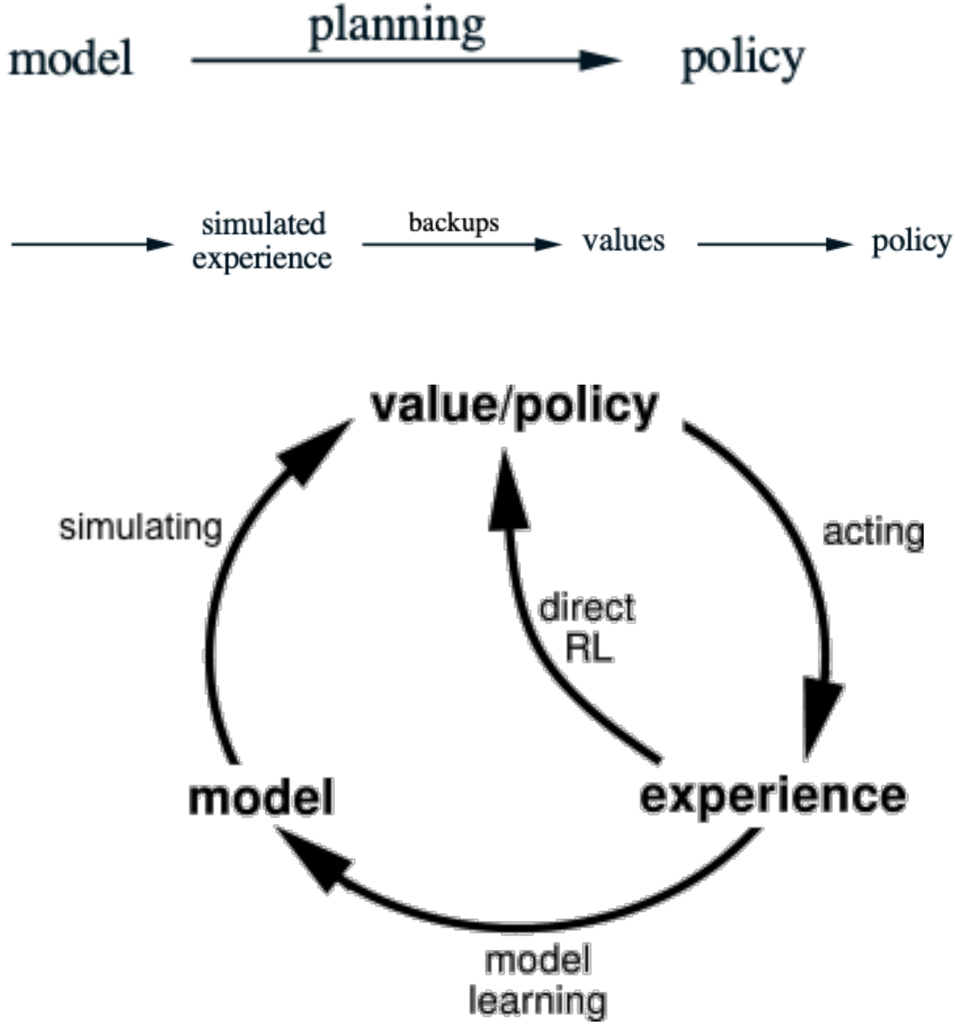

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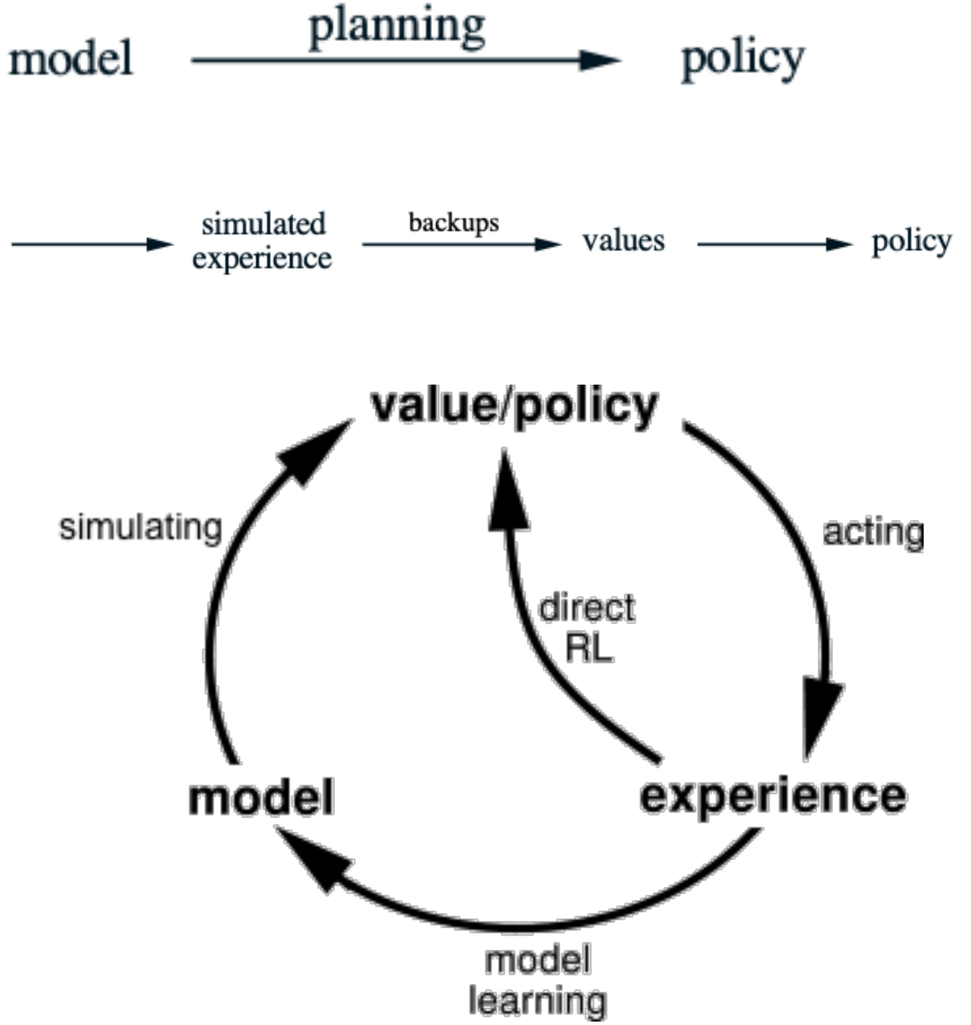
2. **Model learning**:
   a. Update model of the environment $Model(s,a)$



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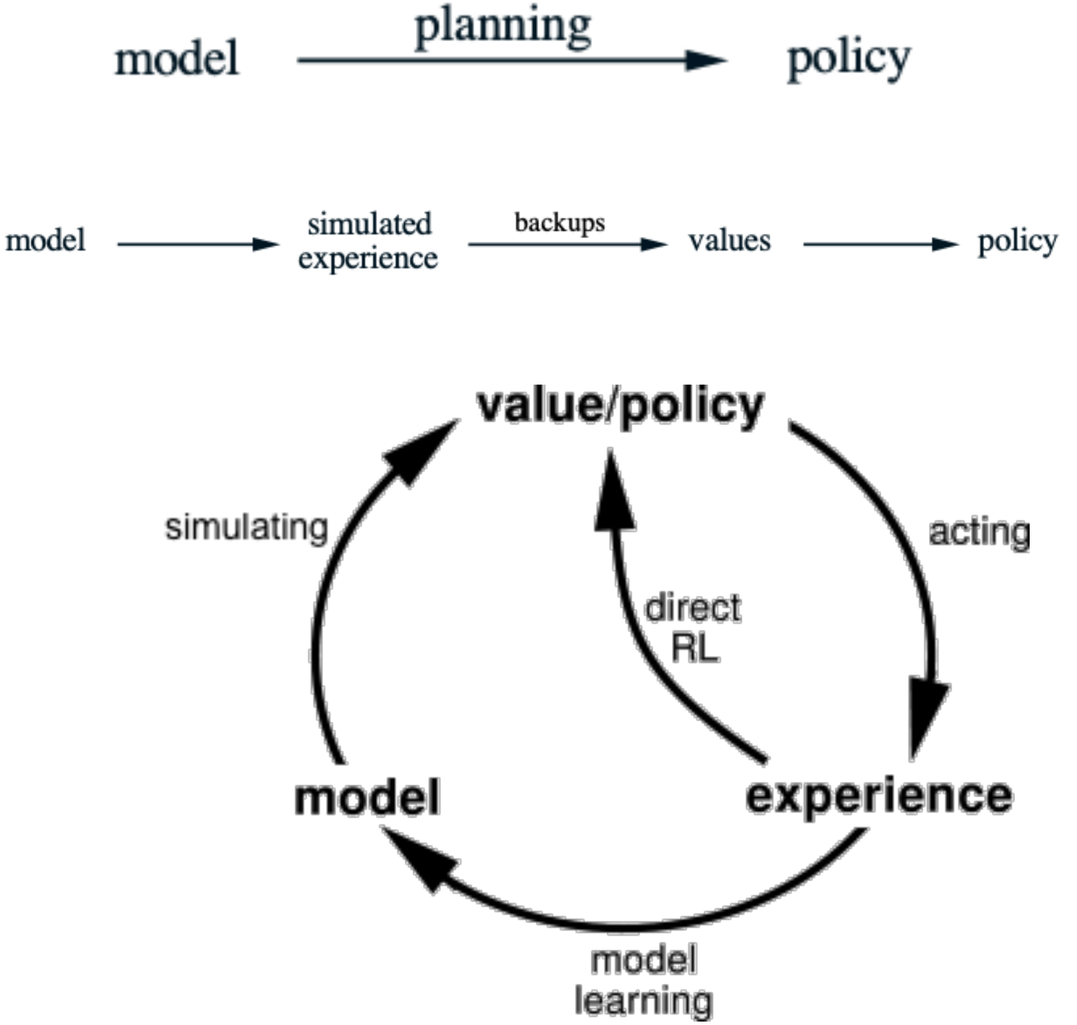

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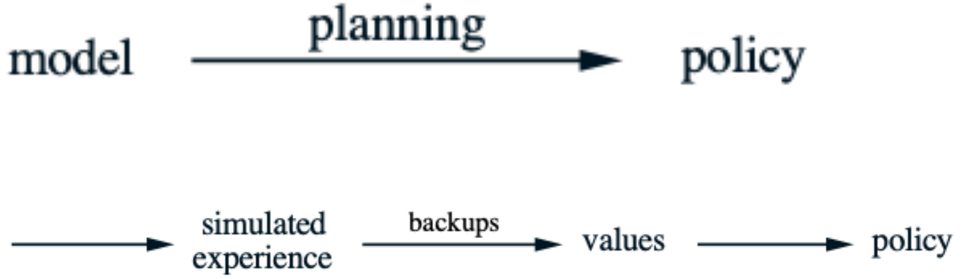

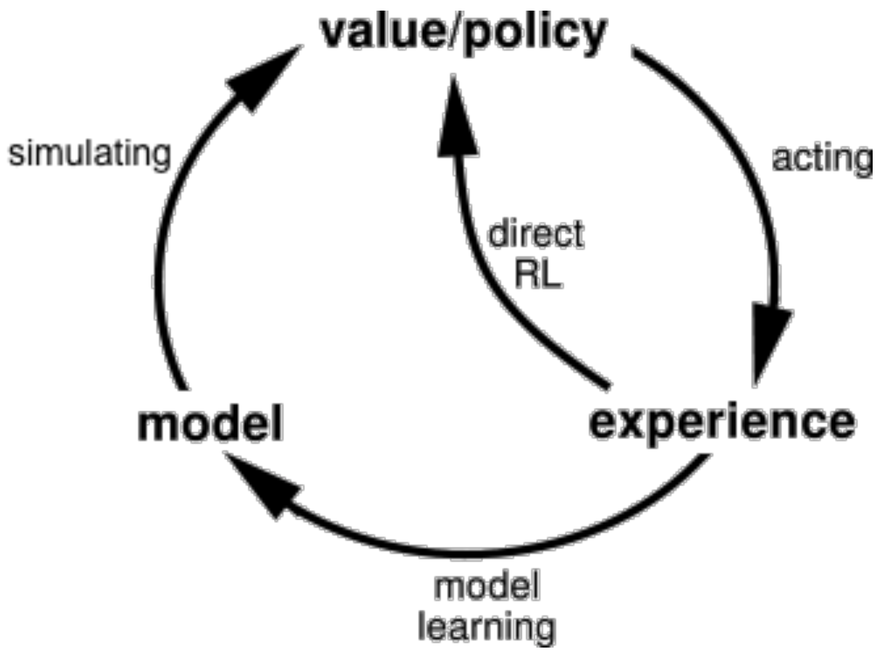

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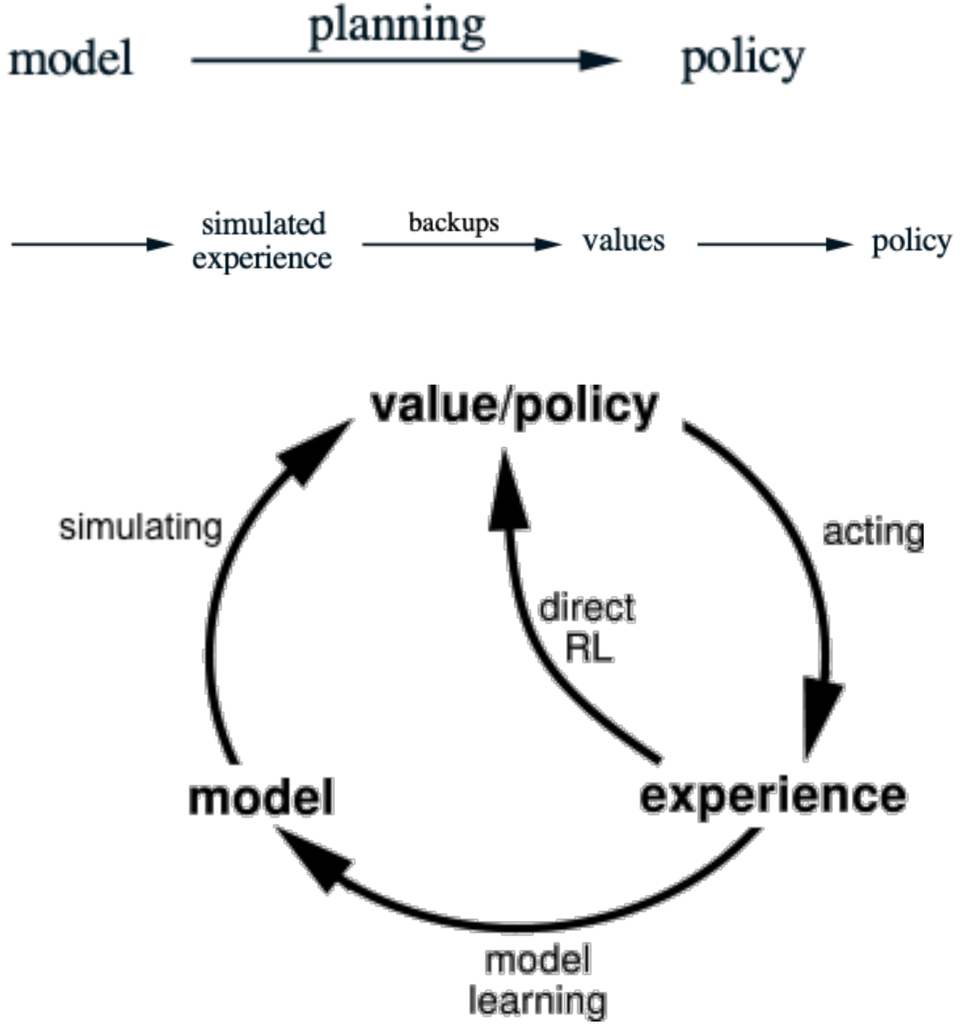

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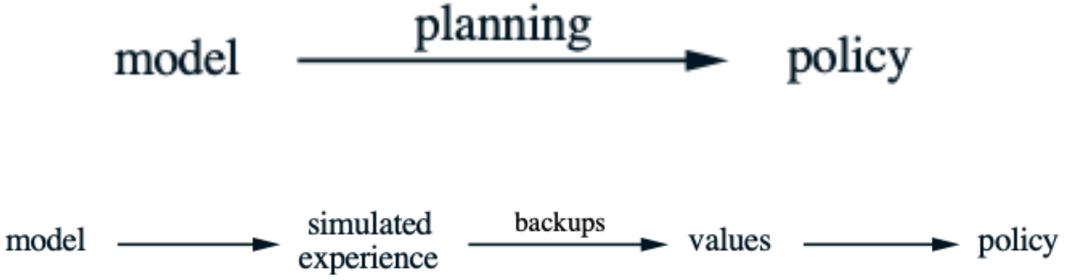
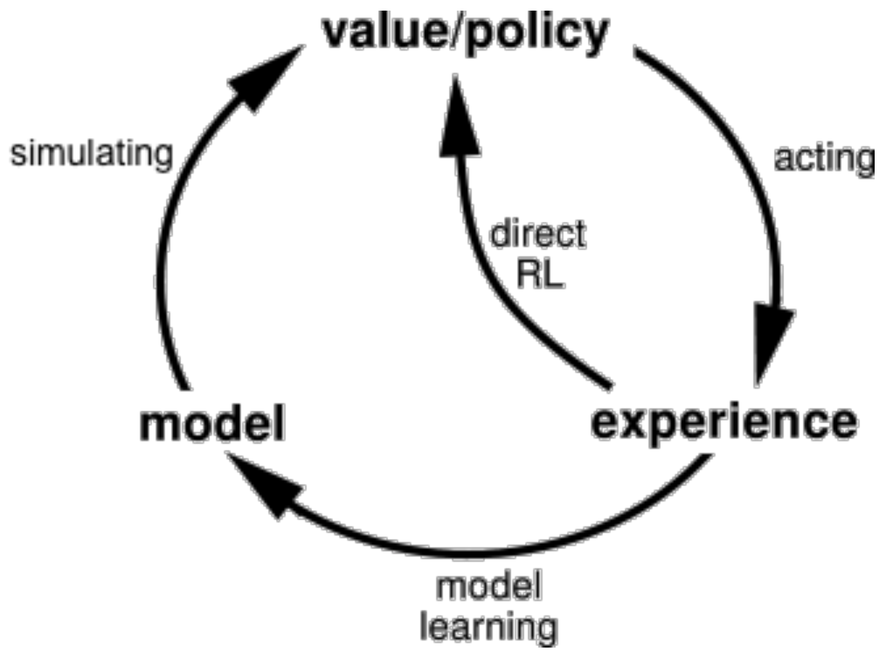
- These simulations can be controlled for better efficiency (e.g., prioritized sweeps of reward-relevant state visitations; Moore & Atkeson, 1993)

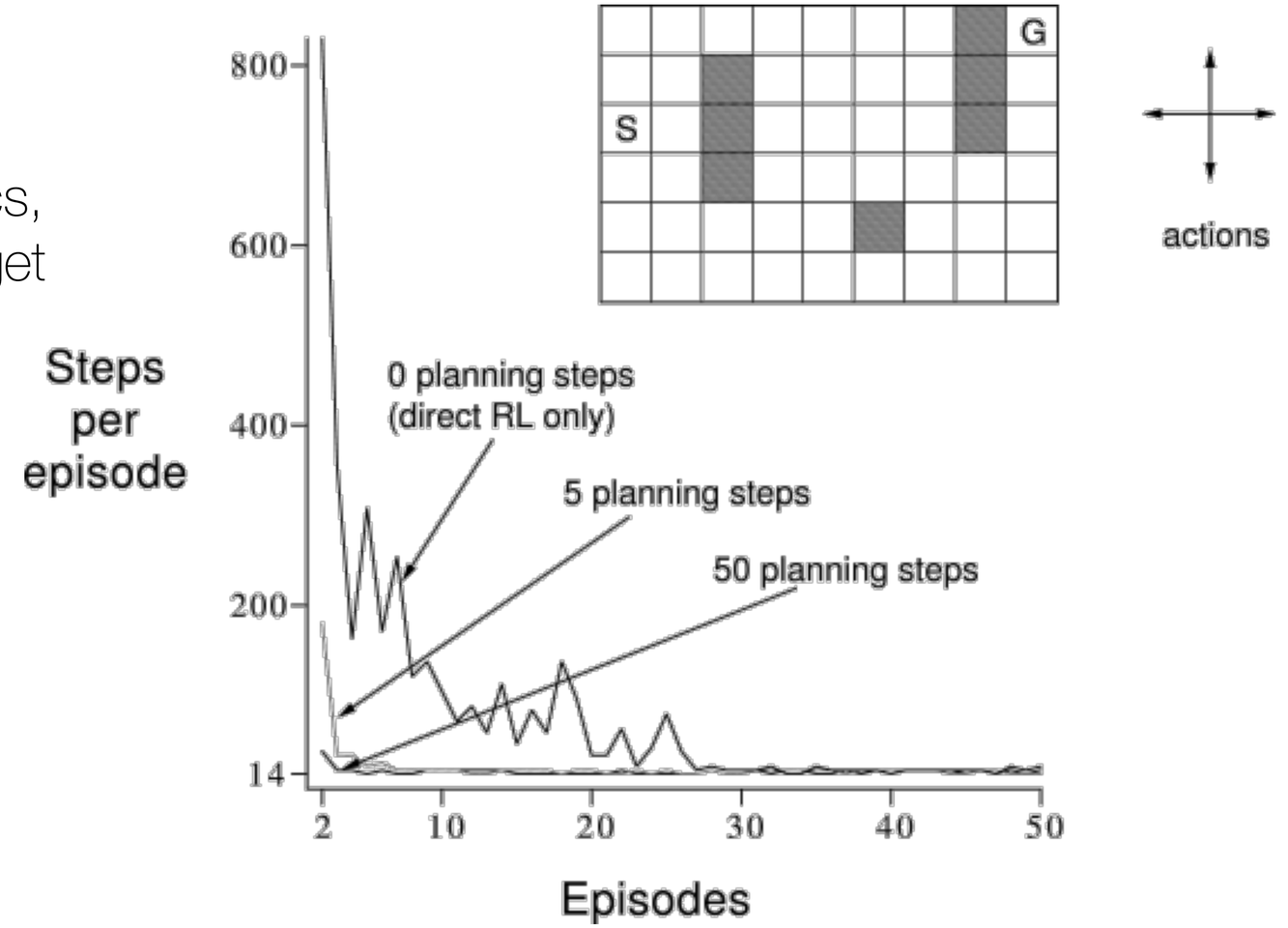




Benefits of Model-based planning

- Model-based planning needs far fewer real interactions with the environment (episodes) to learn better policies
  - Consider settings like self-driving cars, robotics, financial systems… where it is very costly to get real interaction data

Sutton & Barto Fig. 9.5



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- Halfway through only the 2nd episode…
  - Arrows show greedy action in each state and no arrow if all actions are equal

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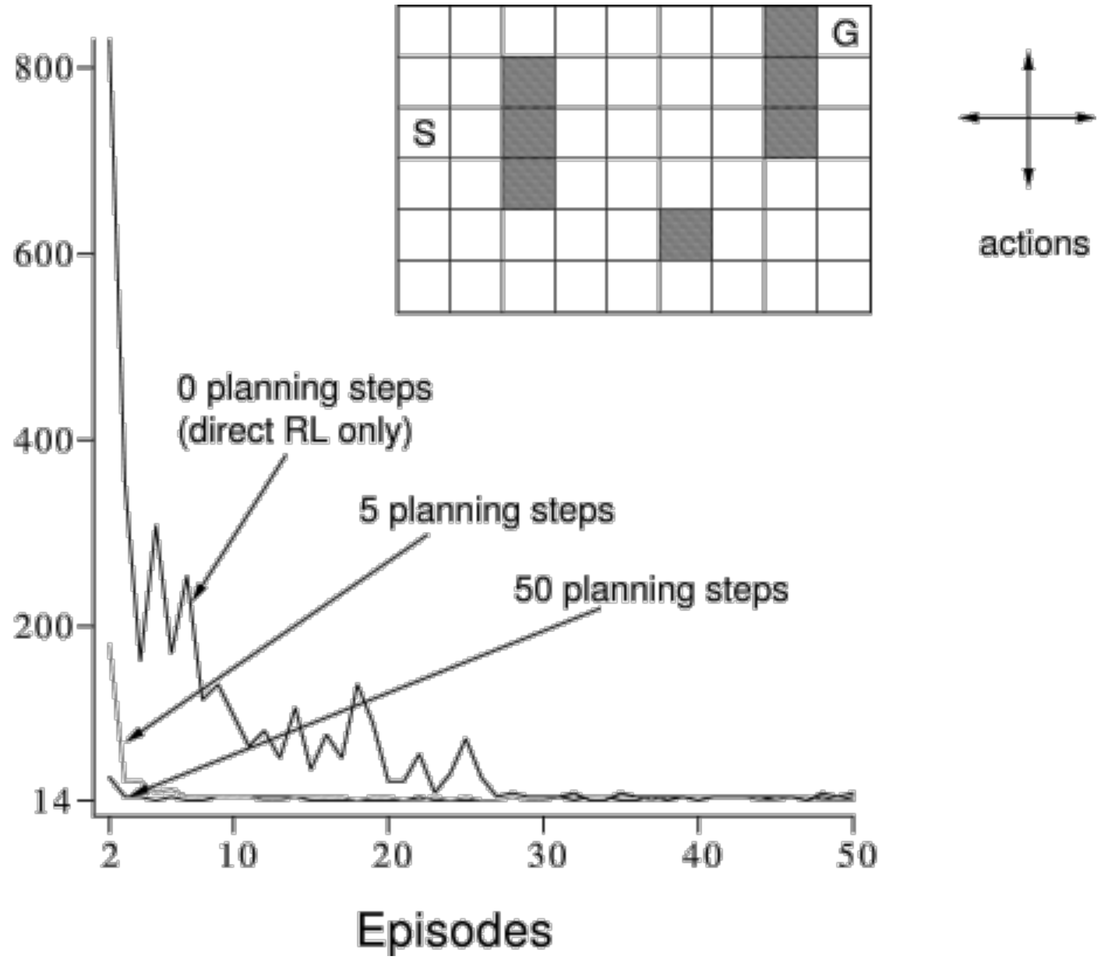
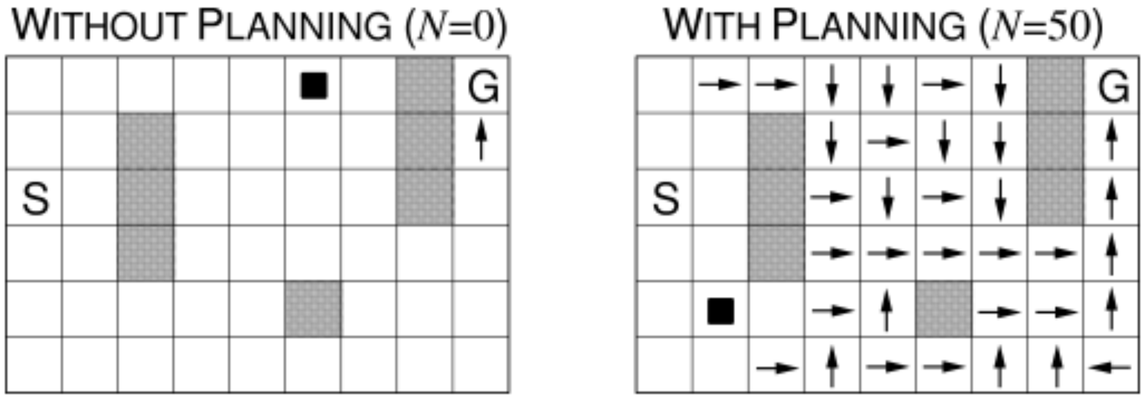
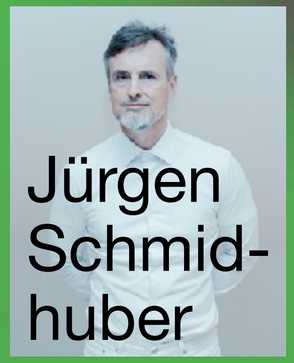




Sutton & Barto Fig. 9.6

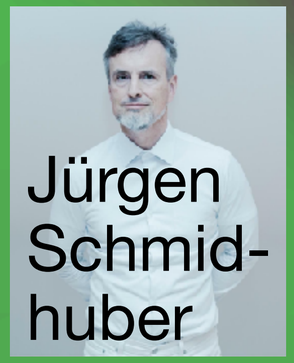


Recurrent World Models Facilitate Policy Evolution

NIPS 2018
Oral Presentation

Thirty-Second Annual Conference on
Neural Information Processing Systems
Montréal, Canada

Interactive demo. Tap screen or use arrow keys to override the agent's decisions.



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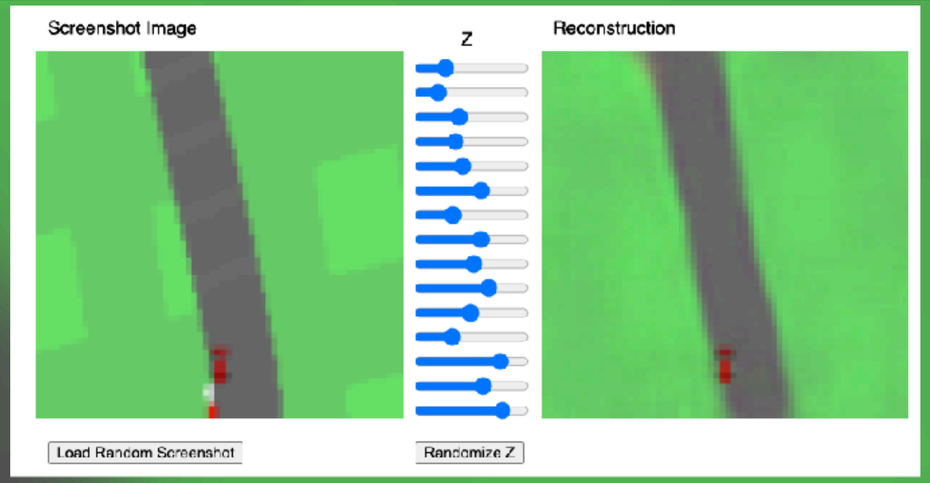

Check out worldmodels.github.io/ for iteractive demos and more details!

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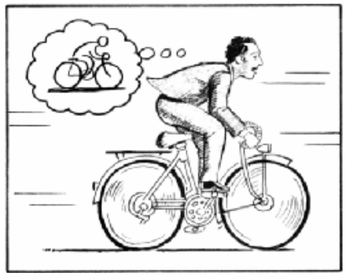
Ha & Schmidhuber (2018)

World models



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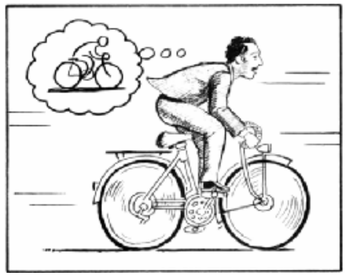

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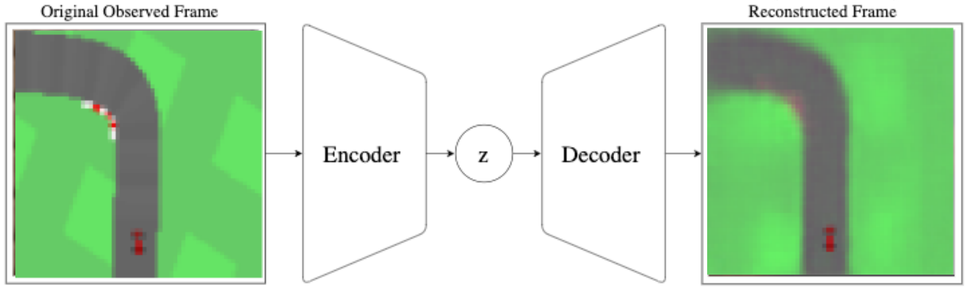
Variational Autoencoder (VAE)



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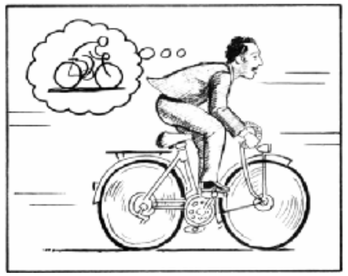

World models

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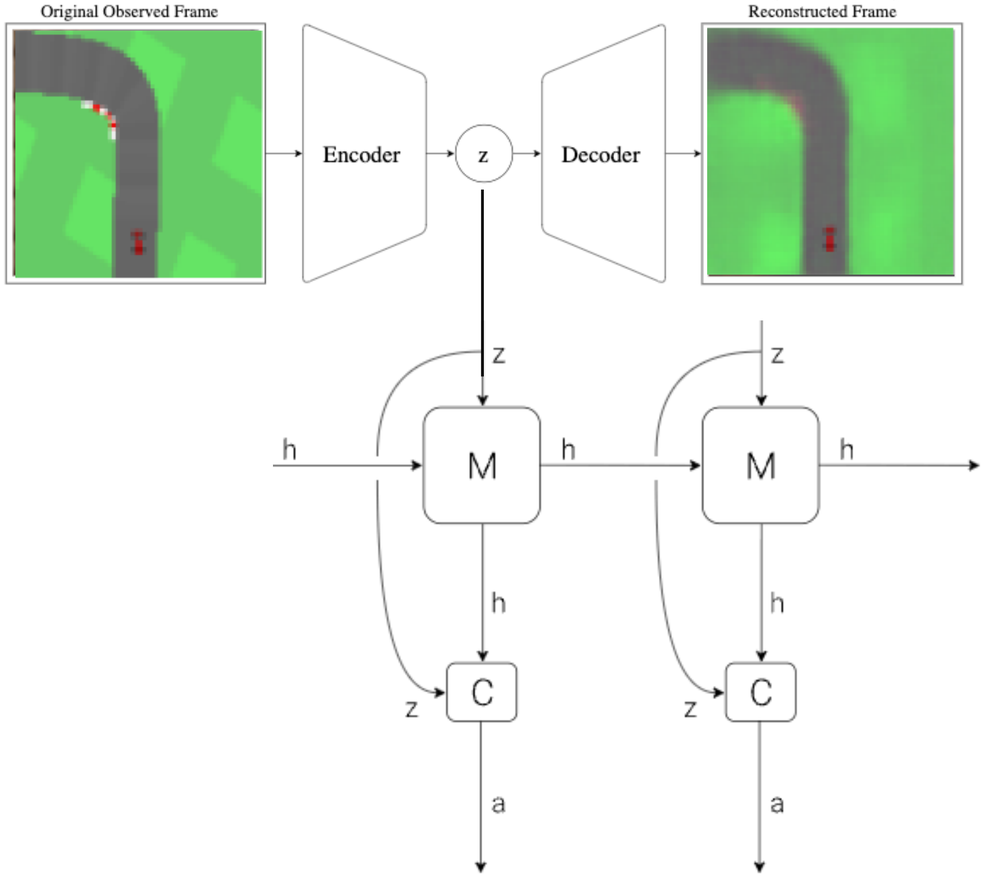

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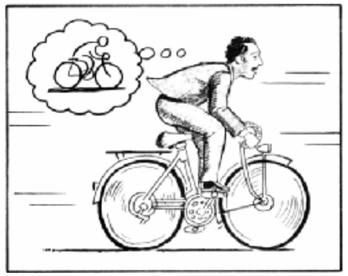

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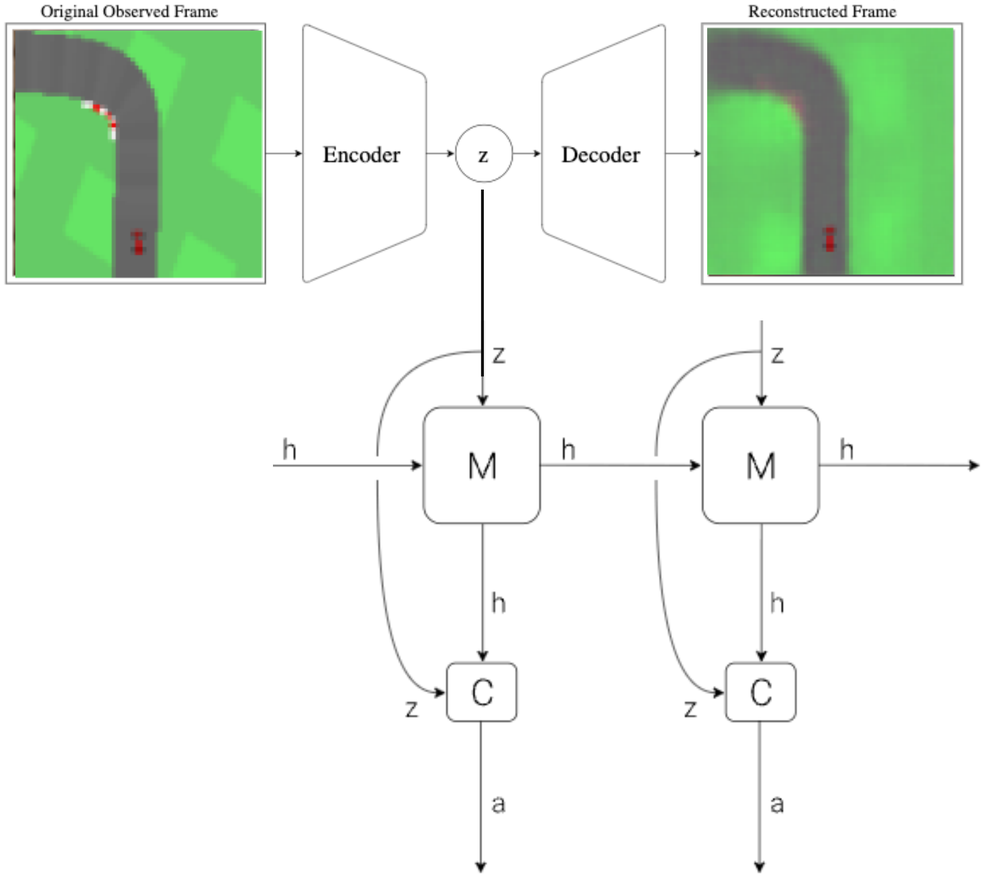

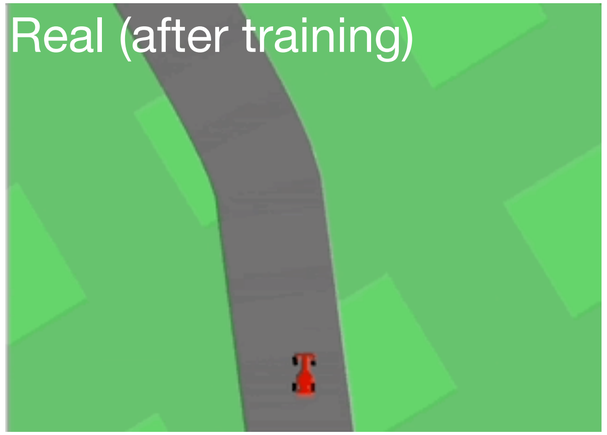

Ha & Schmidhuber (2018)

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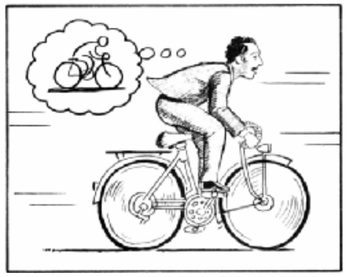

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- Training on dreams by simulating future states and treating them as real
  - Used to update controller weights

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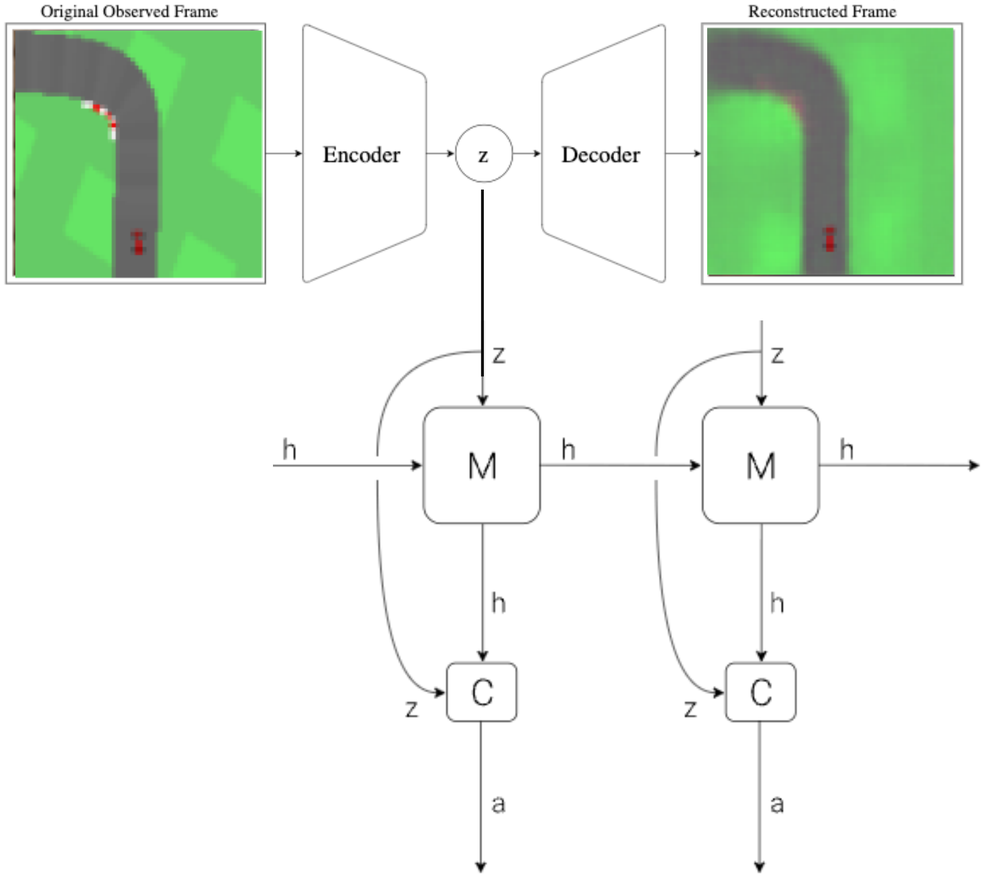

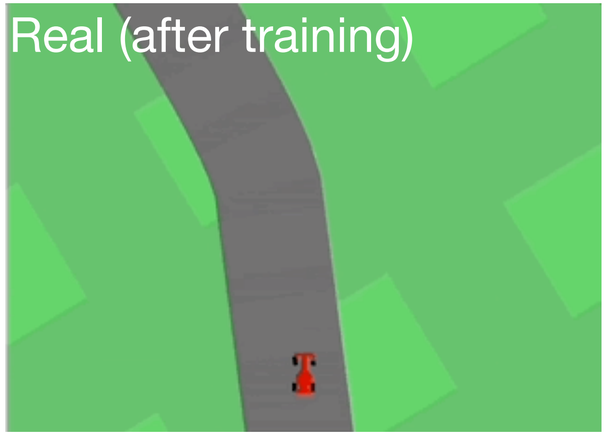

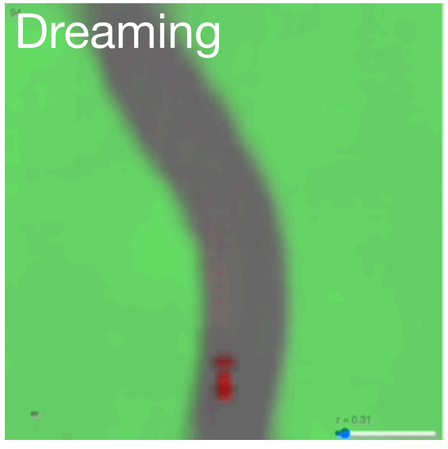


DreamerV3
Hafner et al., (2023)


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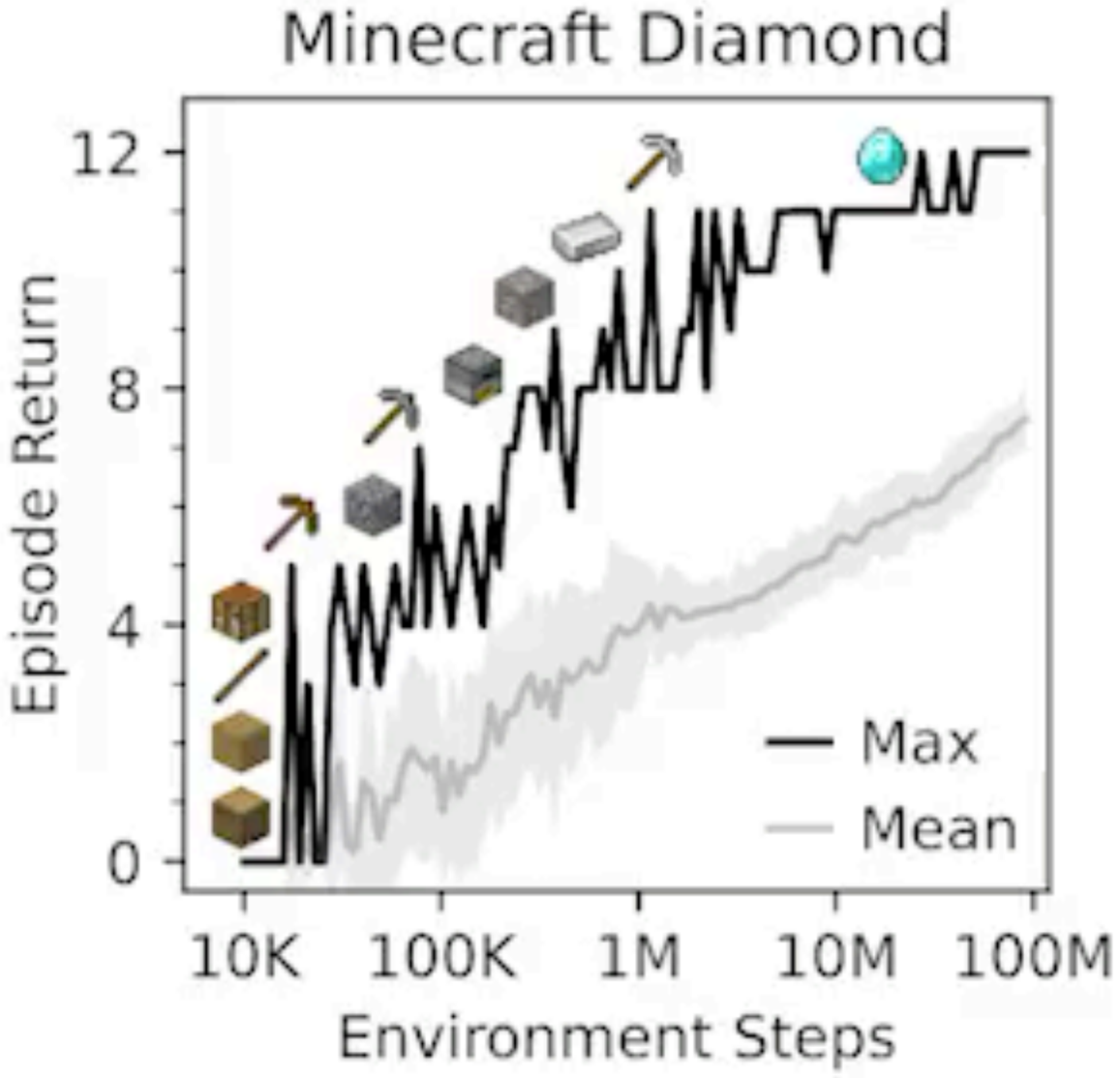
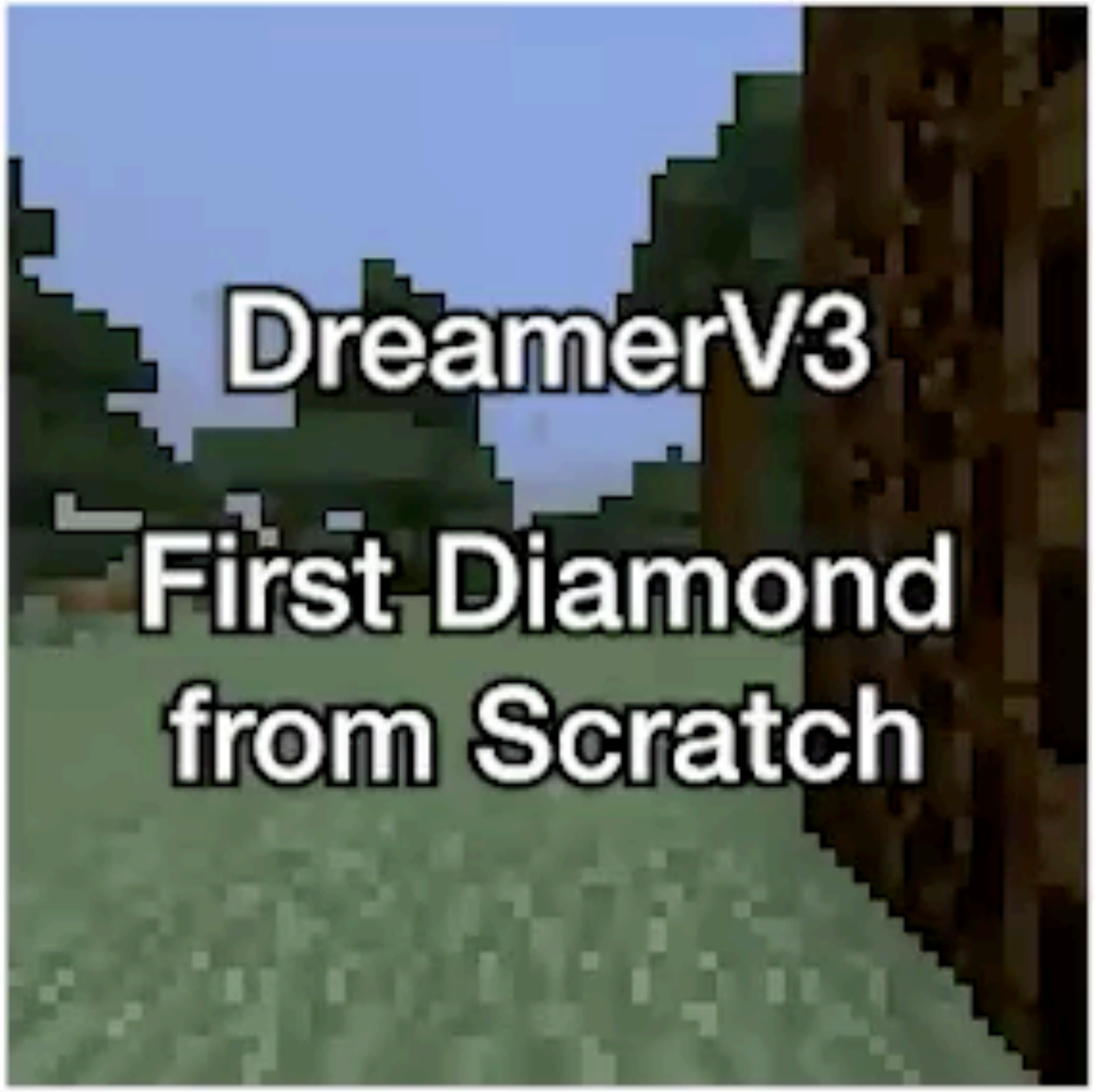
Hafner et al., (2023)

First algorithm to collect diamonds in Minecraft without human data or training curricula





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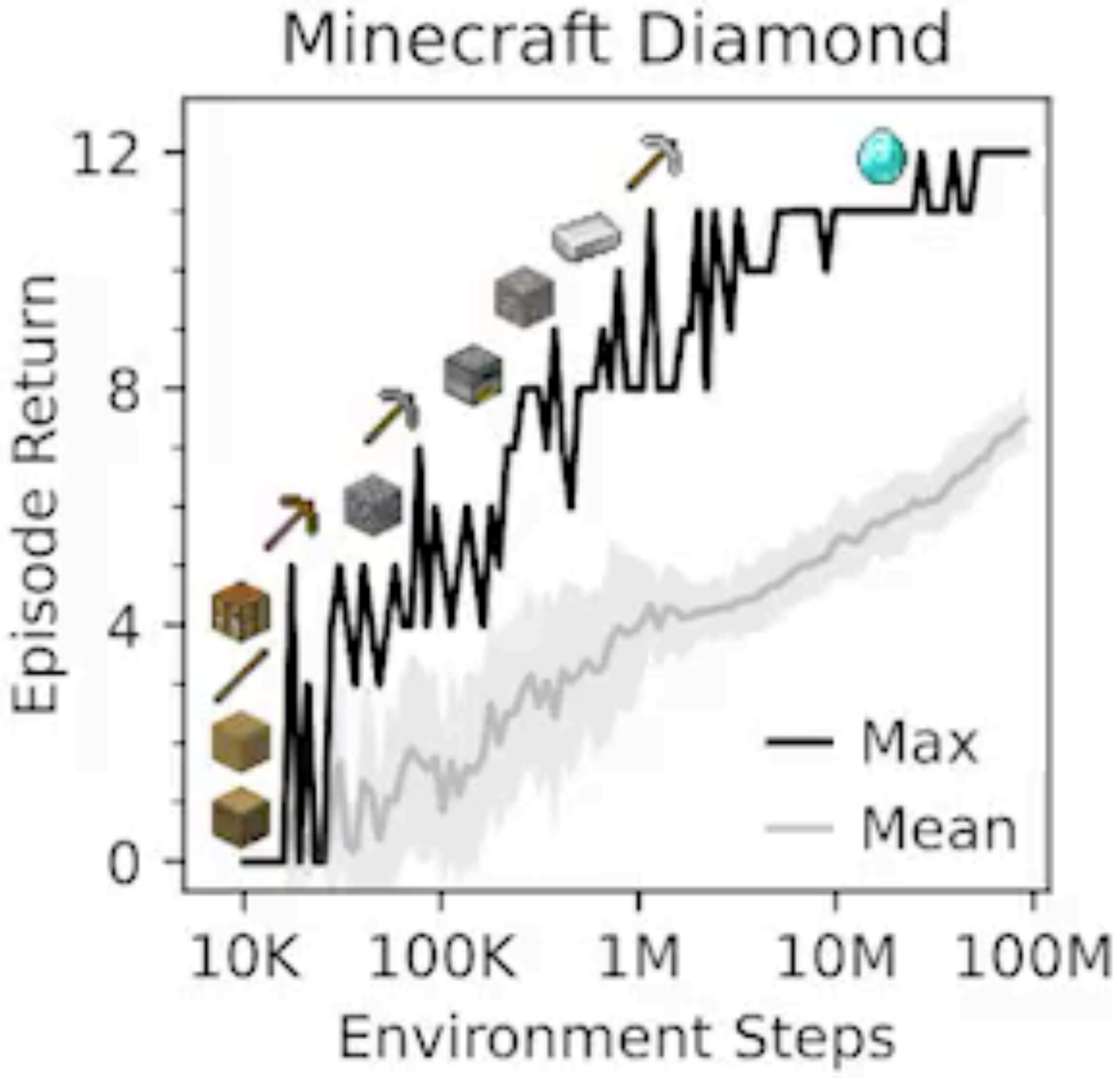
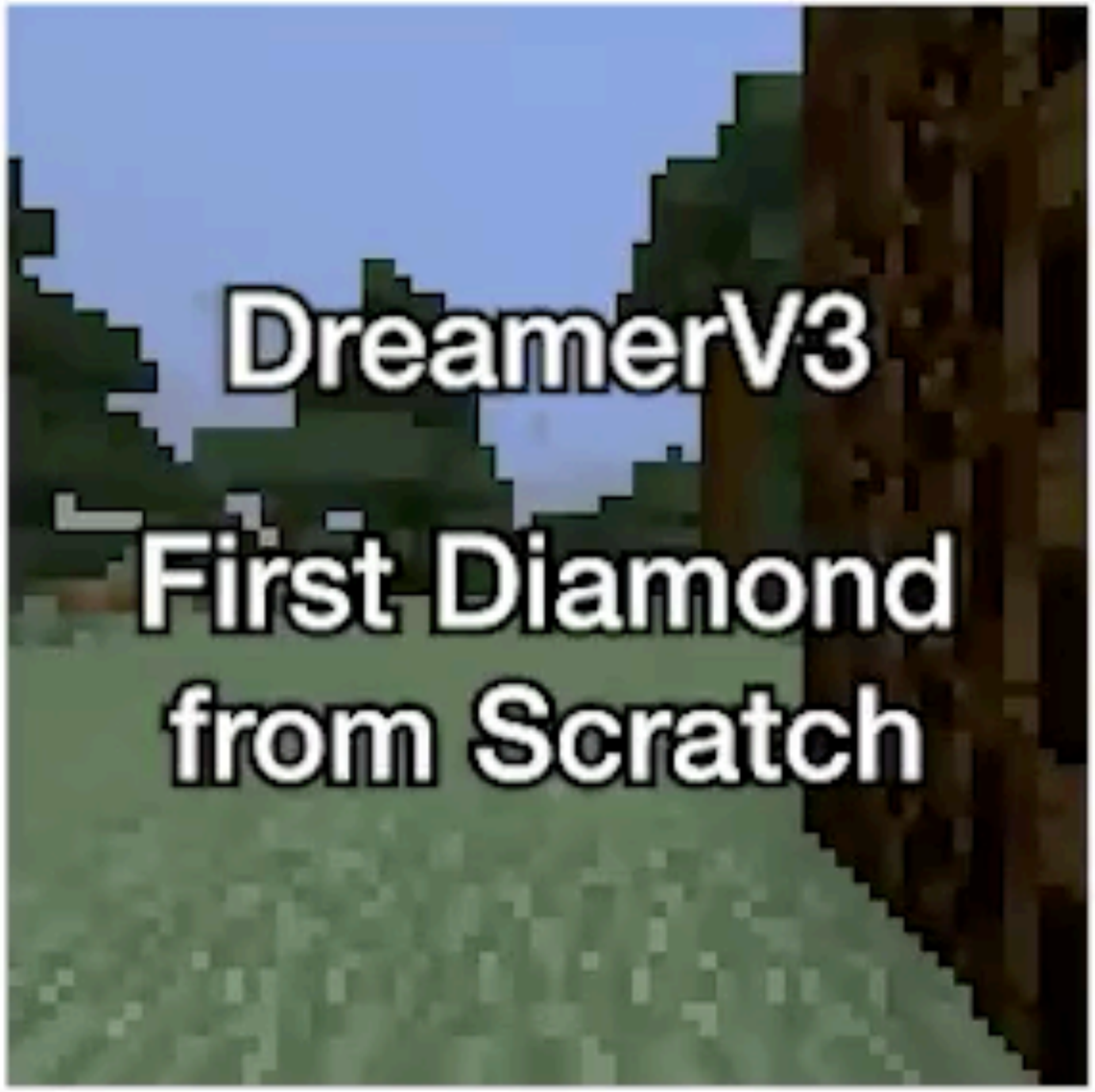




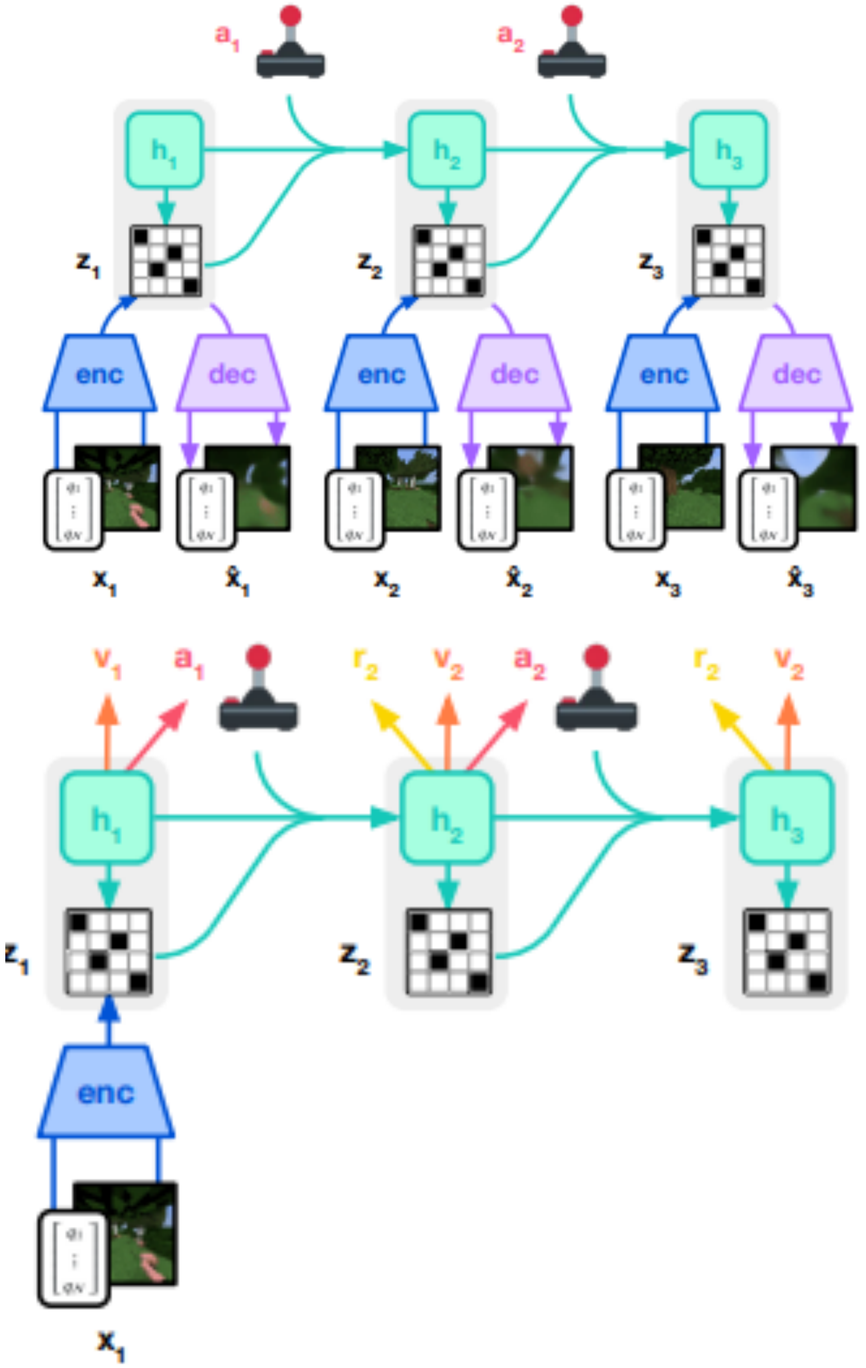
Dreamer Hafner et al., (2023)

Similar concept to World Models

- **Encoder** $z_t \sim q_\phi(z_t \mid h_t, x_t)$ given hidden state h_t and observations x_t
- **Sequence model** $h_{t+1} = f_\phi(h_t, z_t, a_t)$ and **dynamics predictor** $\hat{z}_t \sim p_\phi(\hat{z}_t \mid h_t)$

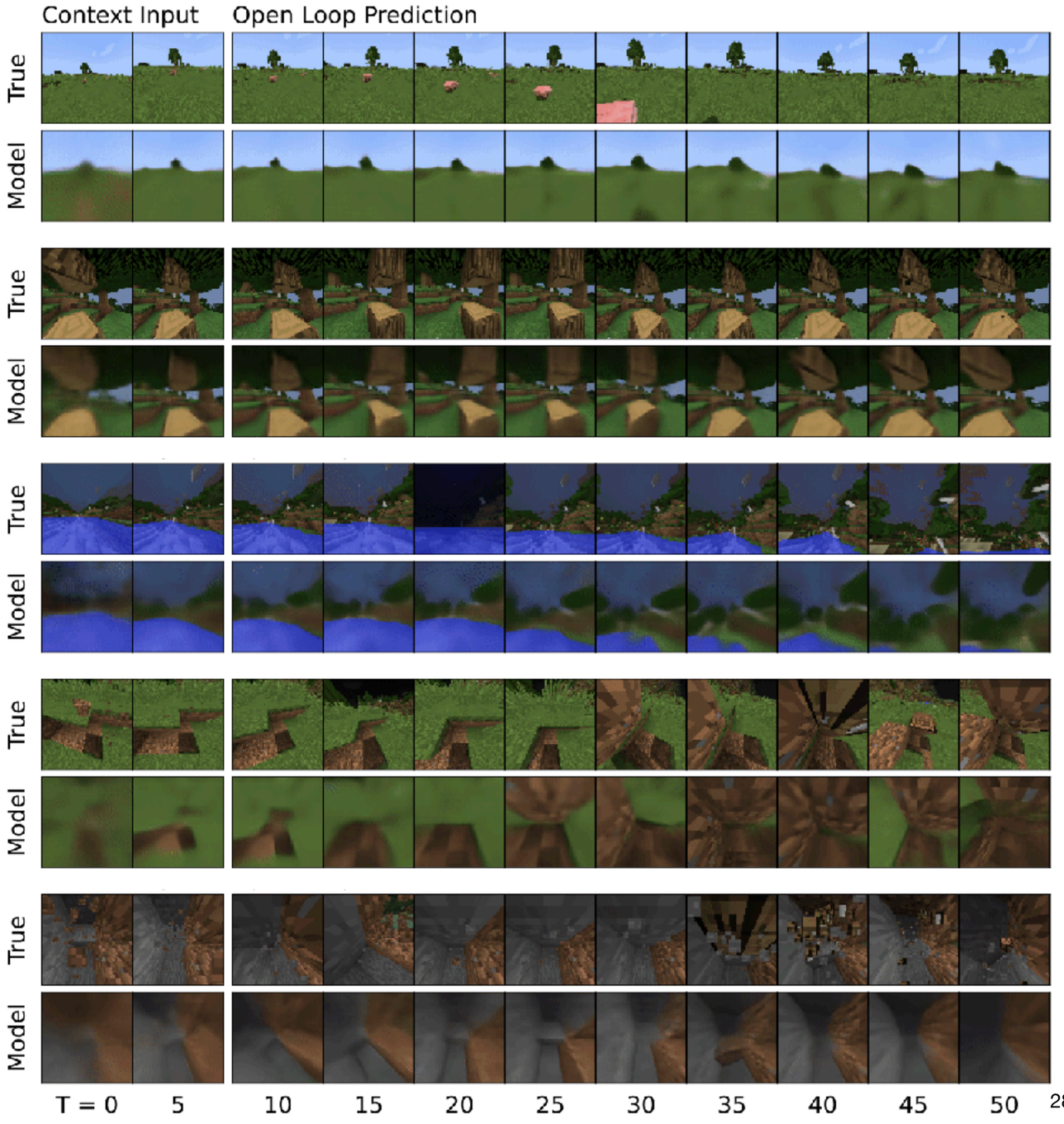
Actor-critic architecture

- **Actor** $a_t \sim \pi_\theta(a_t \mid s_t)$ where $s_t = \{h_t, z_t\}$
- **Critic** $v_\psi(R_t \mid s_t)$



Model-based planning via simulating the future

- Main purpose of the model is to supplement real training experiences (direct RL) by simulating (imagining) future experiences



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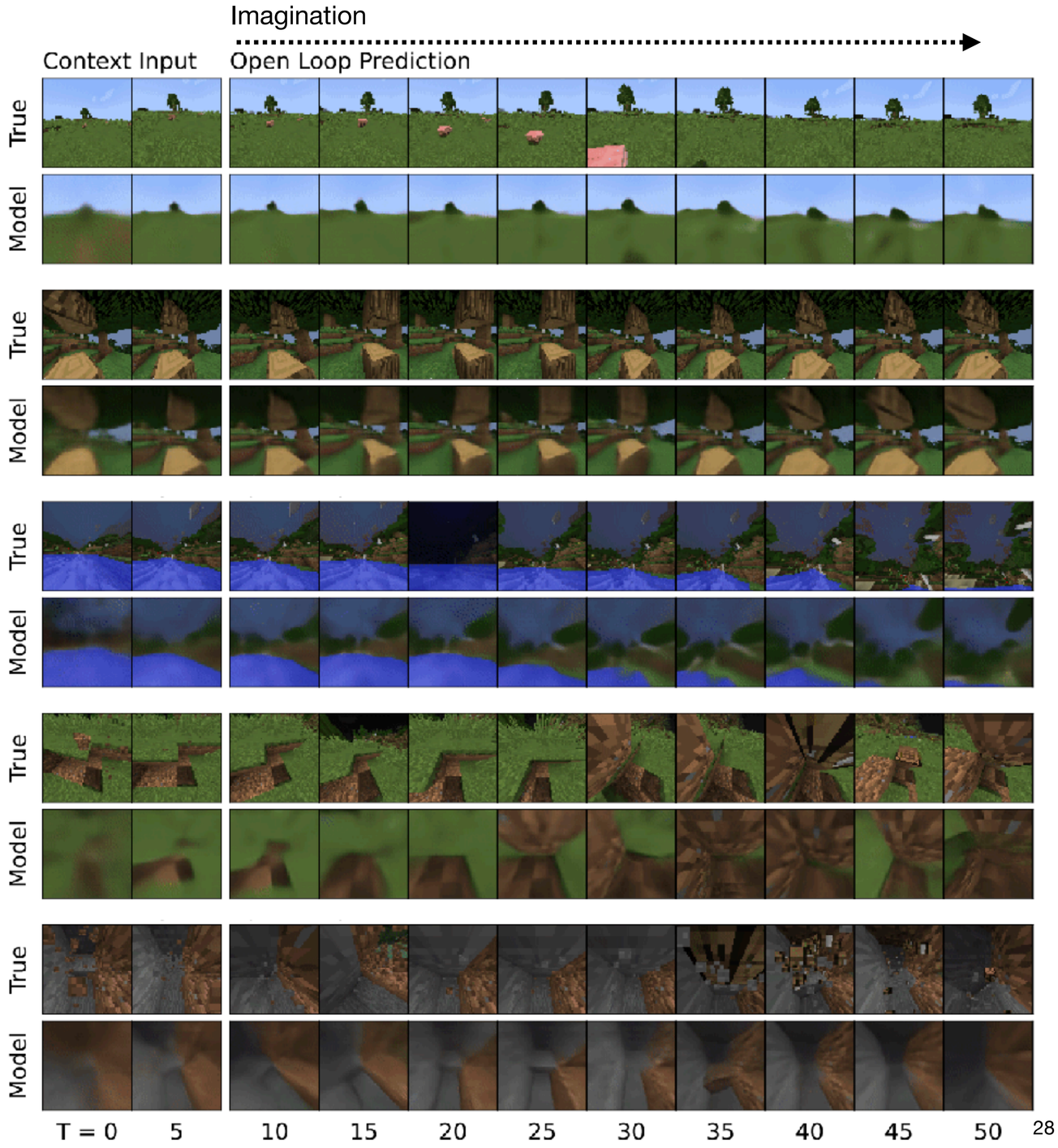

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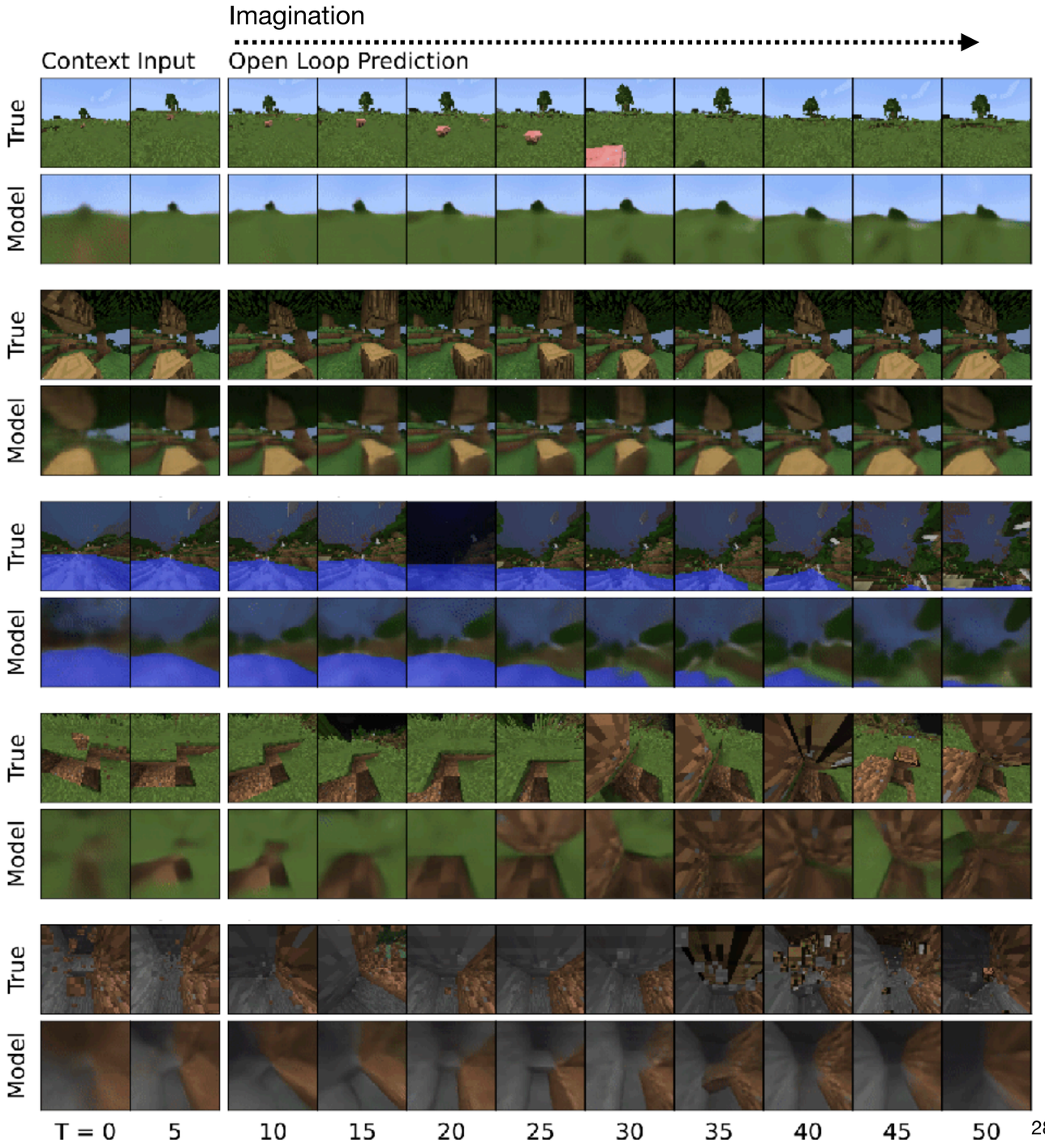

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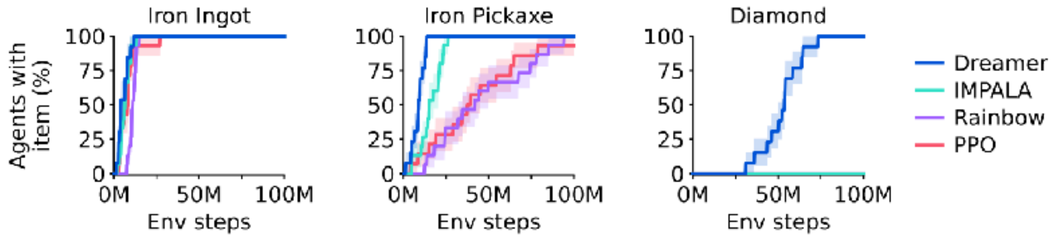

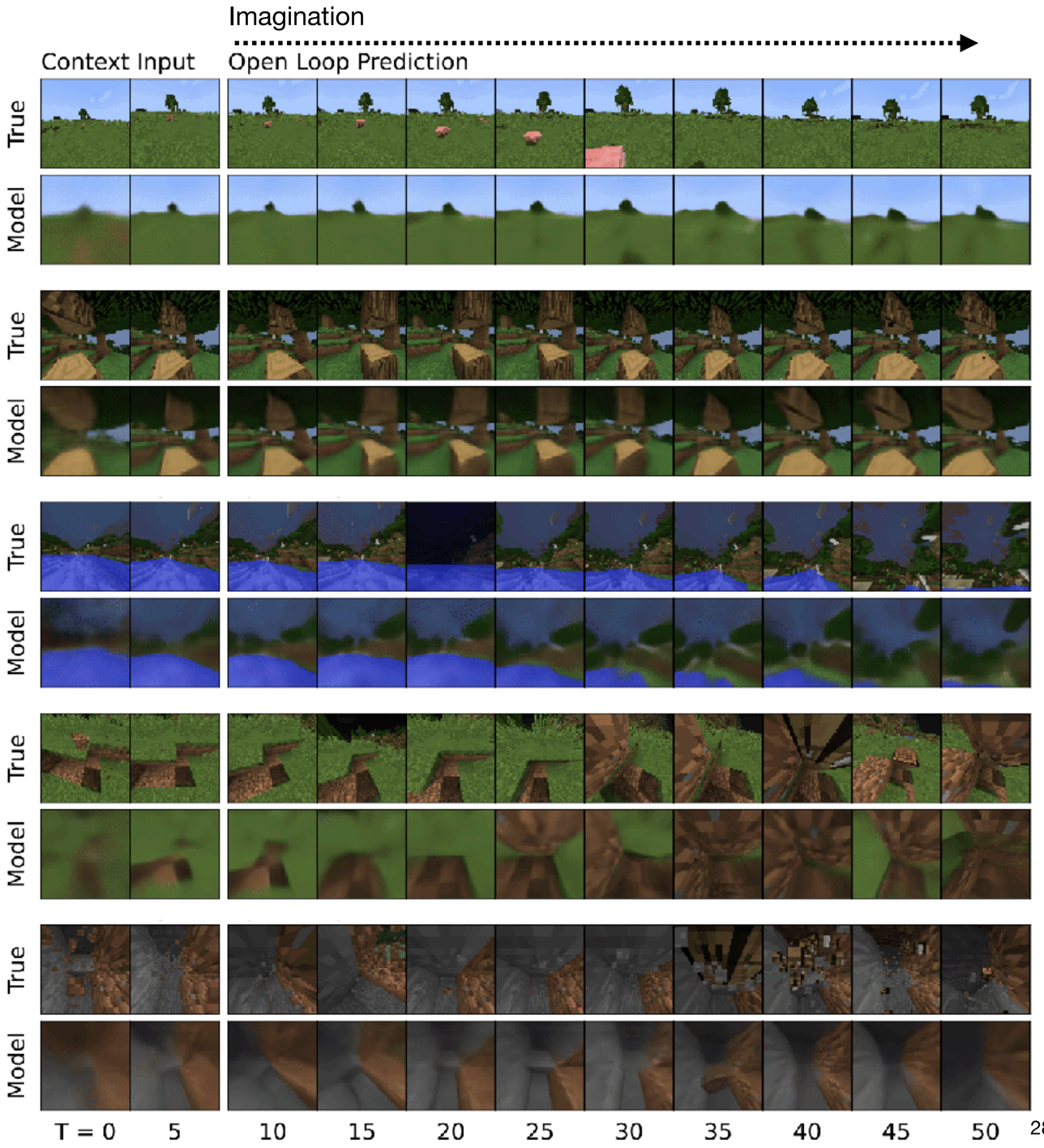

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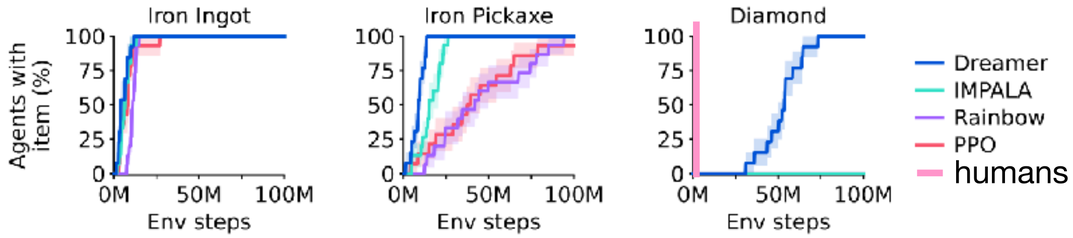

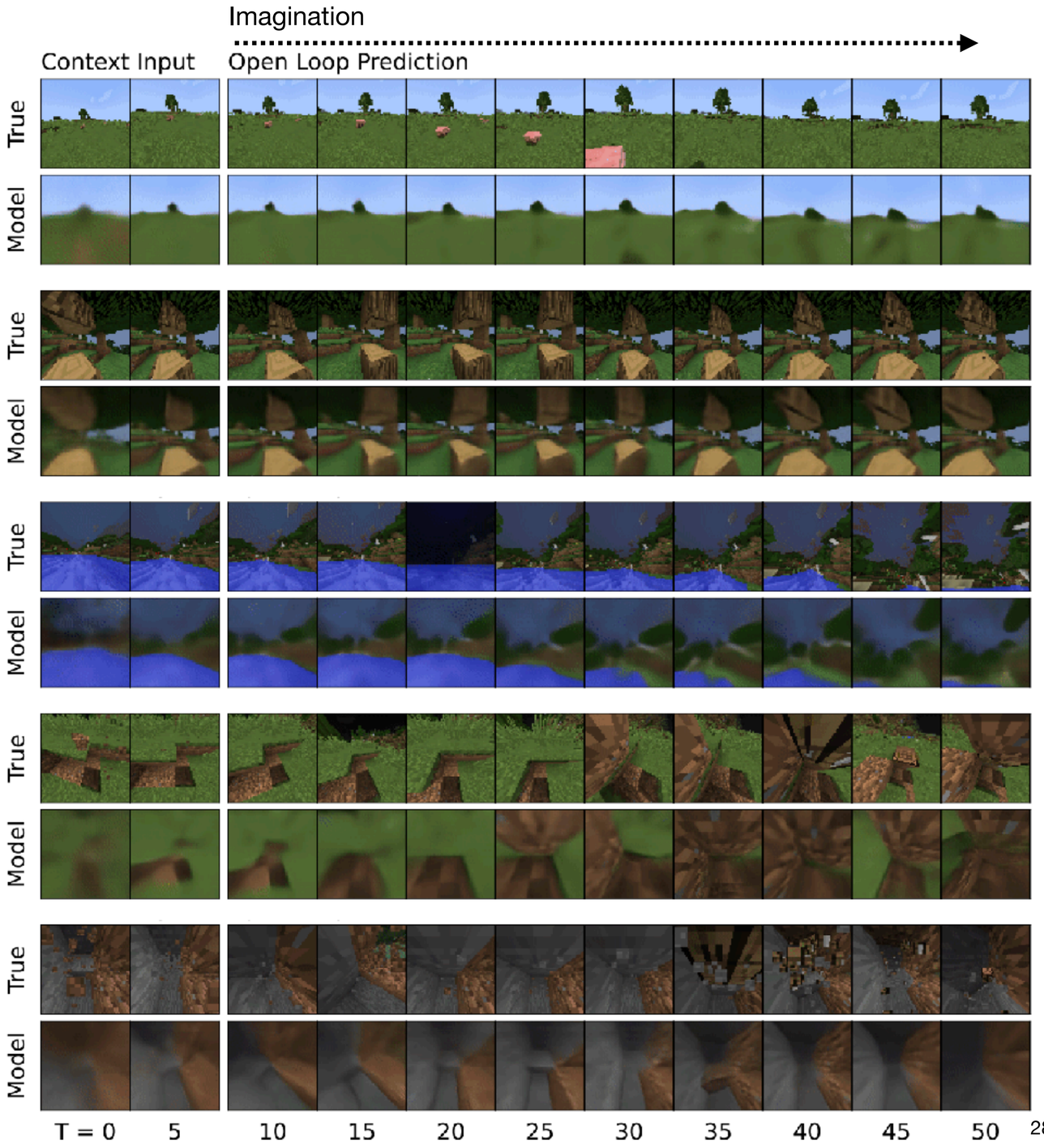

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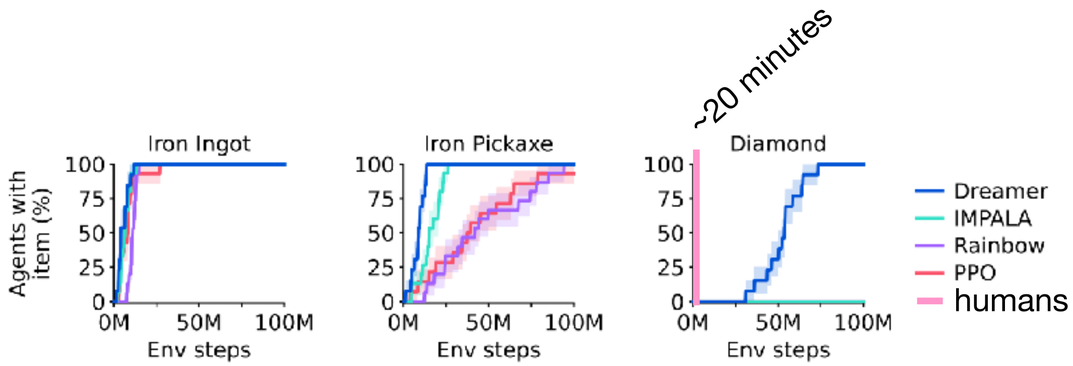

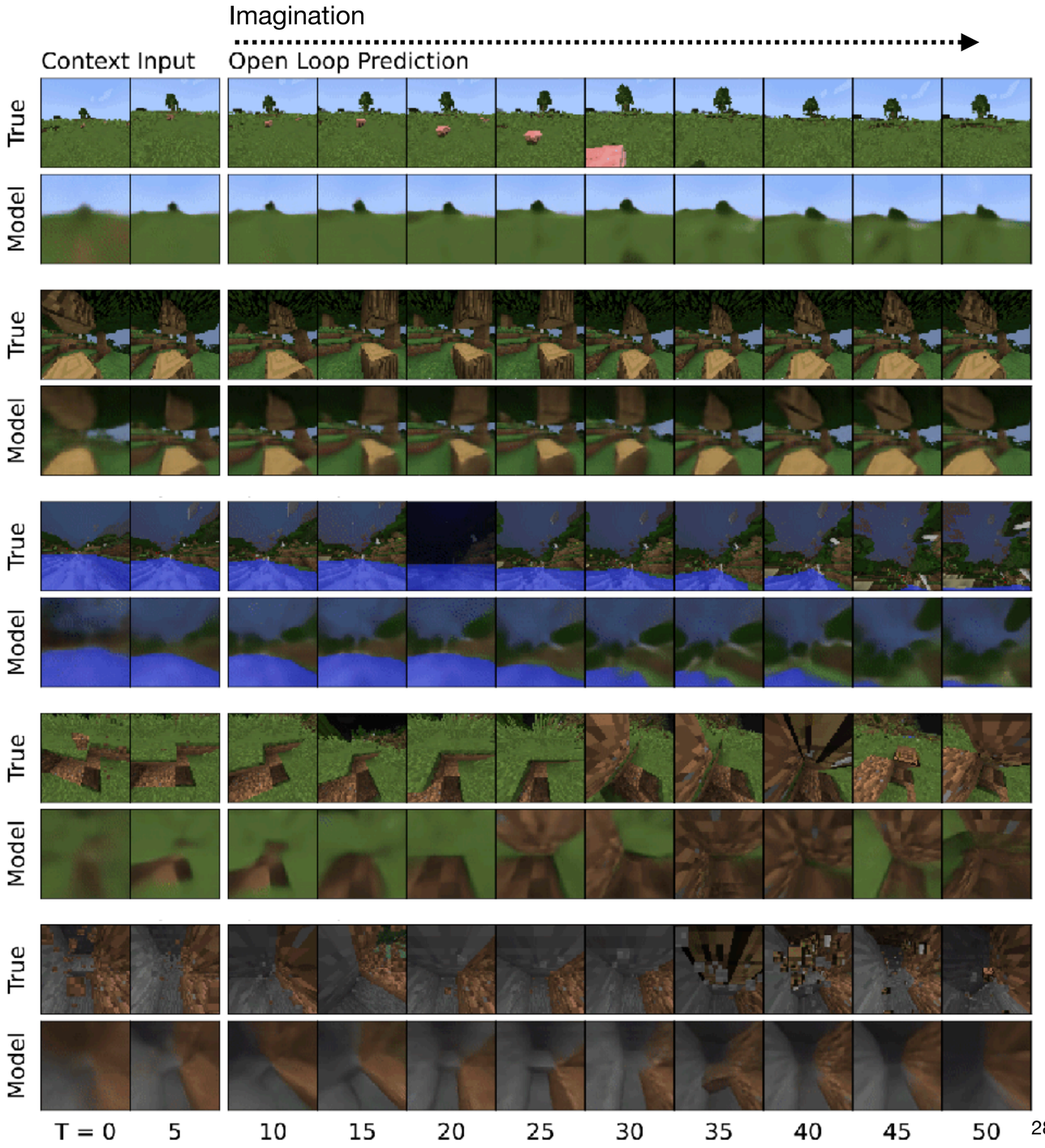

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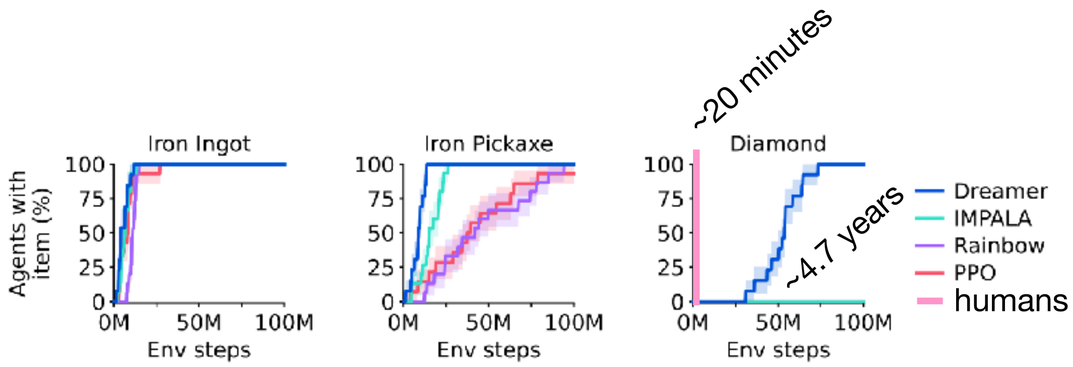
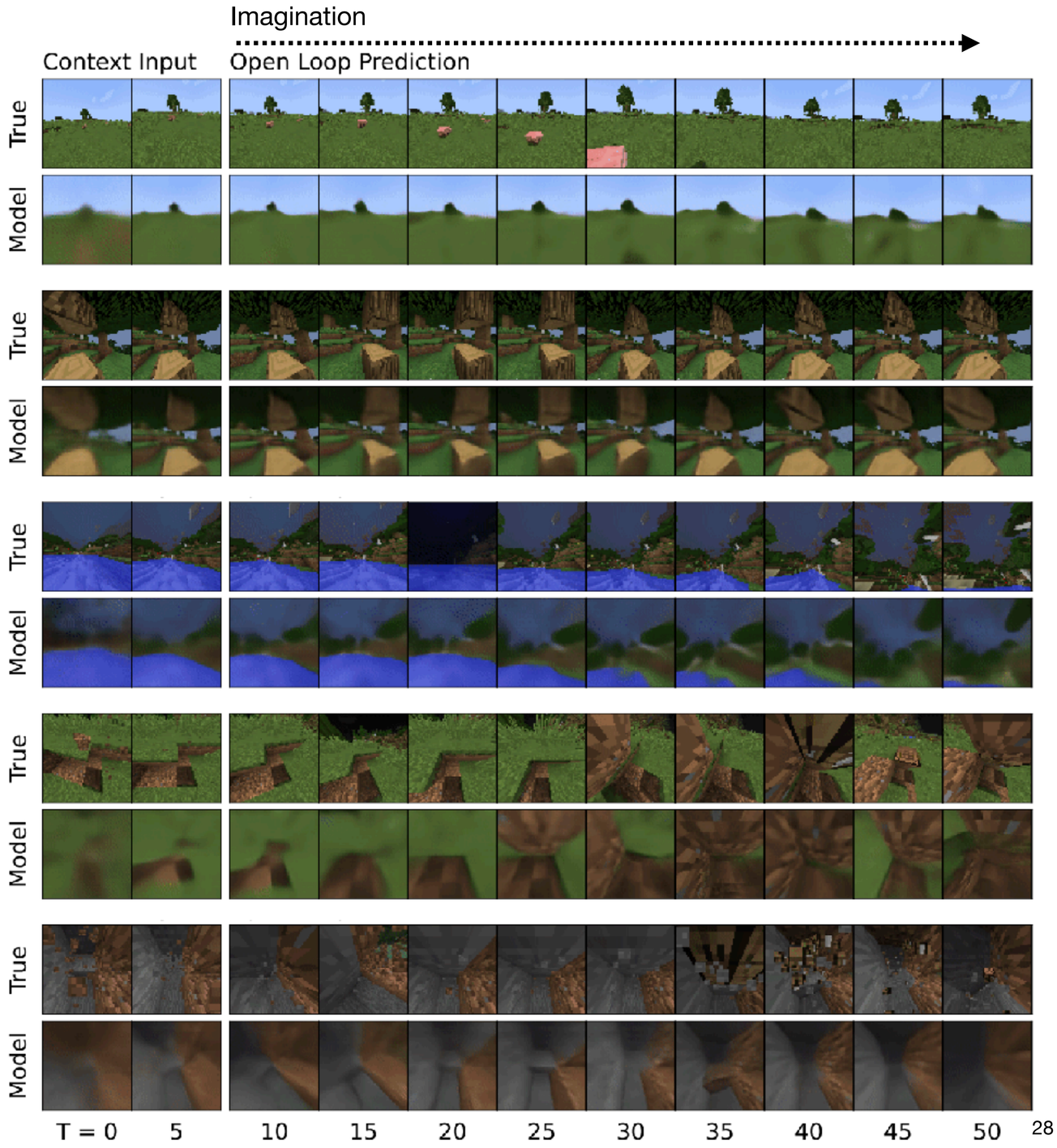




Model-based methods summary

How is the model learned?

- Through trial-and-error learning using delta-rule updates
- With modern ML techniques
  - Encode high-dimensional stimuli into a low-dimensional representation z
  - Learn the temporal dynamics $P(z_{t+1} \mid z_t)$

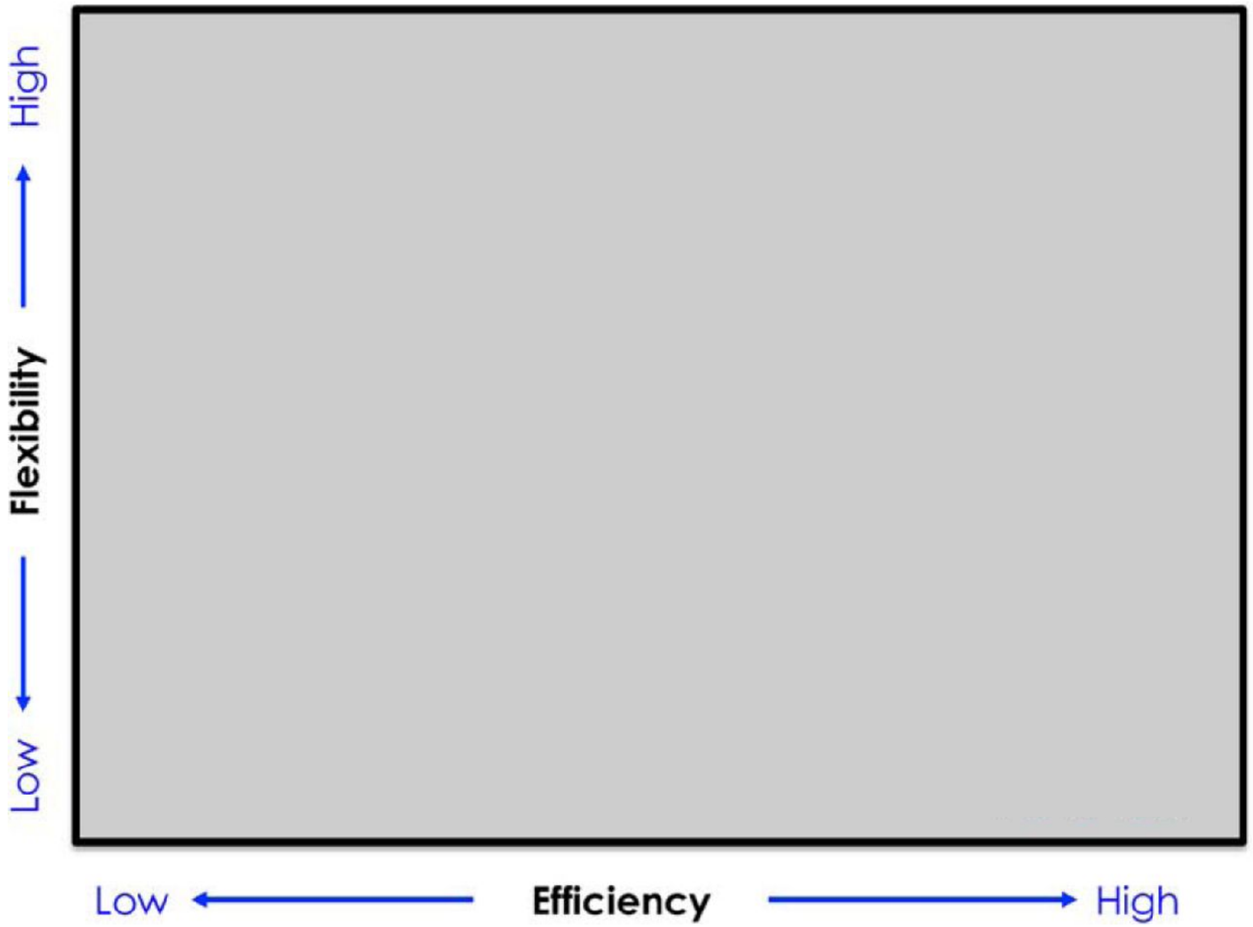
How is the model used?

- Use simulated experiences to augment direct RL (i.e., learning from real experiences)
- Model-free methods (e.g., actor-critic) can also be combined with model-based learning to great effect (Dreamer)

5 minute break

Balancing flexibility and efficiency

- Model-free methods are typically more data efficient (less training examples)
  - But lack flexibility to changes in the environment
- Model-based methods are highly flexible (local changes in environment lead to local changes in model)
  - But typically requires much more data to learn
- Is there nothing in between?



Gershman (2018)

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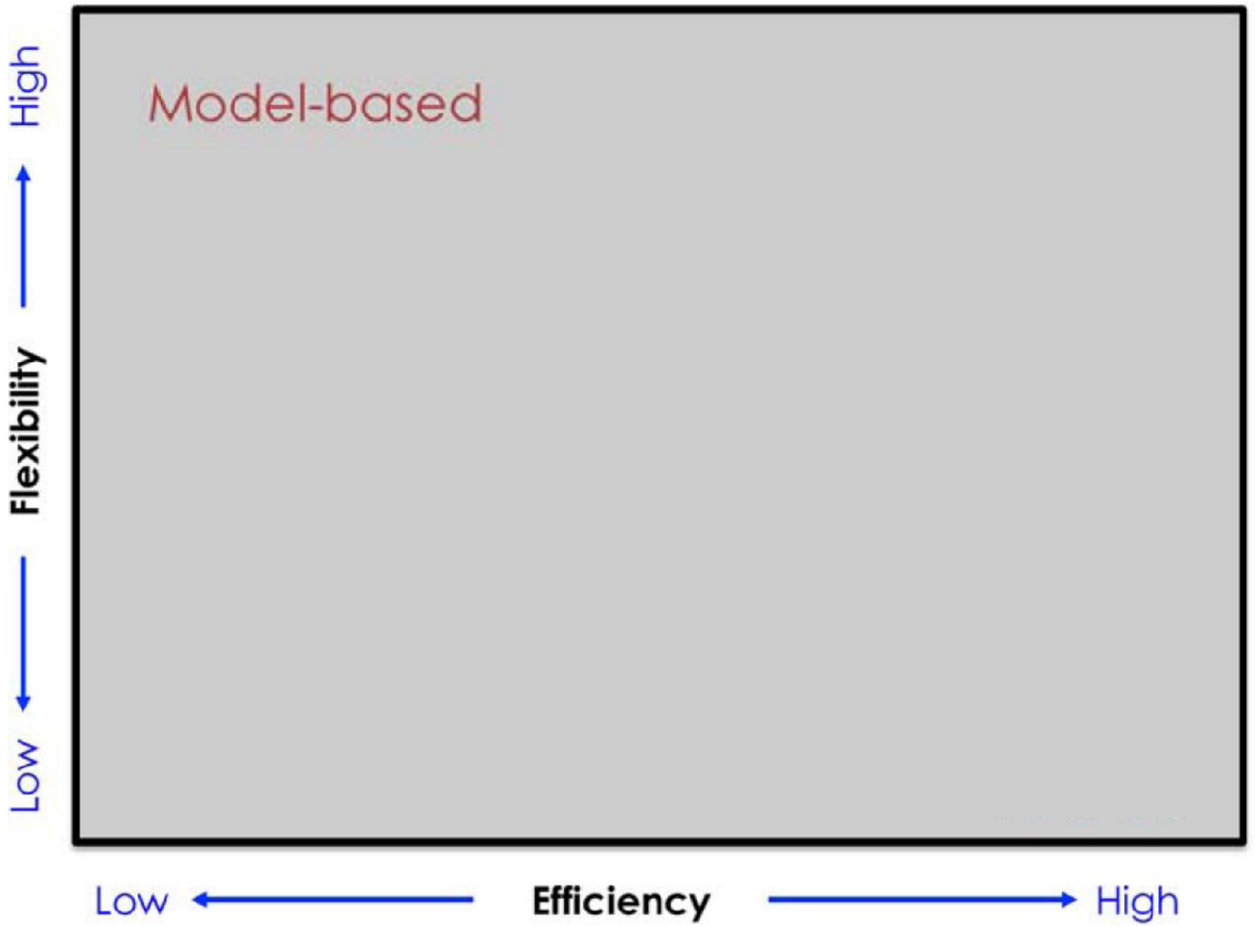

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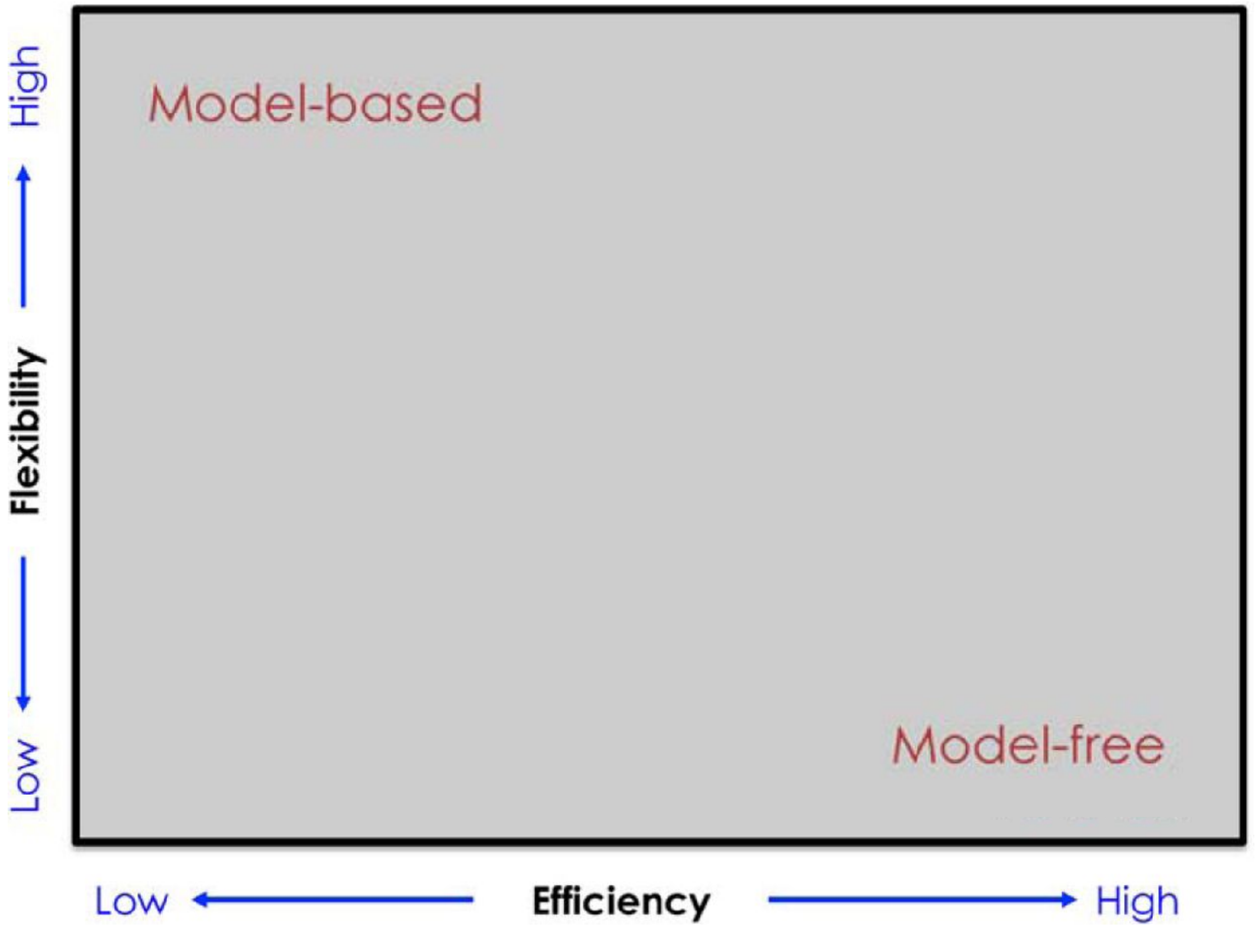

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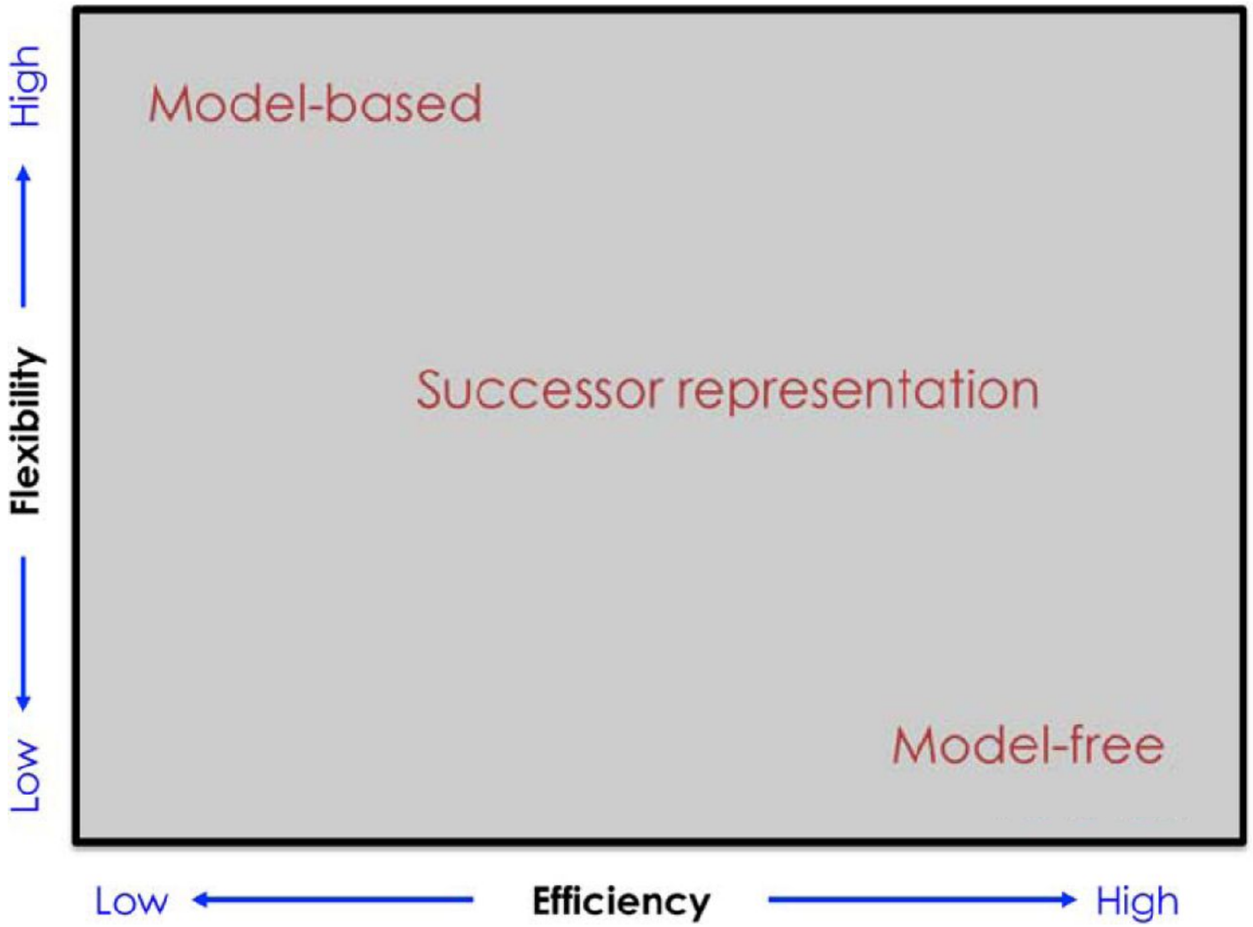
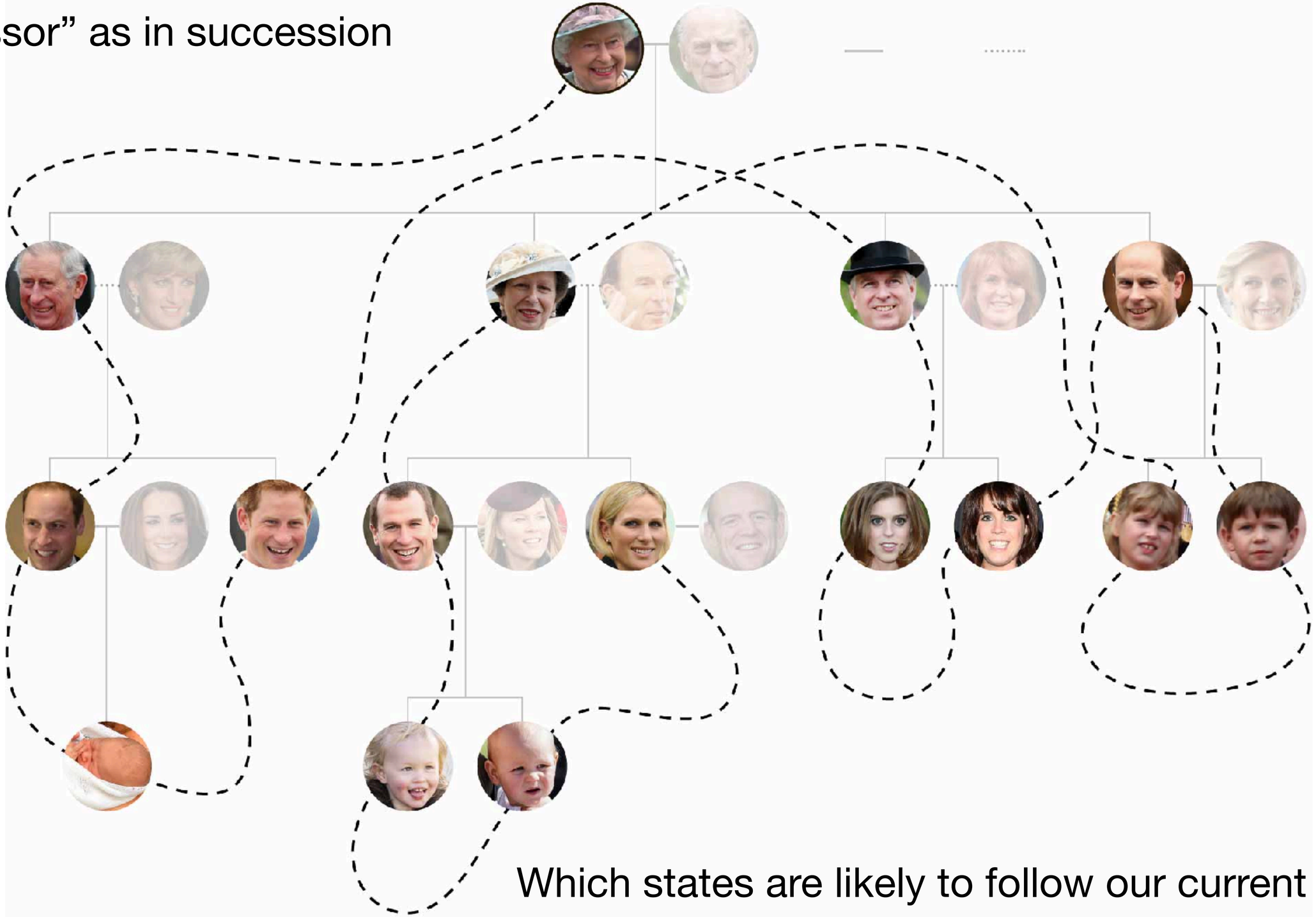


Gershman (2018)

“Successor” as in succession



Which states are likely to follow our current state?

SR as a decomposition of the TD value function

Dayan (1993)

$$V^{\pi}(s) = \mathbb{E}_{a \sim \pi}\left[\sum_{t=0}^{\infty} \gamma^{t} r_{t}\right]$$

Value function from TD Learning

SR as a decomposition of the TD value function

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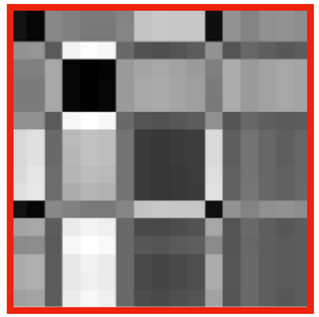
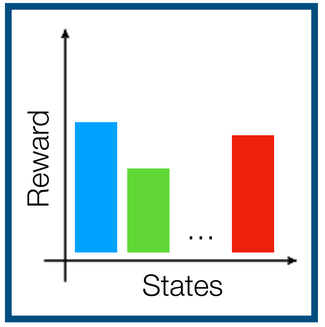
SR decomposition

Successor Representation

S by S matrix of future discounted state occupancies



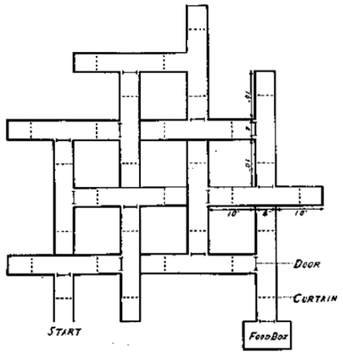


Reward Values

vector of singular rewards for each state

Successor Representation

Not just a map…



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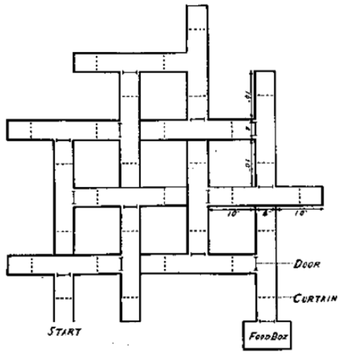
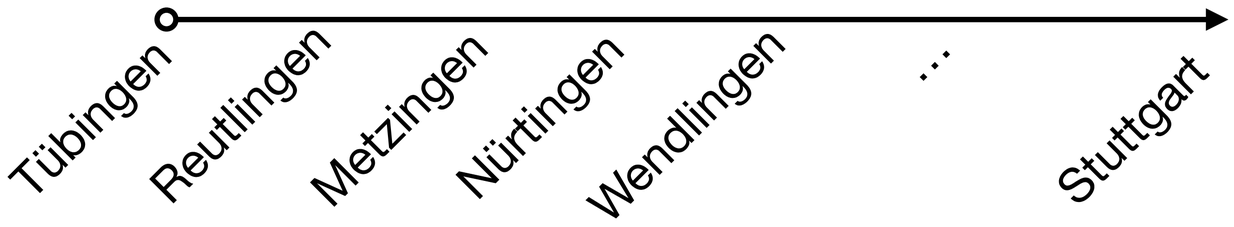


… but a goal-directed representation about which states are likely to encountered given a policy



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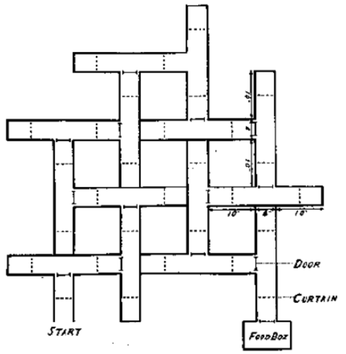

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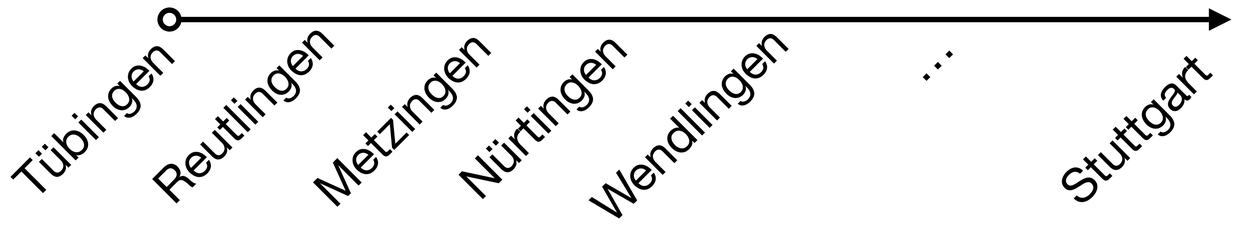

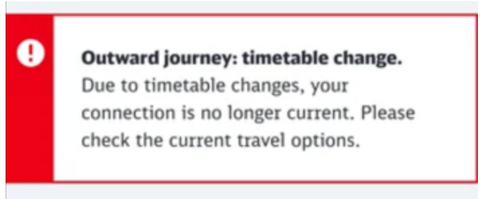

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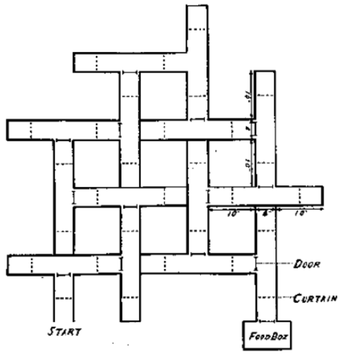

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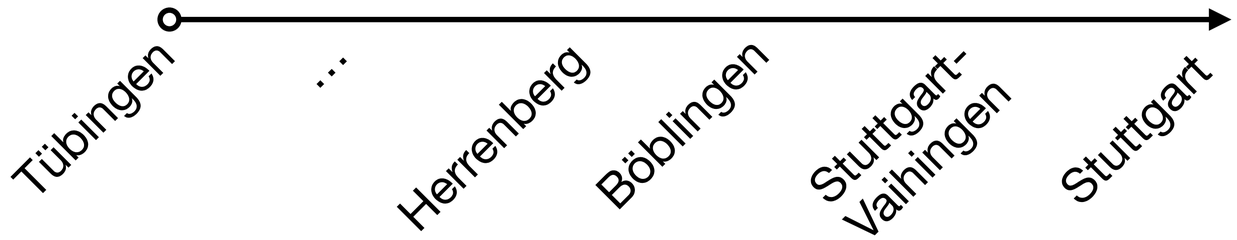

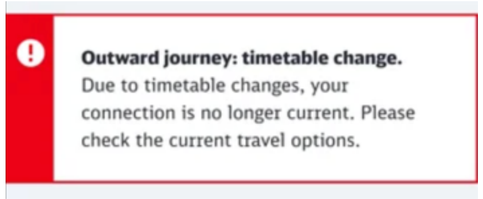

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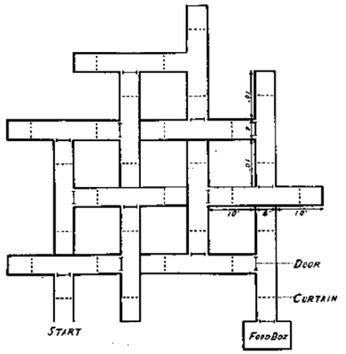

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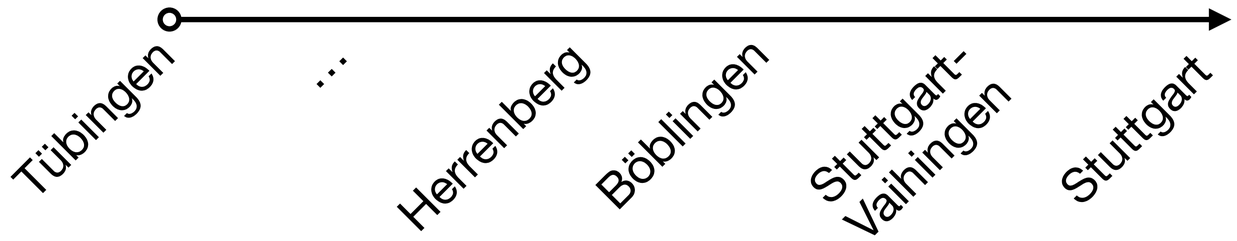

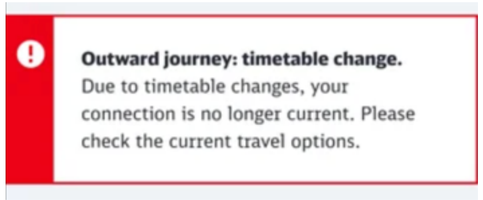

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where $\delta(*)$ is the Kronecker delta and equal to 1 when the argument is true, and 0 otherwise

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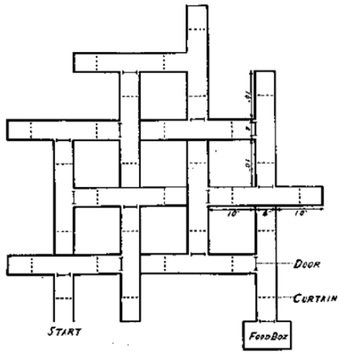

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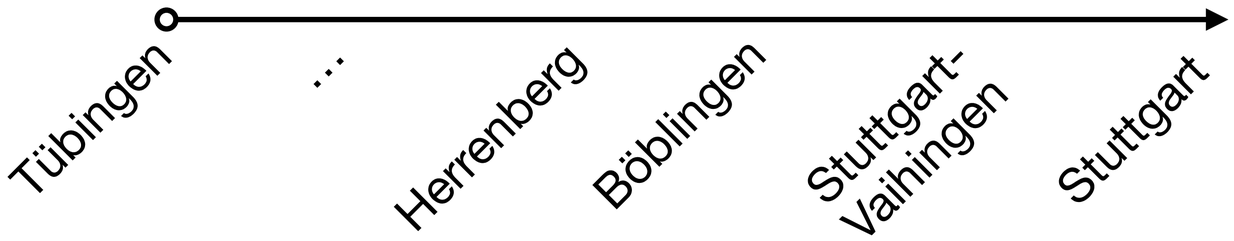

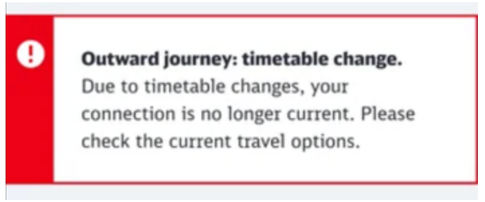

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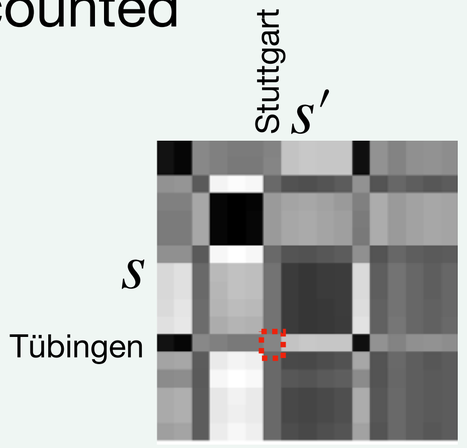

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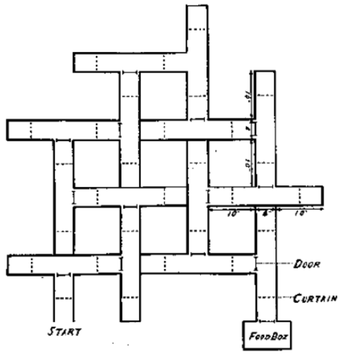

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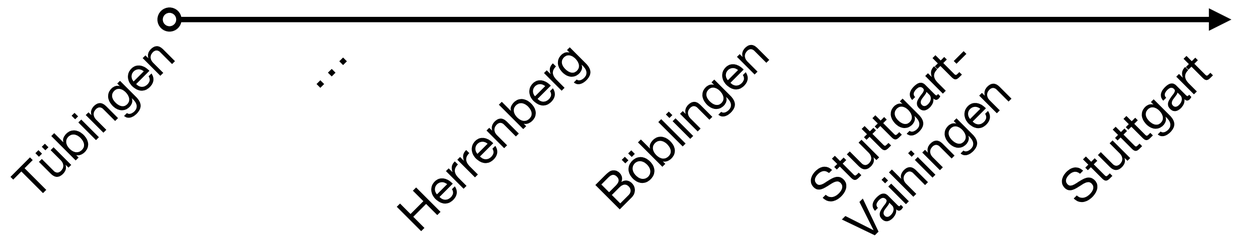

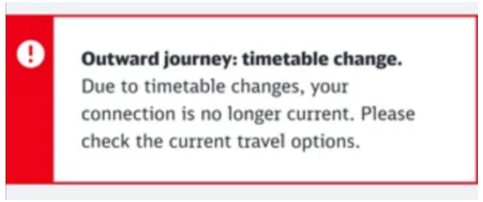

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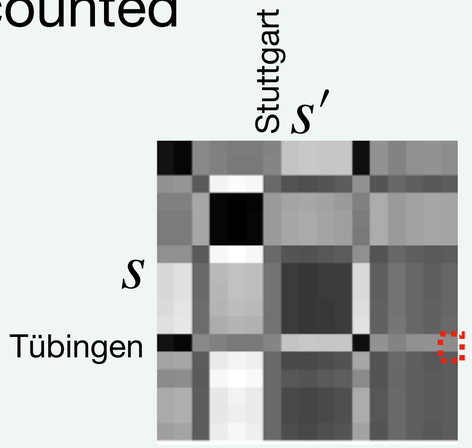

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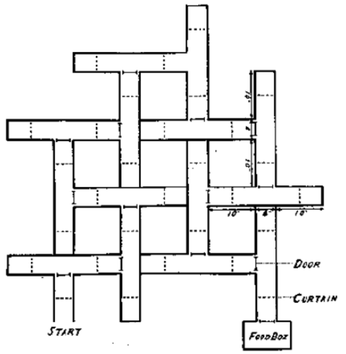

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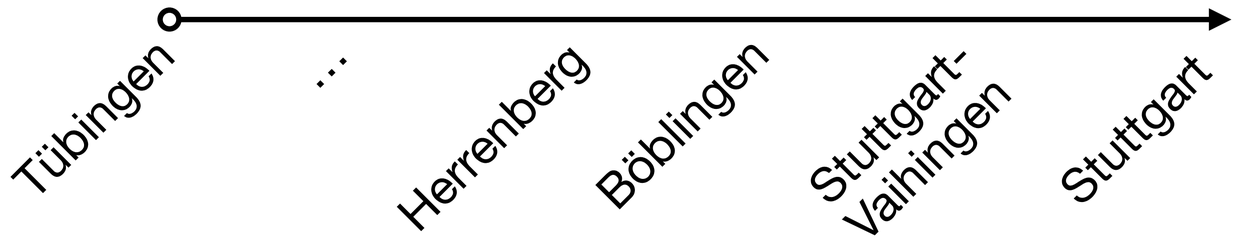

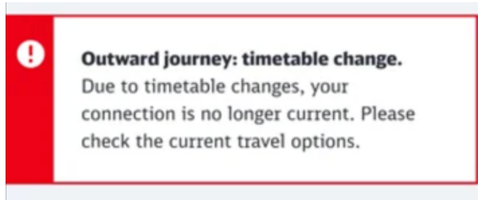

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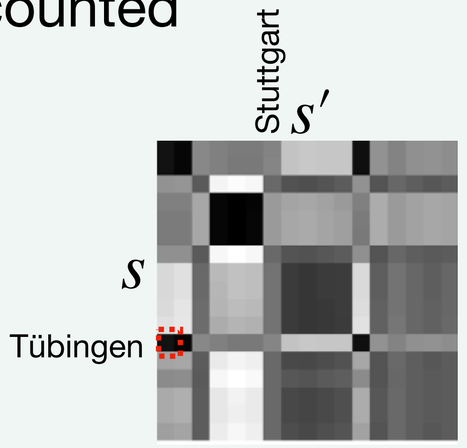

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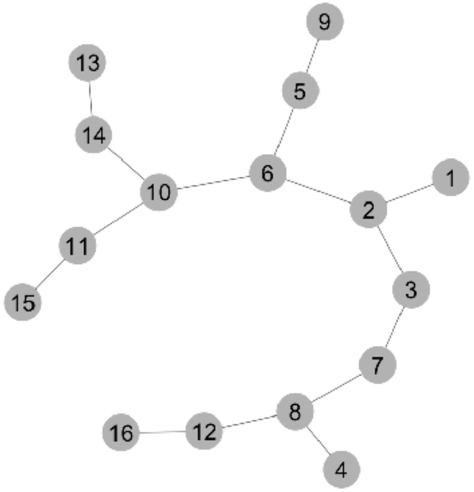
Computing the Successor Representation (off-policy)

If the state space is fully known, we can compute the SR in closed form:



$$M(s, s') = \sum_{t=0}^{\infty} \gamma^t T^t = (I - \gamma T)^{-1}$$

I is the identity matrix, γ is the temporal discount factor

T is the transition matrix under a policy: $T(s, s') = \sum_a \pi(a \mid s) P(s' \mid s, a)$

A further simplifcation that is often used is to assume a random policy, allowsing us to define T using the degree (D) and adjacency (A) matrices

$$T = D^{-1}A$$

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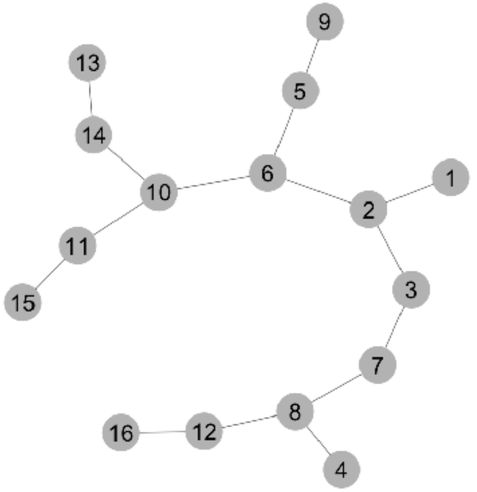

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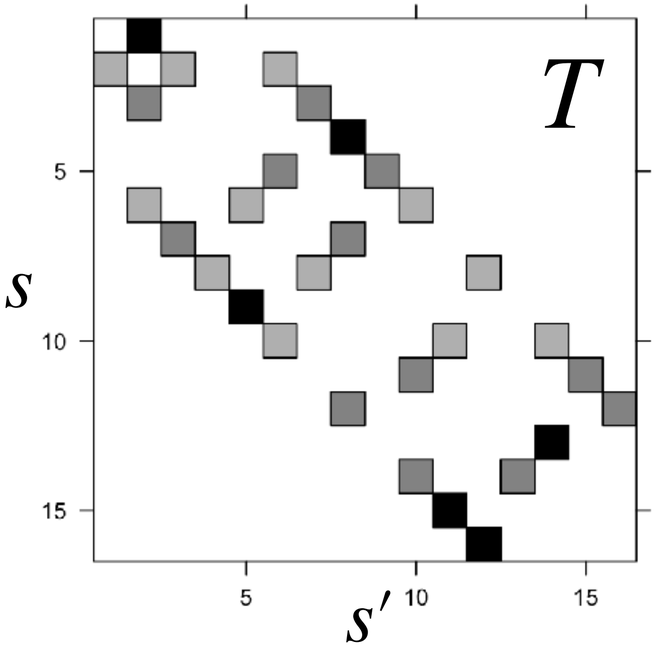

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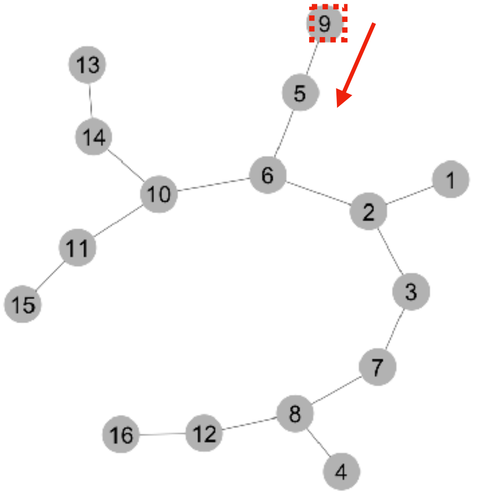

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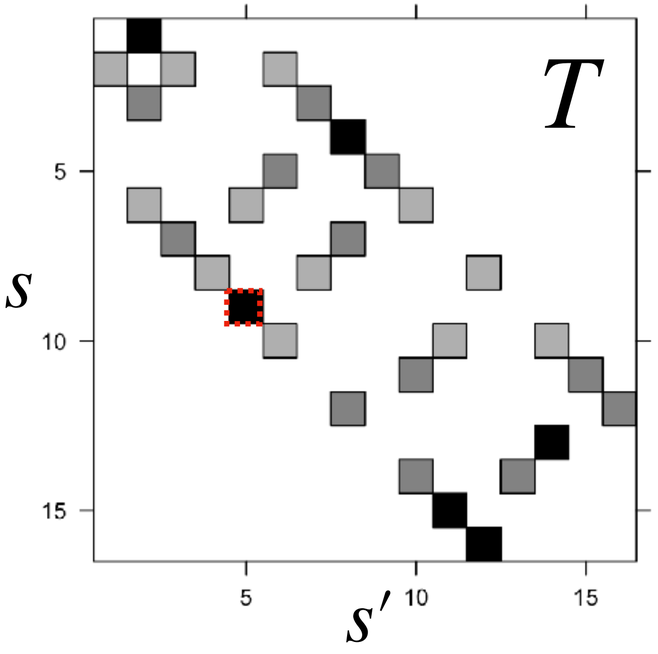

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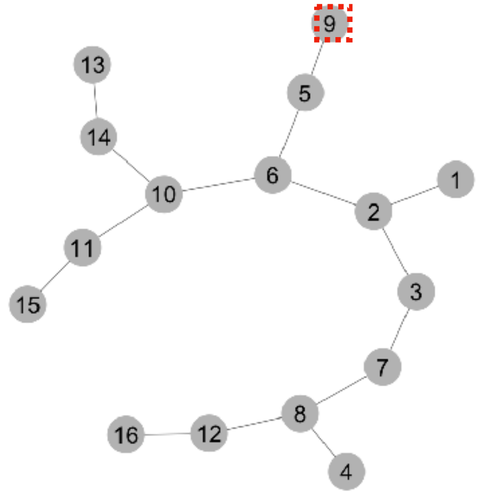
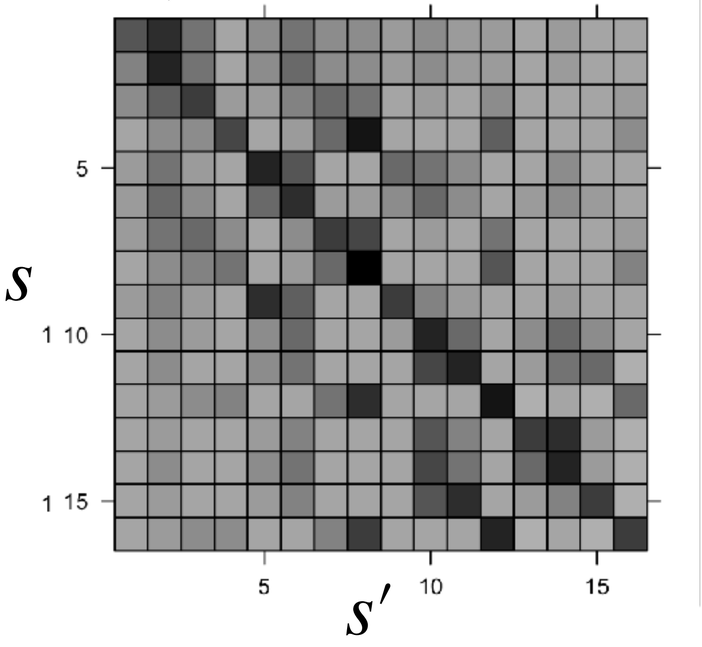


$M_{\gamma=.9}(s, s')$



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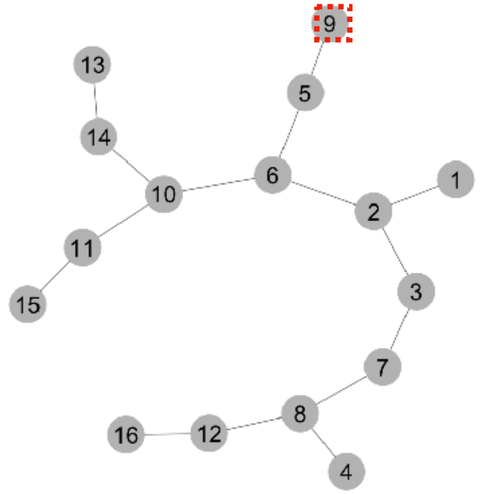
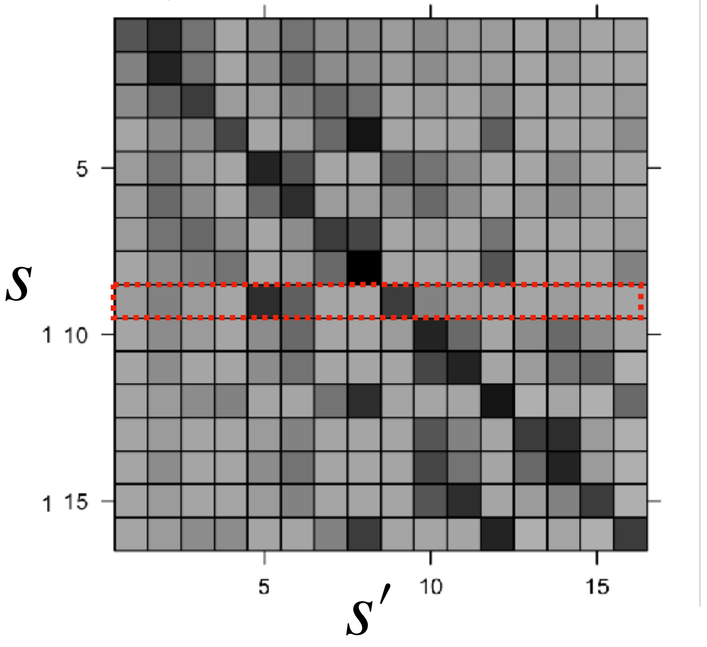
If the state space is fully known, we can compute the SR in closed form:

$$M(s, s') = \sum_{t=0}^{\infty} \gamma^t T^t = (I - \gamma T)^{-1}$$



$M_{\gamma=.9}(s, s')$



I is the identity matrix, γ is the temporal discount factor

T is the transition matrix under a policy: $T(s, s') = \sum_a \pi(a \mid s) P(s' \mid s, a)$

A further simplifcation that is often used is to assume a random policy, allowsing us to define T using the degree (D) and adjacency (A) matrices

$$T = D^{-1}A$$

Computing the Successor Representation (on policy)

If the state space is not known, we can compute the SR using the delta-rule:

$$\hat{M}_{t+1}(s_t, s') = \hat{M}_t(s_t, s') + \alpha \left[\delta(s_t = s') + \gamma \hat{M}_{t+1}(s_t, s') - \hat{M}_t(s_t, s') \right]$$

where α is the learning rate and δ is the kronecker delta $\delta = 1$ when true, 0 otherwise

- This update is identical to the temporal difference learning rule for value functions

- The successor representation is updated based on the *successor* prediction error instead of the *reward* prediction error

Computing the Successor Representation (on policy)

Russek et al., (2017)

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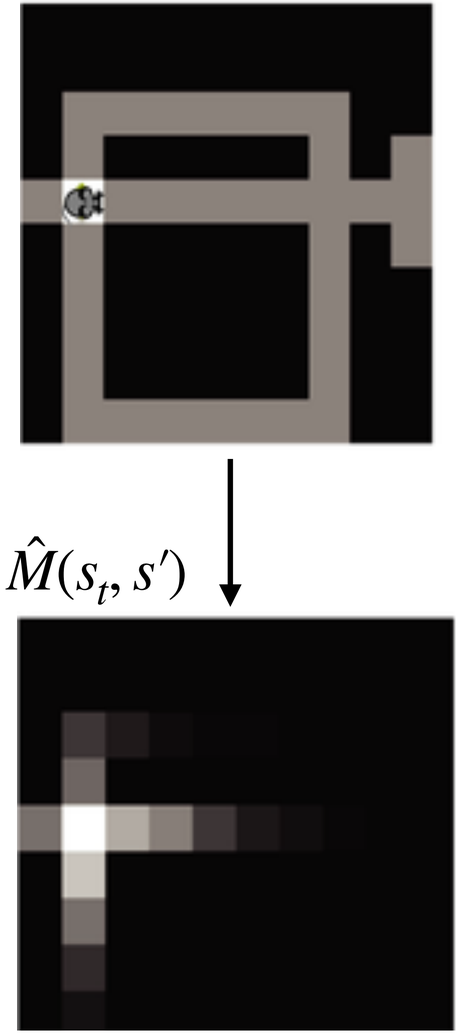

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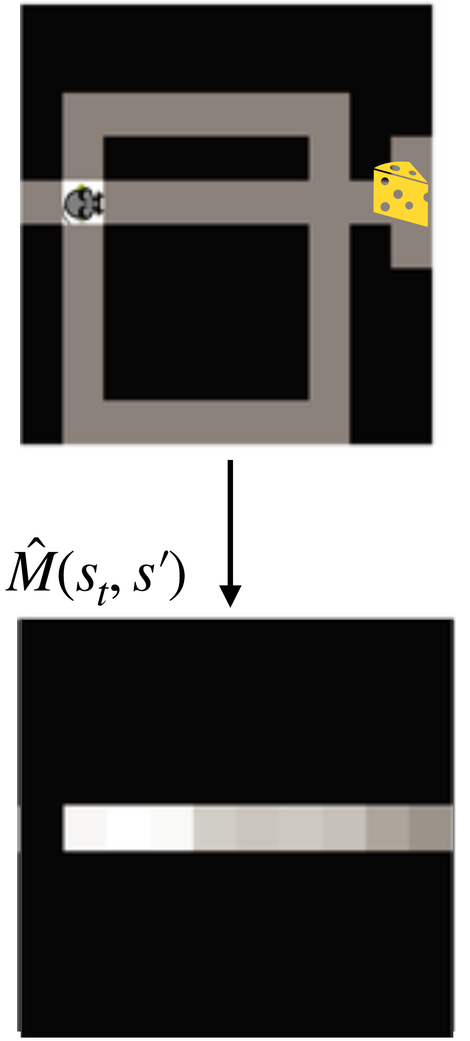
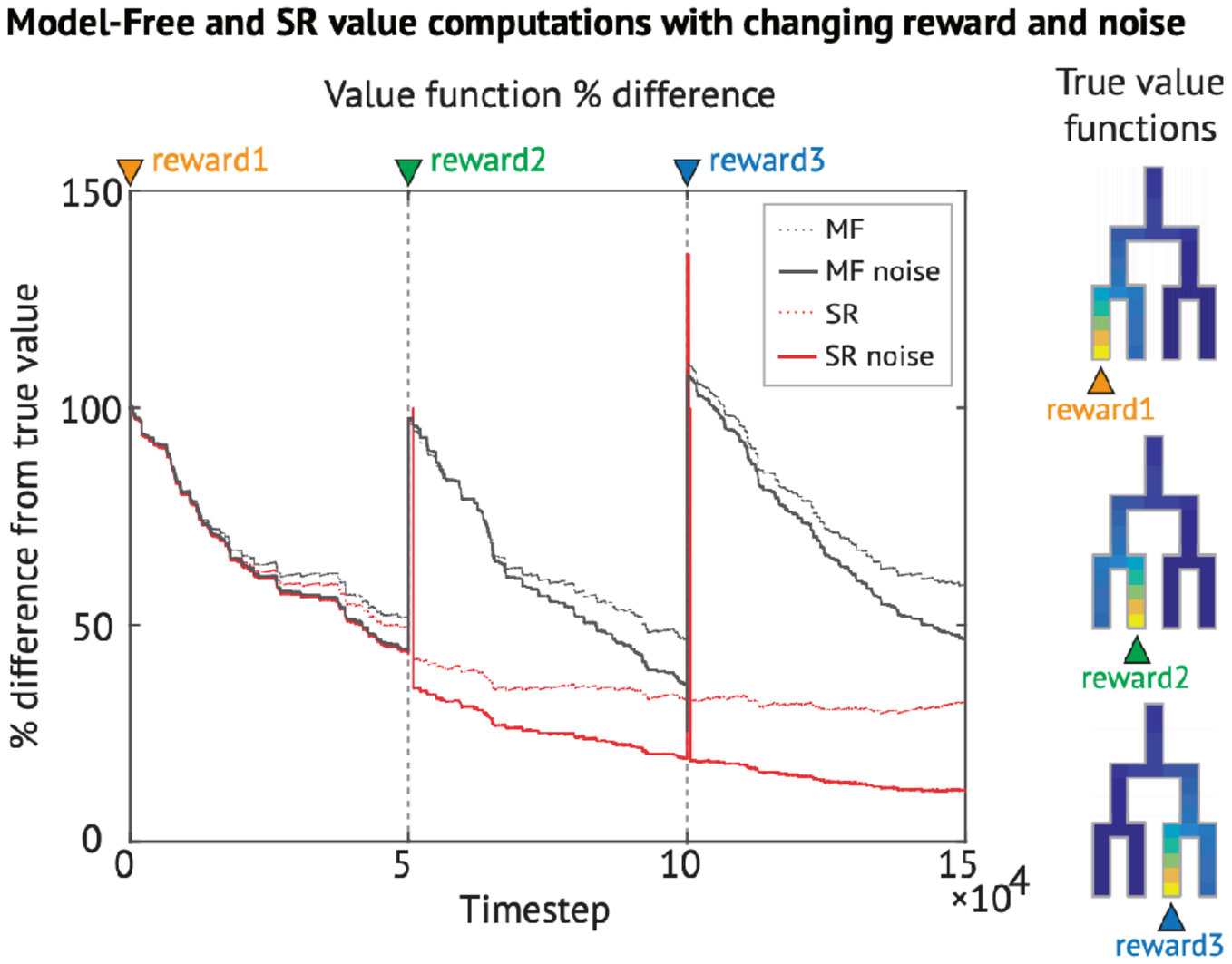


SR generalizes for changes in reward

- If the location of rewards change, only the $r(s')$ part needs to be re-learned while $M(s, s')$ remains the same

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

- This leads to faster generalization to changes in the environment

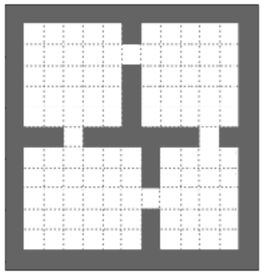


Stachenfeld, Botvinick & Gershman (2017)

The Eigenvalues of the SR

- Eigenvectors capture different dimensions of variability
  - $M = V\Lambda V^{-1}$ where $v_i \in V$ are Eigenvectors and $\lambda_i \in \Lambda$ are the Eigenvalues

Environment



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The Eigenvalues of the SR

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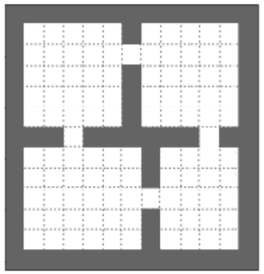

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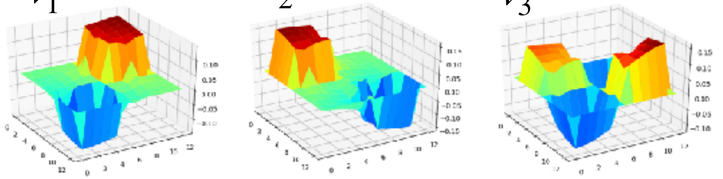
Eigenvectors

v_1 v_2 v_3



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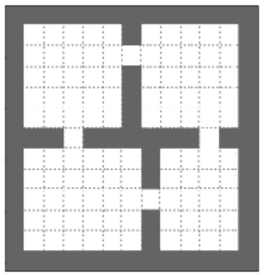

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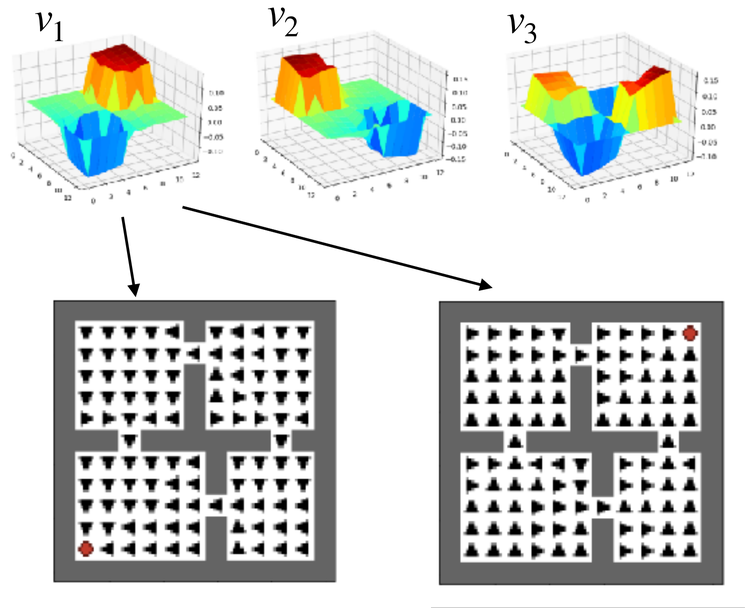

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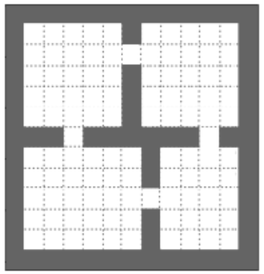

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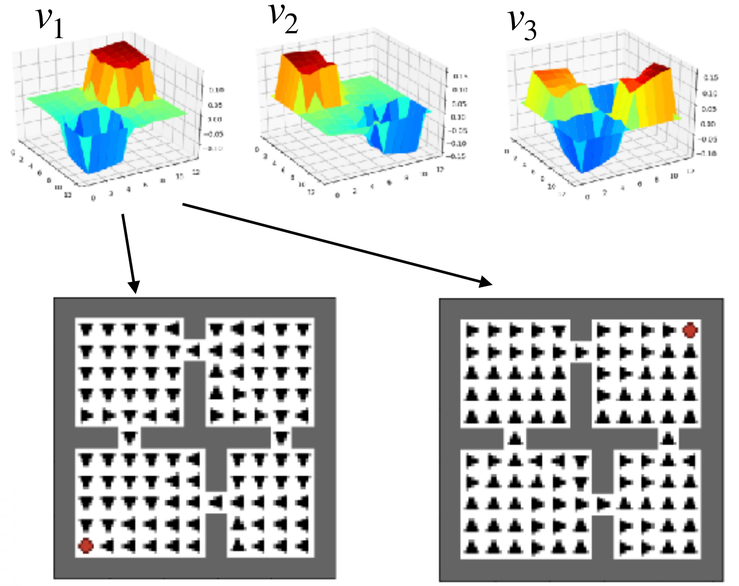

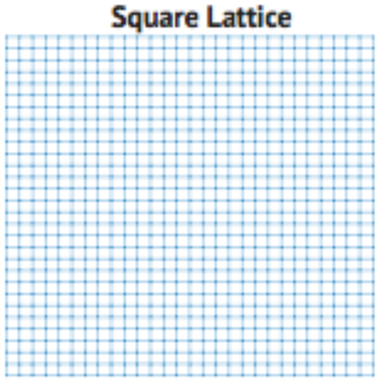

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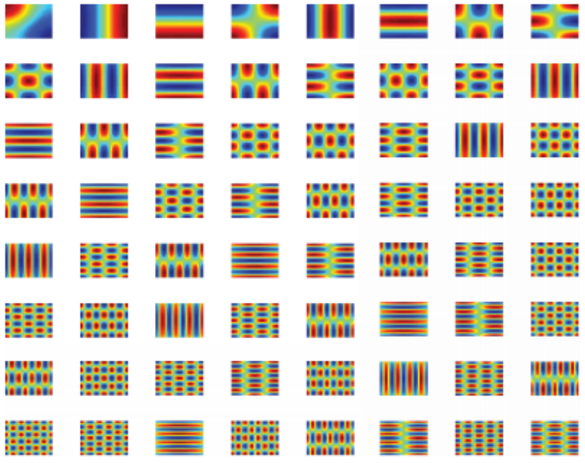

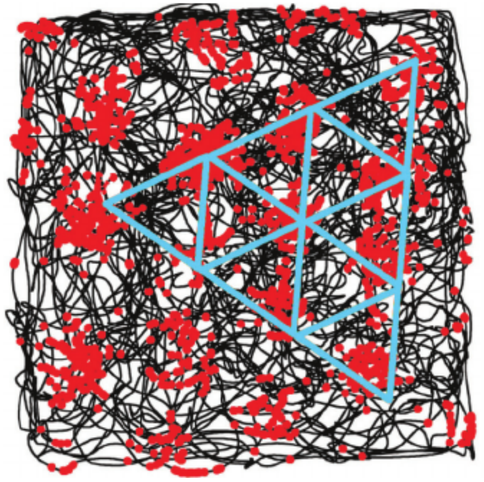

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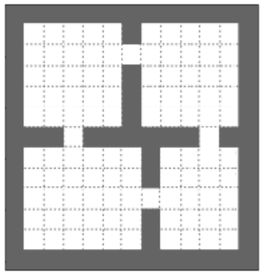

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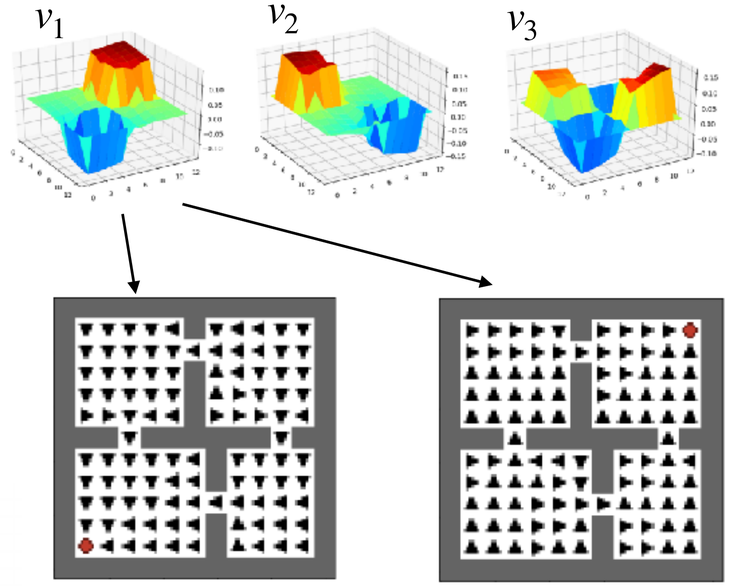

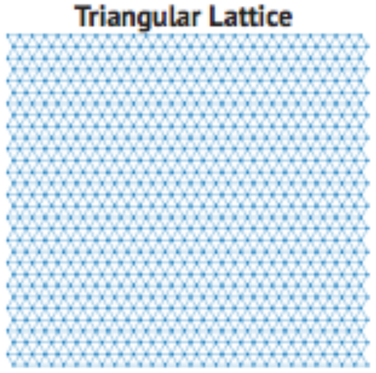

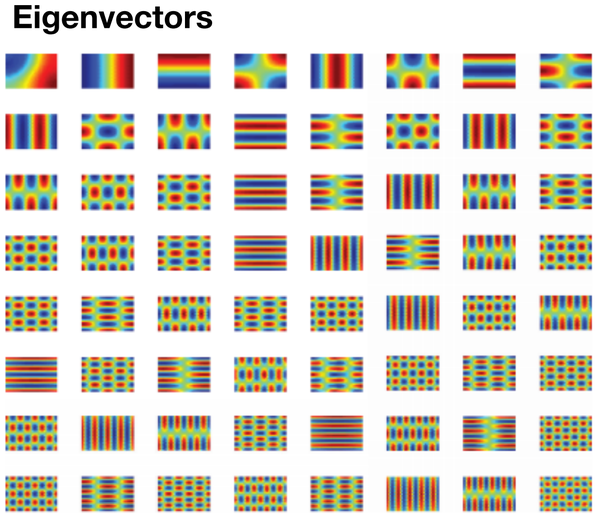

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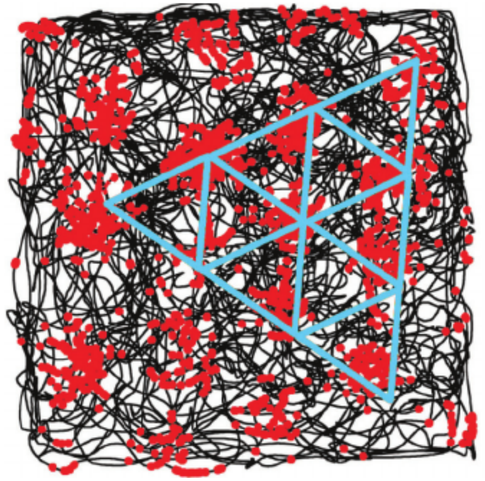

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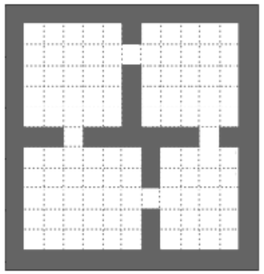

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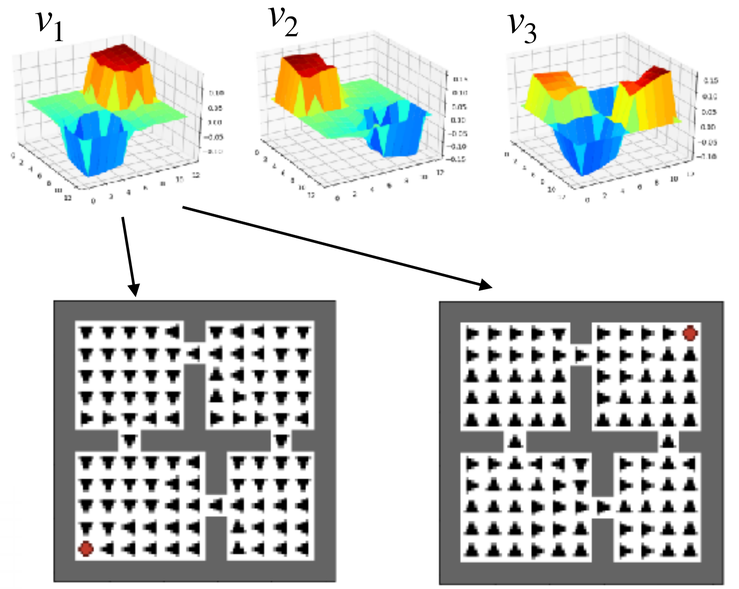

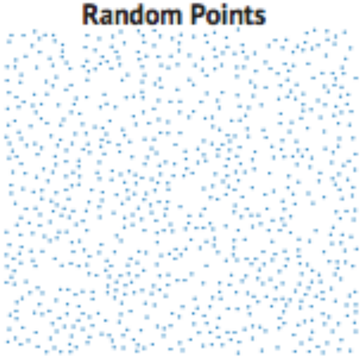

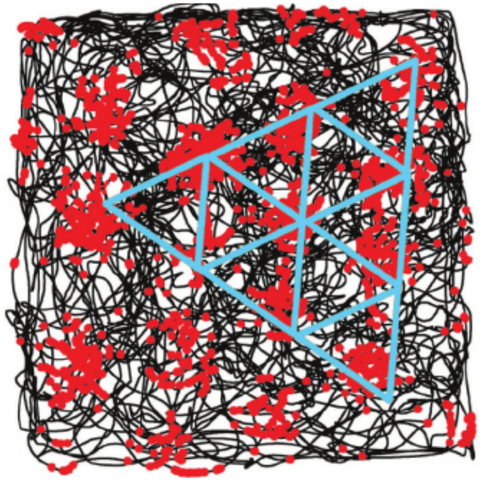

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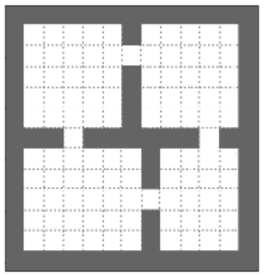

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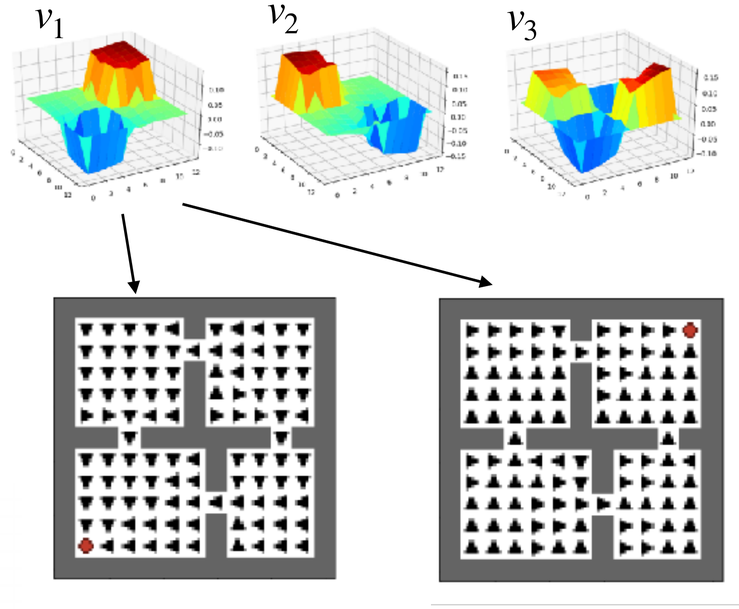

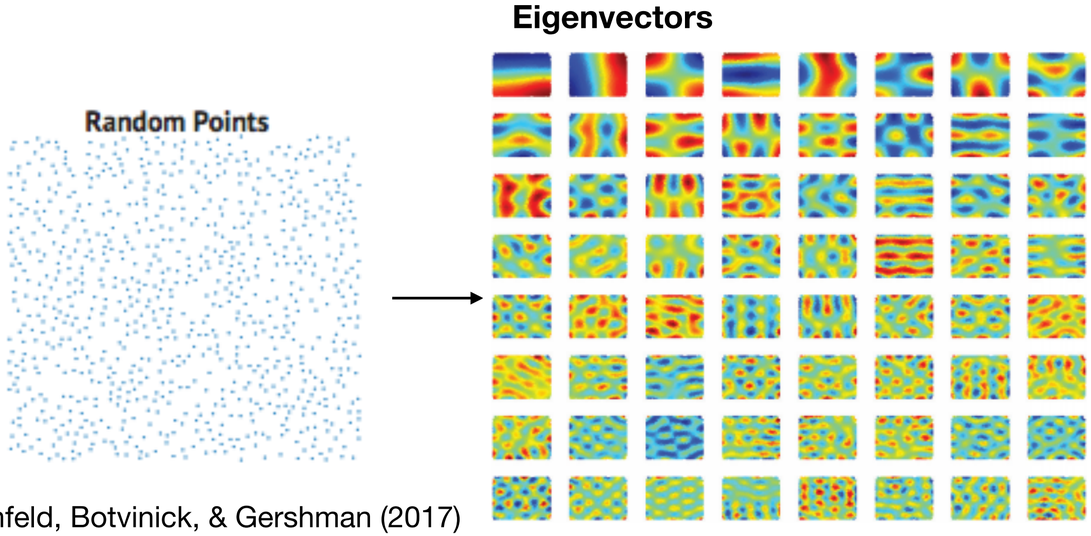

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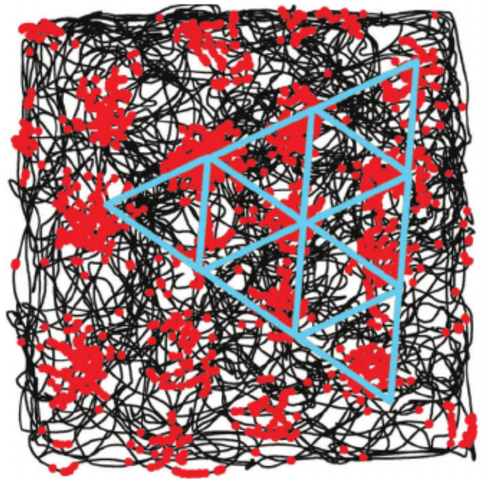
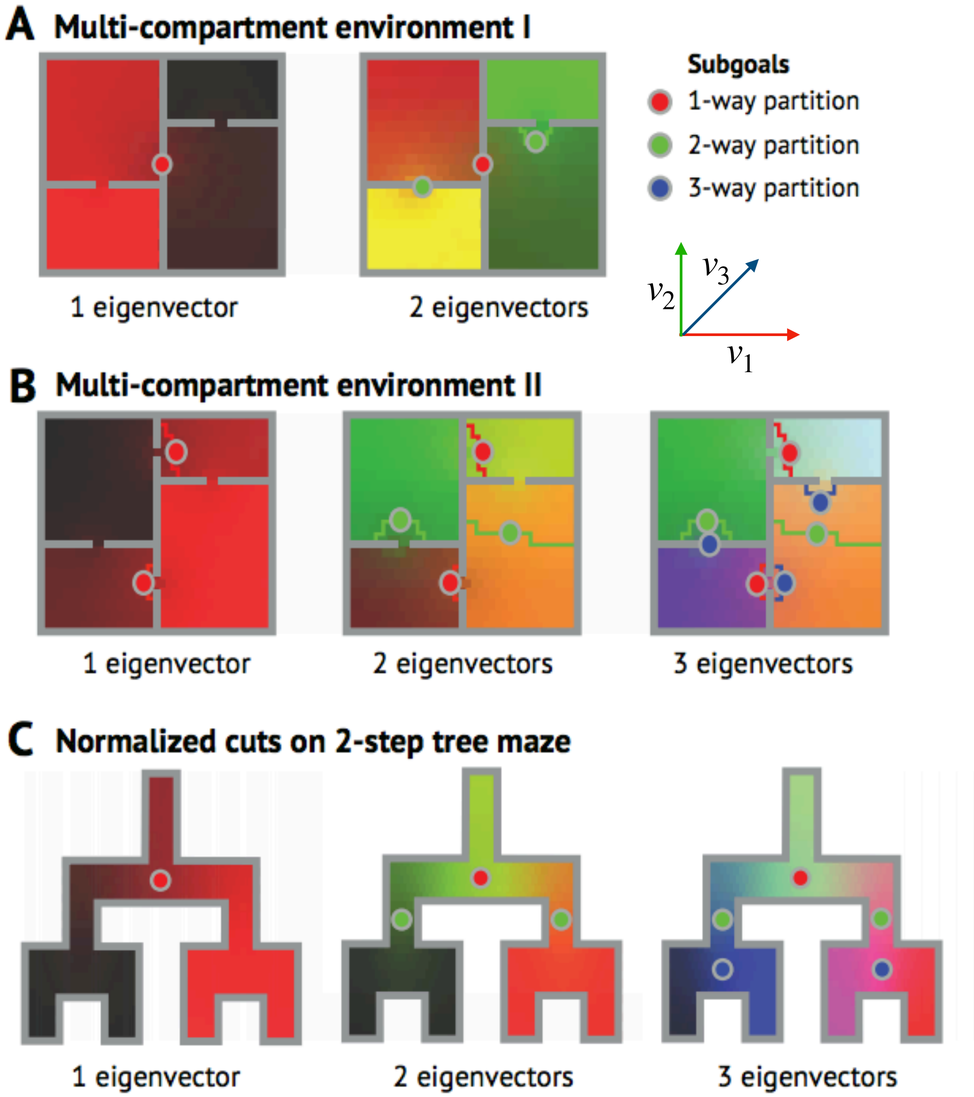


** Not unique to the SR, but any similarity metric that captures transition structure*

SR naturally identifies subgoals

- Eigenvectors capture subgoals (i.e., compartments in the environment)

Stachenfeld, Botvinick, & Gershman (*NatNeuro* 2017)



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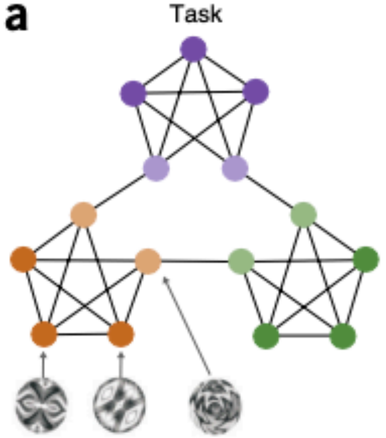
Schapiro *et al.* (2015)



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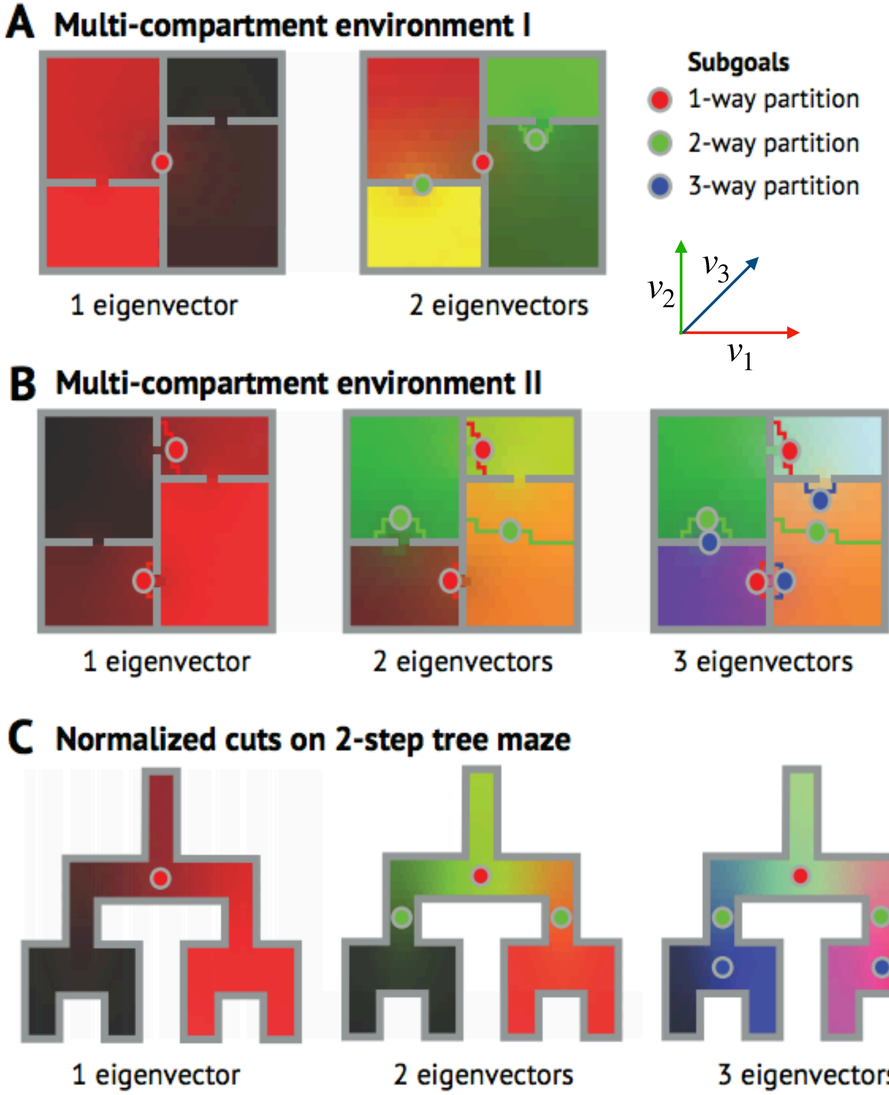

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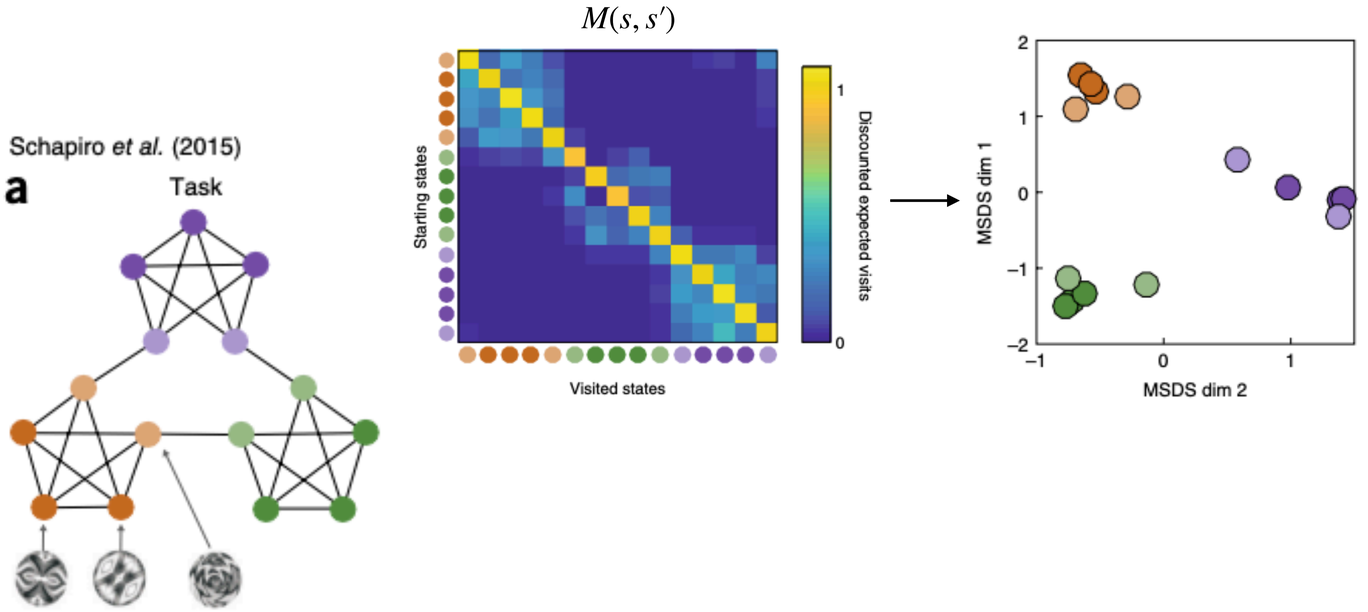

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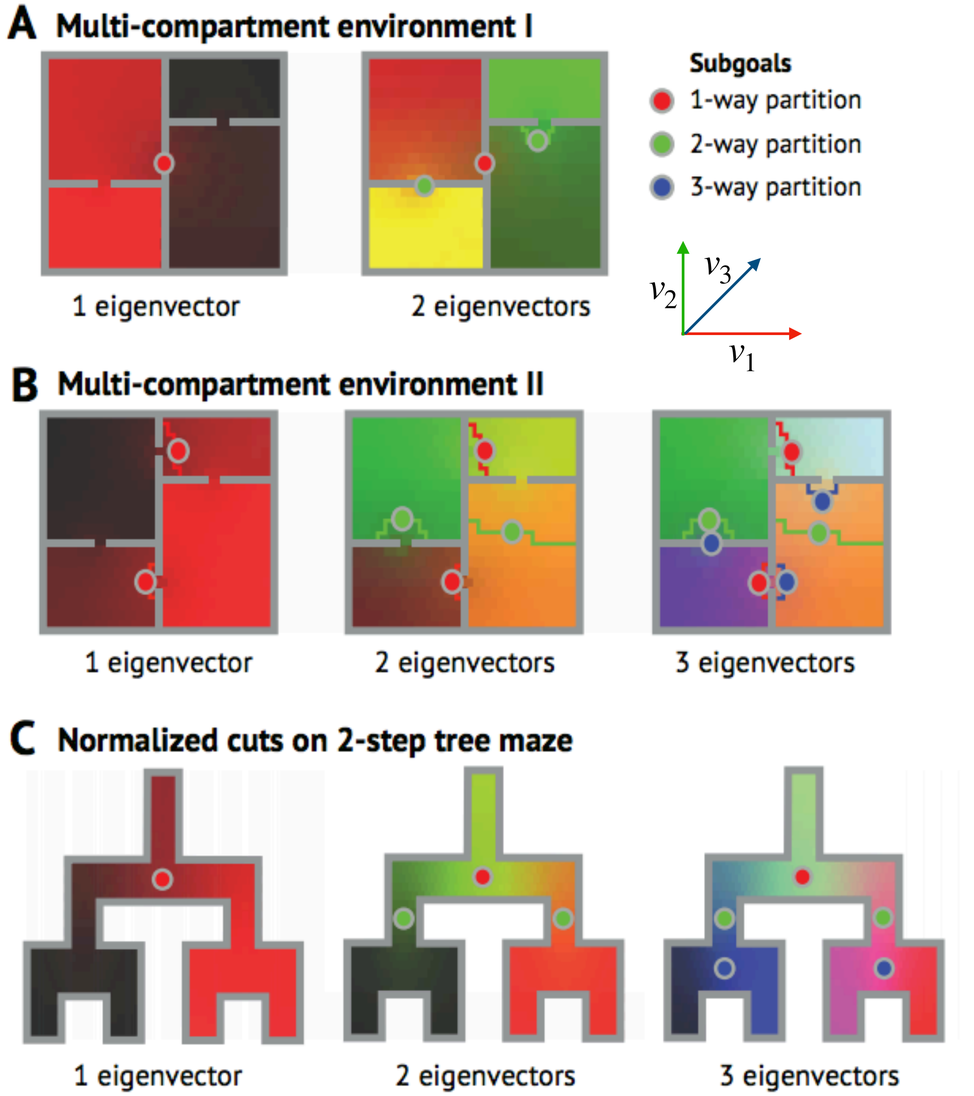

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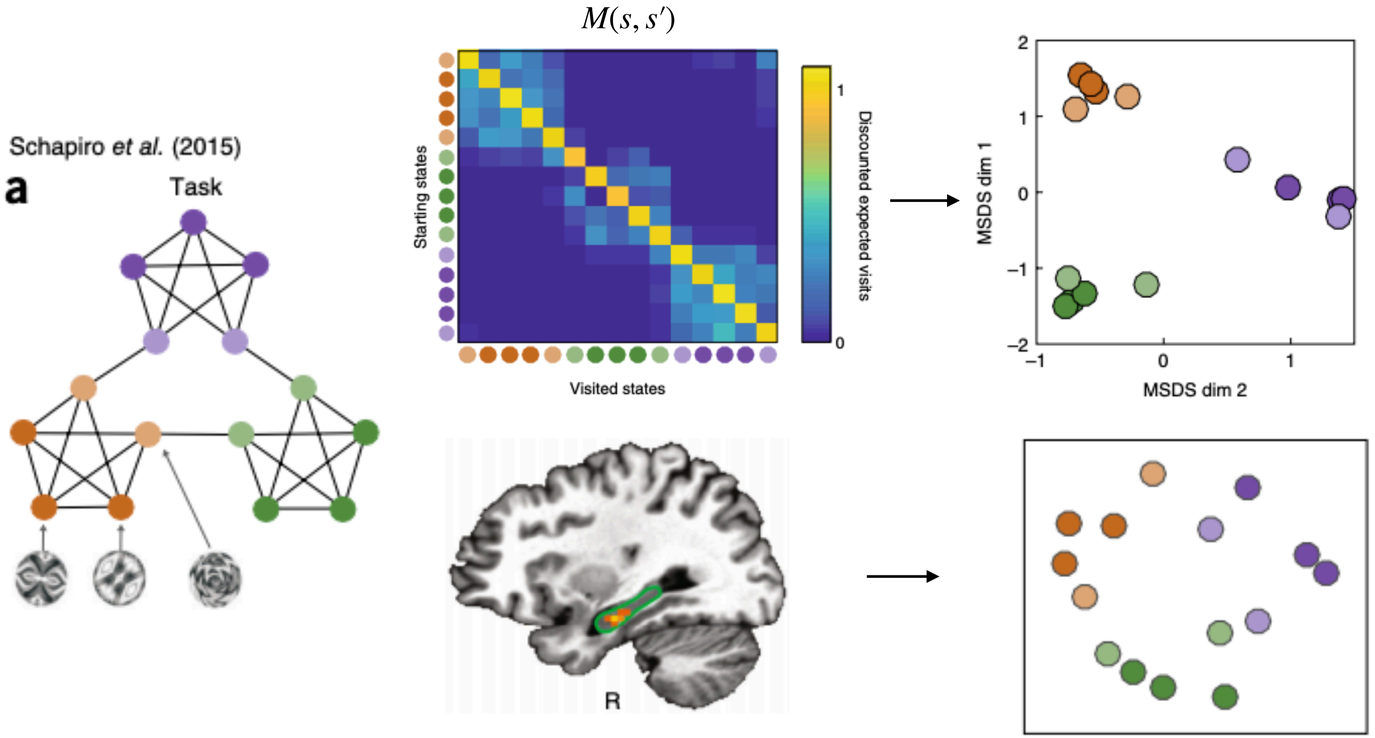

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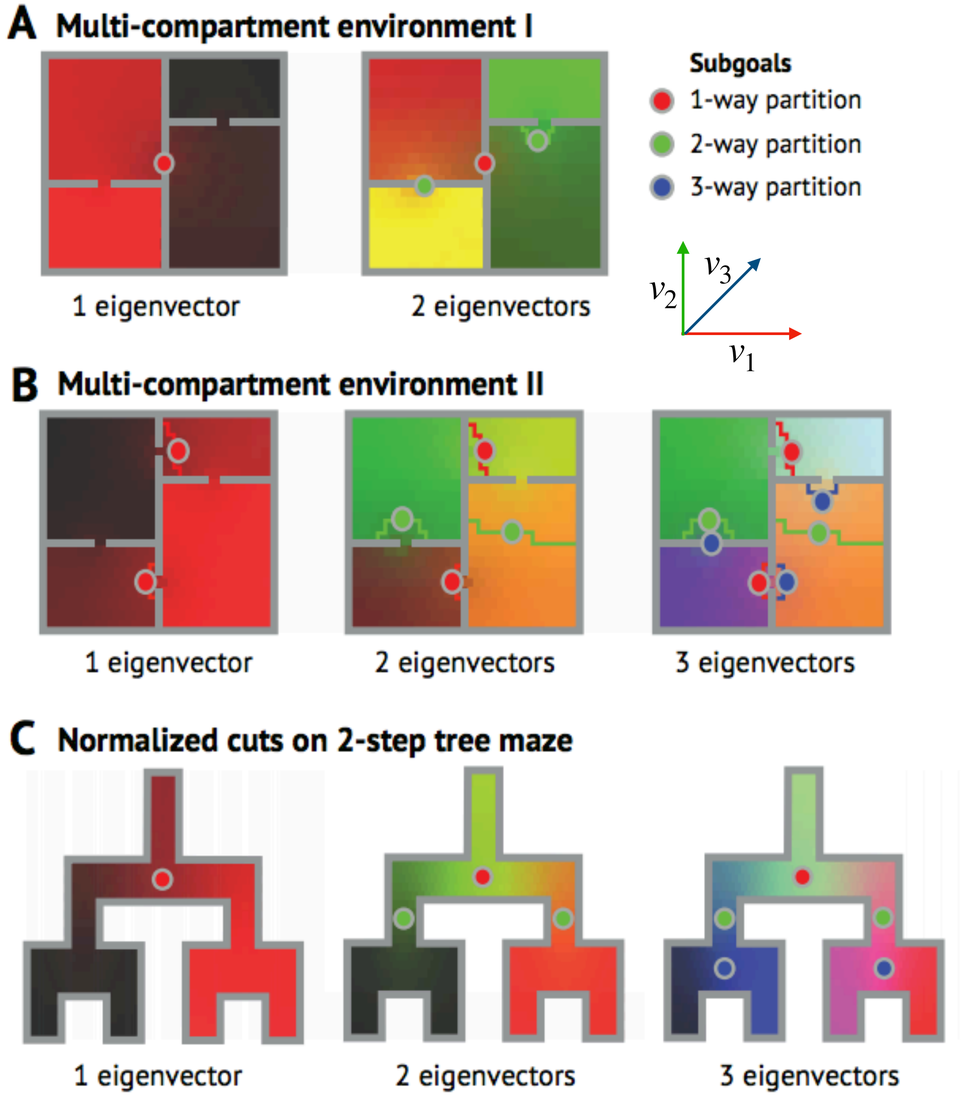
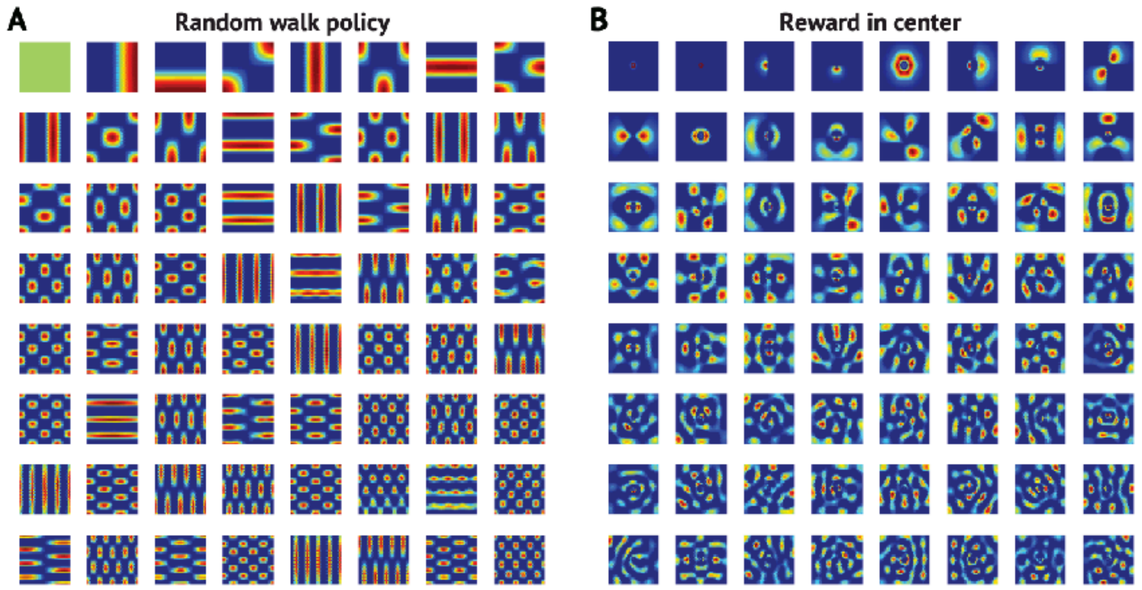


SR is sensitive to policy

- SR learned under different policies learn different representations
- Under a softmax-optimal policy seeking the goal state, states become organized according to their distance from the goal
- But it also makes them less grid-like



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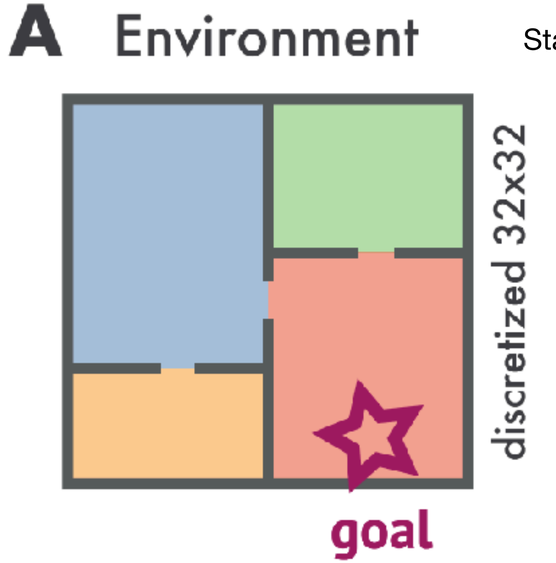
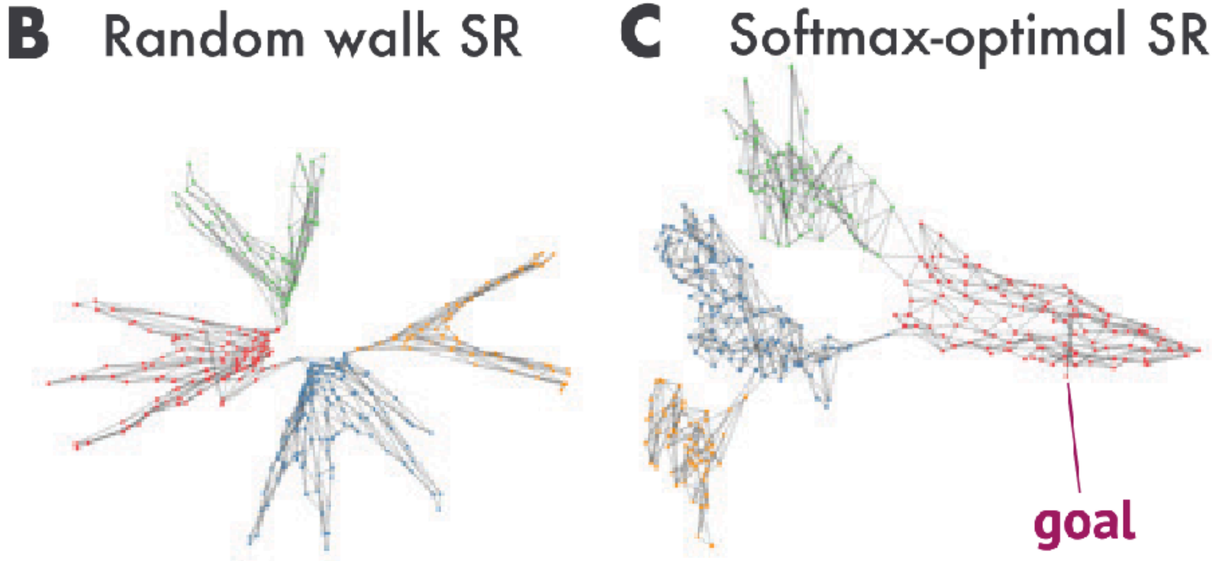


Stachenfeld (Phd thesis, 2018)

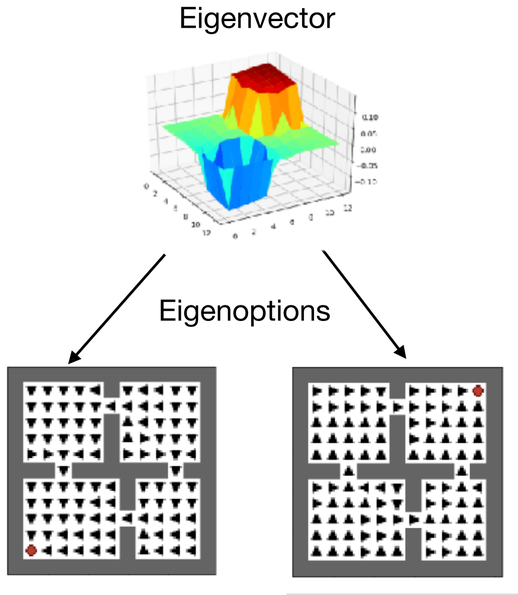


SR for option discovery

- “Options framework” in RL corresponds to learning extended sequences of actions instead of only a single action at a time
  - Options: Make coffee vs. make tea
  - Actions: move left leg, move right leg, …. move wrist 34 degrees
- SR naturally discovers *Eigenoptions*
- More recent work has identified functional sequences of actions this way

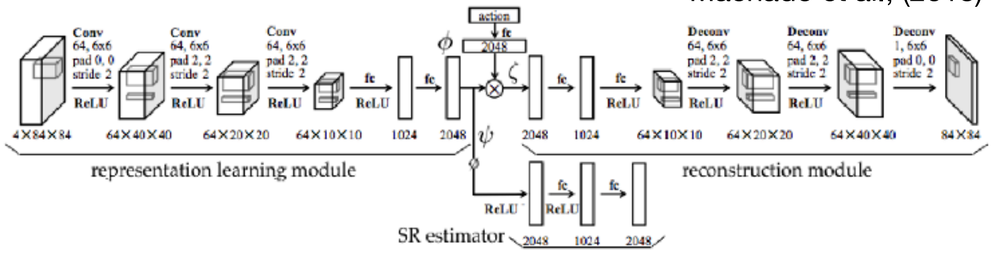
SR for option discovery

- "Options framework" in RL corresponds to learning extended sequences of actions instead of only a single action at a time
  - Options: Make coffee vs. make tea
  - Actions: move left leg, move right leg, …. move wrist 34 degrees
- SR naturally discovers *Eigenoptions*
- More recent work has identified functional sequences of actions this way



SR for option discovery

Machado et al., (2018)



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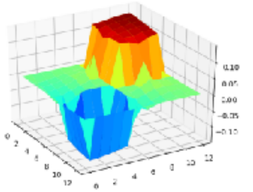
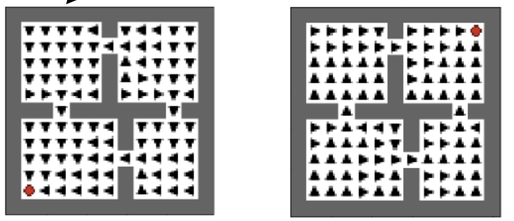
Eigenvector



Eigenoptions



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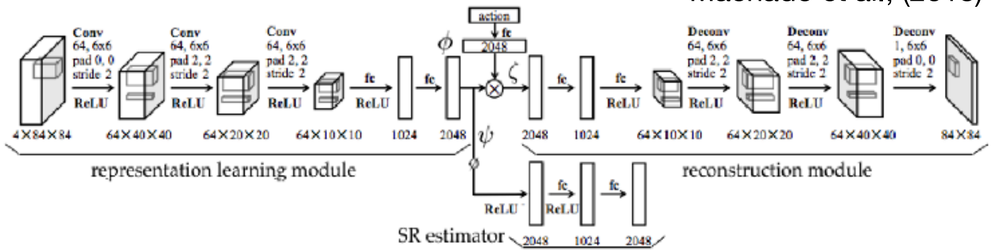

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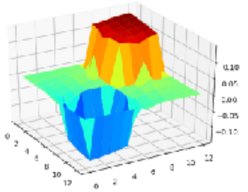

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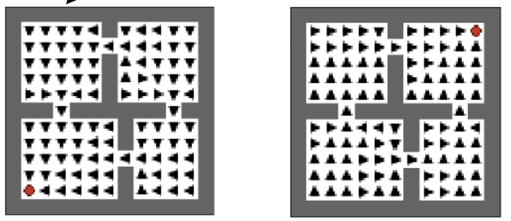
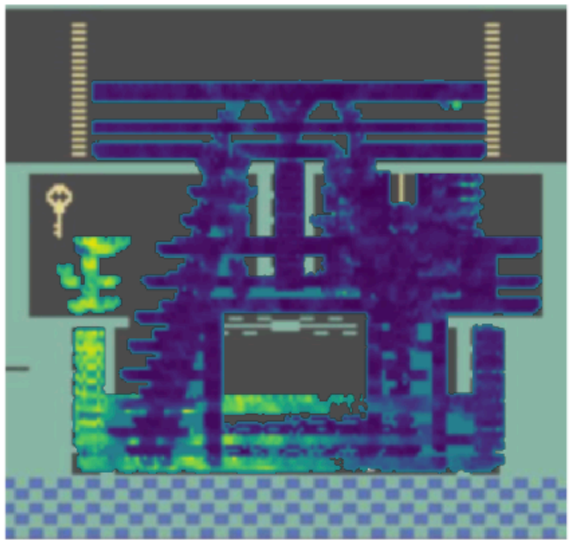
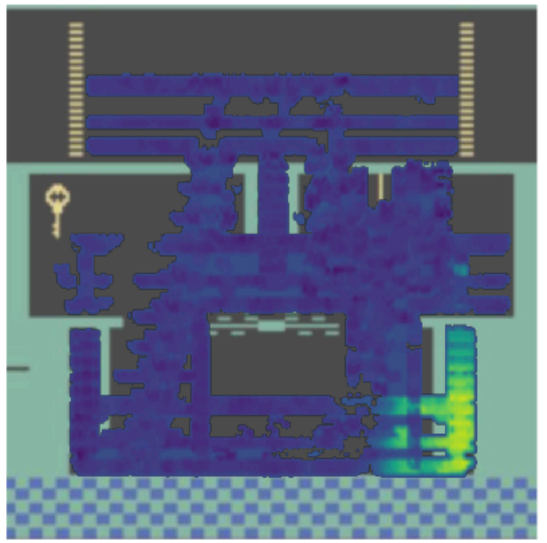


Montezuma's Revenge

Eigenfunction #1



Eigenfunction #2



Klissarov & Machado (2023)

Summary

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  - **Value-based** Deep Q-Learning
  - **Policy-based** Policy Gradient
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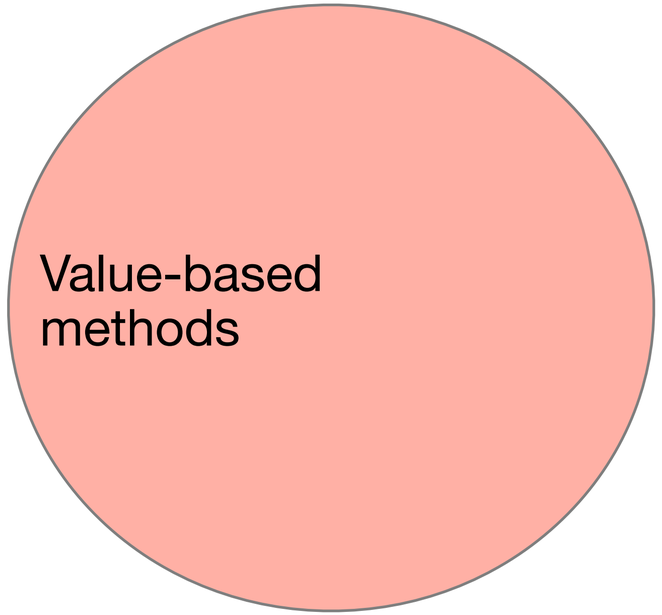

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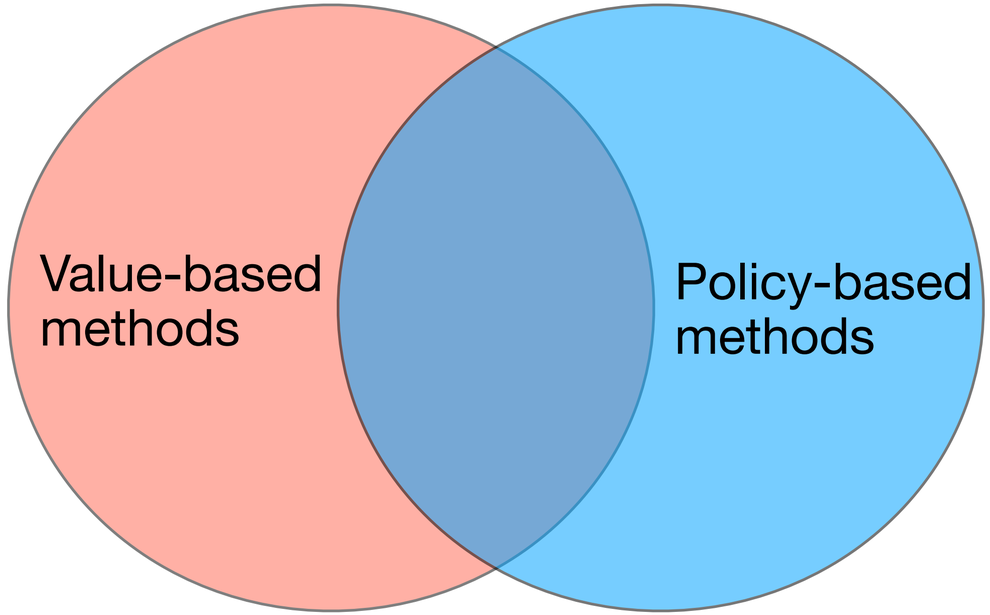

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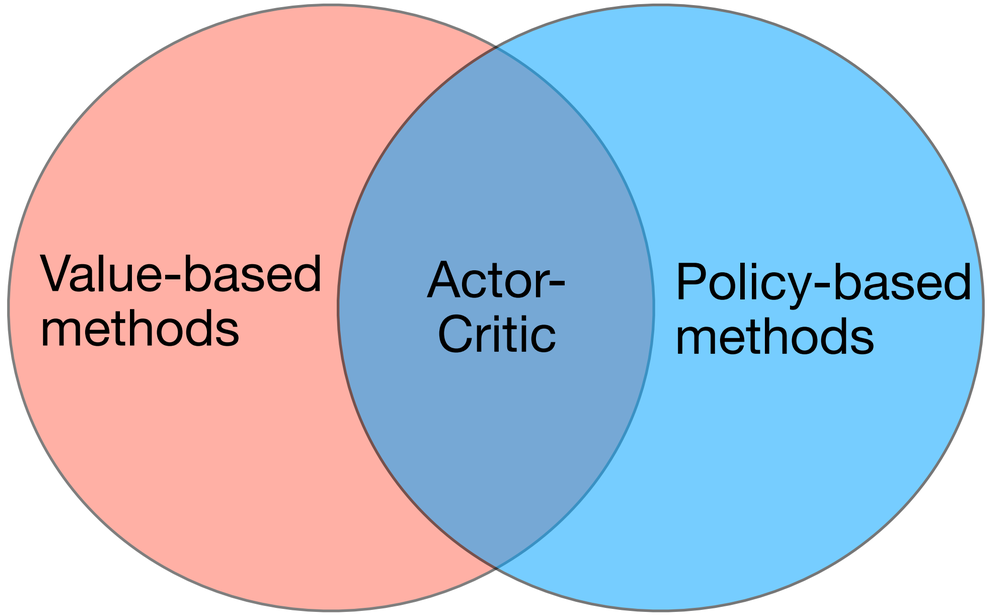

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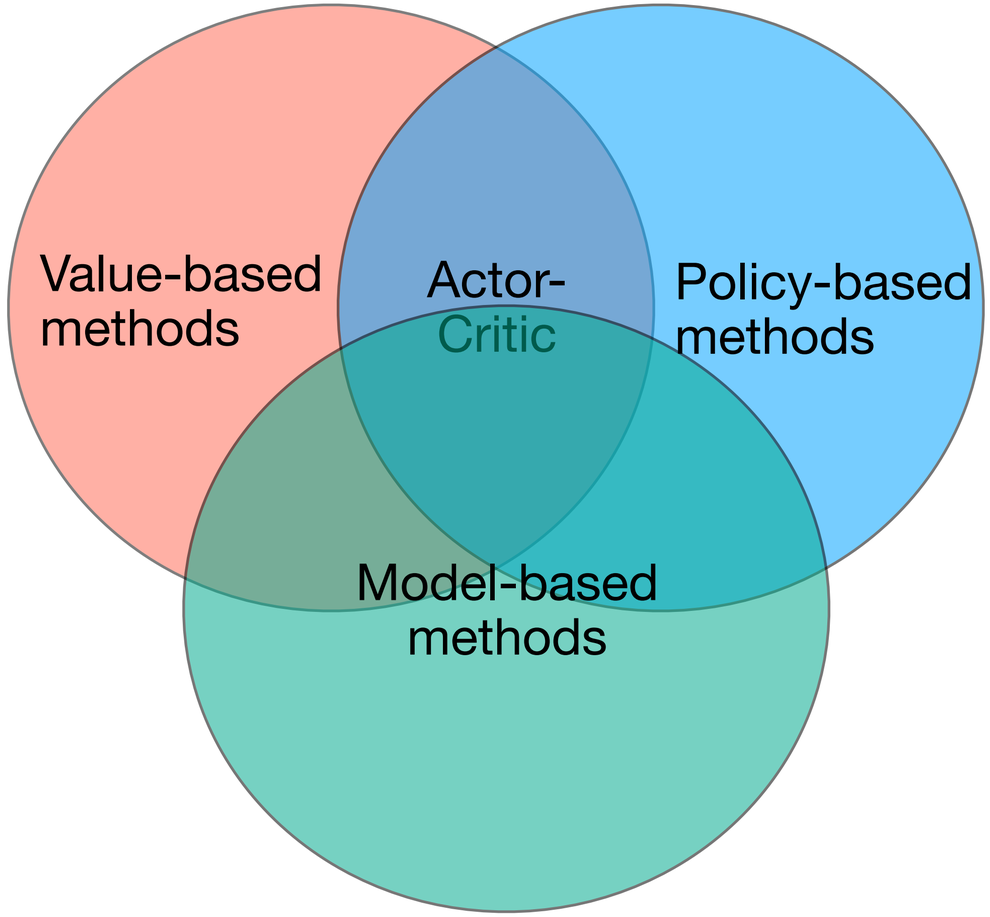

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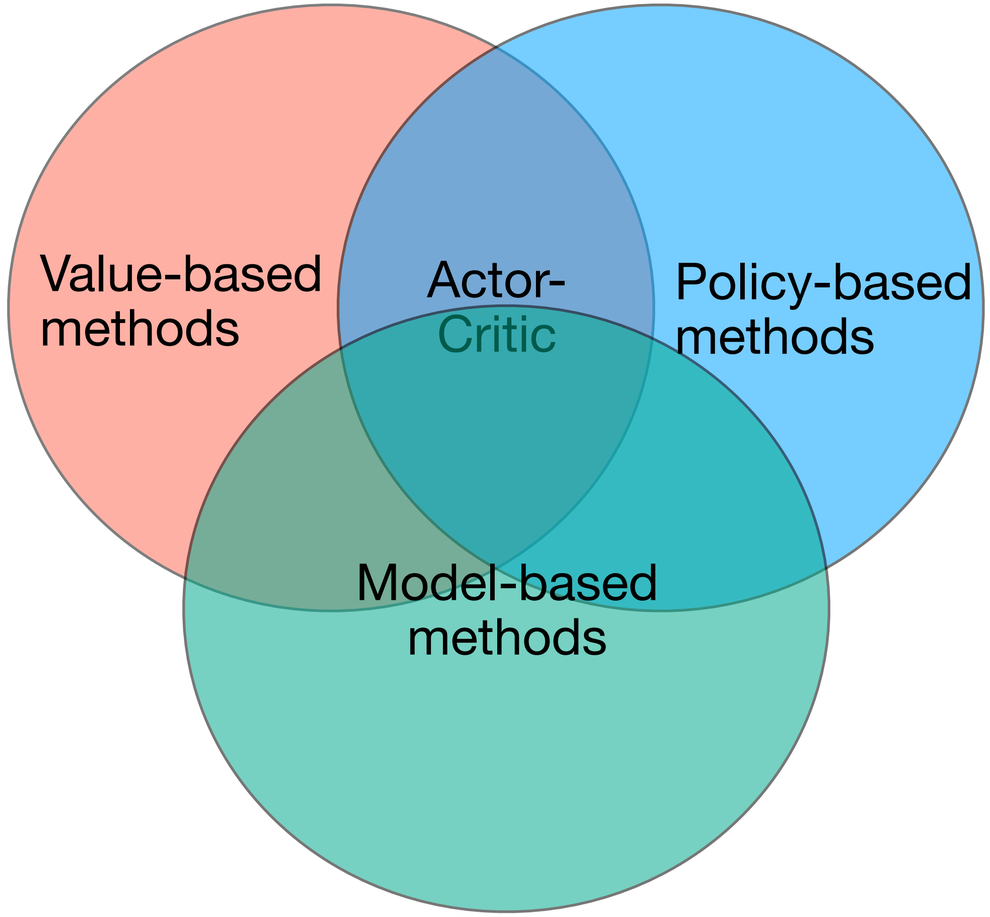
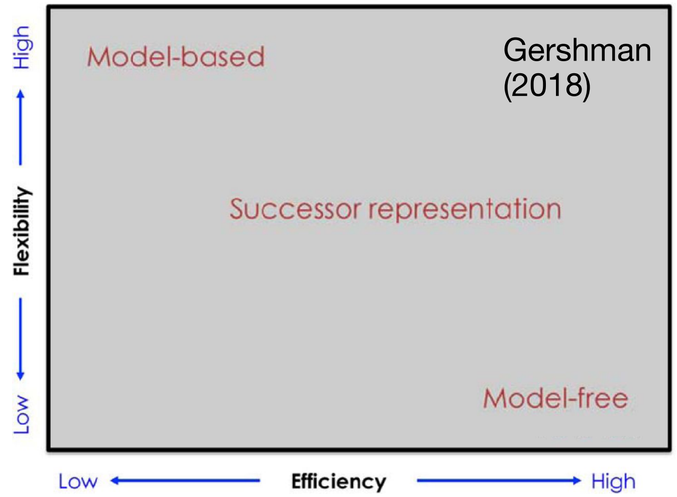


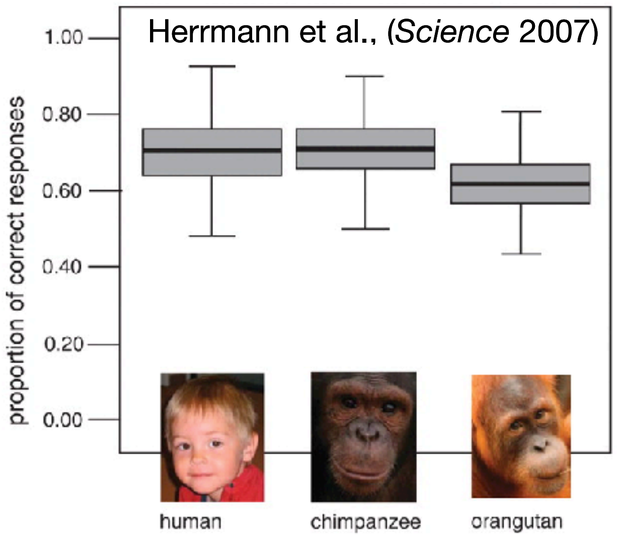


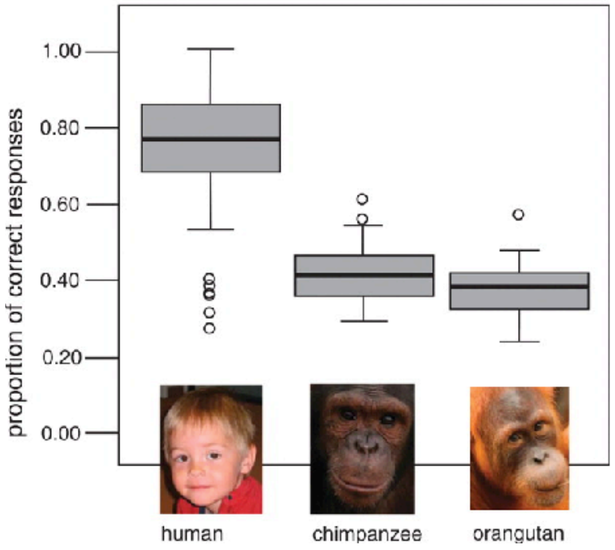
Next week: Social learning

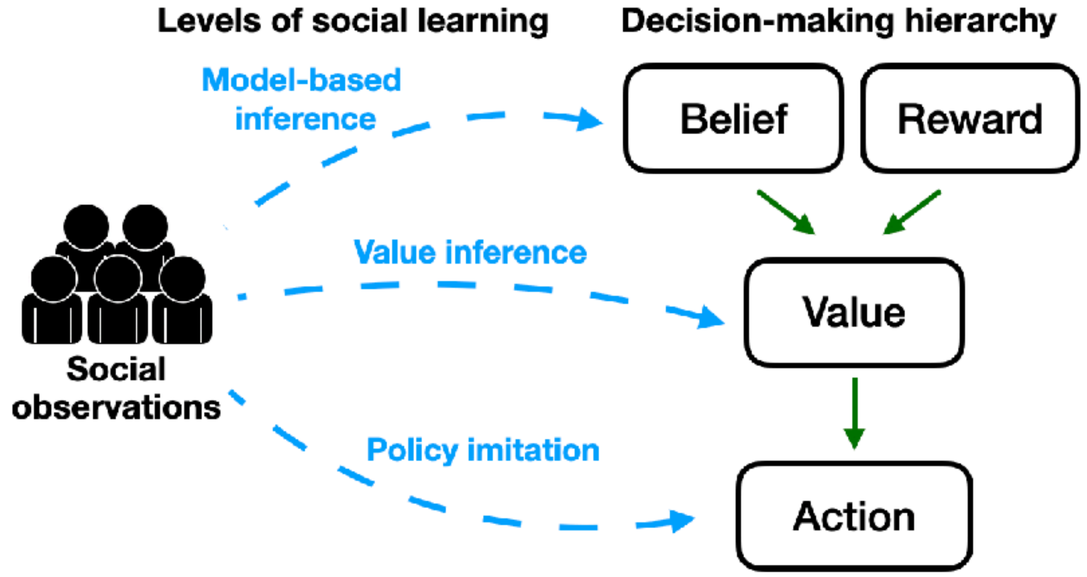
Alexandra Witt

Physical

Social







Wu et al., (2022)

Witt et al., (*PNAS* 2024)