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TÜBINGEN AI CENTER
BMBF Competence Center for Machine Learning



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CyberValley



Intelligente Systeme

ADVANCING MACHINE INTELLIGENCE WITH ROBUST MACHINE LEARNING

Generalization in Reinforcement Learning

Charley Wu

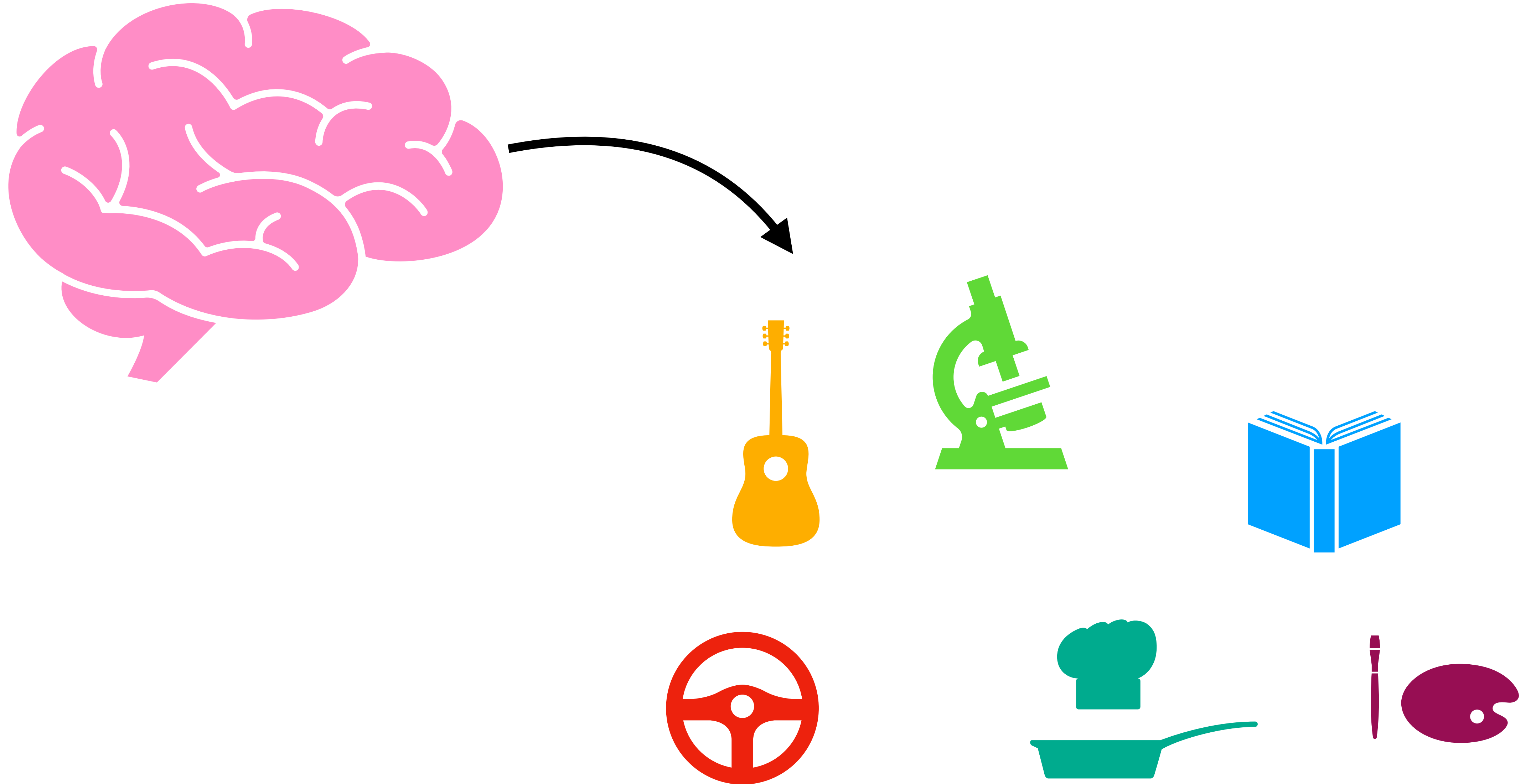
Human and Machine Cognition Lab

hmc-lab.com

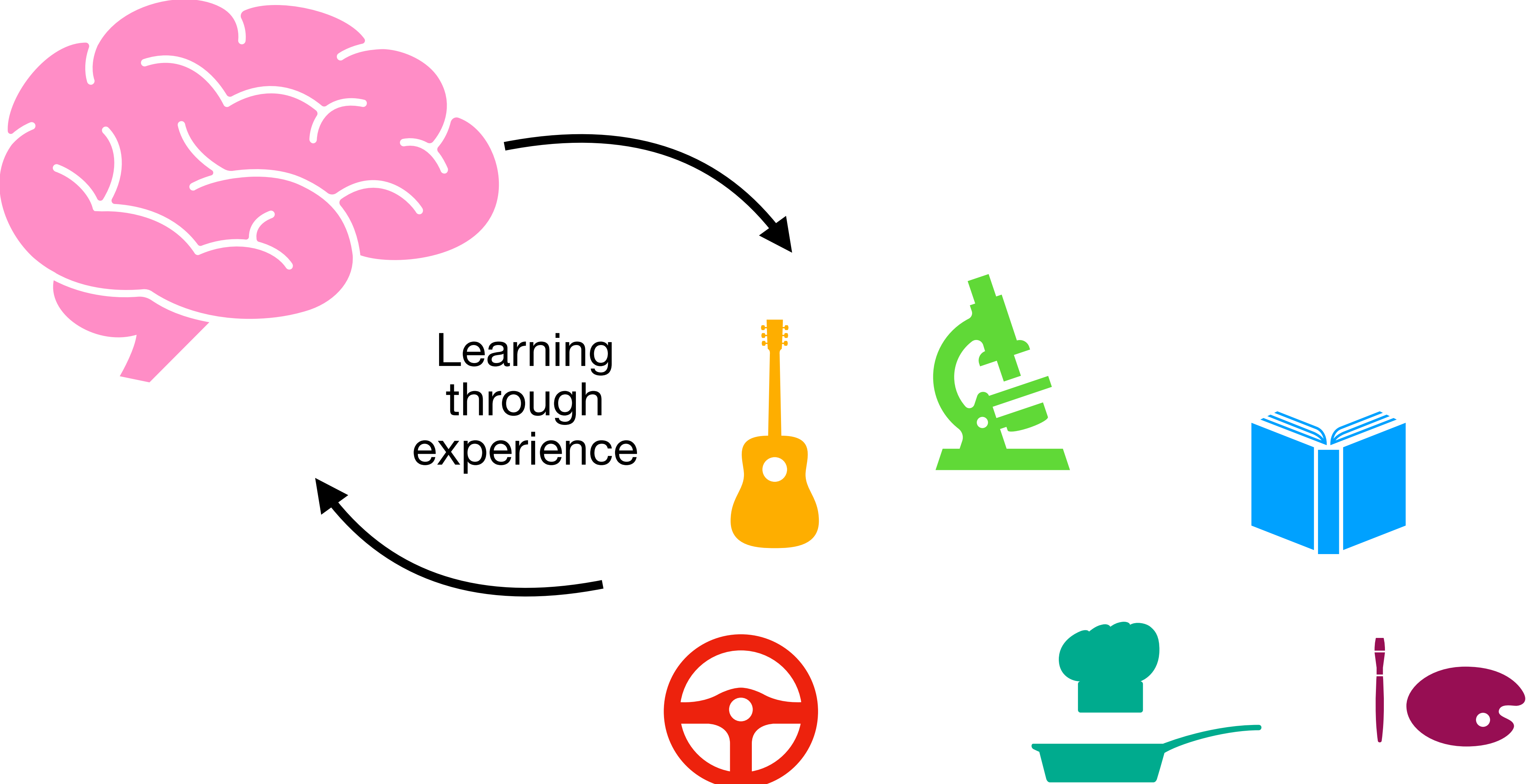
Brains control behavior



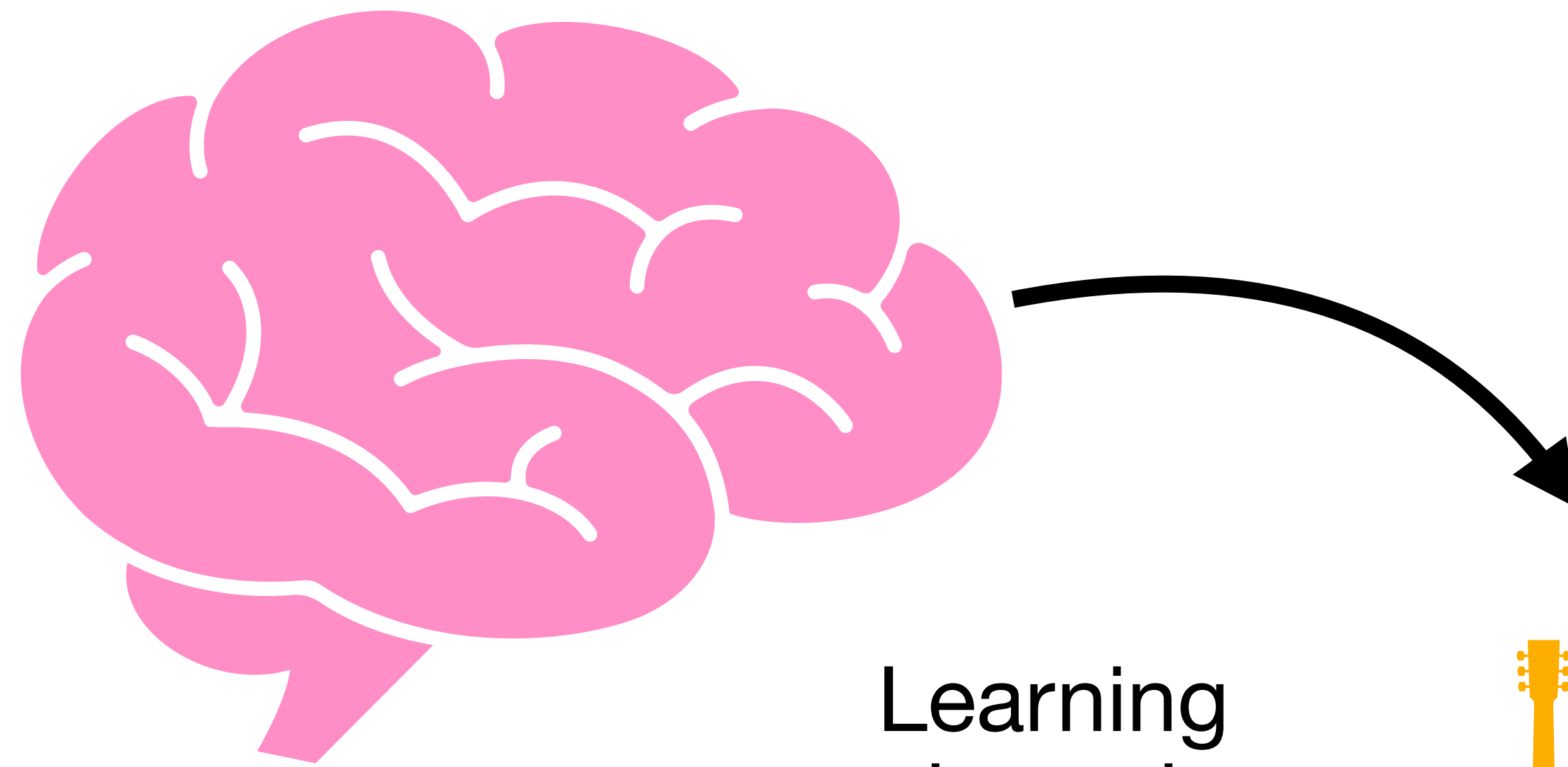
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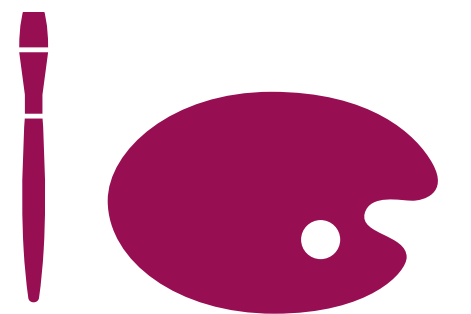
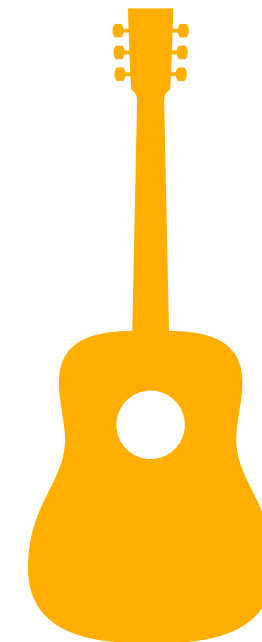
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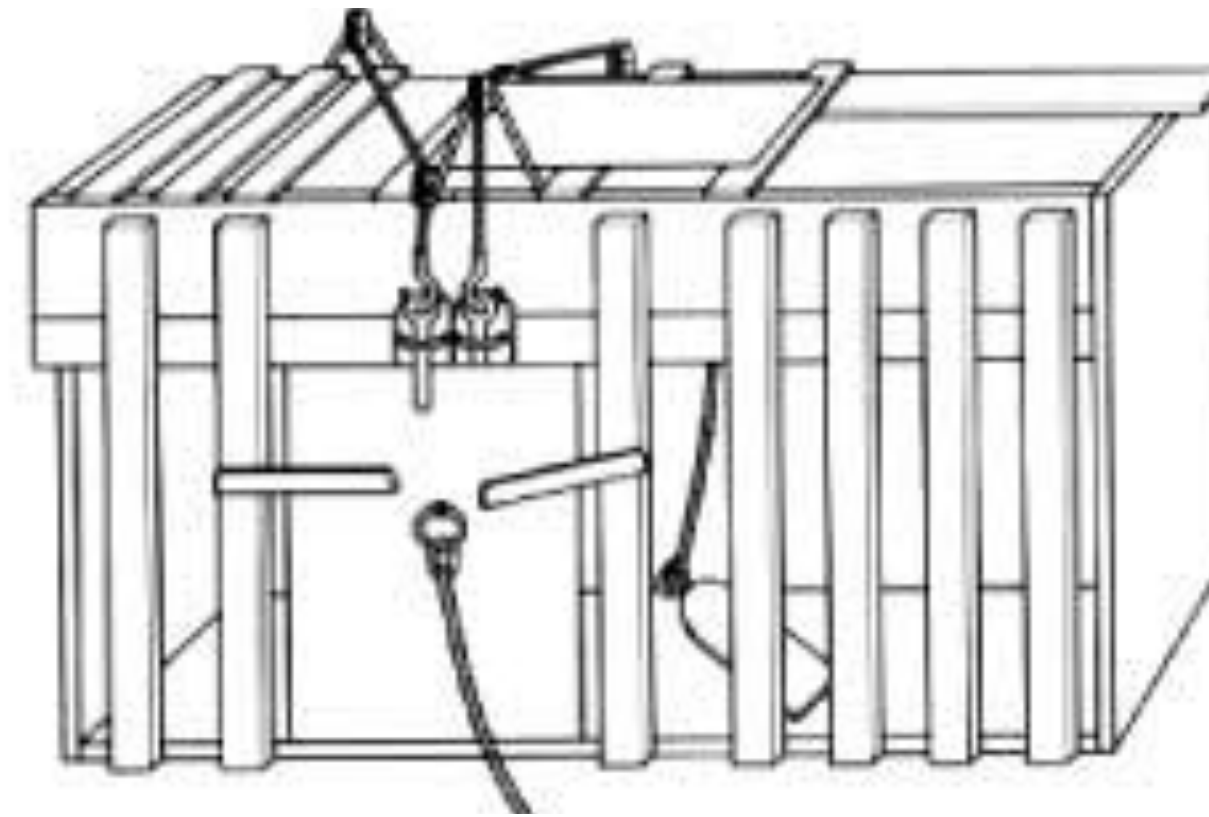


Learning
through
experience



But how?

Thorndike's (1898) Law of Effect

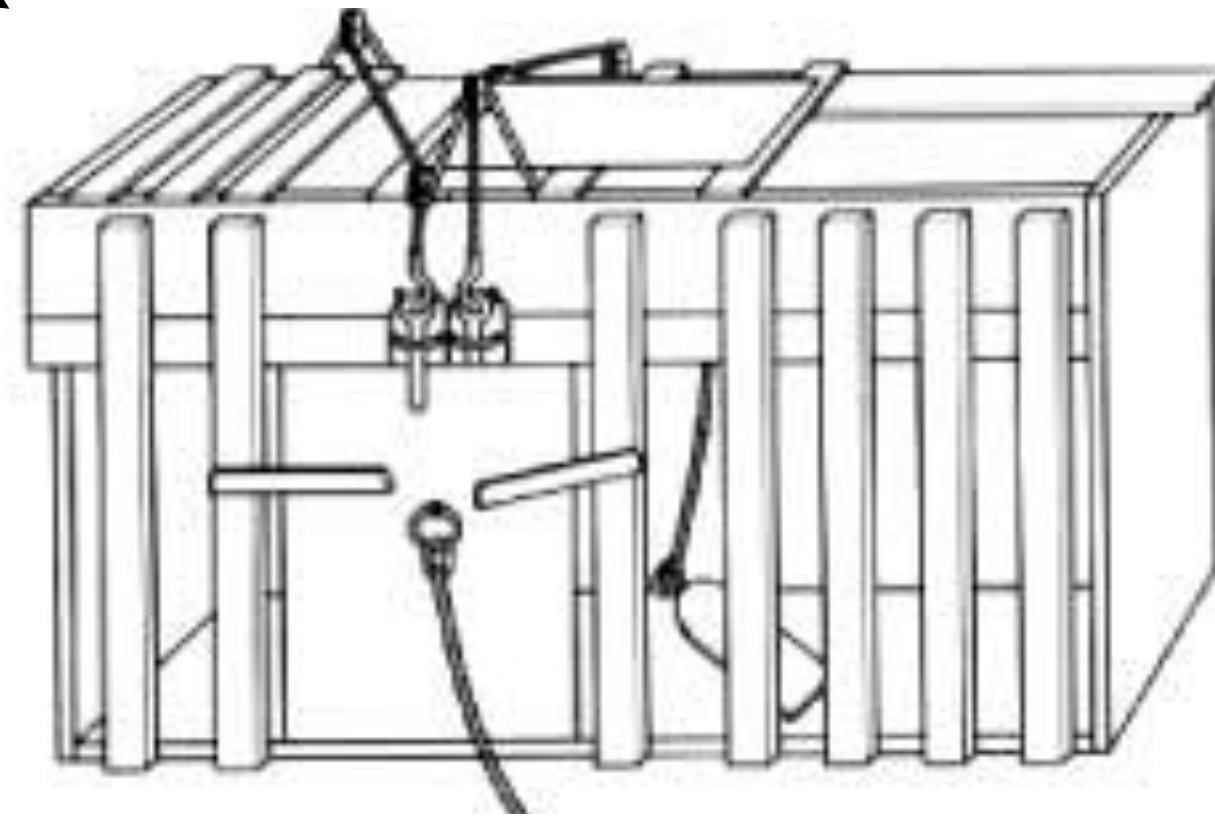


Puzzle Box

Thorndike's (1898) Law of Effect



Cat

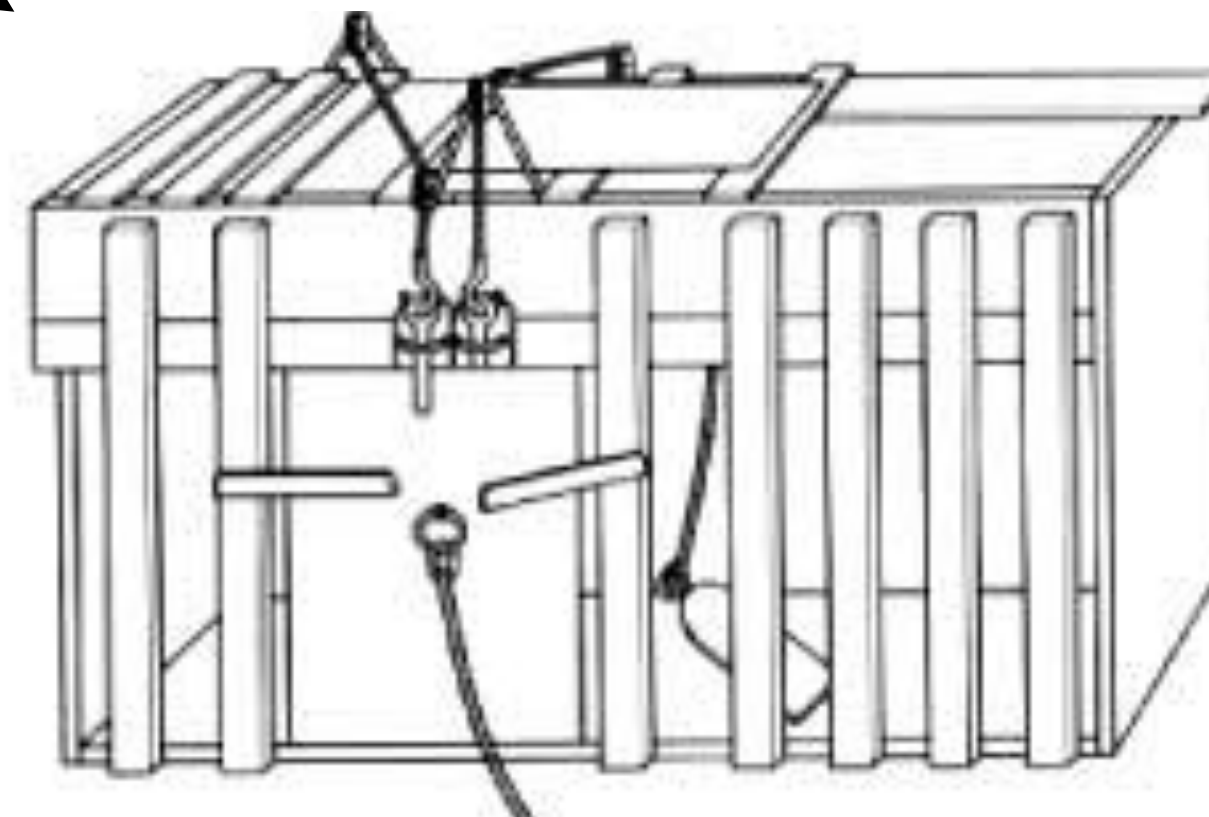


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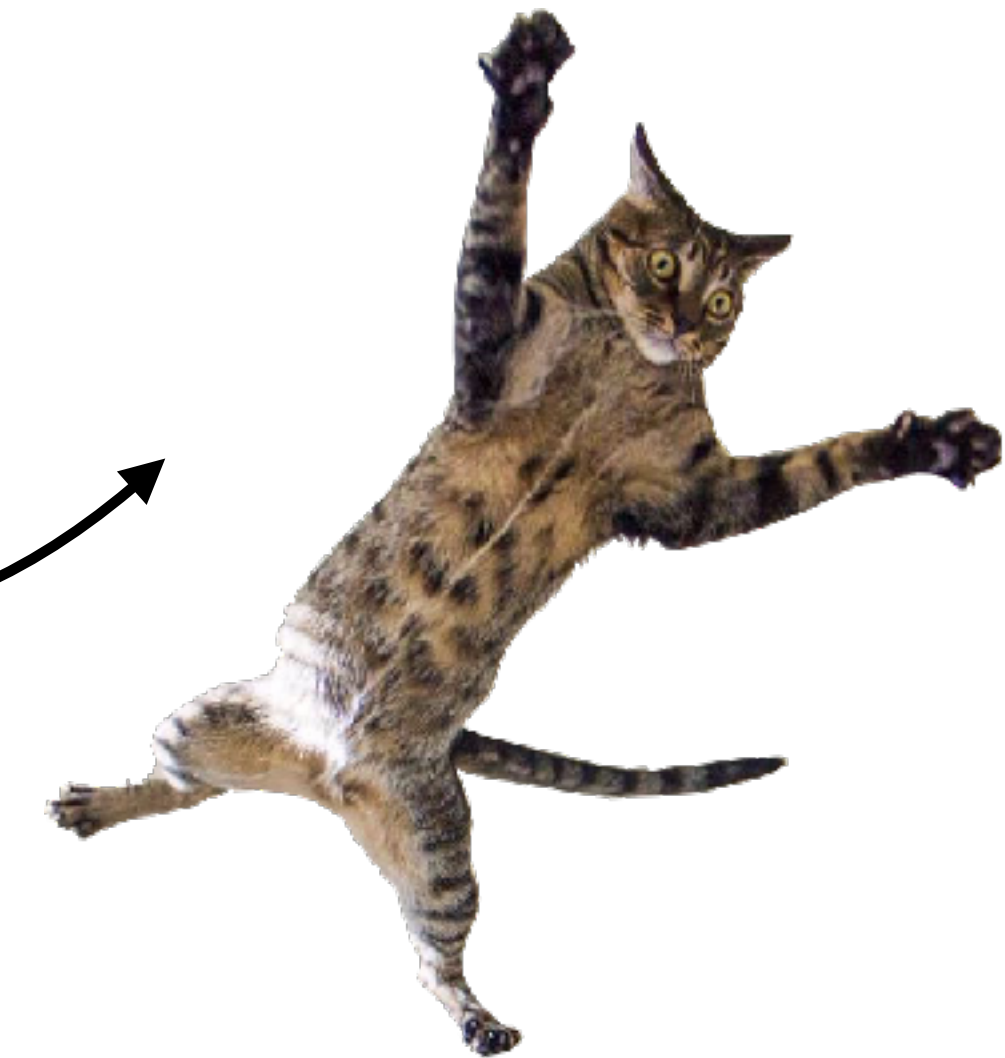
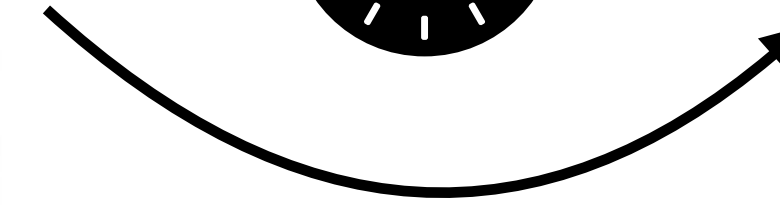
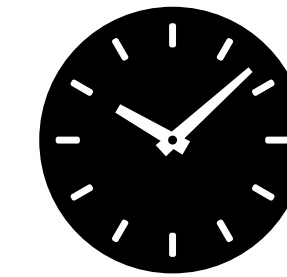
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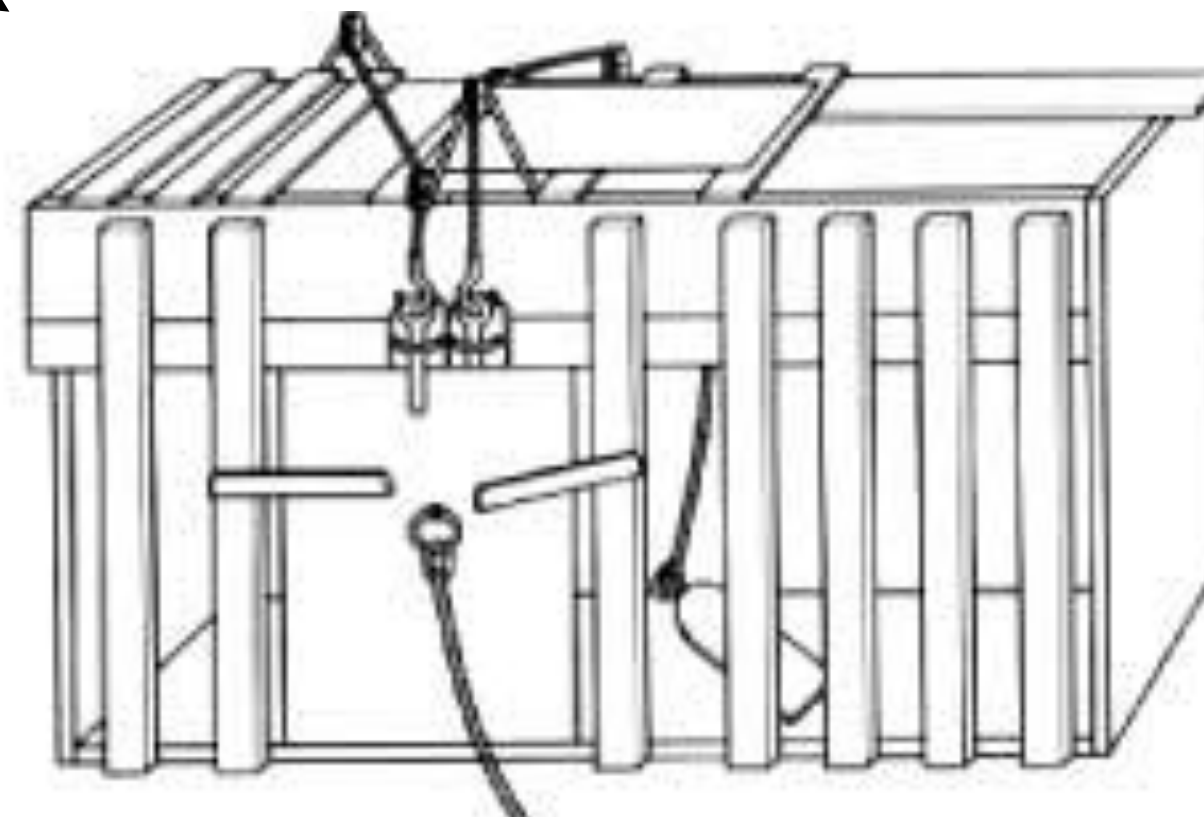


Time to escape

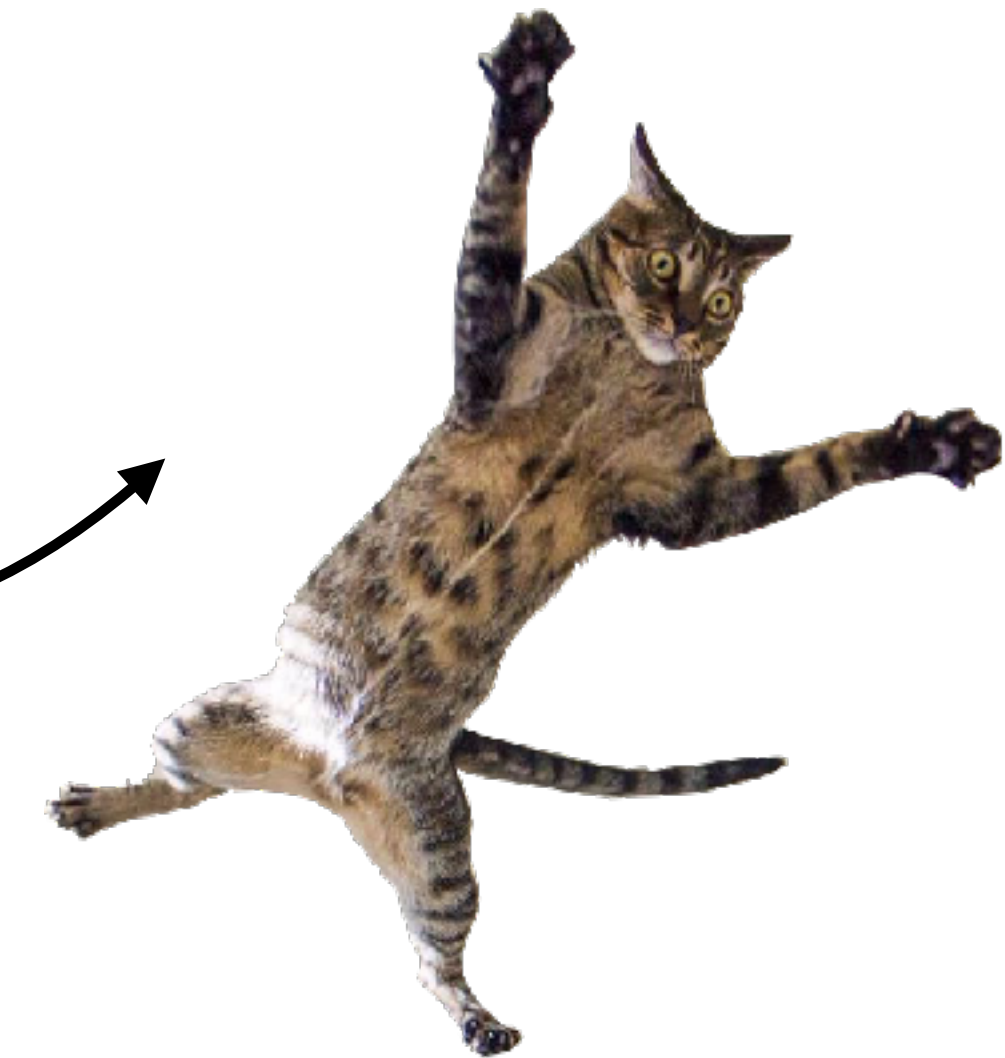
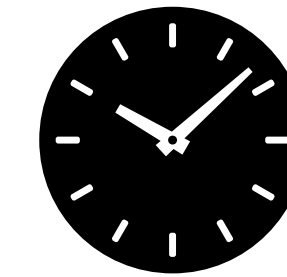
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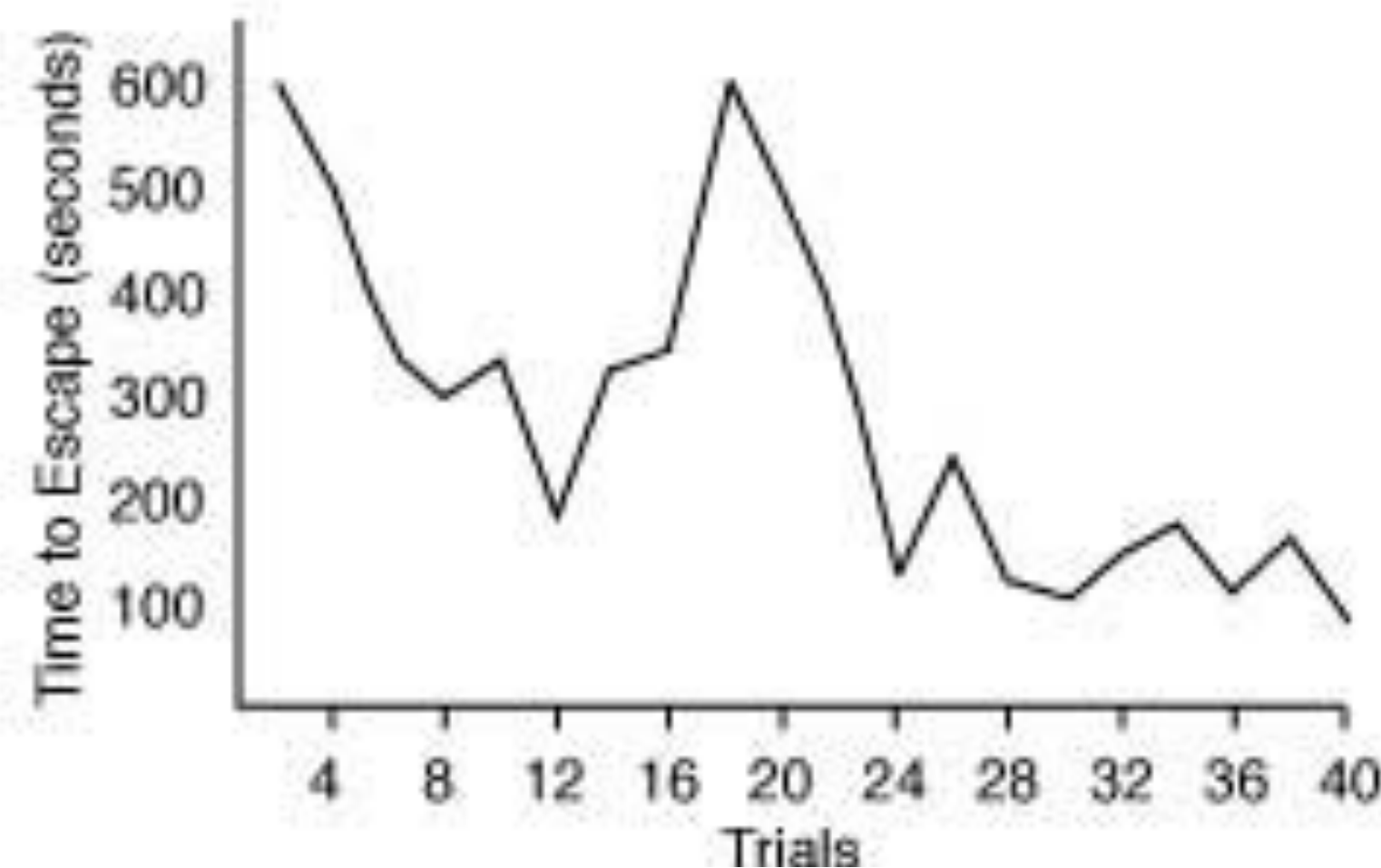
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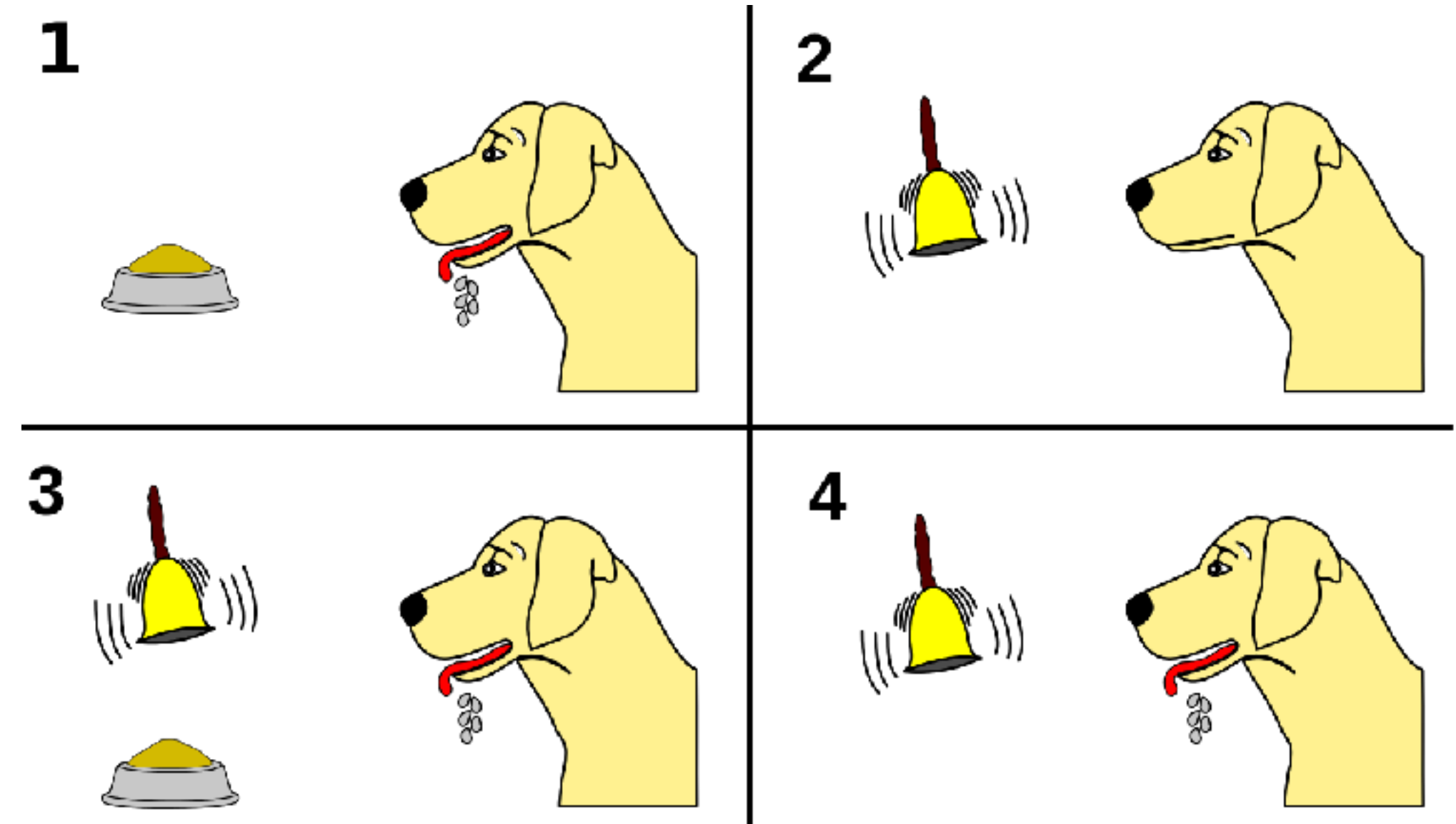


Actions associated with satisfaction are strengthened, while those associated with discomfort become weakened.

Classical and Operant Conditioning

Classical Condition (Pavlov, 1927)

Learning as the *passive* coupling of stimulus (bell ringing) and response (salivation), anticipating future rewards



Operant Condition (Skinner, 1938)

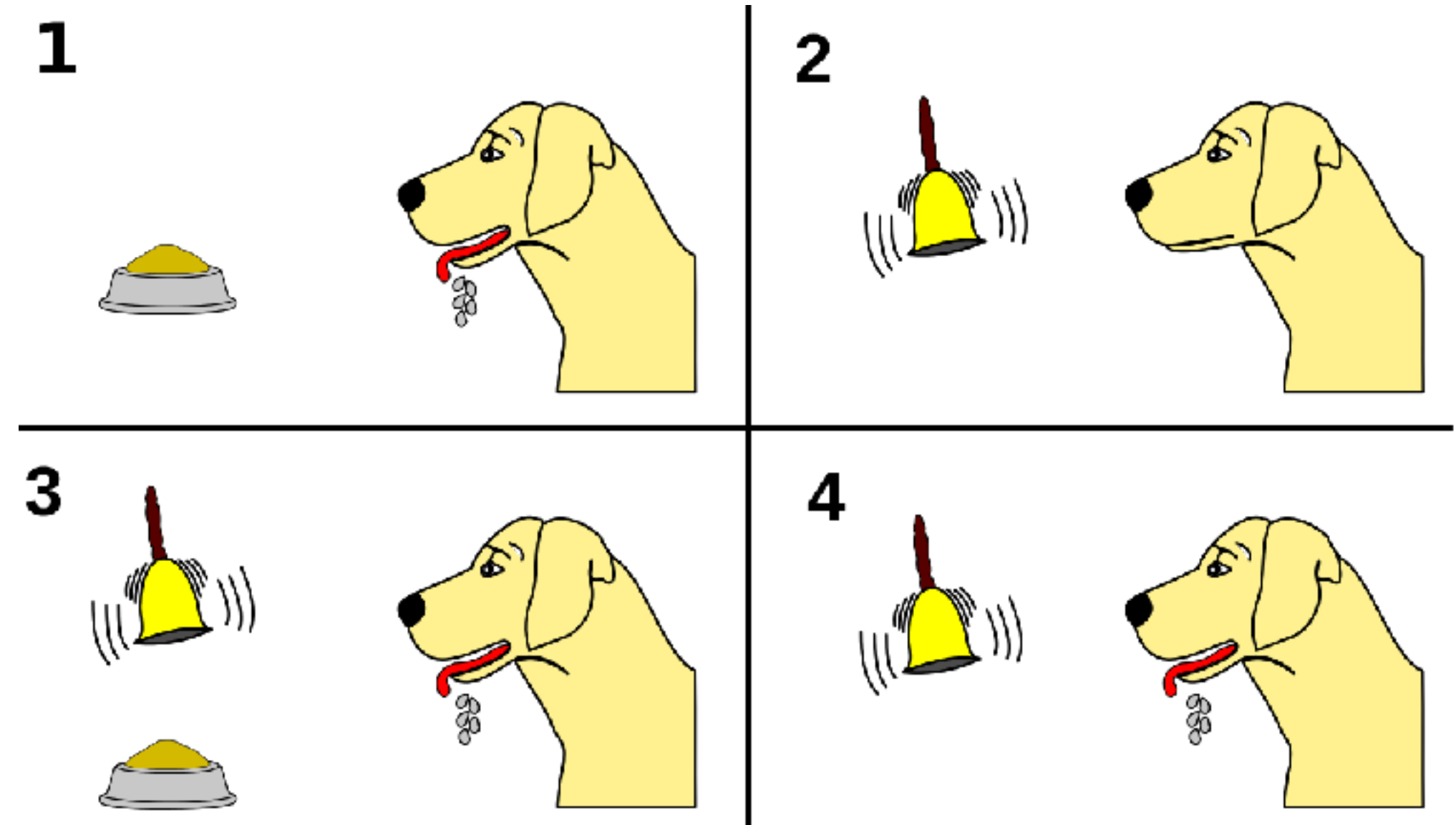
Skinner (1938): Learning as the *active* shaping of behavior in response to rewards or punishments



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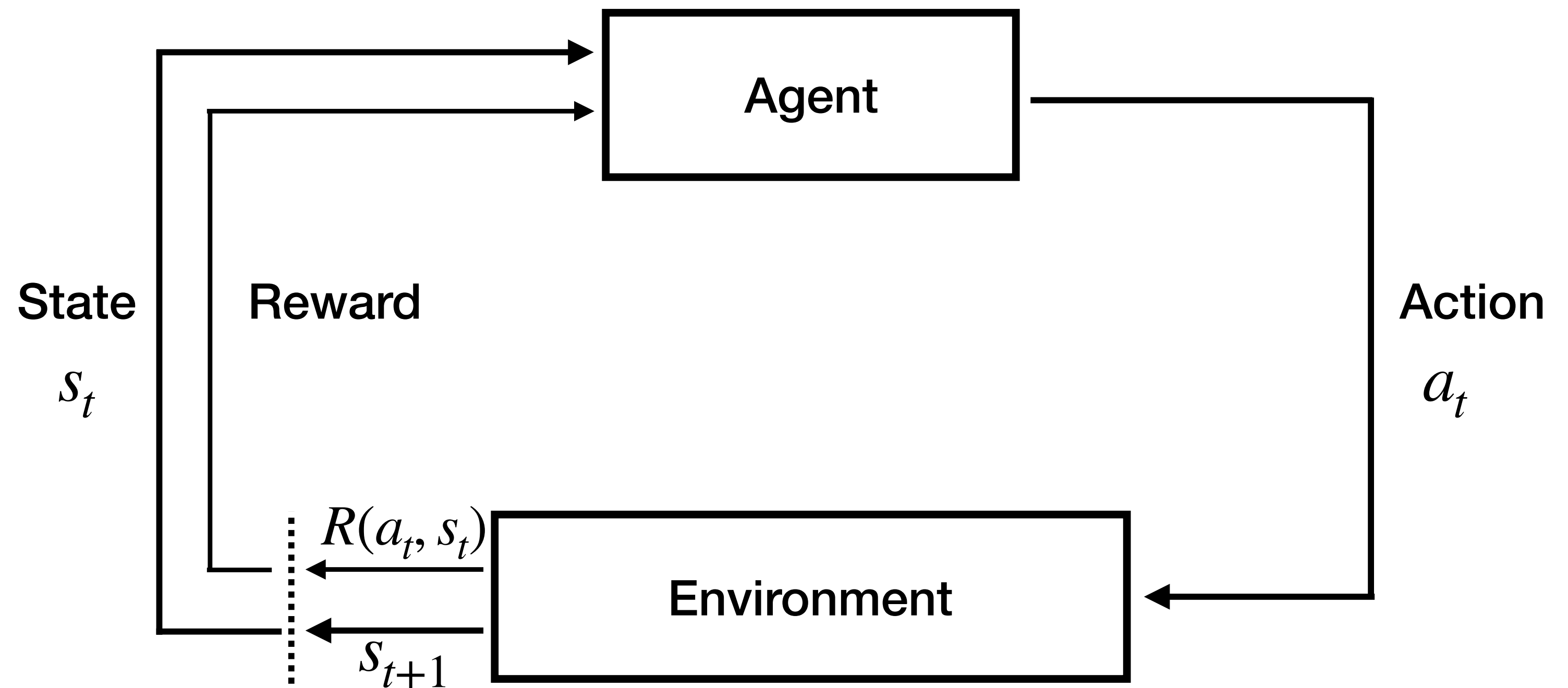
Reinforcement Learning

The Environment:

- governs the transition between states
- provides rewards

The Agent:

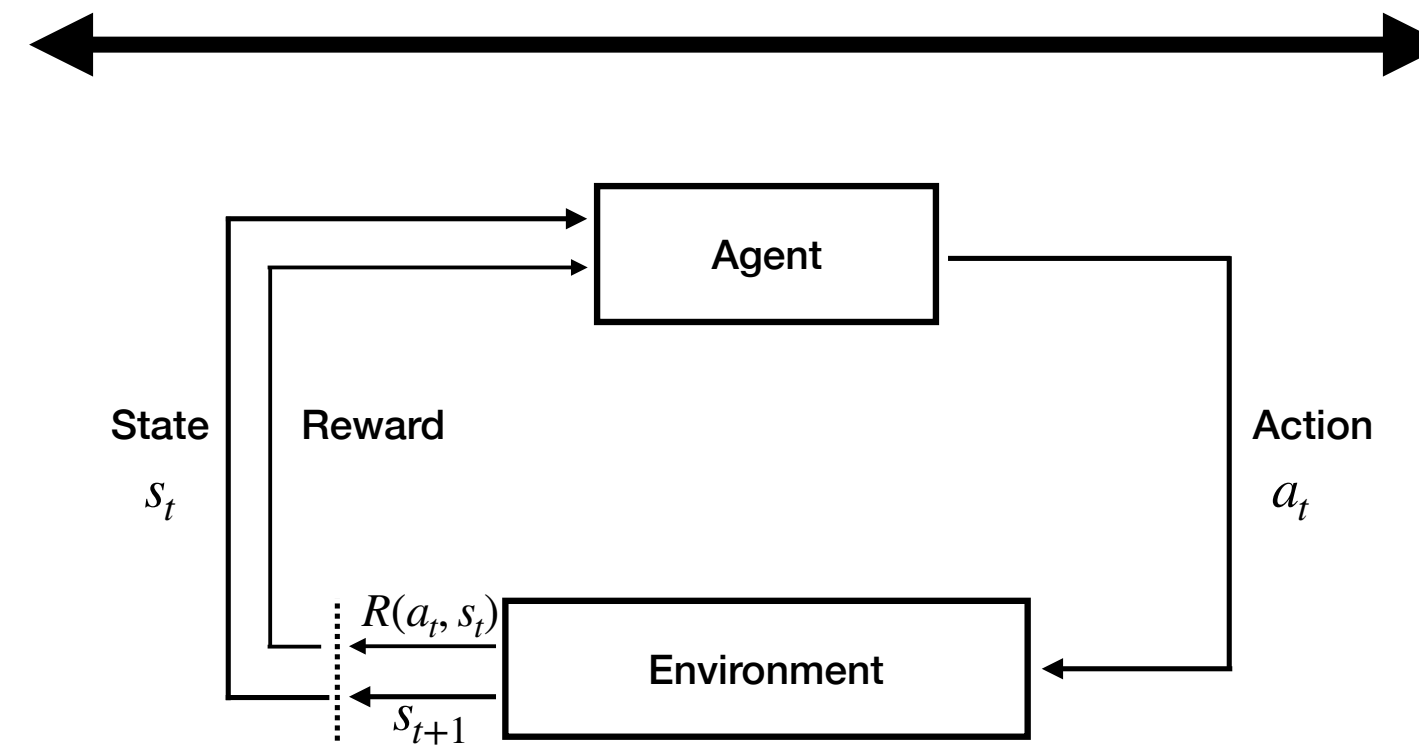
- Learns a *value function* mapping actions onto rewards
- Implements a policy, selecting actions based on their value



Neuroscience



Reinforcement Learning



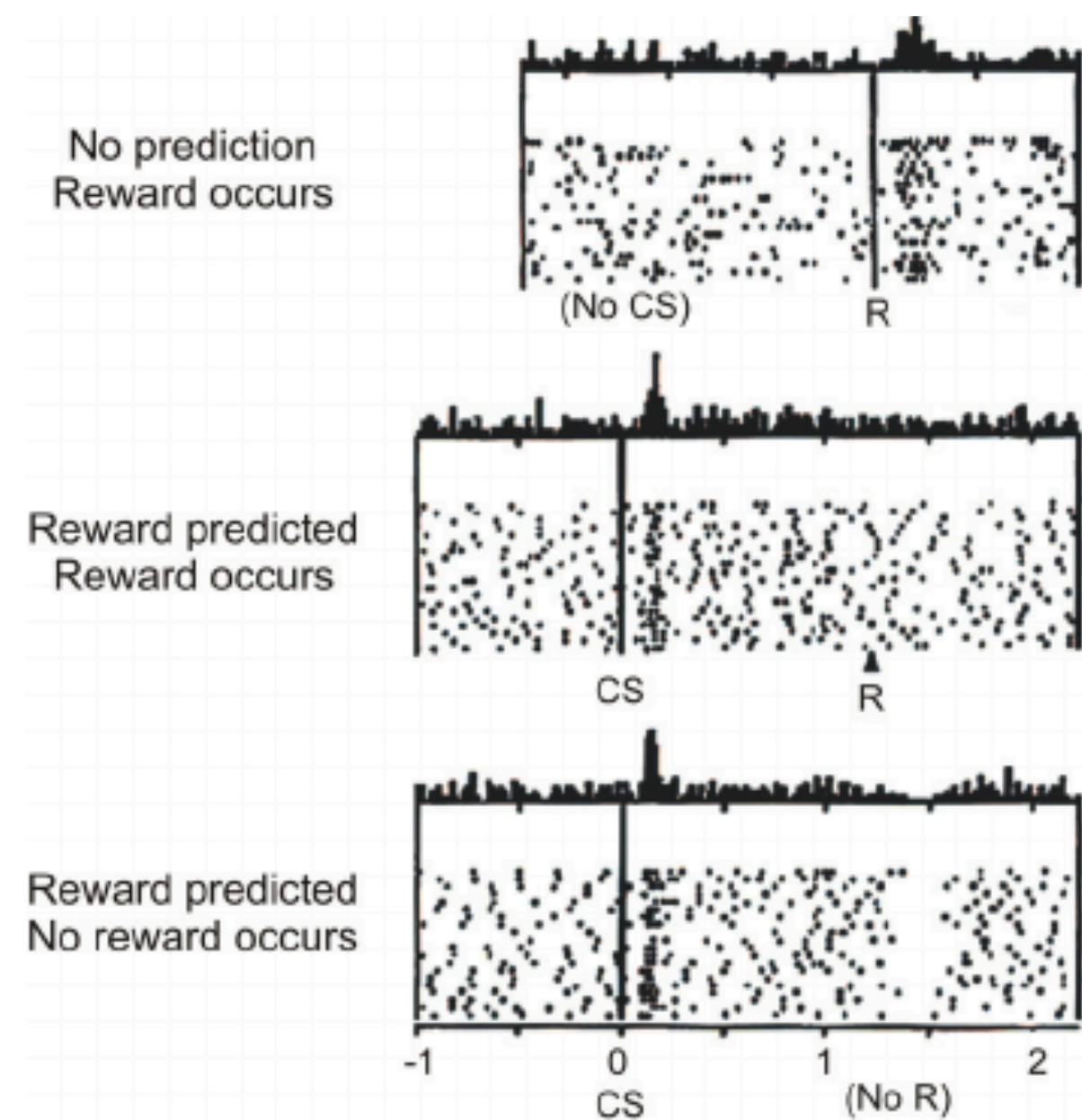
AI and Machine Learning



Neuroscience

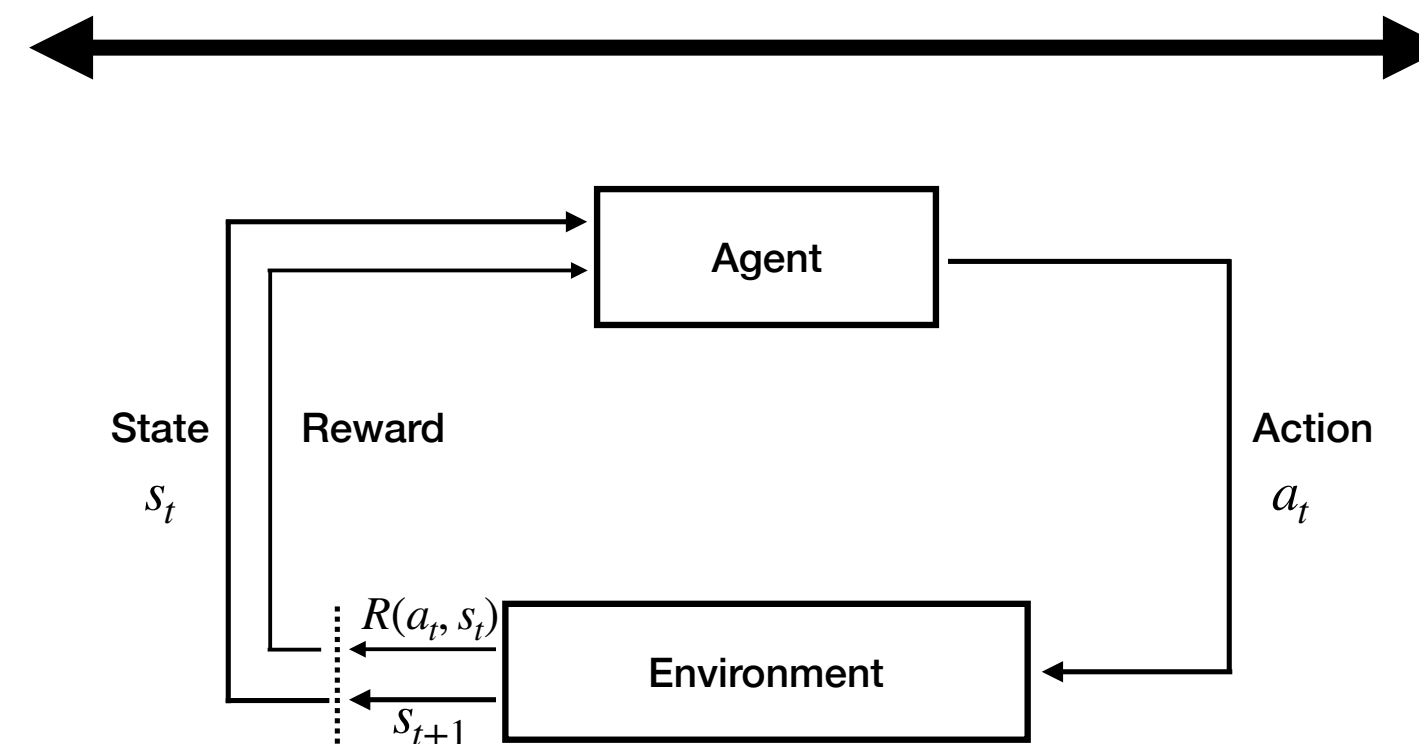


Dopamine Reward Prediction Error



Schultz et al. (1997)

Reinforcement Learning



Temporal Difference Learning

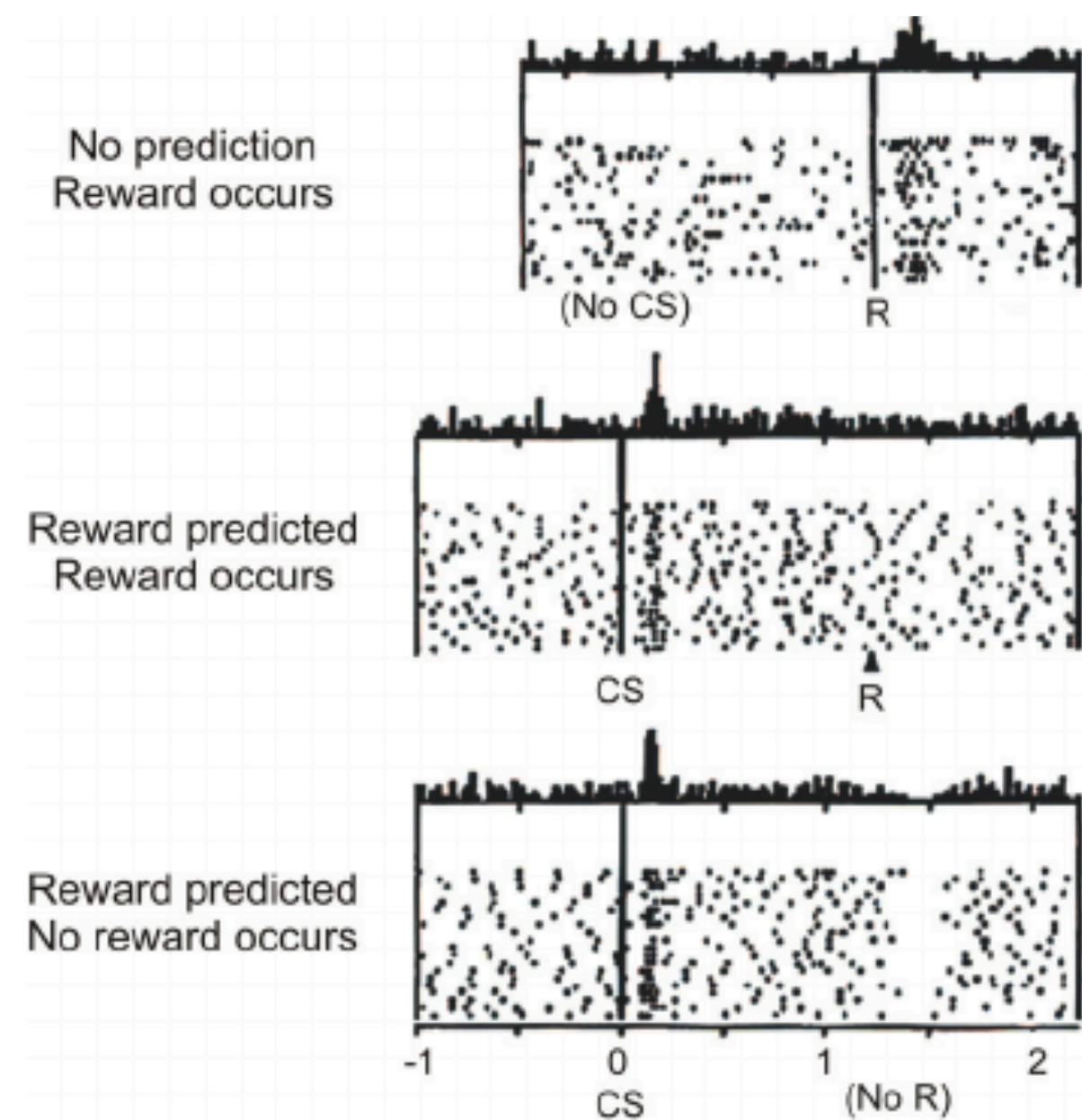
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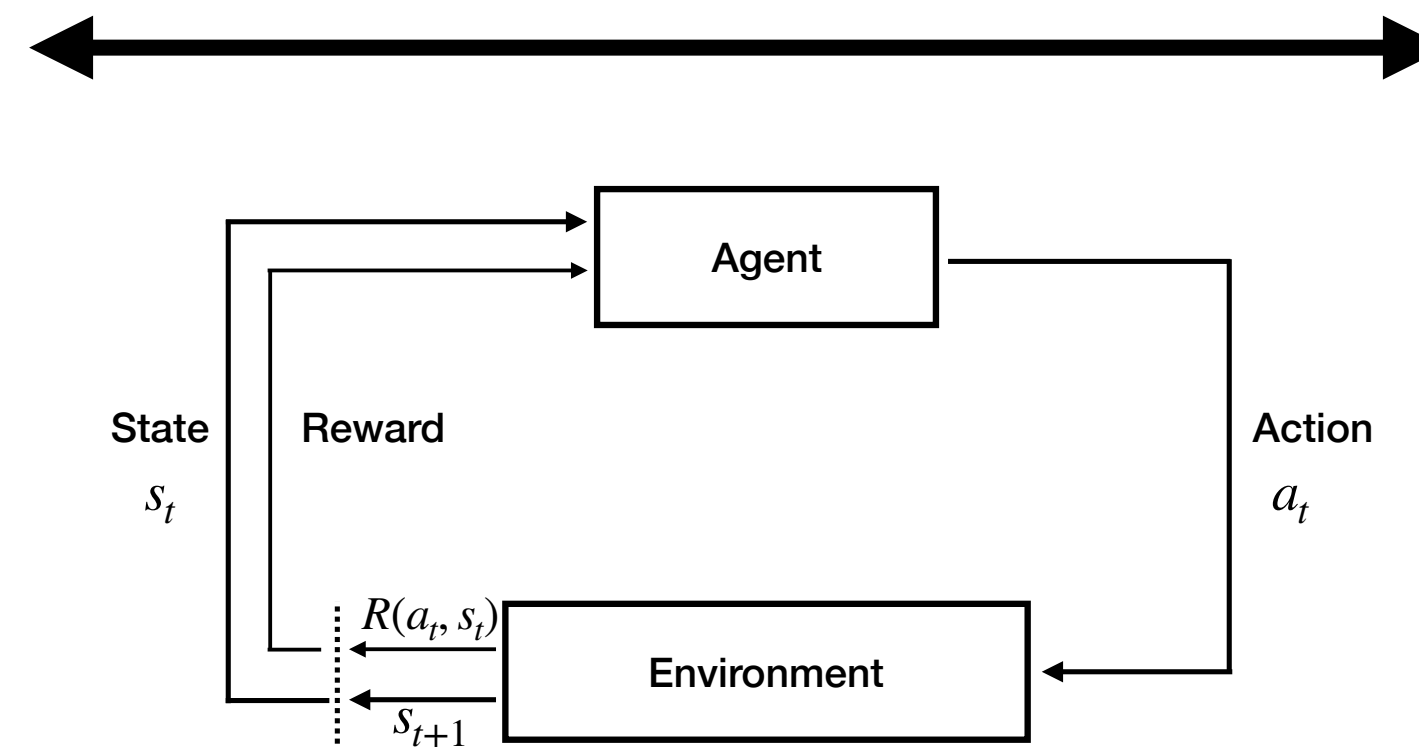


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Temporal Difference Learning

Monte Carlo Tree Search

AI and Machine Learning



AlphaGo



Silver et al. (2016)

Outline

Part 1. Overview of Reinforcement Learning

- Value functions and policies
- Tabular methods vs. value-function approximation
- Multi-armed Bandit problem
- Models of human learners

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~~~~~ Break ~~~~~

# Outline

## Part 1. Overview of Reinforcement Learning

- Value functions and policies
- Tabular methods vs. value-function approximation
- Multi-armed Bandit problem
- Models of human learners

~~~~~ Break ~~~~~

Part 2. Generalization guided learning

- Search in vast spaces (Wu et al., *NHB* 2018)
- Learning like a child (Schulz et al., *PsychSci* 2019; Meder et al., *DevSci* 2021; Giron et al., *in prep*)
- Connecting spatial and conceptual search (Wu et al., *PLoS CompBio* 2020)
- Graph-structured generalization (Wu et al., *CBB* 2020)

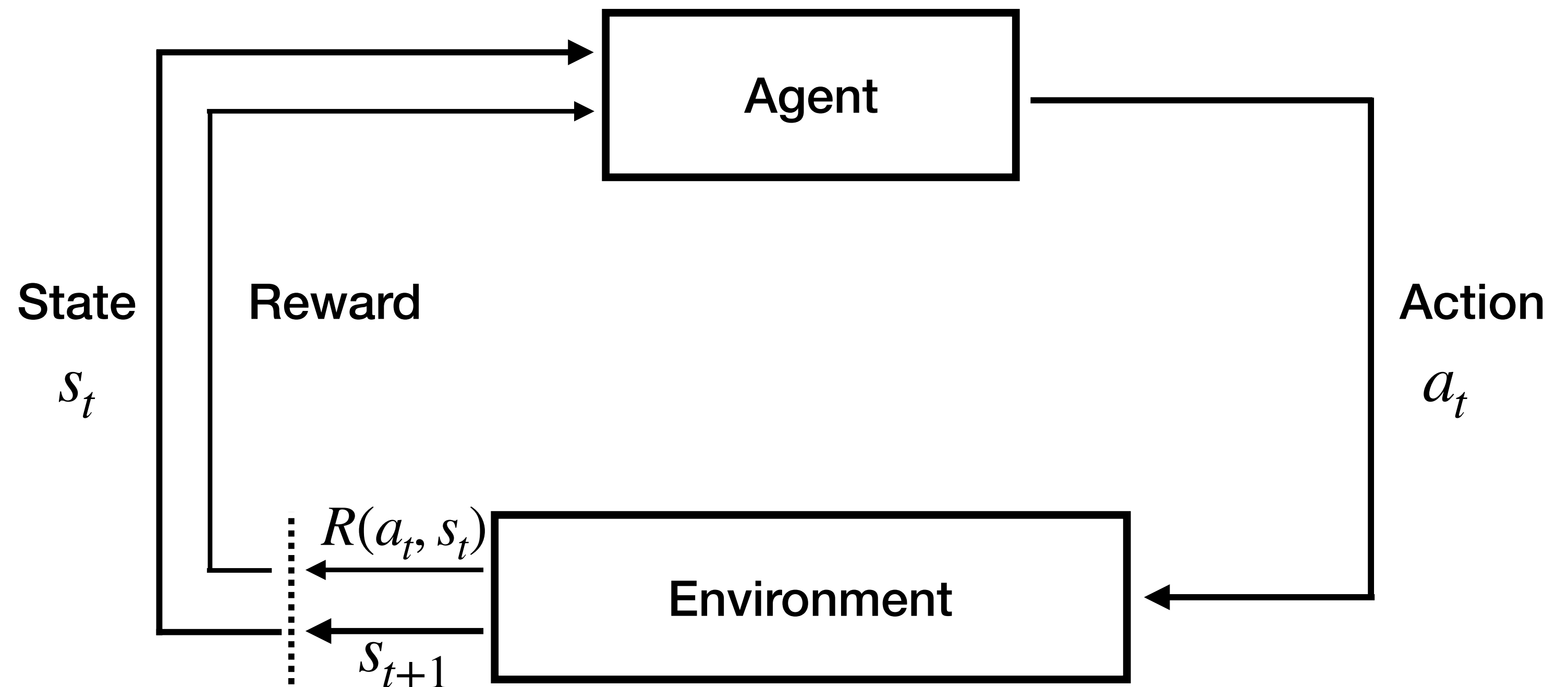
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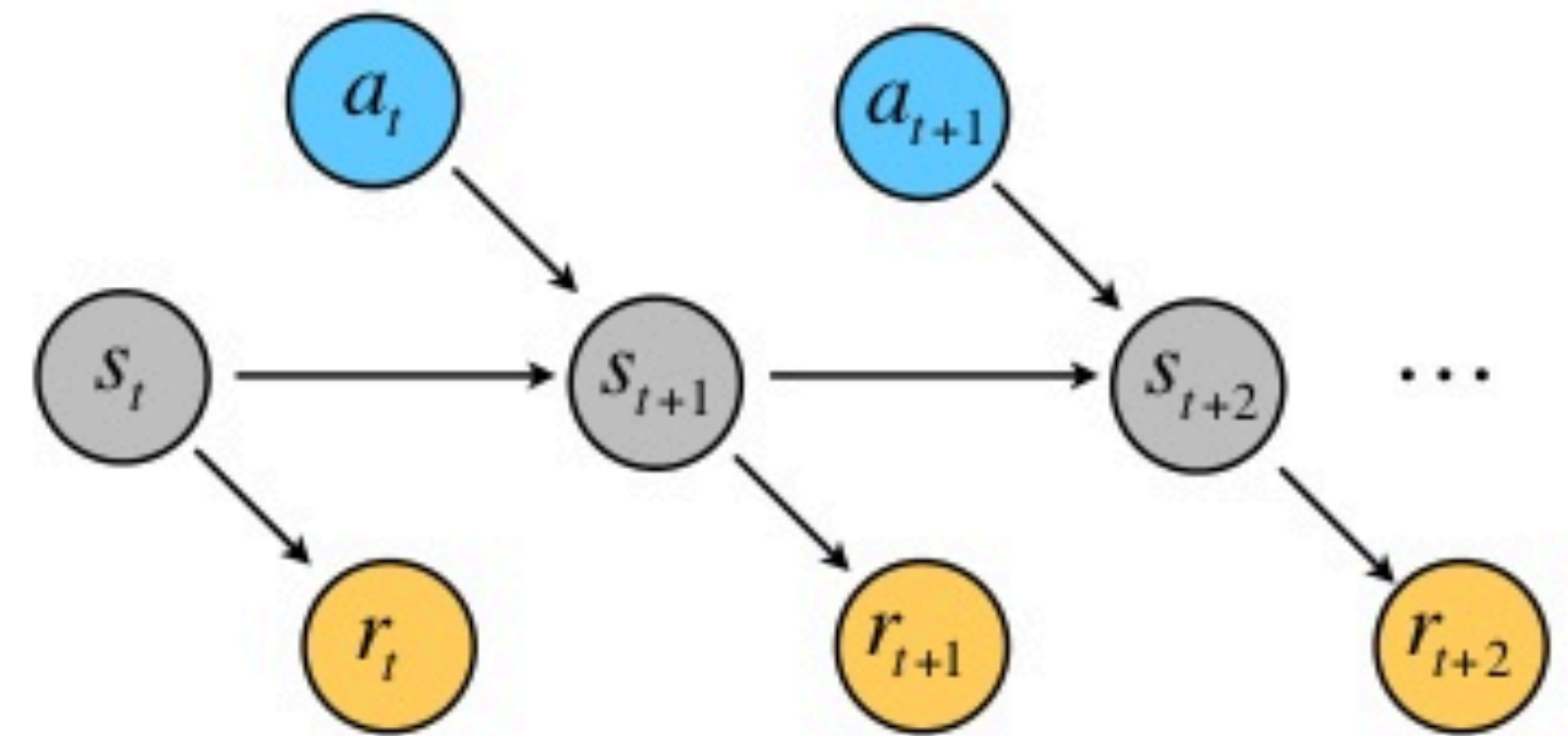
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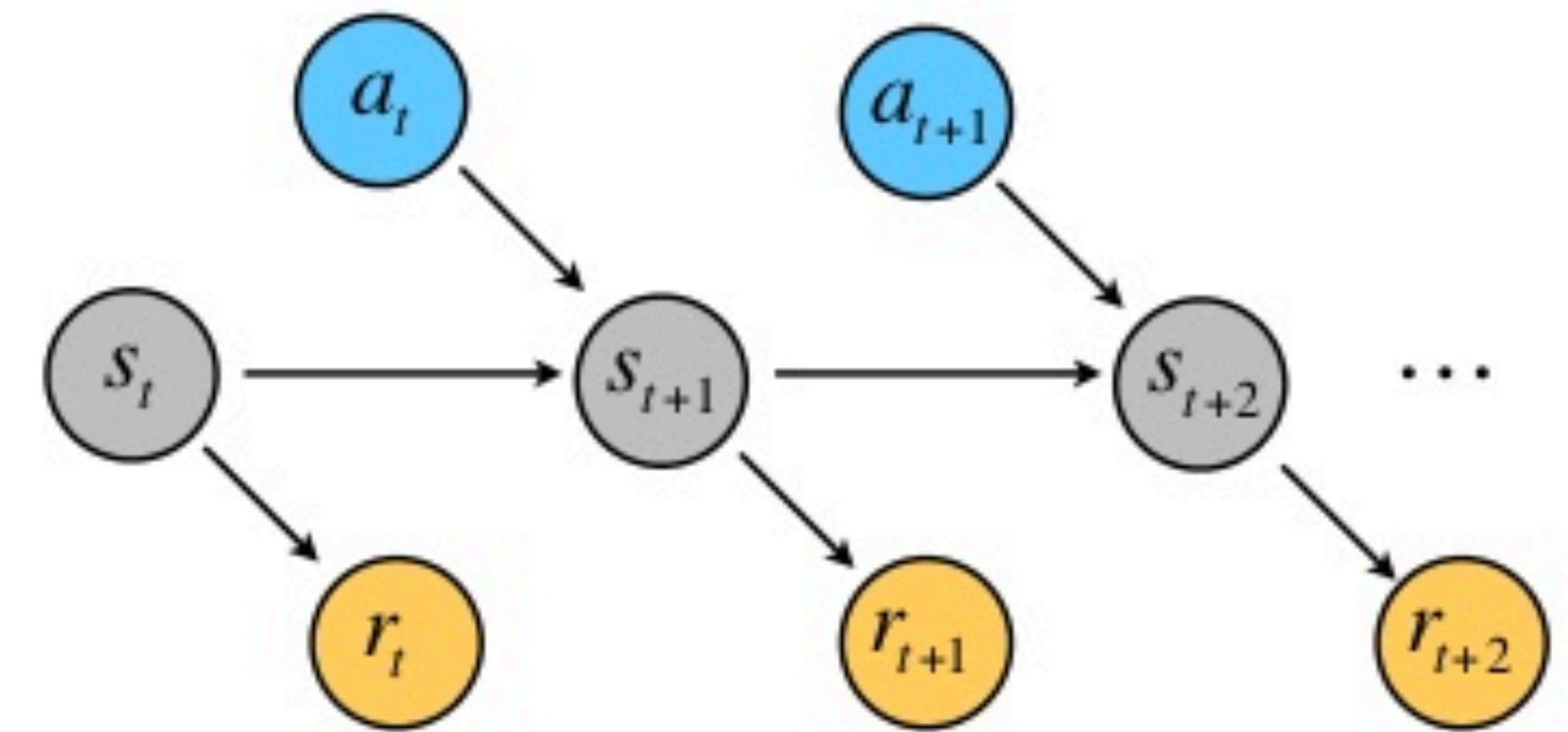
Environment

Markov Decision Process (MDP)

- Simplifying assumption that the system is fully defined by only the previous state (i.e., Markov Principle): $P(s_{t+1} \mid s_t, a_t)$



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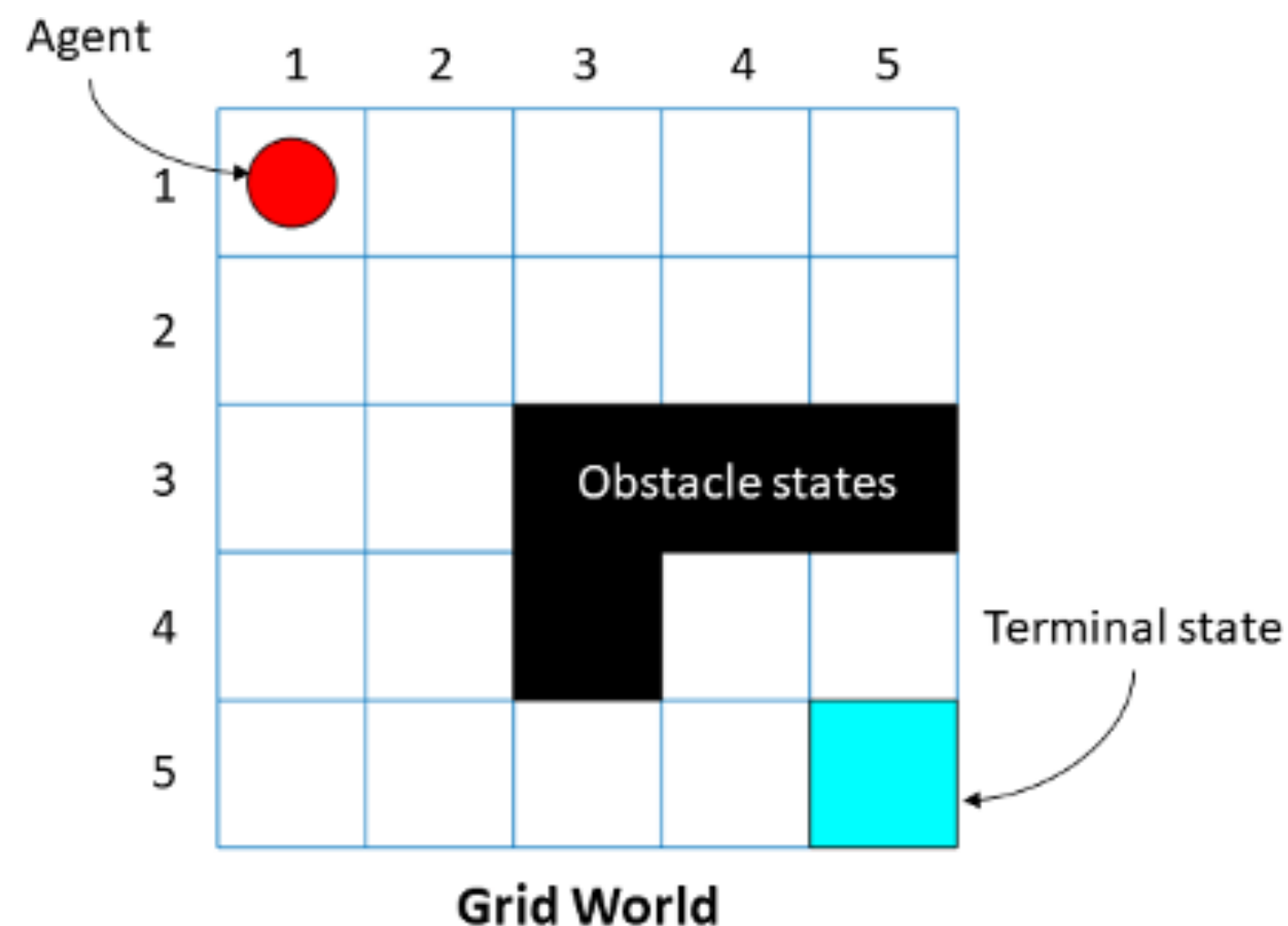


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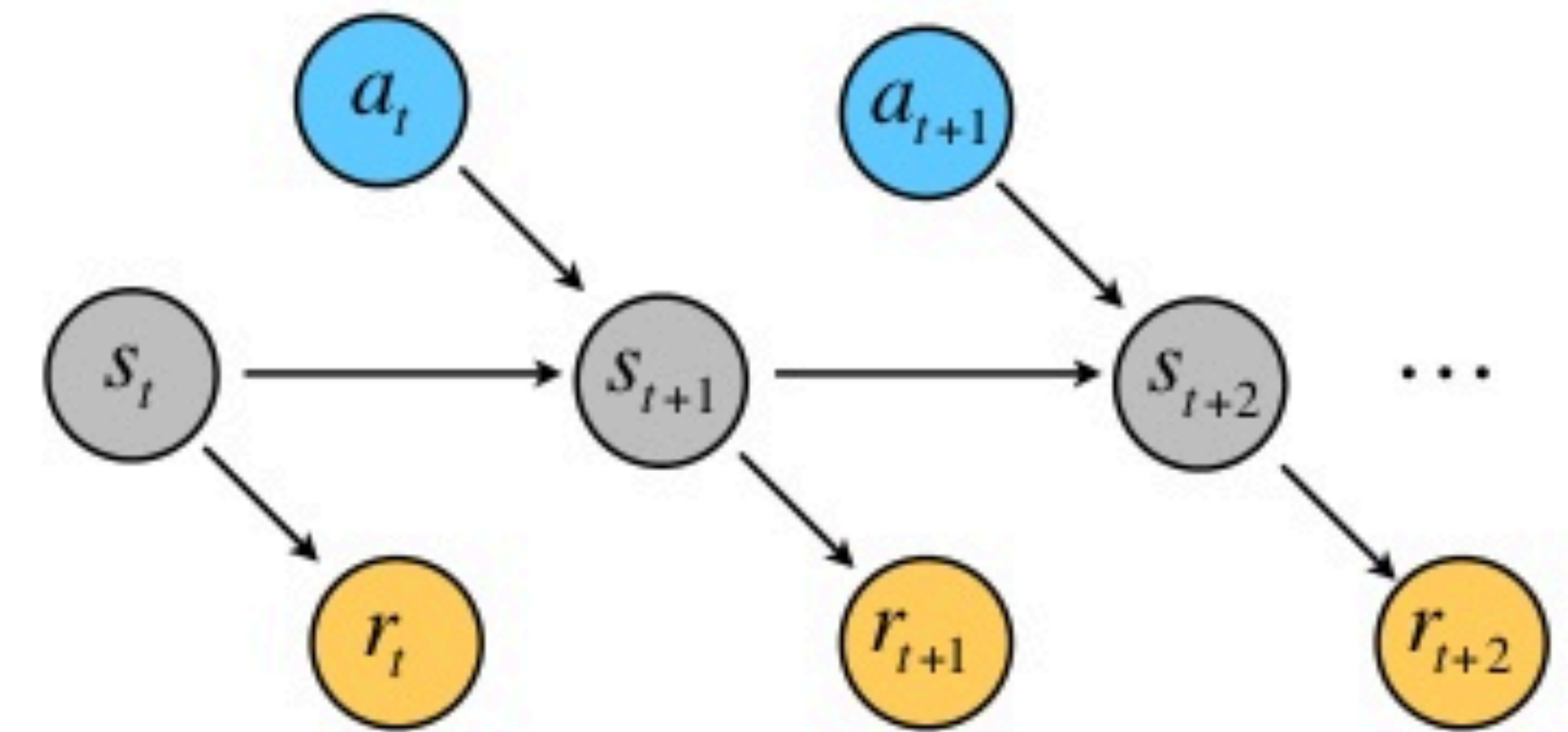
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What are the states?

- Discrete locations, pixels on a screen, a set of feature values, etc...



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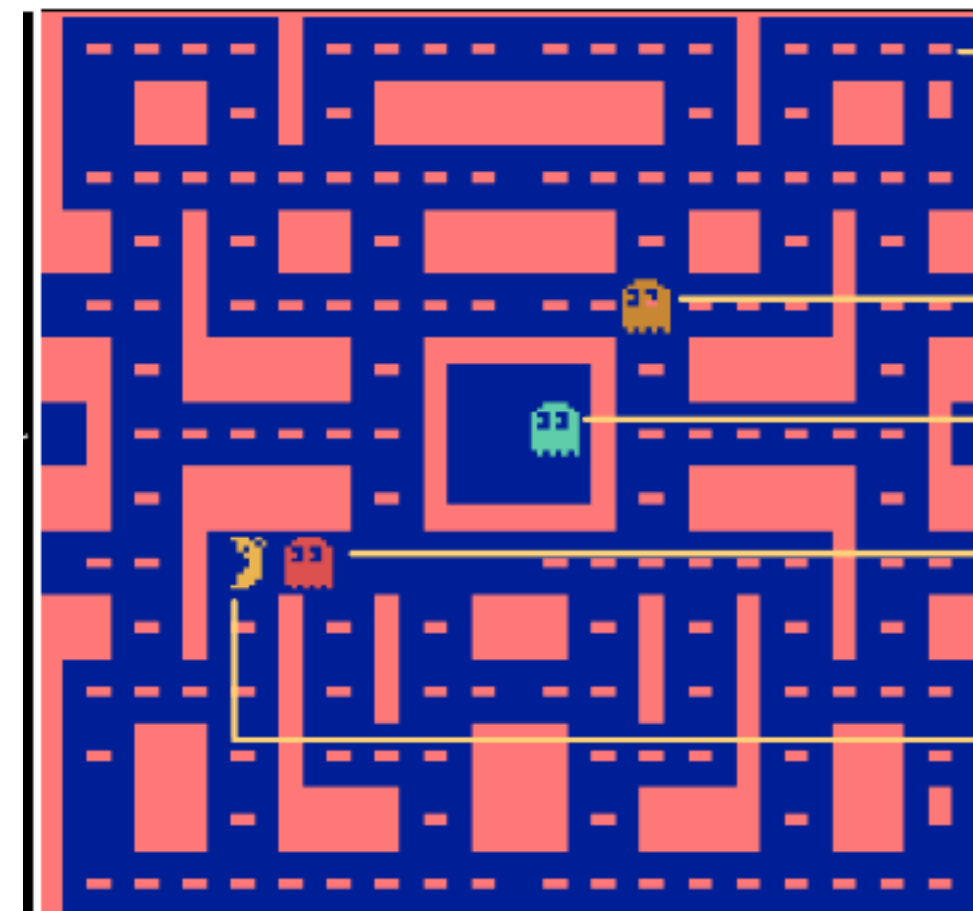
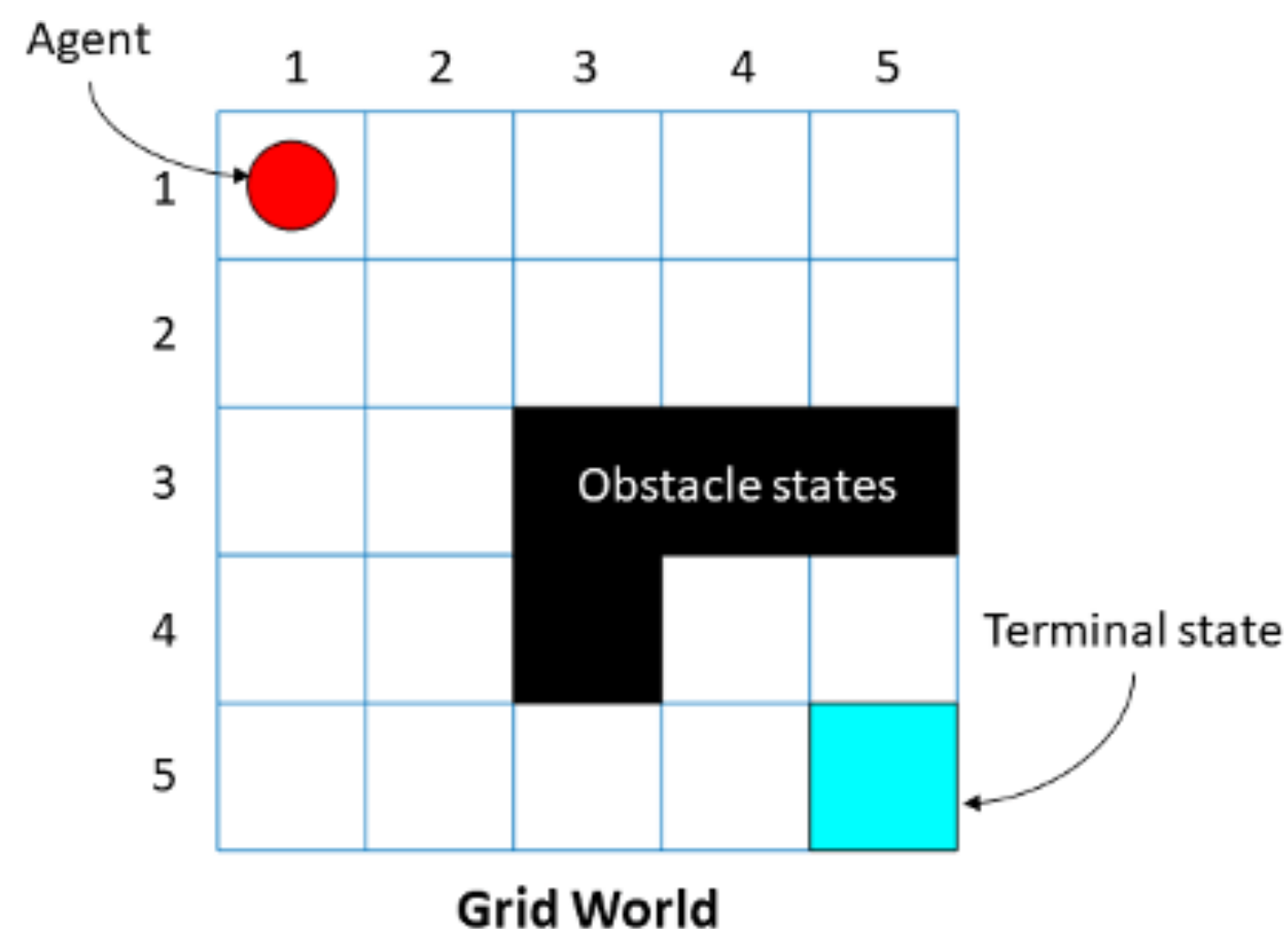


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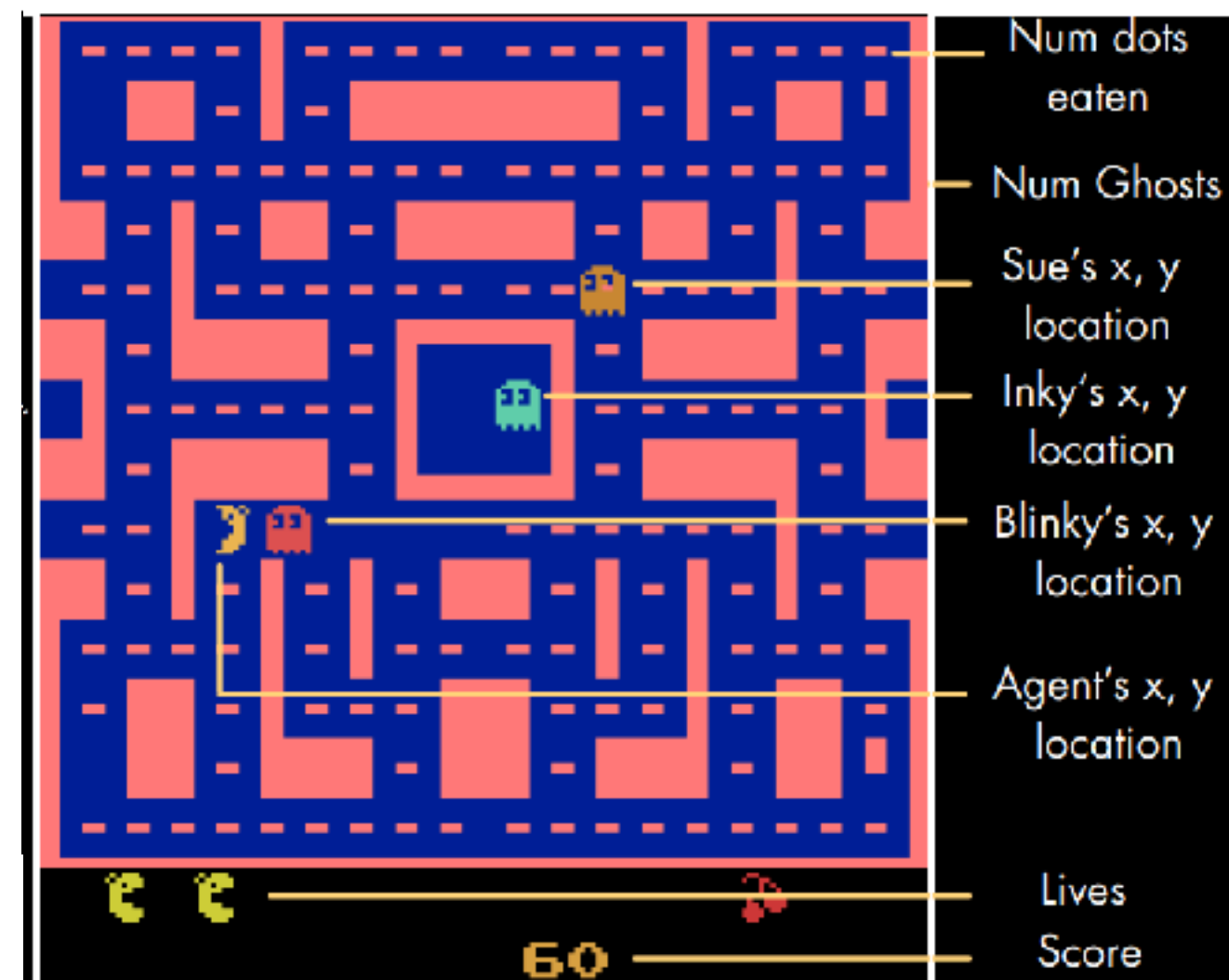
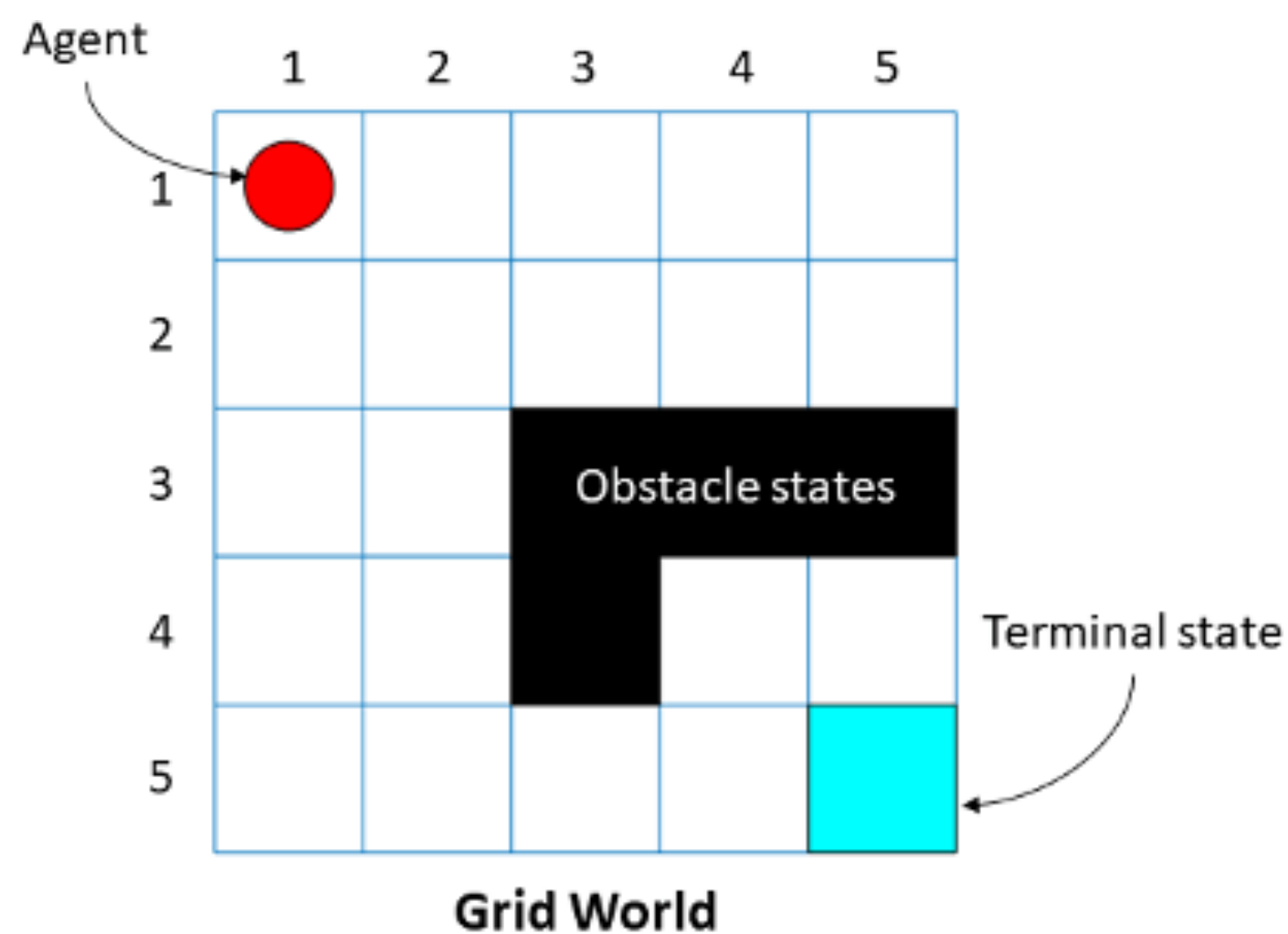
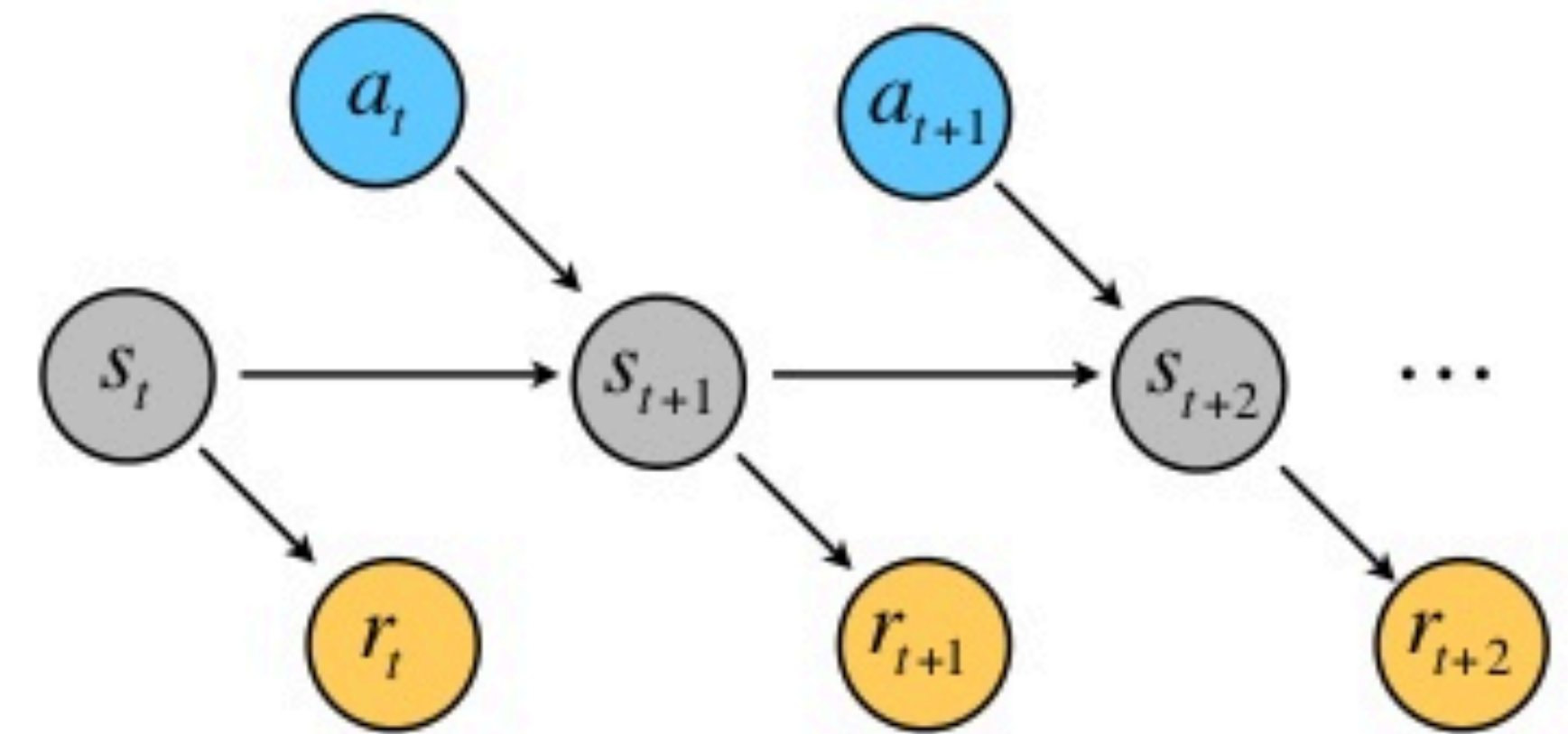
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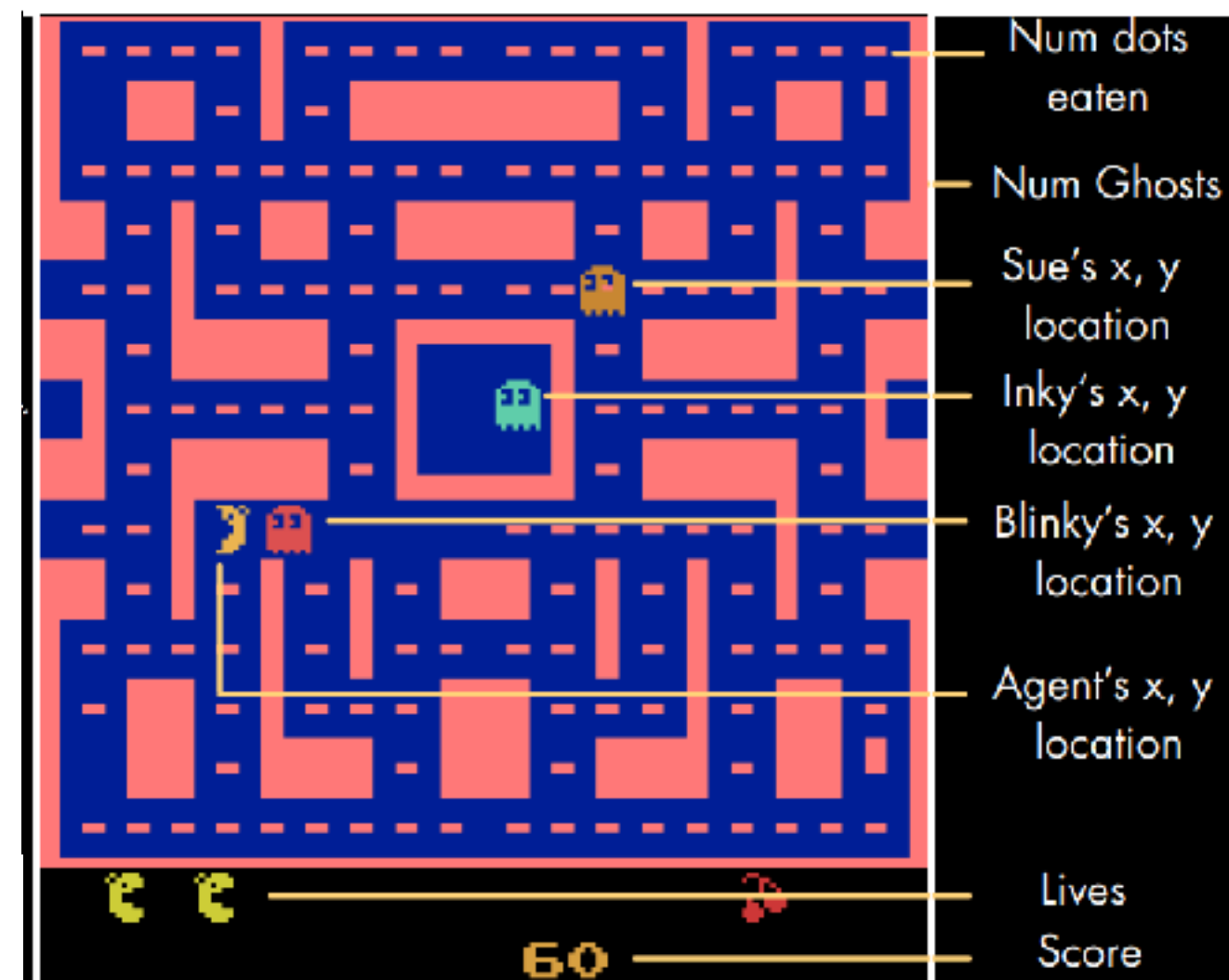
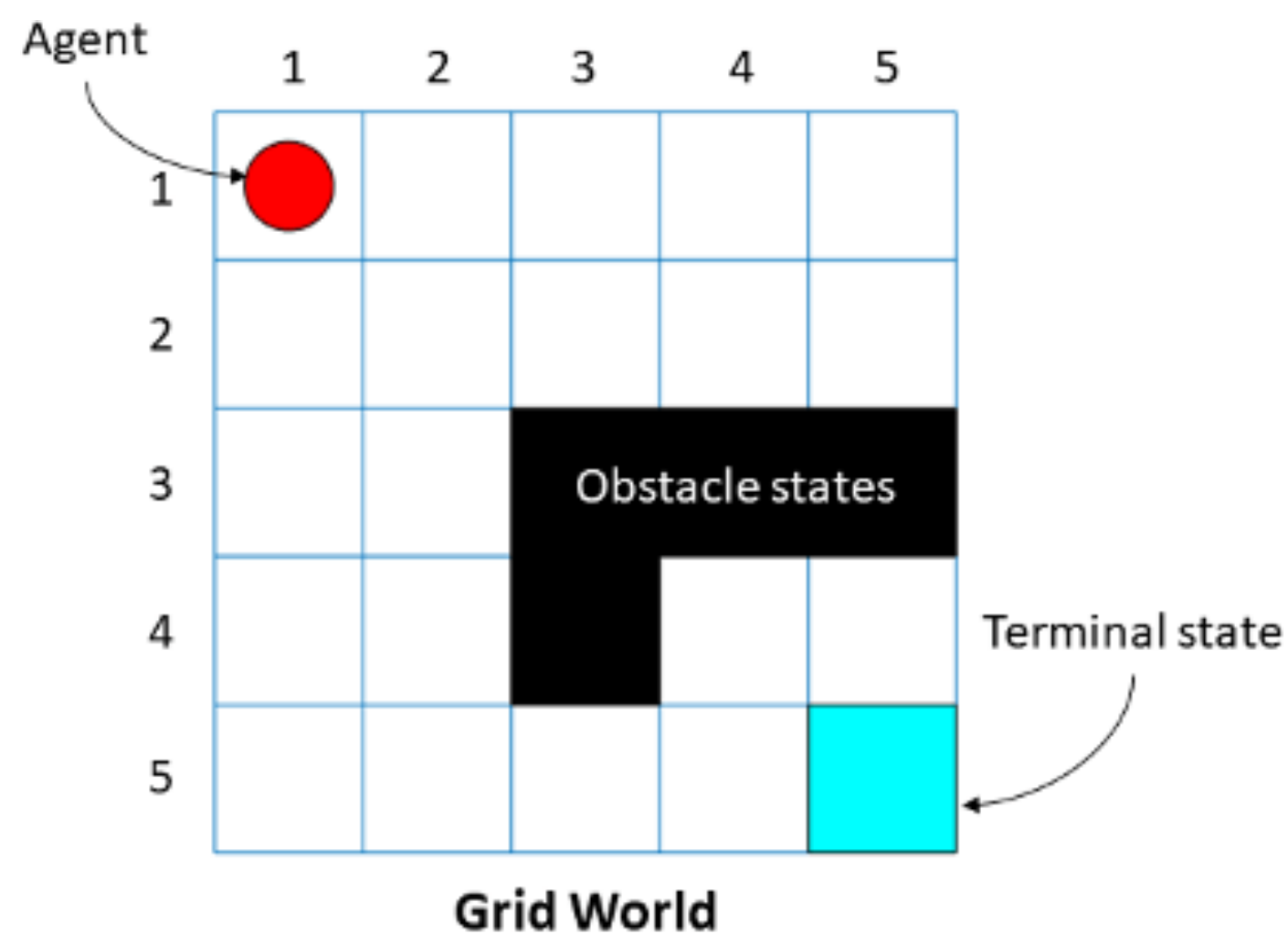
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Partially Observable MDP (POMDP)



Agent



Agent

- **Experiences Rewards**

- **Learns a Policy**

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- How good is a given state? $r_t = R(s_t)$



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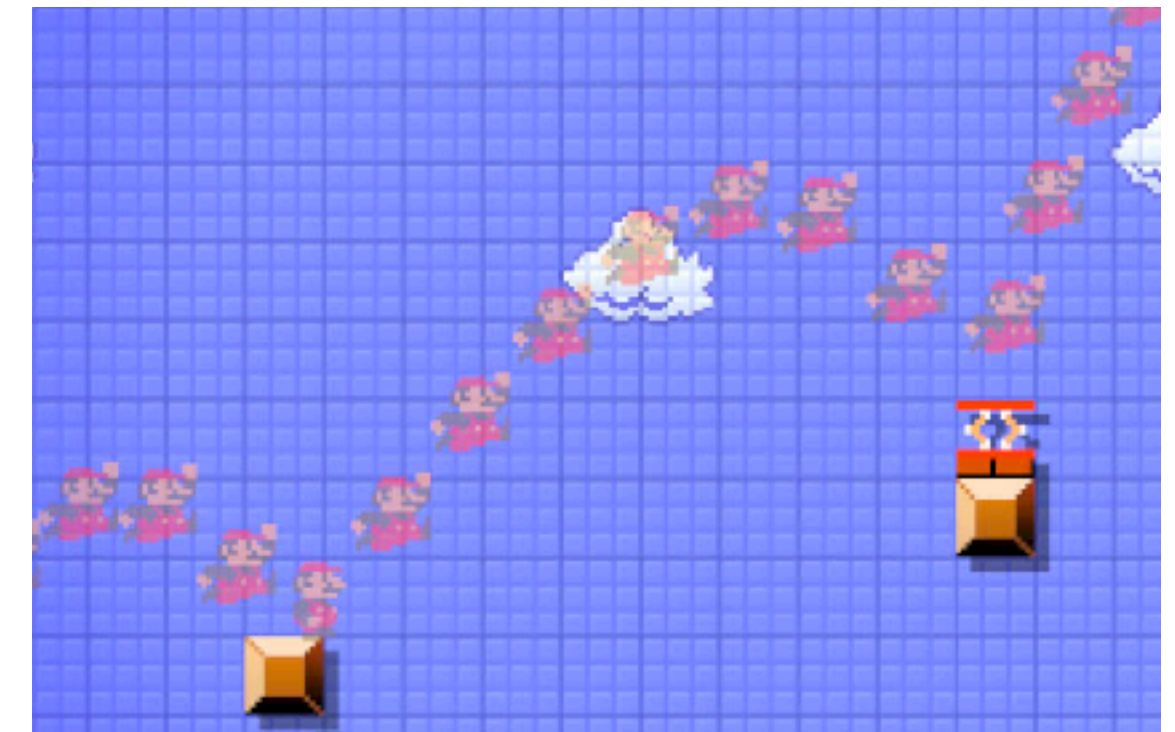


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- How good is a *trajectory* $\tau = (s_0, a_0, s_1, a_1, \dots)$:
$$R(\tau) = \sum_{t=0}^{\infty} \gamma^k r_t$$
 where $\gamma \in [0,1]$ is the temporal discount



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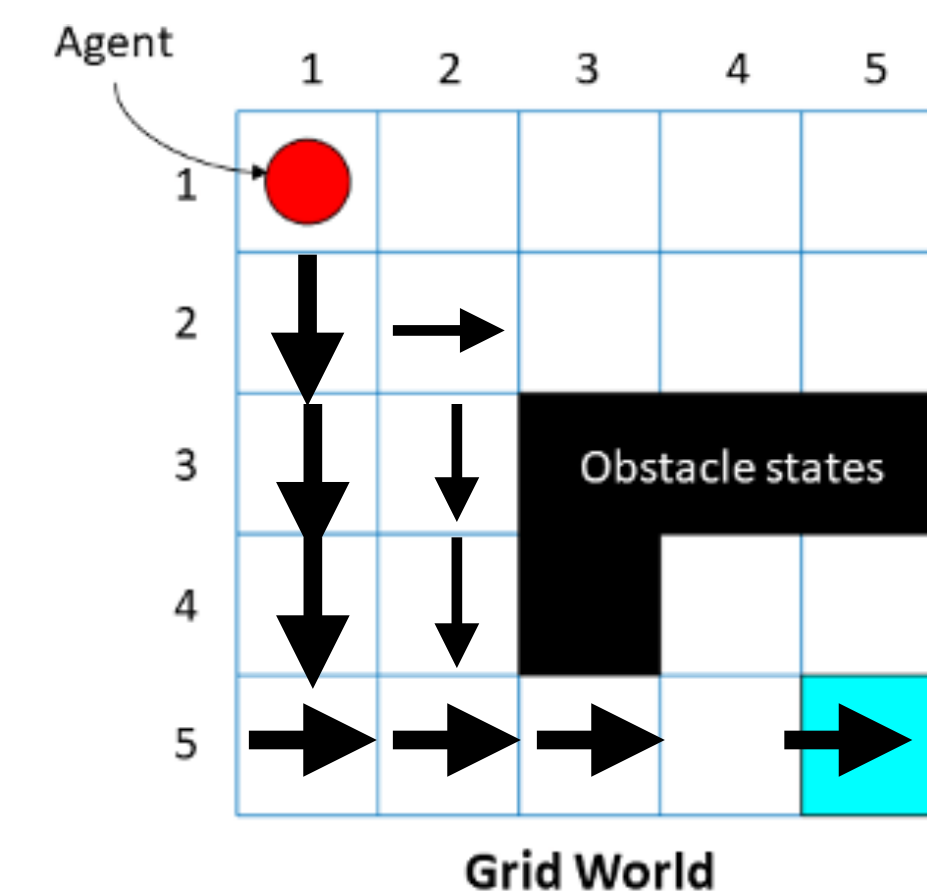
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- **Learns a Policy**

- π defines how to act, where $\pi(a | s)$ is the probability of selecting action a in state s
- sample trajectories from the policy $\tau \sim \pi$



The RL Problem

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Select a policy π^* that maximizes expected rewards

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For this, we need to define a **value function**:

- The expected discounted returns under a policy:

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$$V_{\pi}(s) = \sum_a \pi(a \mid s) \sum_{s'} P(s' \mid s, a) [R(s', a) + \gamma V_{\pi}(s')]$$

- The expectation over a policy is equivalent to summing up all actions and their new state transitions, weighted by their probability
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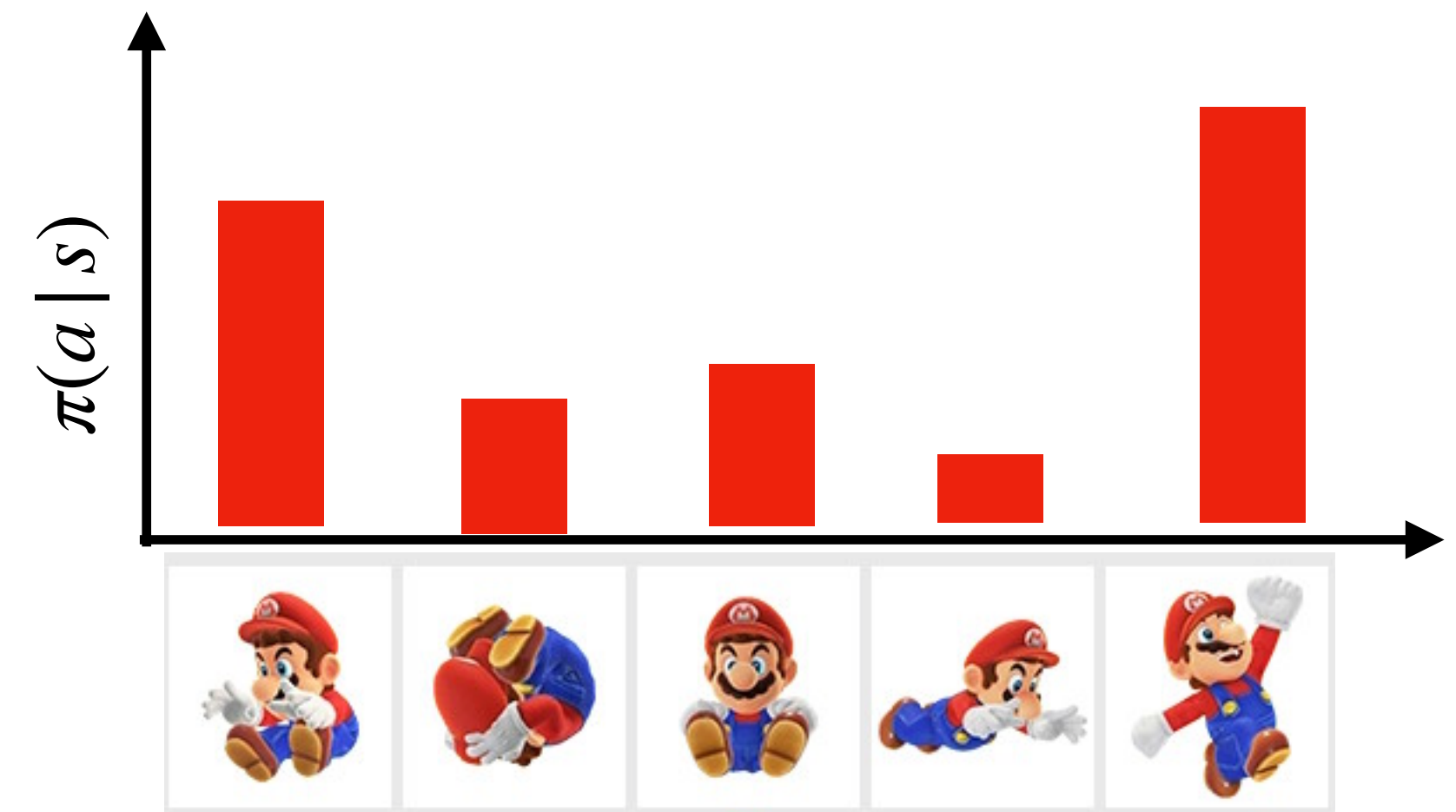
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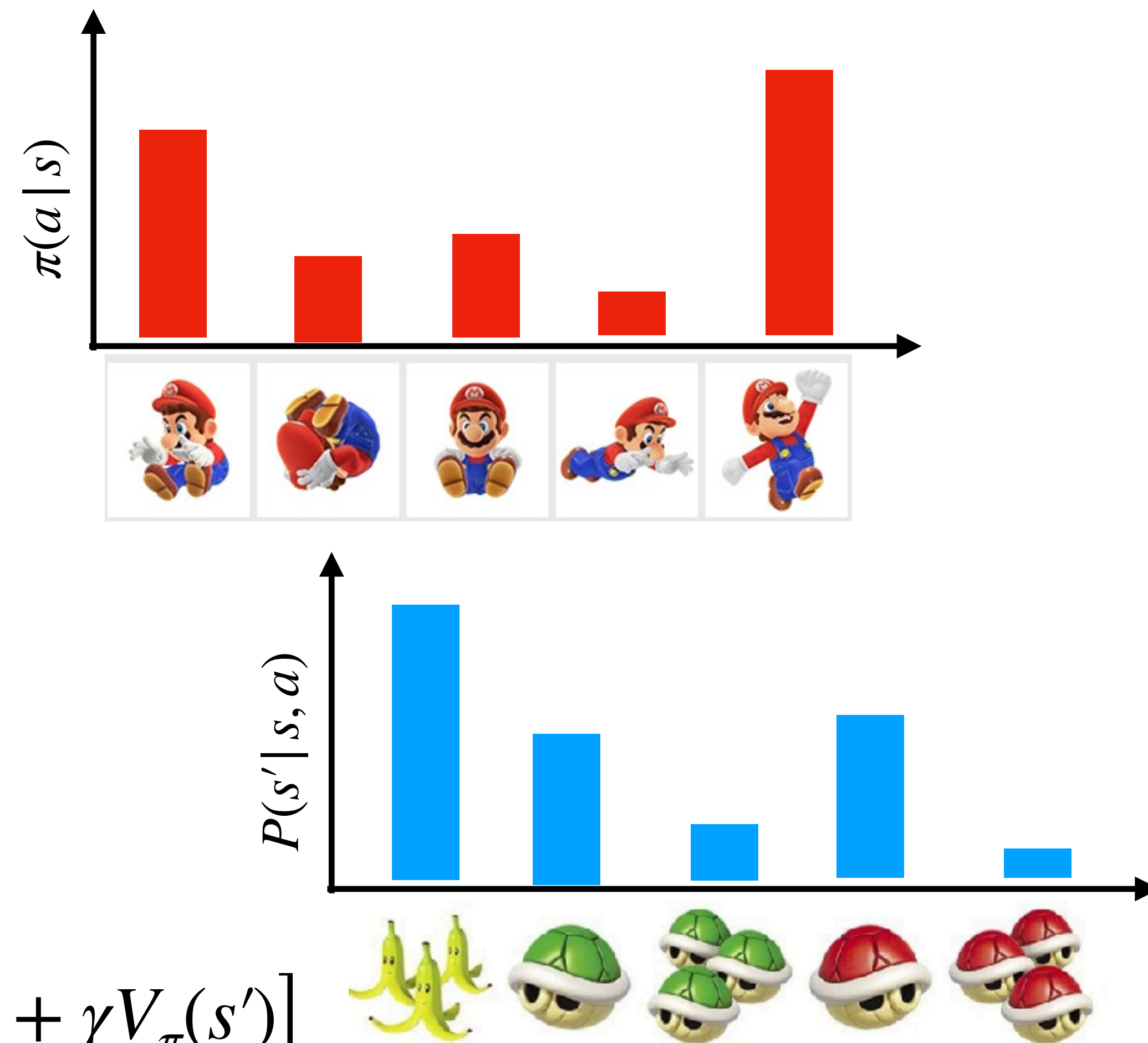
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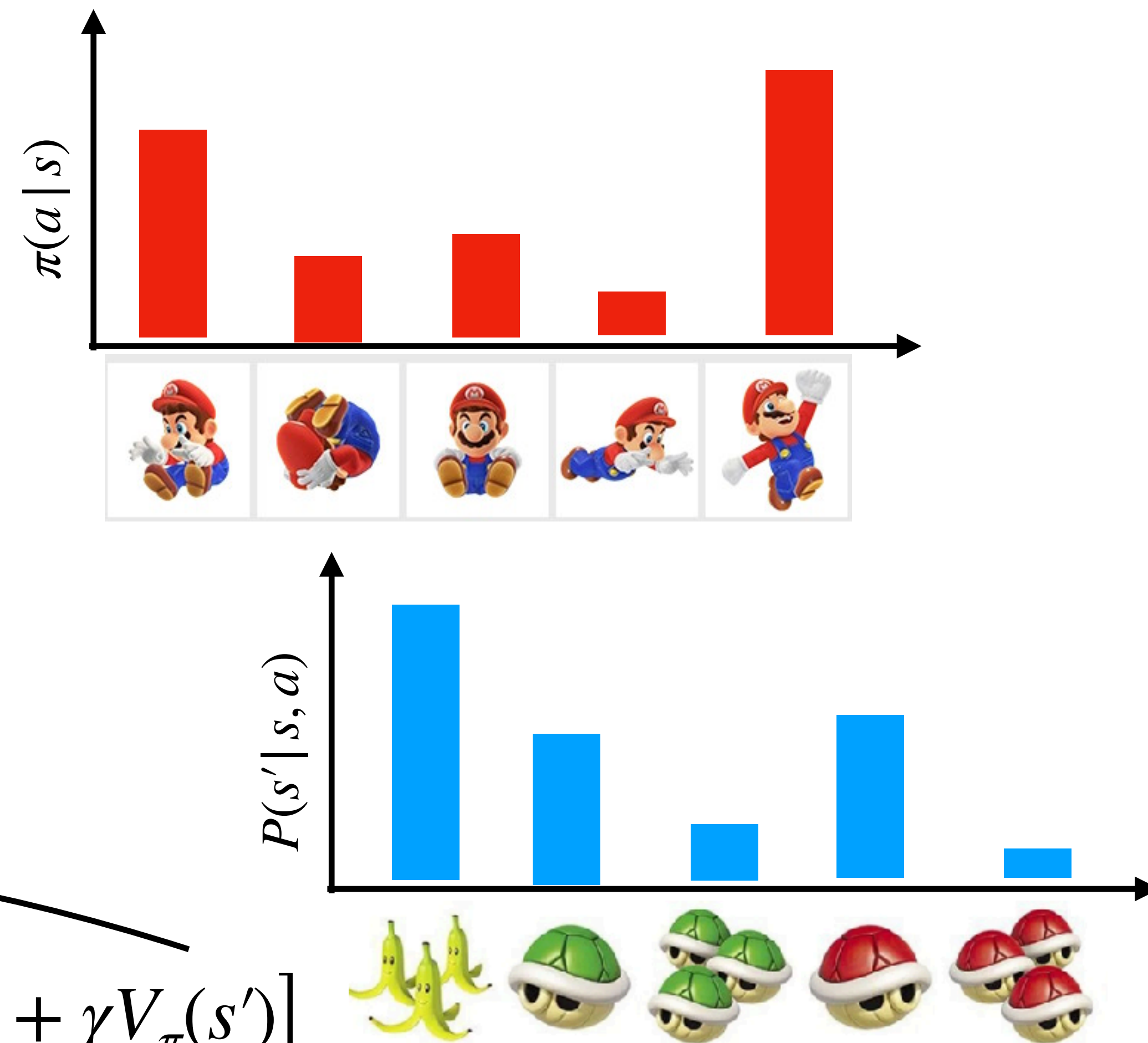
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Finding an optimal policy via Bellman Equations

- Bellman equations are a concept from dynamic programming that provide a recursive method for optimization:

$$V_{\pi}(s) = \sum_a \pi(a | s) \sum_{s'} P(s' | s, a) [R(s', a) + \gamma V_{\pi}(s')]$$

- Theoretically, we can define an optimal value function:

$$V_*(s) = \max_a \sum_{s'} P(s' | s, a) [R(s, a) + \gamma V_*(s')]$$

- Optimal policy:

$$\pi_* = \arg \max_a V_*(s)$$

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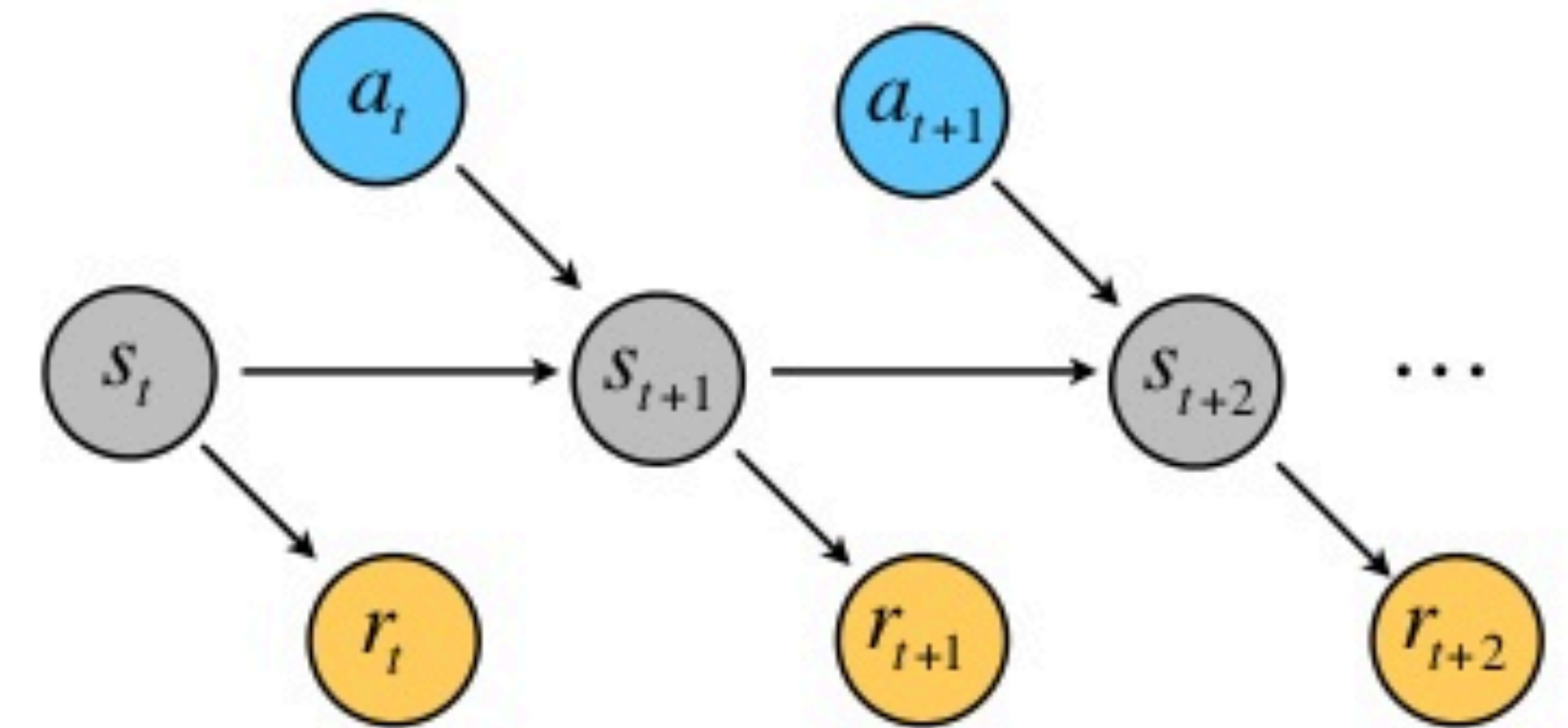
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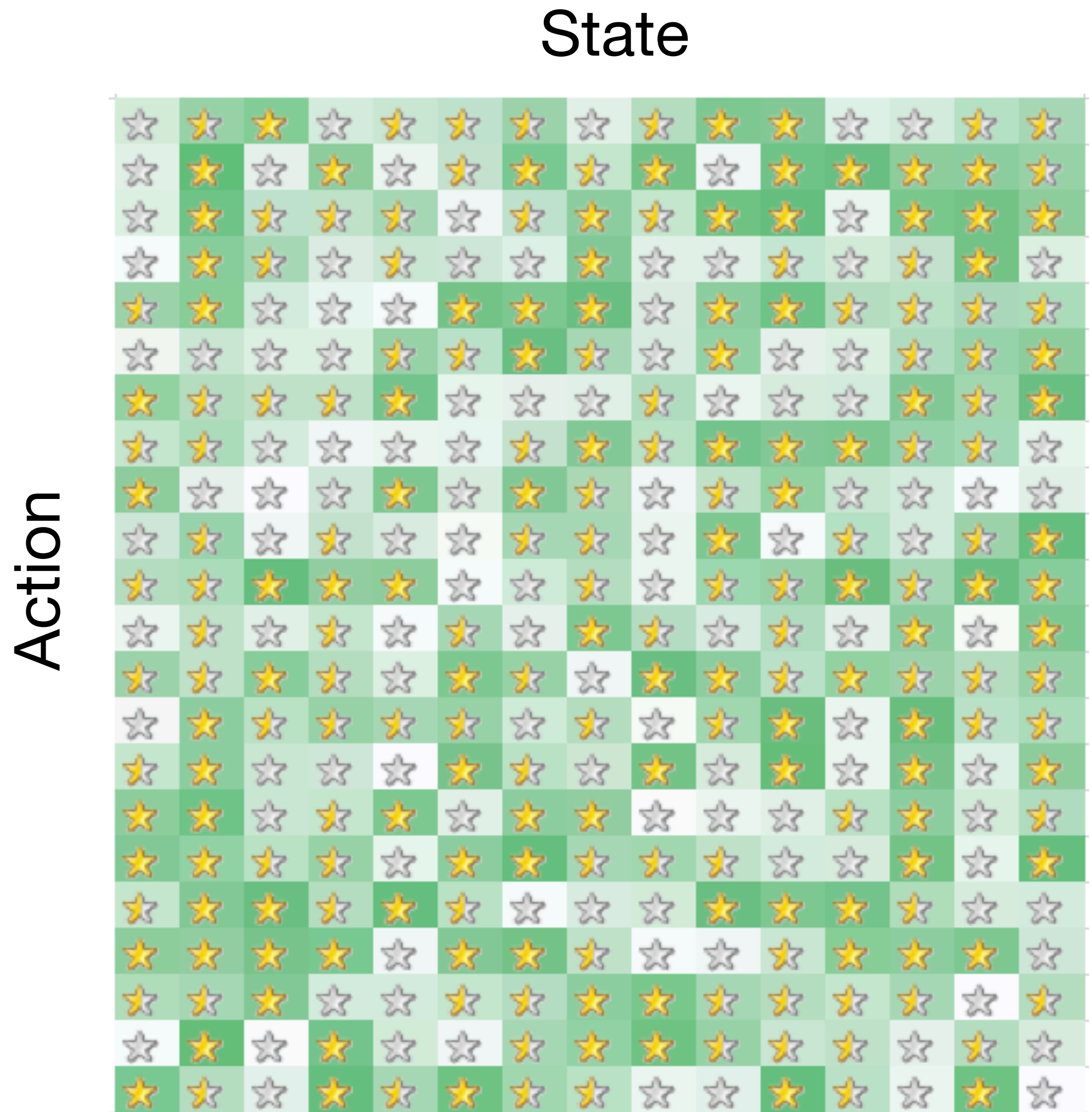
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Tabular methods

- Based on methods from Dynamic programming (Bellman, 1957), Tabular methods were first proposed as solutions for RL problems by Minsky (1961)
- Think of a giant lookup table, where we store a value representation
- Value iteration and policy iteration are examples
- Caveat: solutions require repeat visits to each state, which is infeasible in most real-world problems



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State

Action

| | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| ☆ | ☆ | ☆ | ☆ | ☆ | ? | ? | ? | ? | ? | ? | ? | ? | ? | ? |
| ☆ | ☆ | ☆ | ☆ | ☆ | ? | ? | ? | ? | ? | ? | ? | ? | ? | ? |
| ☆ | ☆ | ☆ | ☆ | ☆ | ? | ? | ? | ? | ? | ? | ? | ? | ? | ? |
| ☆ | ☆ | ☆ | ☆ | ☆ | ? | ? | ? | ? | ? | ? | ? | ? | ? | ? |
| ☆ | ☆ | ☆ | ☆ | ☆ | ? | ? | ? | ? | ? | ? | ? | ? | ? | ? |
| ☆ | ☆ | ☆ | ☆ | ☆ | ? | ? | ? | ? | ? | ? | ? | ? | ? | ? |
| ? | ? | ? | ? | ? | ? | ? | ? | ? | ? | ? | ? | ? | ? | ? |
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| ? | ? | ? | ? | ? | ? | ? | ? | ? | ? | ? | ? | ? | ? | ? |
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| ? | ? | ? | ? | ? | ? | ? | ? | ? | ? | ? | ? | ? | ? | ? |
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| ? | ? | ? | ? | ? | ? | ? | ? | ? | ? | ? | ? | ? | ? | ? |

Value iteration

Iteratively visit all states and update the value function until a “good enough” solution has been reached.

1. Initialize the value function as $V_0(s) = 0$ for all states

2. For all s in \mathcal{S} :

$$V_{k+1}(s) = \max_{a \in A} \sum_{s'} P(s' | s, a) [R(s, a) + \gamma V_k(s')]$$

until $\max_{s \in \mathcal{S}} |V_k(s) - V_{k-1}(s)| < \theta$ Bellman residual

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V_k converges on V_* as $k \rightarrow \infty$, and perhaps sooner, but with many costly sweeps through the state space

Policy Iteration

Alternate between evaluating a policy and then improving the policy.

Start with π_0 (typically a random policy), and then iterate for all $s \in \mathcal{S}$ in each step

- **Policy Evaluation**

$$V_{\pi_k}(s) = \mathbb{E}_{\pi_k} \left[R(s', a) + \gamma V_{\pi_k}(s') \right]$$

- **Policy Improvement**

$$\pi_{k+1} = \arg \max_a \sum_{s'} P(s' | s, a) \left[R(s, a) + \gamma V_{\pi_k} \right]$$

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$$V_{\pi_k}(s) = \mathbb{E}_{\pi_k} \left[R(s', a) + \gamma V_{\pi_k}(s') \right]$$

- **Policy Improvement**

$$\pi_{k+1} = \arg \max_a \sum_{s'} P(s' | s, a) \left[R(s, a) + \gamma V_{\pi_k} \right]$$

Policy can converge faster than value function, but still requires visiting all states $2n$ times and lacks convergence guarantees



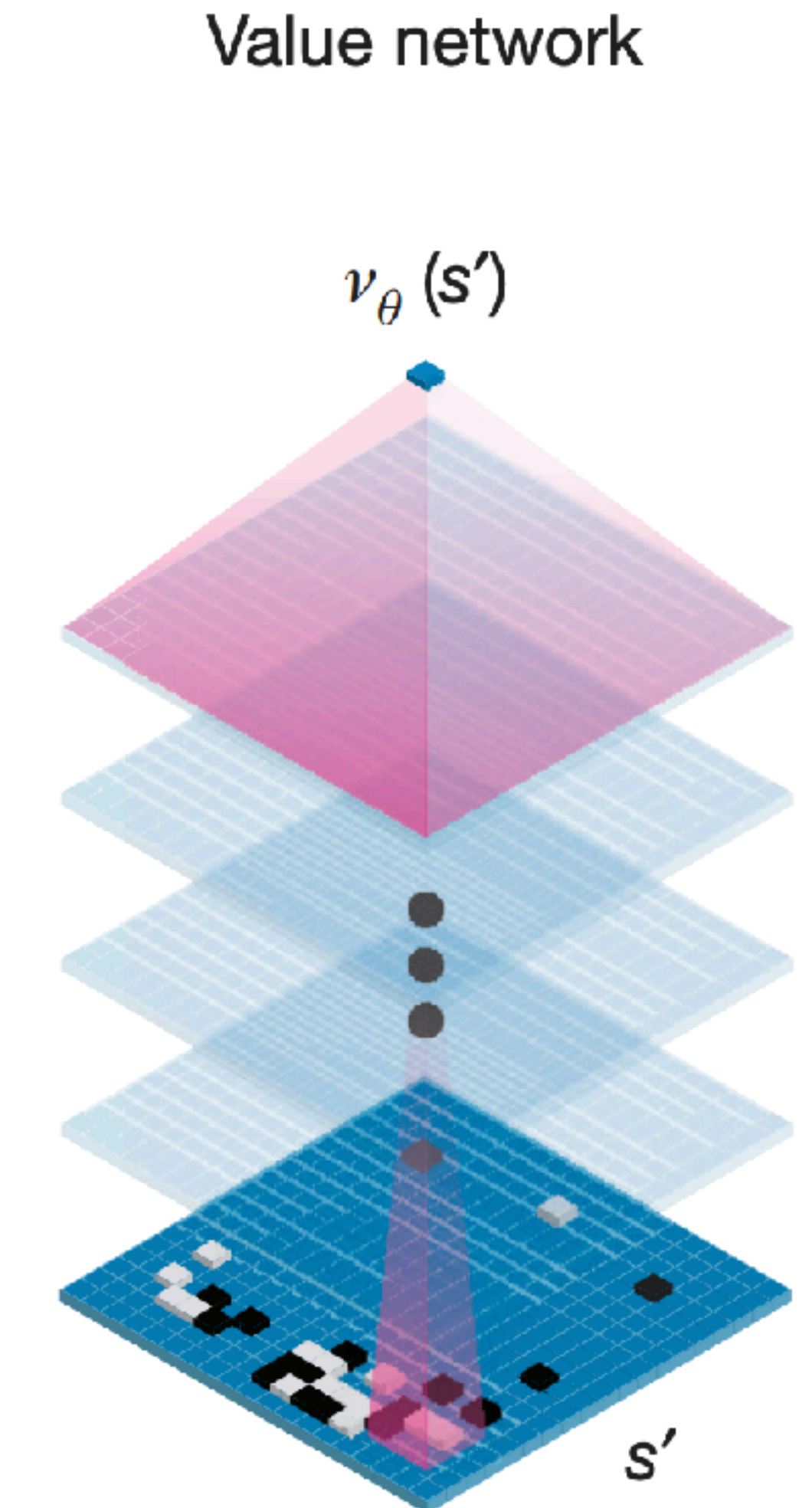
Value function approximation

Instead of learning the value for each state independently, learn a value function mapping each state to some value:

$$f : s \in \mathcal{S} \rightarrow V_{\theta}(s)$$

... a variety of methods are available including:

- linear function approximation (e.g., regression)
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- Gaussian process regression (non-parametric)



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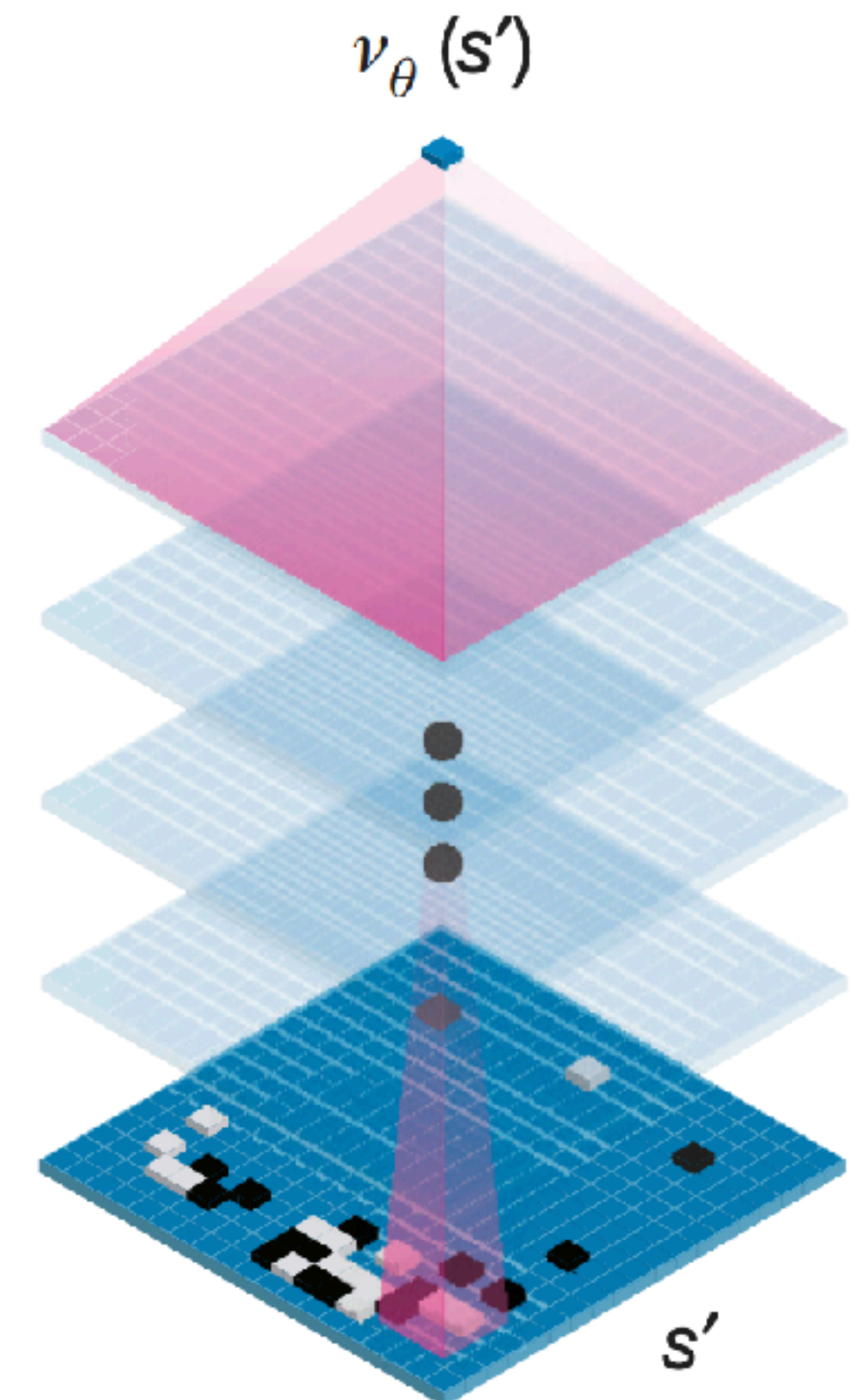
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Value network



Silver et al. (2016)

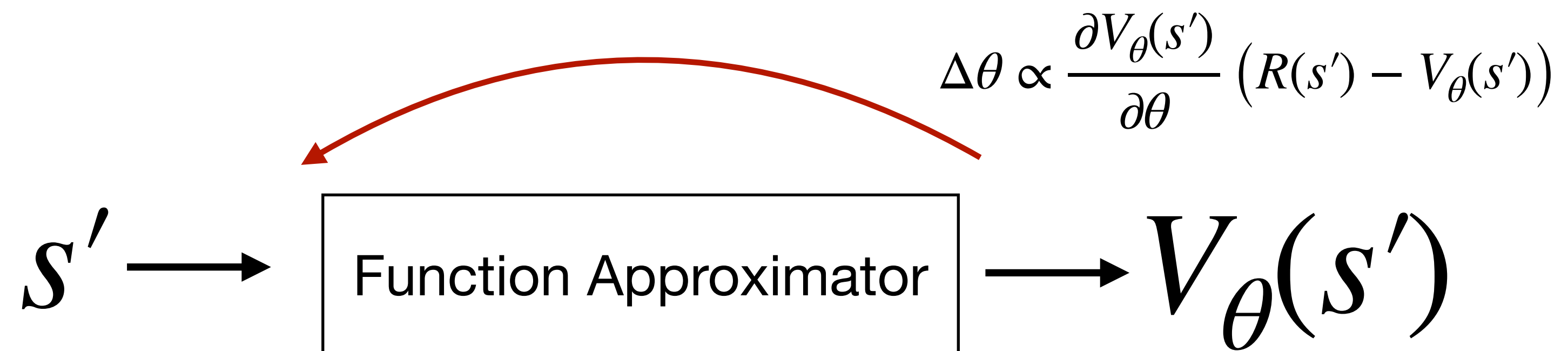
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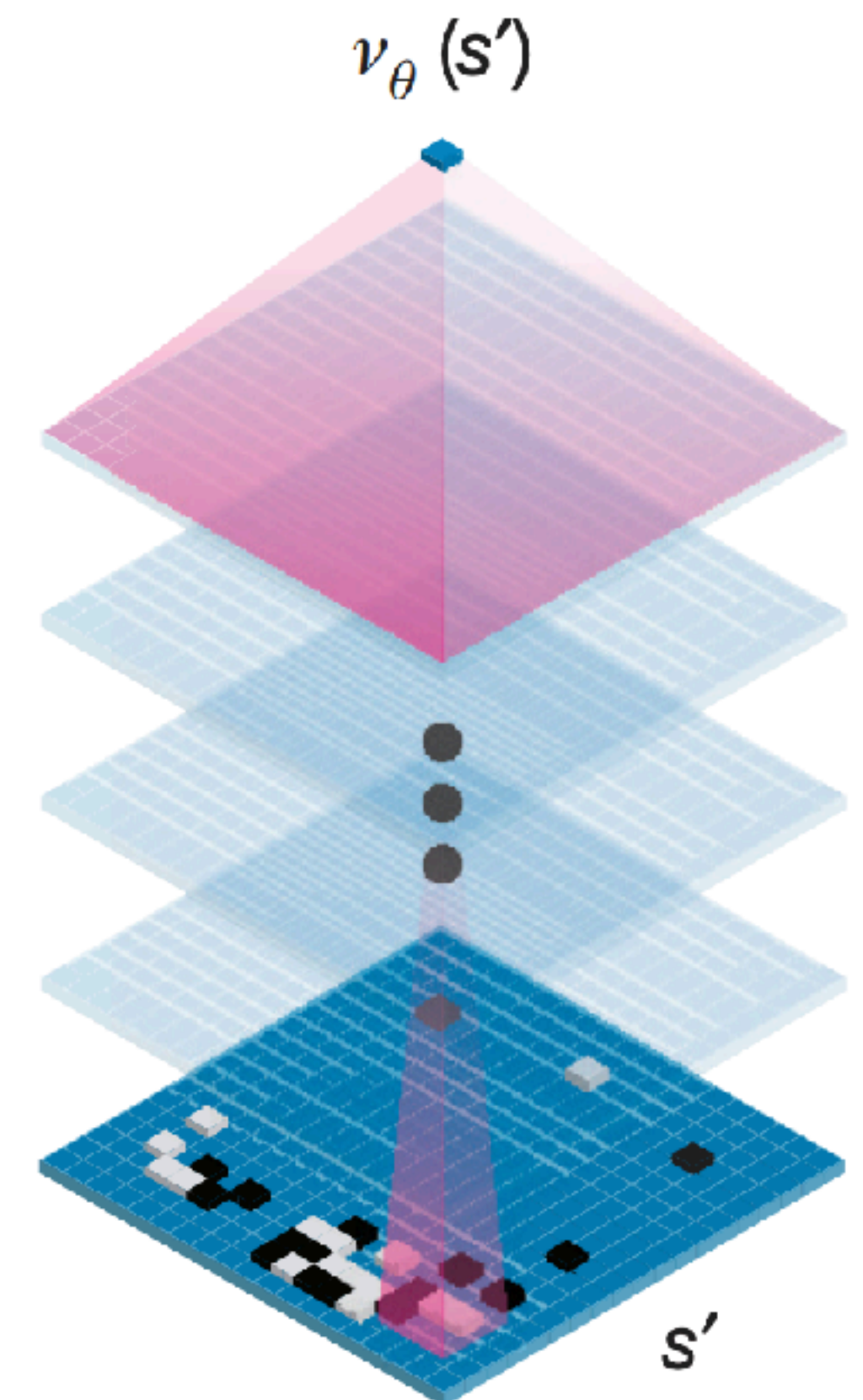
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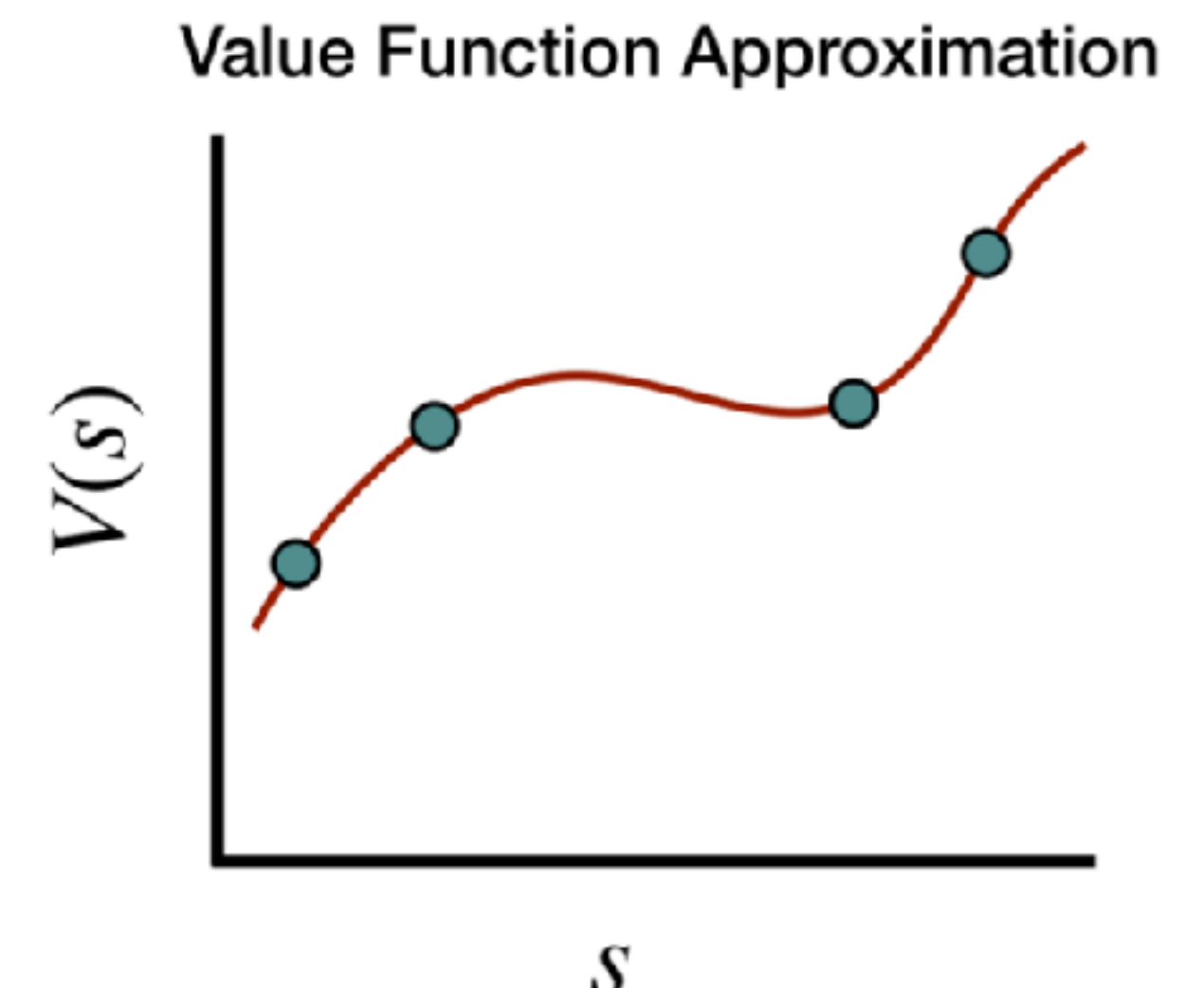
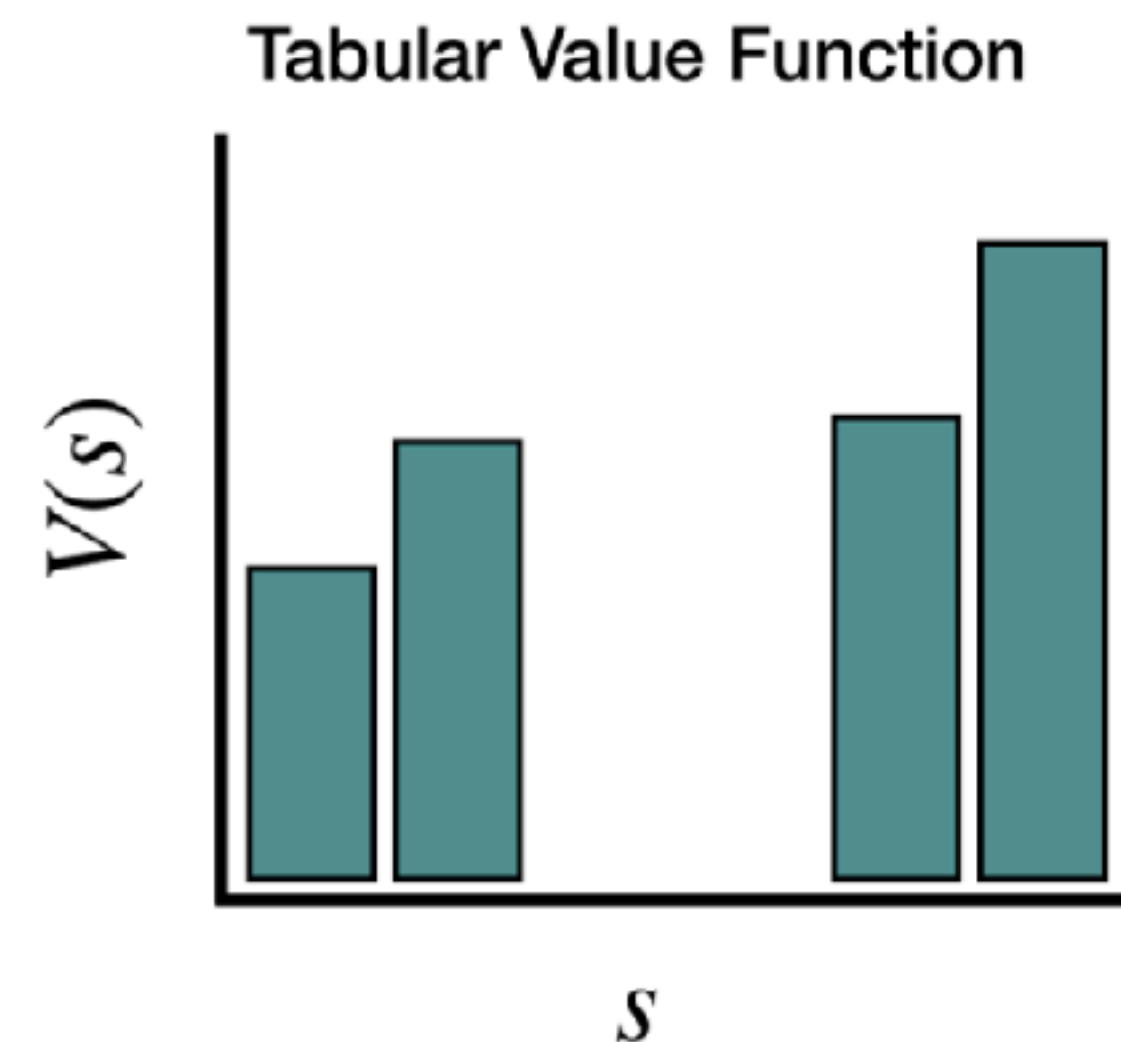
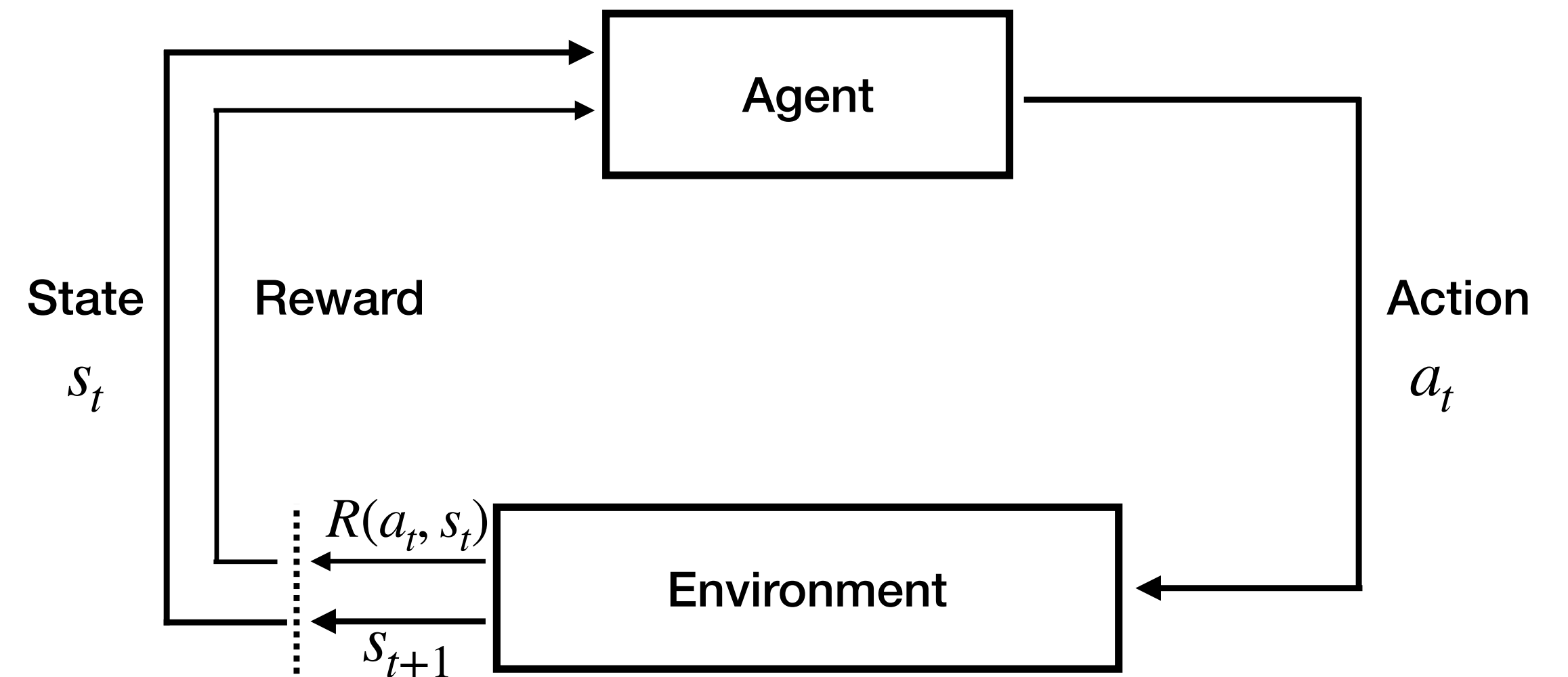
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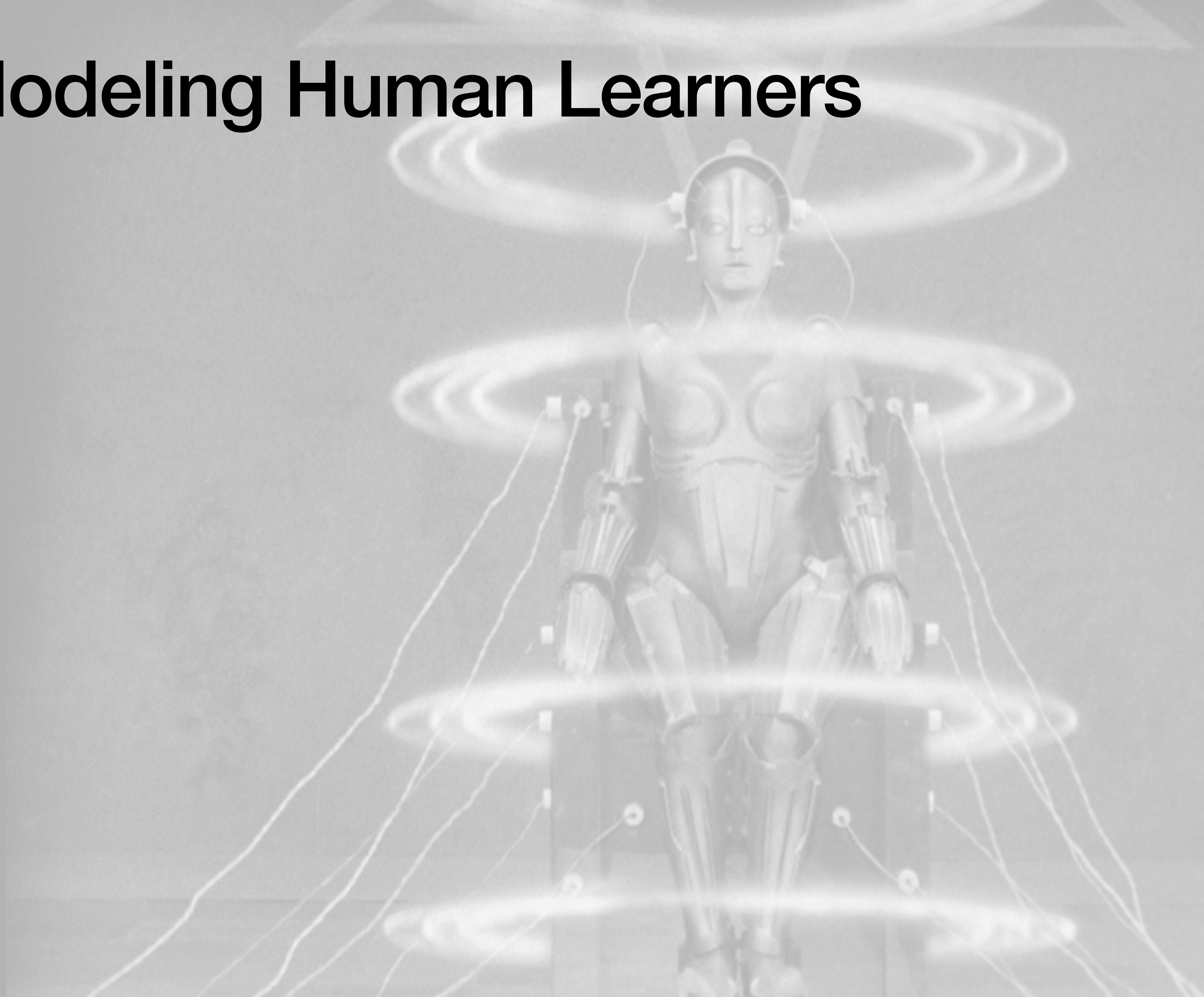
Silver et al. (2016)

Quick recap

- RL framework defines interactions between an **agent** and the **environment**
 - The environment defines the transitions between states and provides rewards
 - The agent learns a value function and then turns this into a policy
- Traditional solutions to RL problems can be broadly classified into either **tabular methods** or **value function approximation**



Modeling Human Learners



Multi-armed bandit

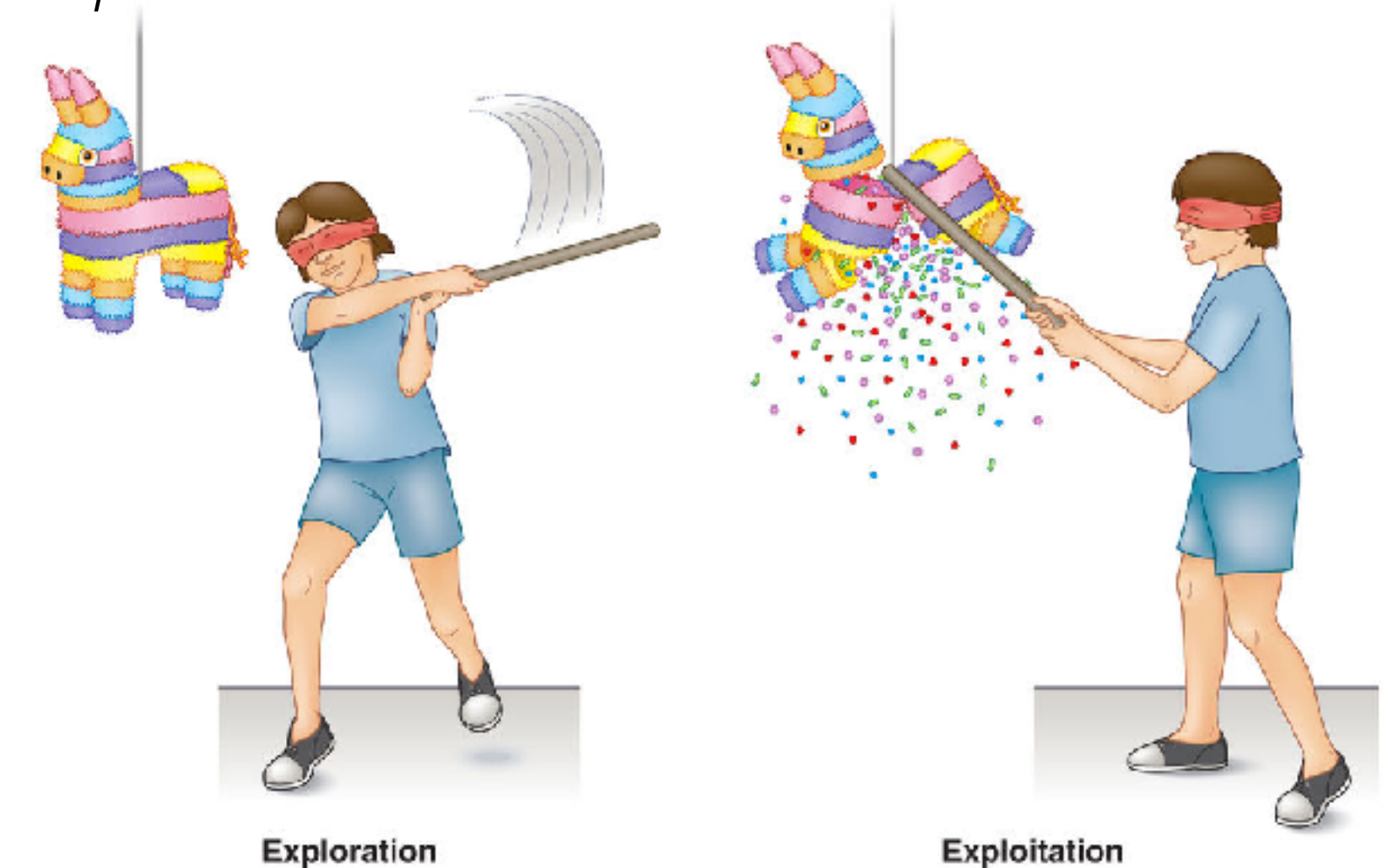
Multi-armed bandit

- Colorful metaphor for a row of slot machines



Multi-armed bandit

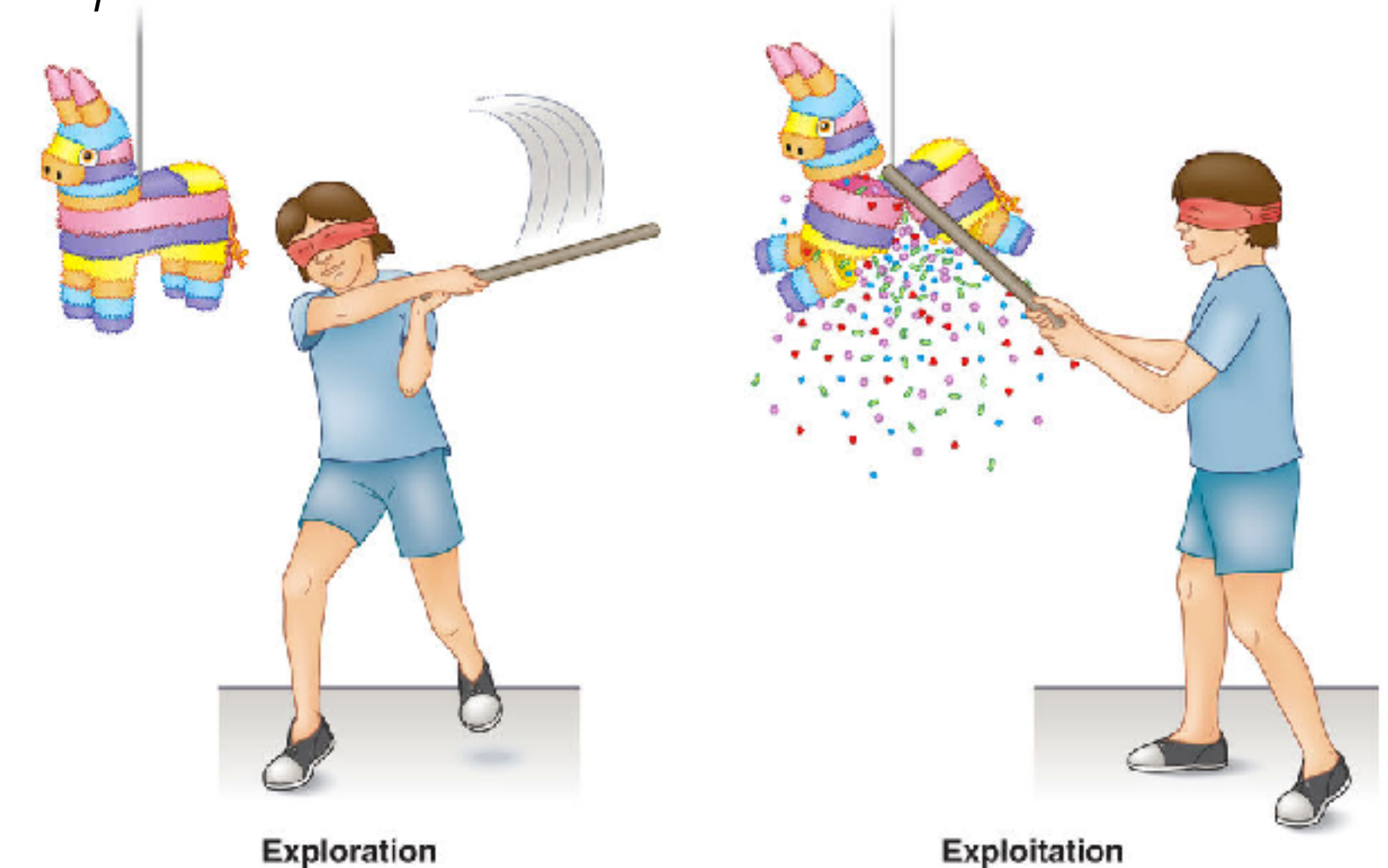
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 - No need to discount future states
 - Instead of state-value function $V(s)$ we can represent the value of an action $V(a)$ or more properly, using an action-value function $Q(s, a)$



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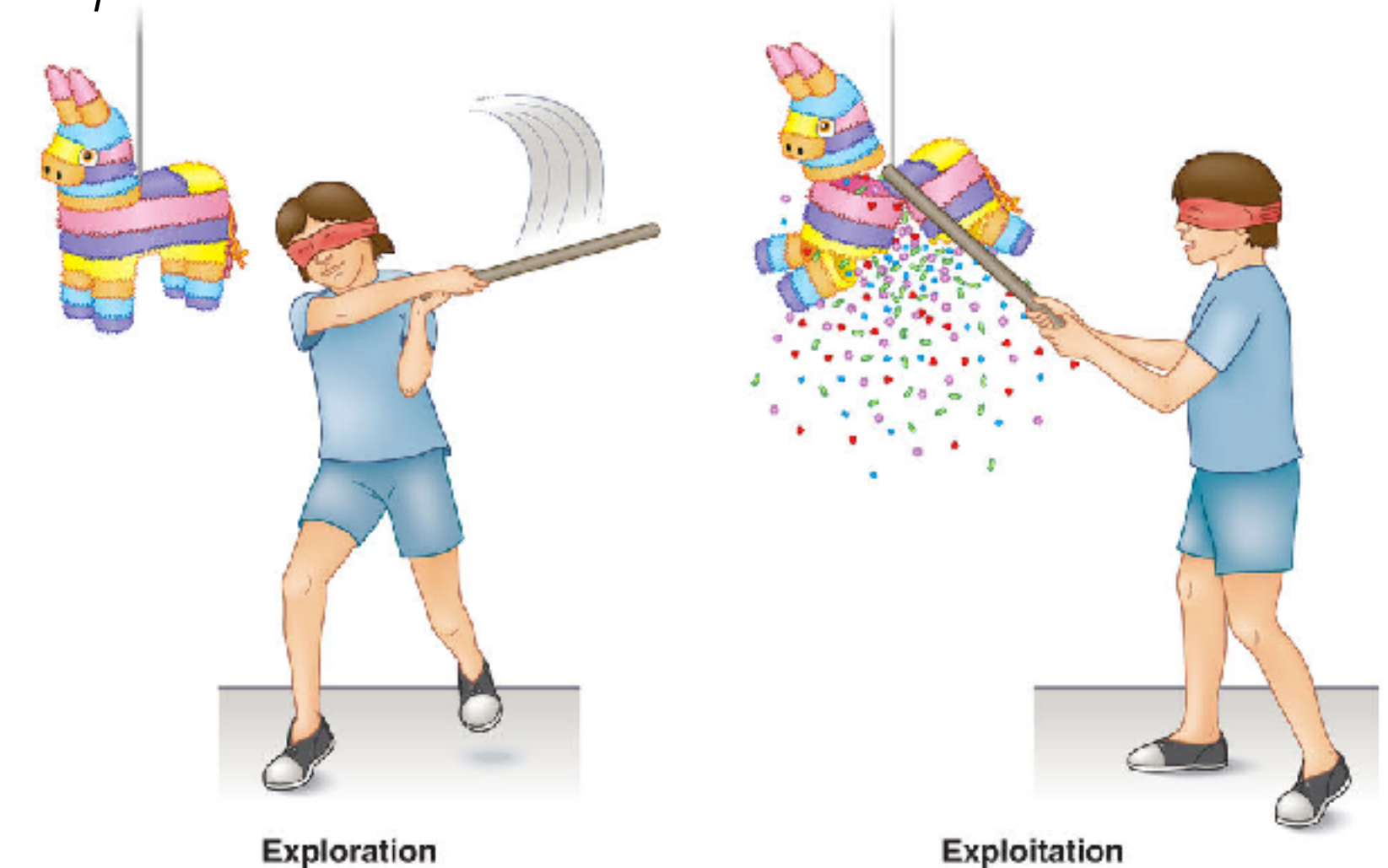
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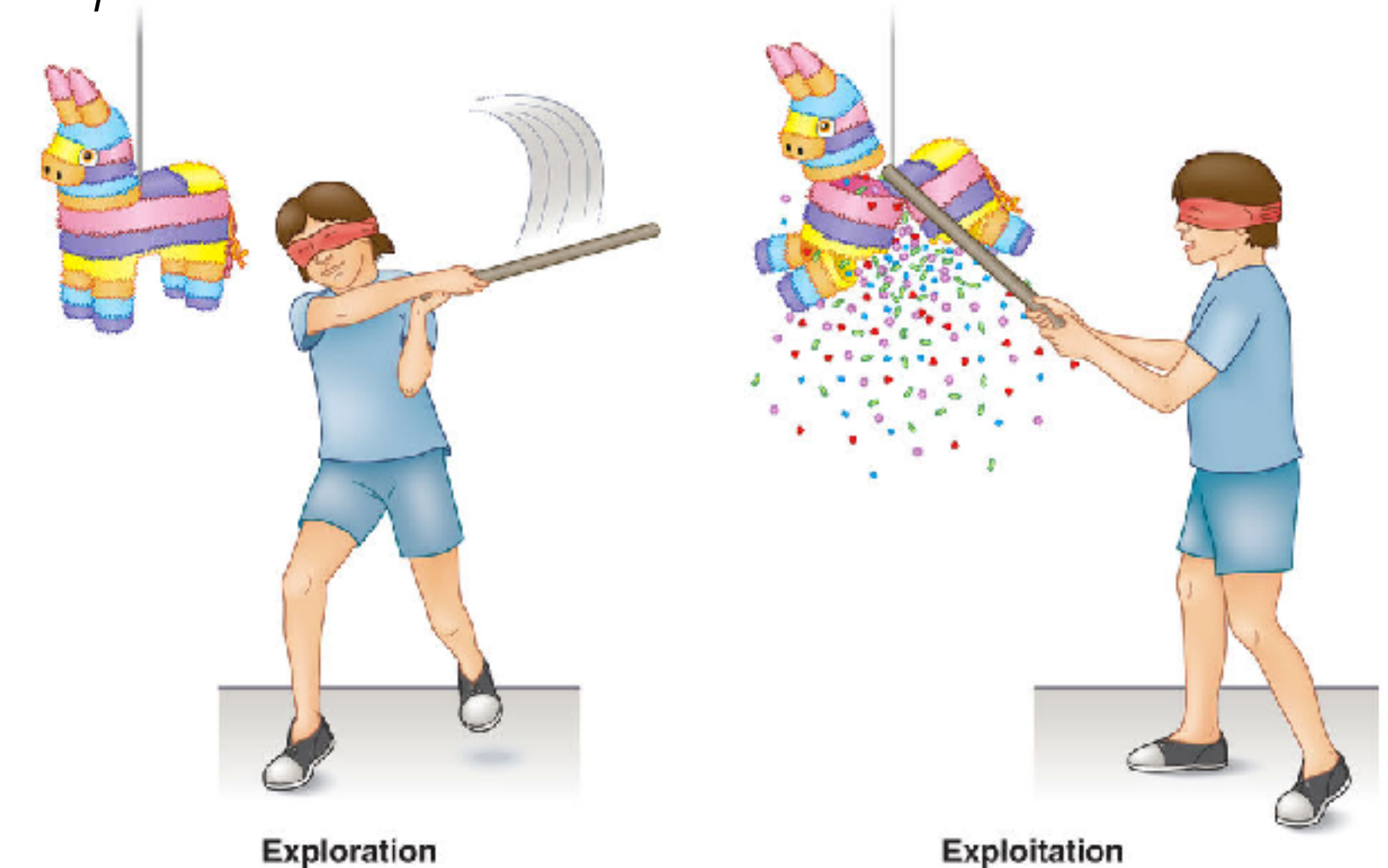
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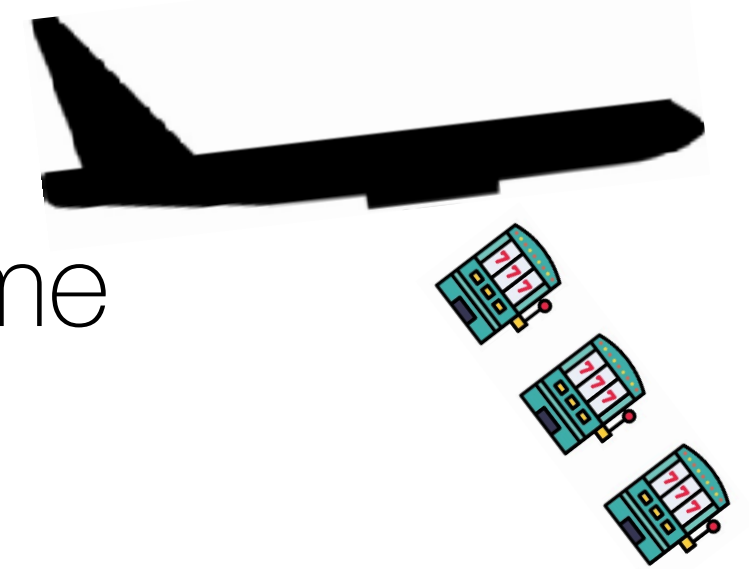
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Brief aside: State-Value function vs. Action-value function

So far, I've focused on describing state-value functions:

$$V_{\pi}(s) = \mathbb{E}_{\tau \sim \pi}[R(\tau) \mid s_0 = s]$$

However, you can also describe a RL model using the action-value function:

$$Q_{\pi}(s, a) = \mathbb{E}_{\tau \sim \pi}[R(\tau) \mid s_0 = s, a_0 = a]$$

Both are equivalent under:

$$V_{\pi}(s) = \sum_{a \in A} \pi(a \mid s) * Q_{\pi}(s, a)$$

Rescorla-Wagner and Q-learning: the Delta Rule

Rescorla-Wagner and Q-learning: the Delta Rule

Rescorla-Wagner (1972) model

- Learning as an active process of making predictions about the world
- Predict the value of stimulus \mathbf{x}_t with a linear combination of weights \mathbf{w}_t :

$$V(\mathbf{x}_t) = \mathbf{w}_t^\top \mathbf{x}_t$$

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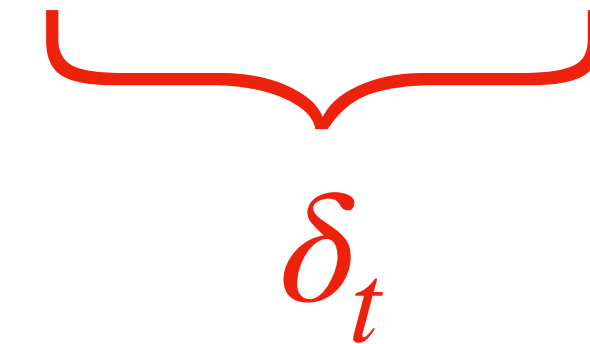
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δ_t

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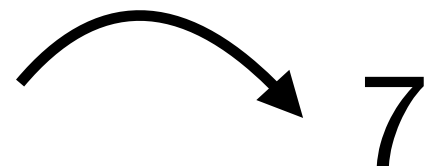
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7

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Temporal Difference Learning

For simplicity, I'm omitting the temporal difference (TD) error, which looks like:

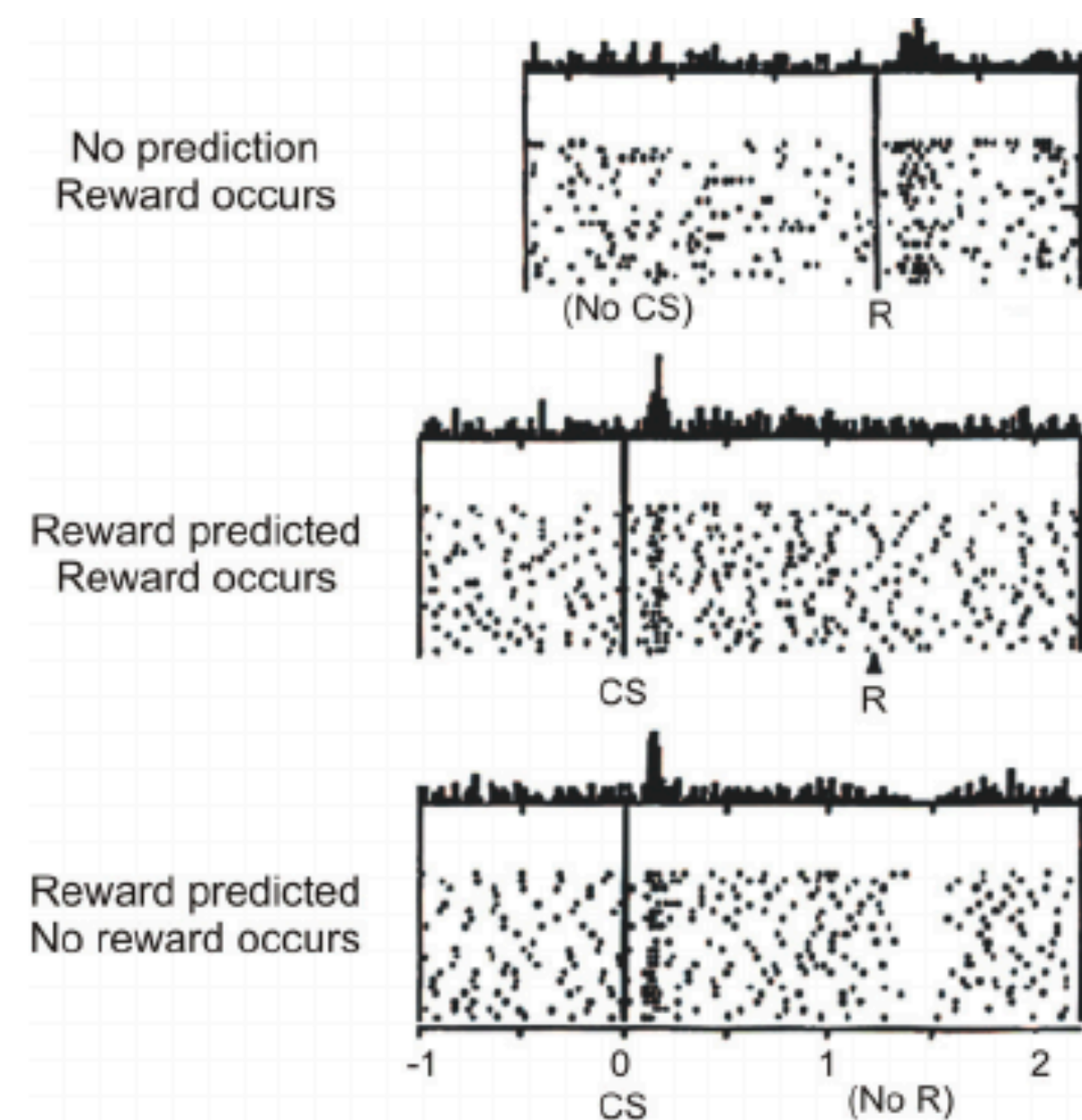
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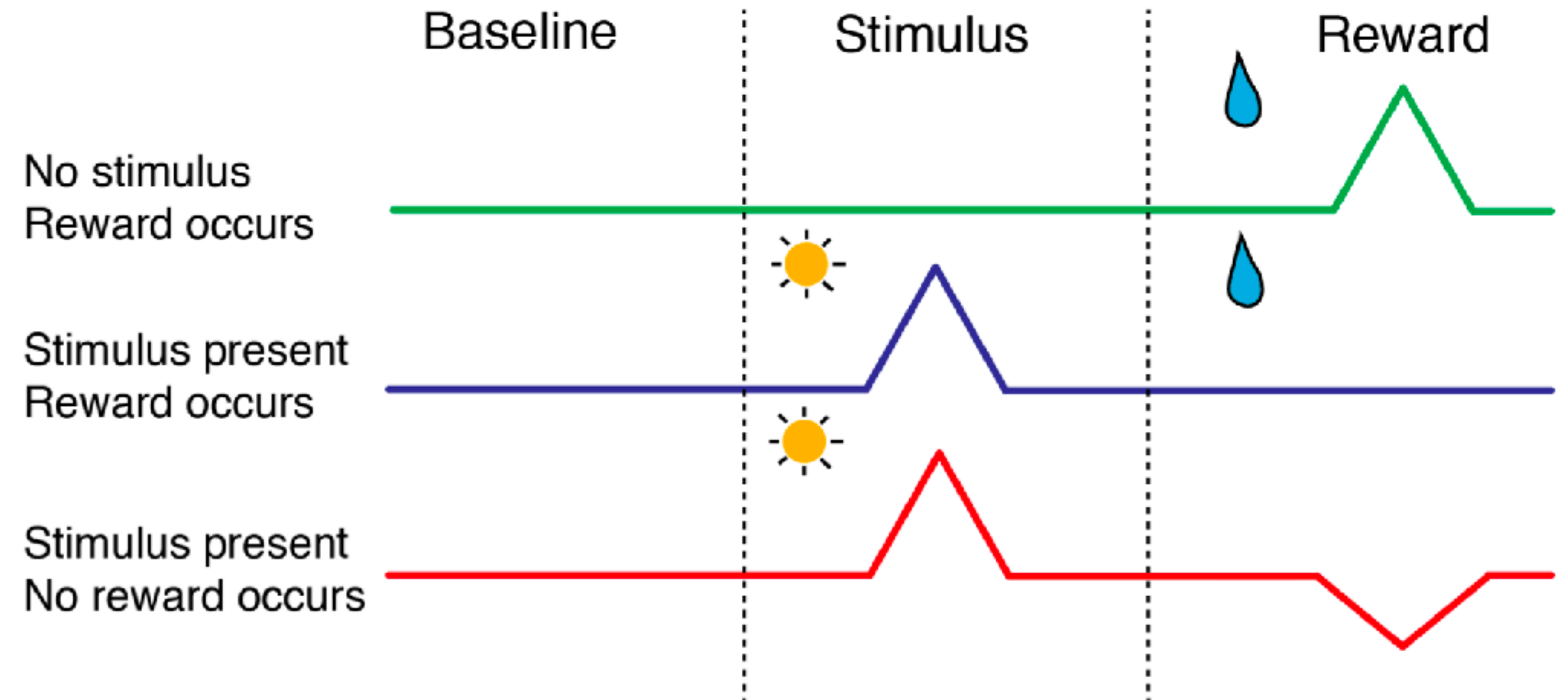
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Dopamine Reward Prediction Error



Schultz et al. (1997)



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$$\text{action} = \begin{cases} \max_a Q(a) & \text{with } p(1 - \epsilon) \\ \text{random action} & \text{with } p(\epsilon) \end{cases}$$

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Q-values

$$\begin{bmatrix} 1.3 \\ 5.1 \\ 0.7 \\ 1.1 \end{bmatrix}$$

$$\rightarrow \frac{\exp(Q(a_i)/\tau)}{\sum_j^n \exp(Q(a_j)/\tau)} \rightarrow$$

Probabilities

$$\begin{bmatrix} 0.002 \\ 0.90 \\ 0.05 \\ 0.02 \end{bmatrix}$$

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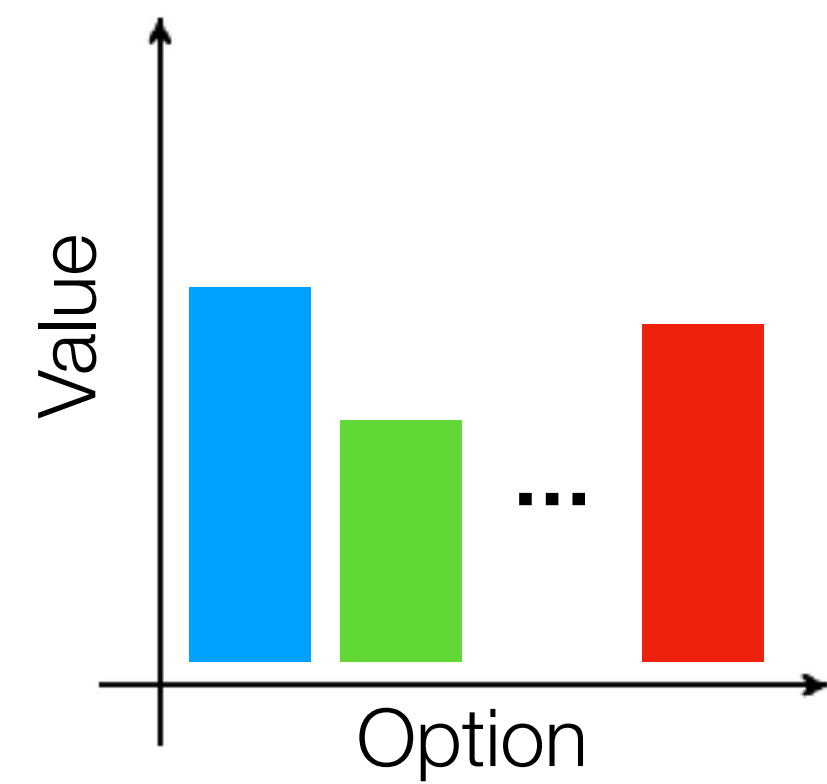
ϵ and τ model forms of exploration, but don't distinguish between experienced vs. inexperienced options

Bayesian reinforcement learning

We can describe a Bayesian variant of the RW model using a Kalman filter:

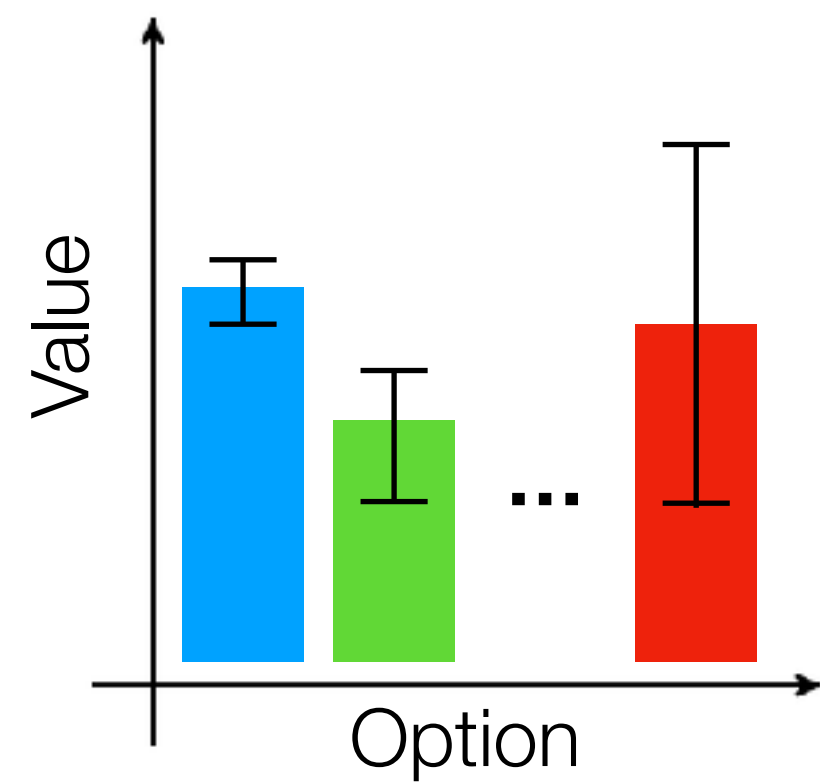
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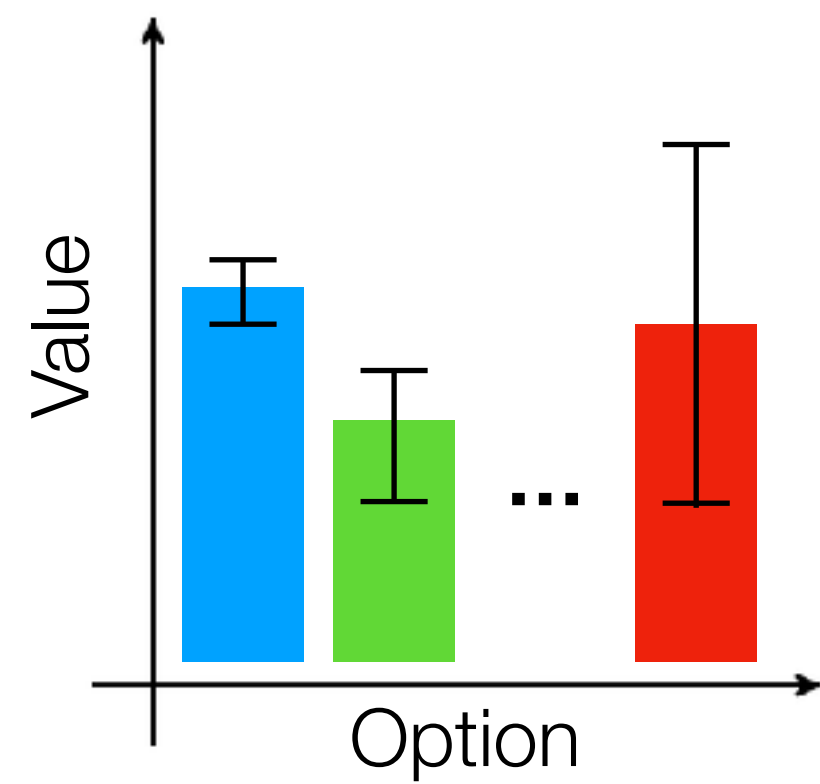
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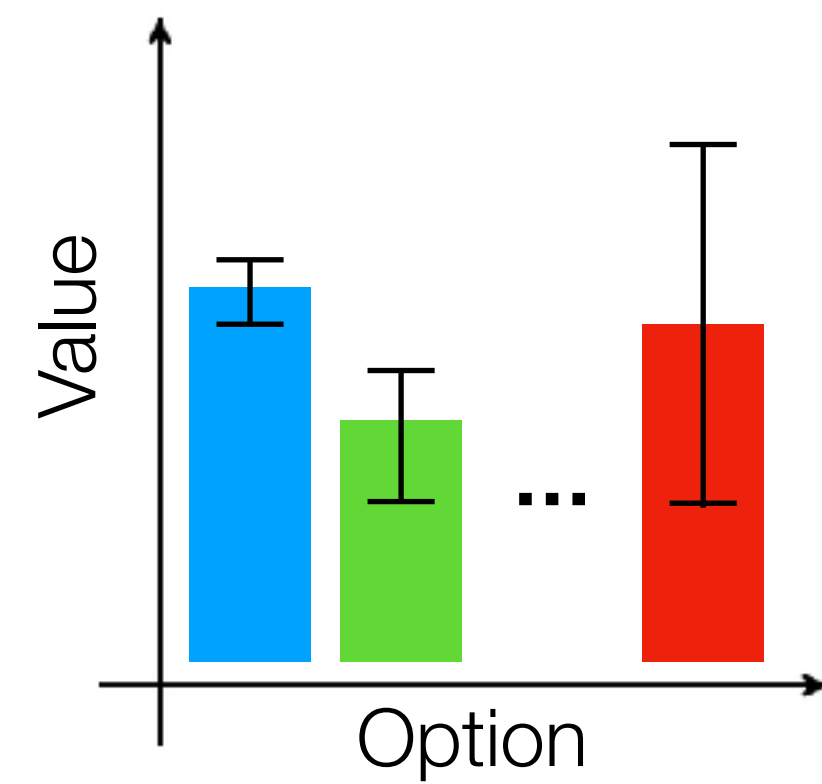


Normally distributed posterior over rewards, where the mean is $Q_{i,t}$:

$$p(r_{i,t} | \mathcal{D}_{t-1}) = \mathcal{N}(Q_{i,t}, \sigma_{i,t}^2) \quad \text{where } \mathcal{D}_t = [a_0, r_0, a_1, r_1, \dots] \text{ collect previous choices and rewards}$$

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$$\text{Mean: } Q_{i,t+1} = Q_{i,t} + k_{i,t} [r_{i,t} - Q_{i,t}]$$

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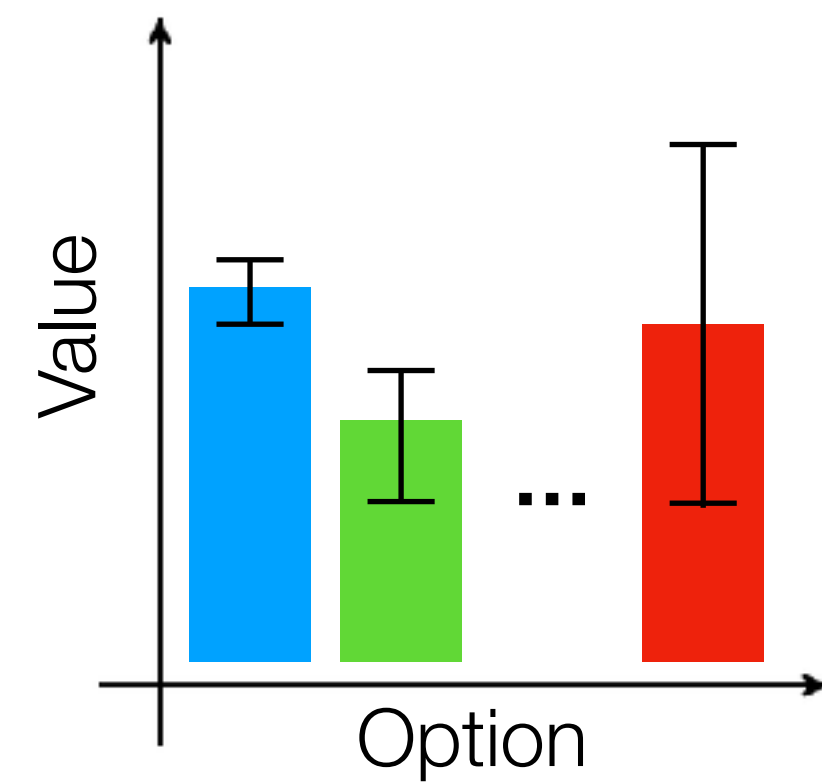
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Error variance σ_ϵ^2 is a free parameter

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Strictly, this is a KF variant known as a Bayesian mean tracker (BMT), assuming stationary rewards

Error variance σ_ϵ^2 is a free parameter

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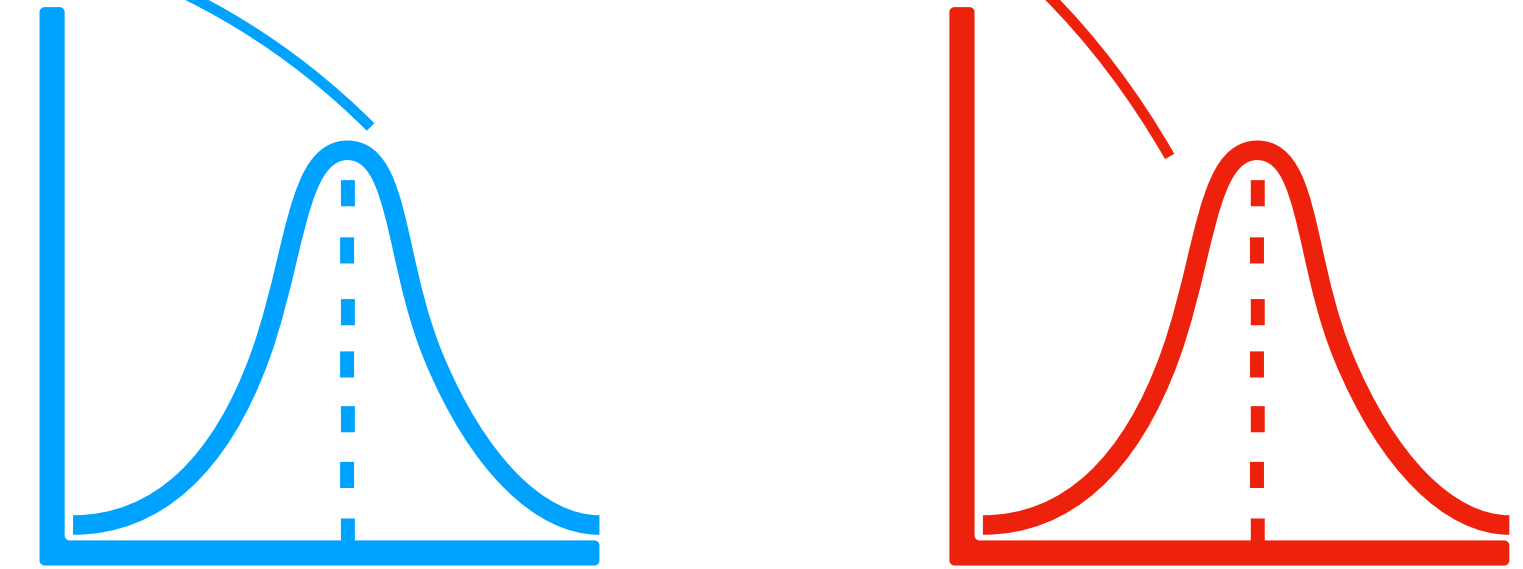
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Monte Carlo Samples



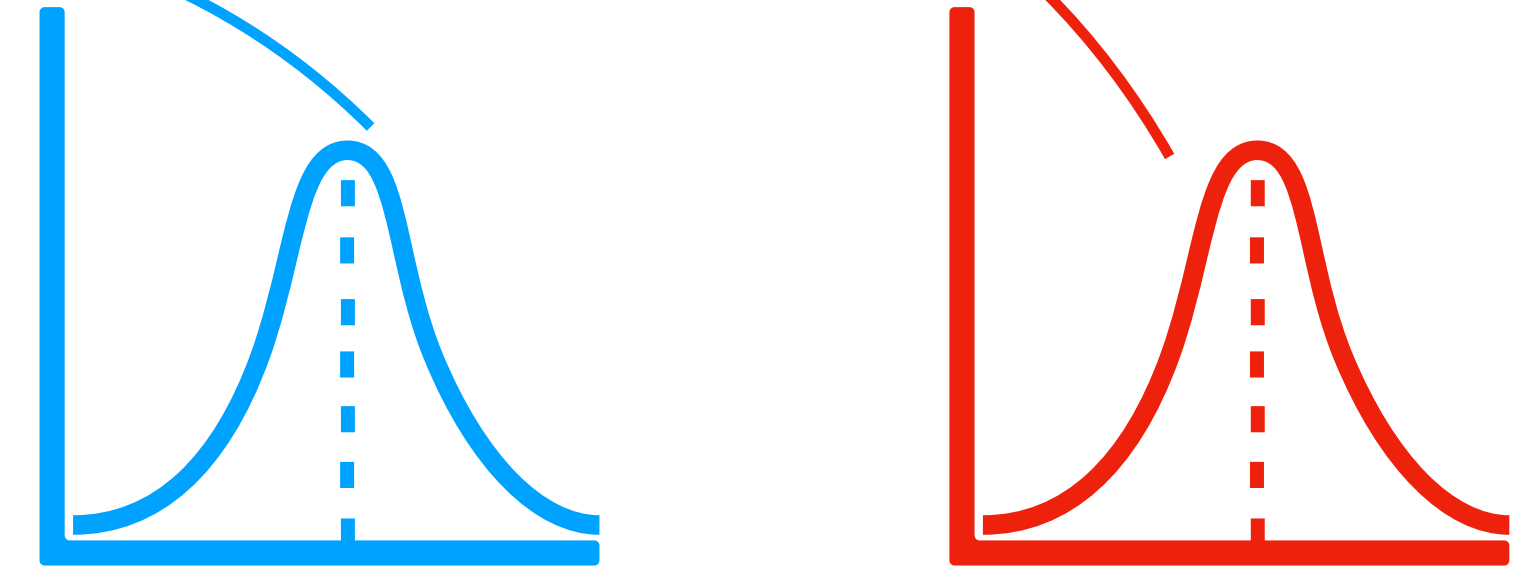
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$$P(a_i) = P(r_i > r_{j \neq i})$$

Monte Carlo Samples



Upper Confidence Bound Sampling:

$$UCB(a_i) = Q_i + \beta \sqrt{\sigma_i^2}$$

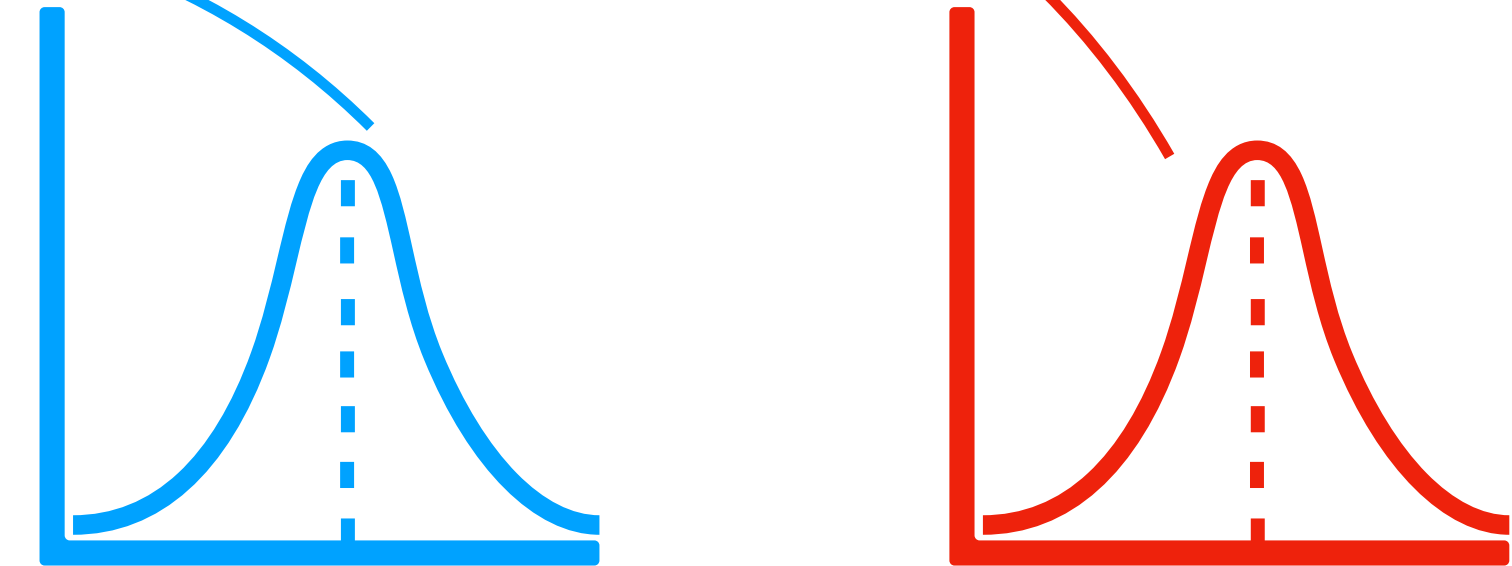
Policies for Bayesian models

We can now use uncertainty estimates to inform our policy and explore more efficiently.

Thompson Sampling:

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Monte Carlo Samples

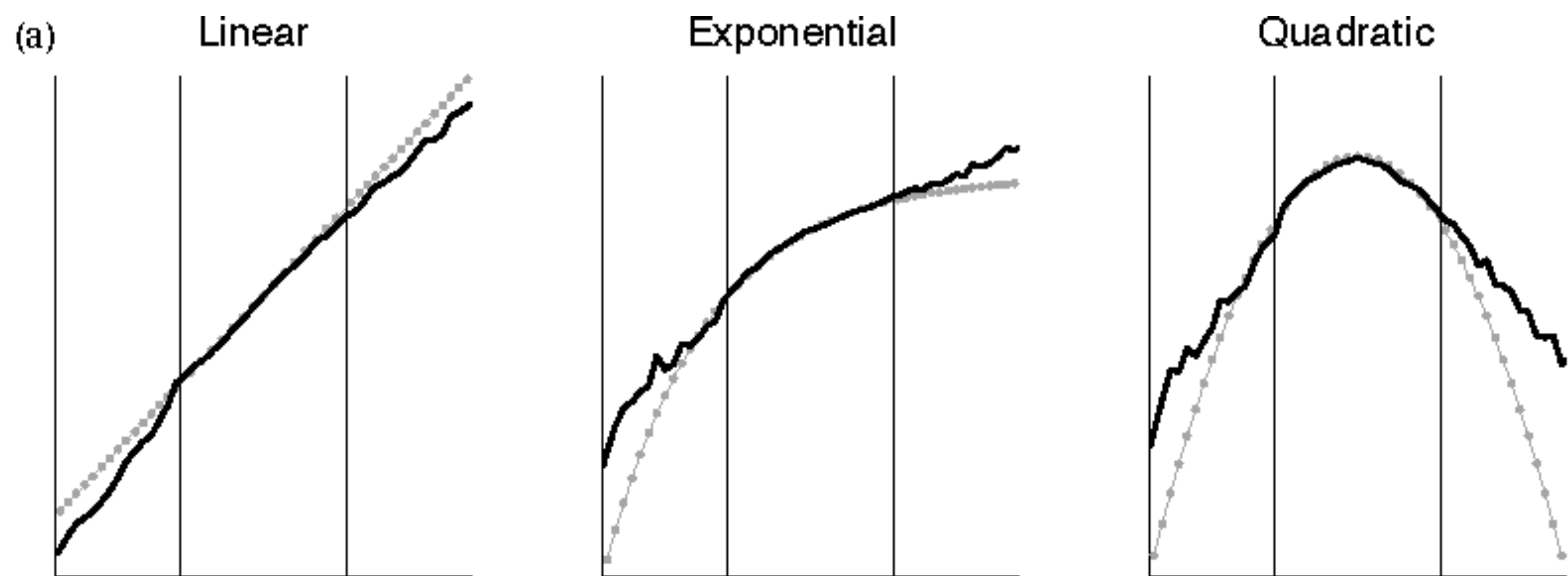


Upper Confidence Bound Sampling:

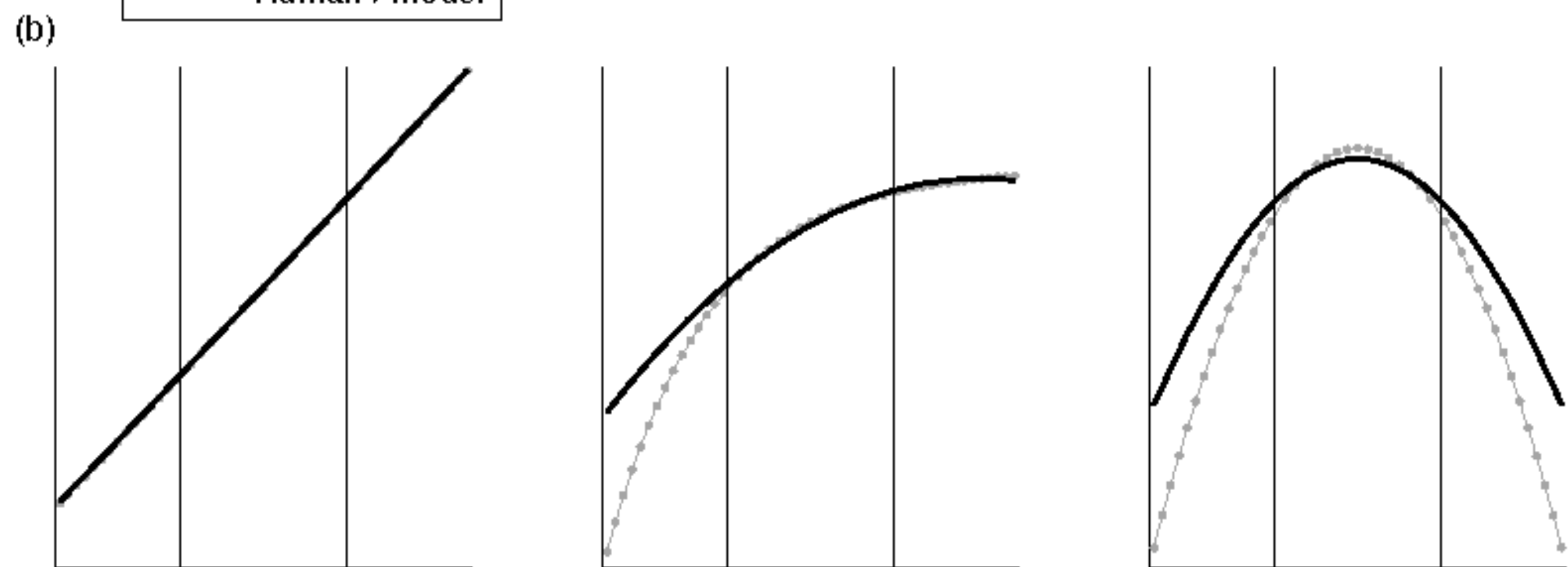
$$UCB(a_i) = Q_i + \beta \sqrt{\sigma_i^2}$$

β models exploration directed towards uncertain choices

Function approximation?



—•— Function
— Human / Model



(c)

| Model | Linear | Exponential | Quadratic |
|--------|--------|-------------|-----------|
| EXAM | .999 | .997 | .961 |
| Linear | .999 | .989 | .470 |
| Quad | .997 | .997 | .901 |
| RBF | .999 | .997 | .882 |
| LQ | .999 | .997 | .886 |
| LR | .999 | .997 | .892 |
| RQ | .998 | .994 | .878 |
| LRQ | .999 | .995 | .877 |

Summary

Summary

RL framework for learning value functions and policies

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- Tabular methods vs. value function approximation

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- Can we understand something about the efficiency of human learning?

Summary

RL framework for learning value functions and policies

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Modeling human learners with RL models

- Can we understand something about the efficiency of human learning?
 - How humans navigate the exploration-exploitation dilemma

Summary

RL framework for learning value functions and policies

- Tabular methods vs. value function approximation
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Modeling human learners with RL models

- Can we understand something about the efficiency of human learning?
 - How humans navigate the exploration-exploitation dilemma
- RW and Q-learning resemble tabular methods that have access to random or noisy exploration

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RL framework for learning value functions and policies

- Tabular methods vs. value function approximation
- Exhaustive iteration over states vs. predictions about novel states

Modeling human learners with RL models

- Can we understand something about the efficiency of human learning?
 - How humans navigate the exploration-exploitation dilemma
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Summary

RL framework for learning value functions and policies

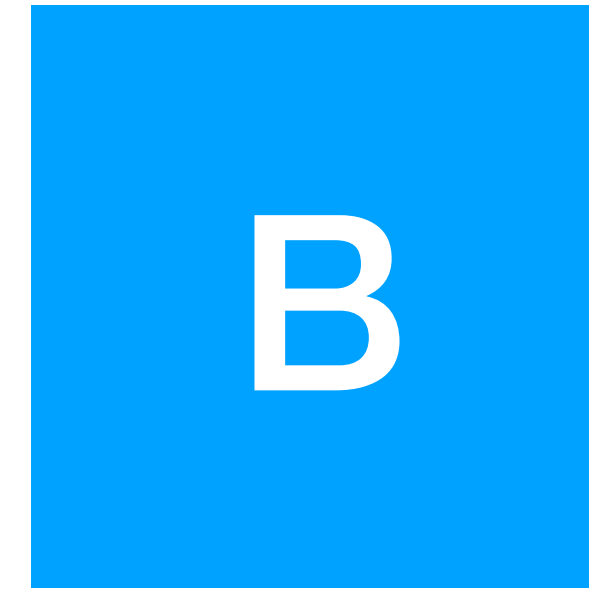
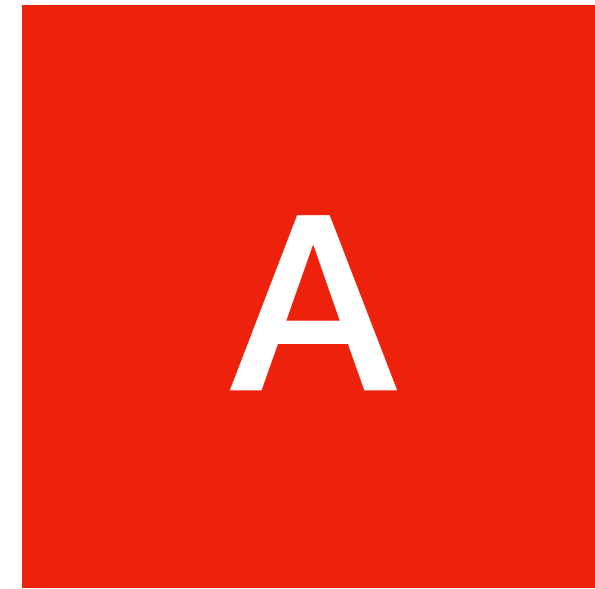
- Tabular methods vs. value function approximation
- Exhaustive iteration over states vs. predictions about novel states

Modeling human learners with RL models

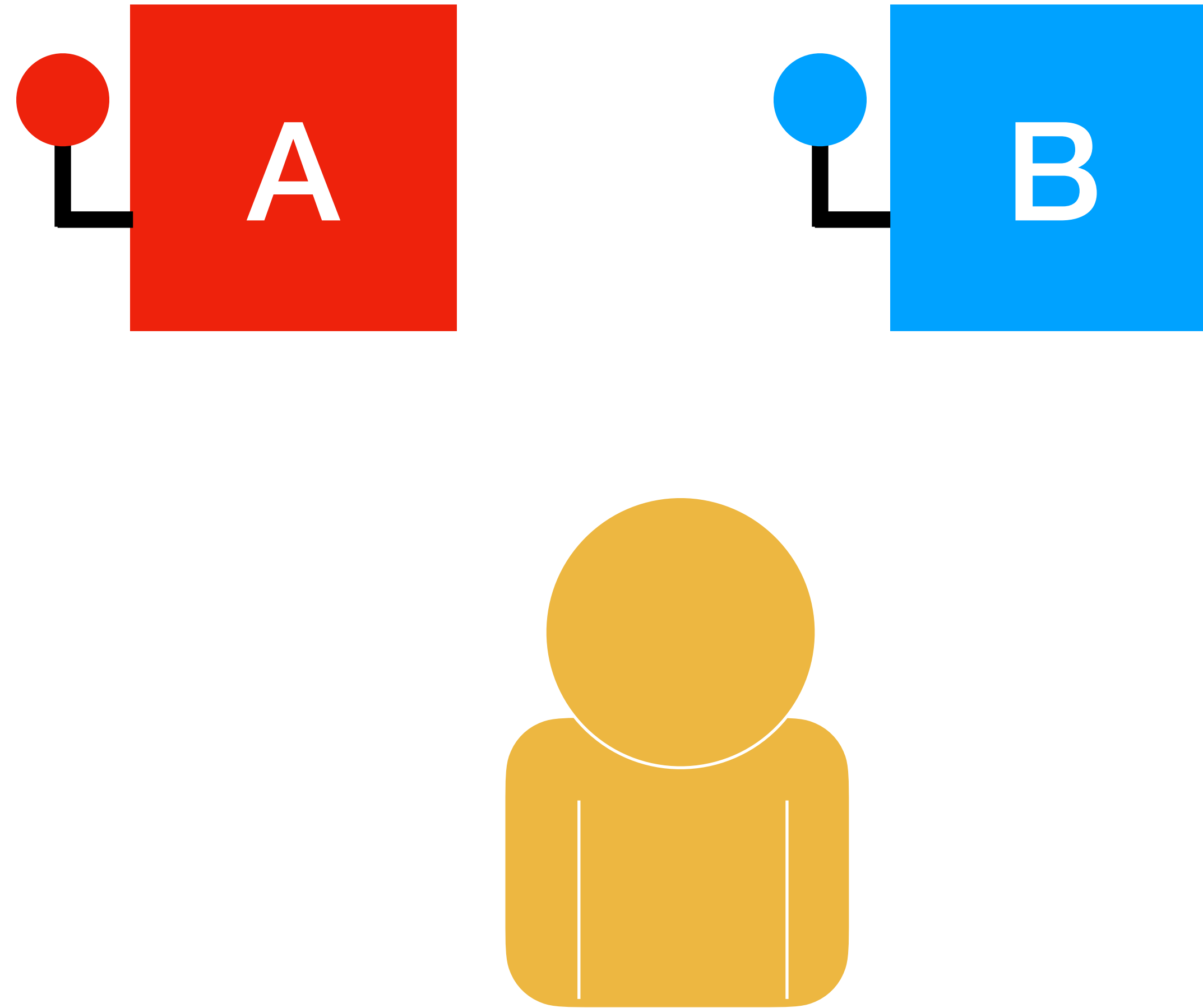
- Can we understand something about the efficiency of human learning?
 - How humans navigate the exploration-exploitation dilemma
- RW and Q-learning resemble tabular methods that have access to random or noisy exploration
- Kalman filter is a Bayesian model, which can use uncertainty-informed exploration
- But what about function approximation?

Break

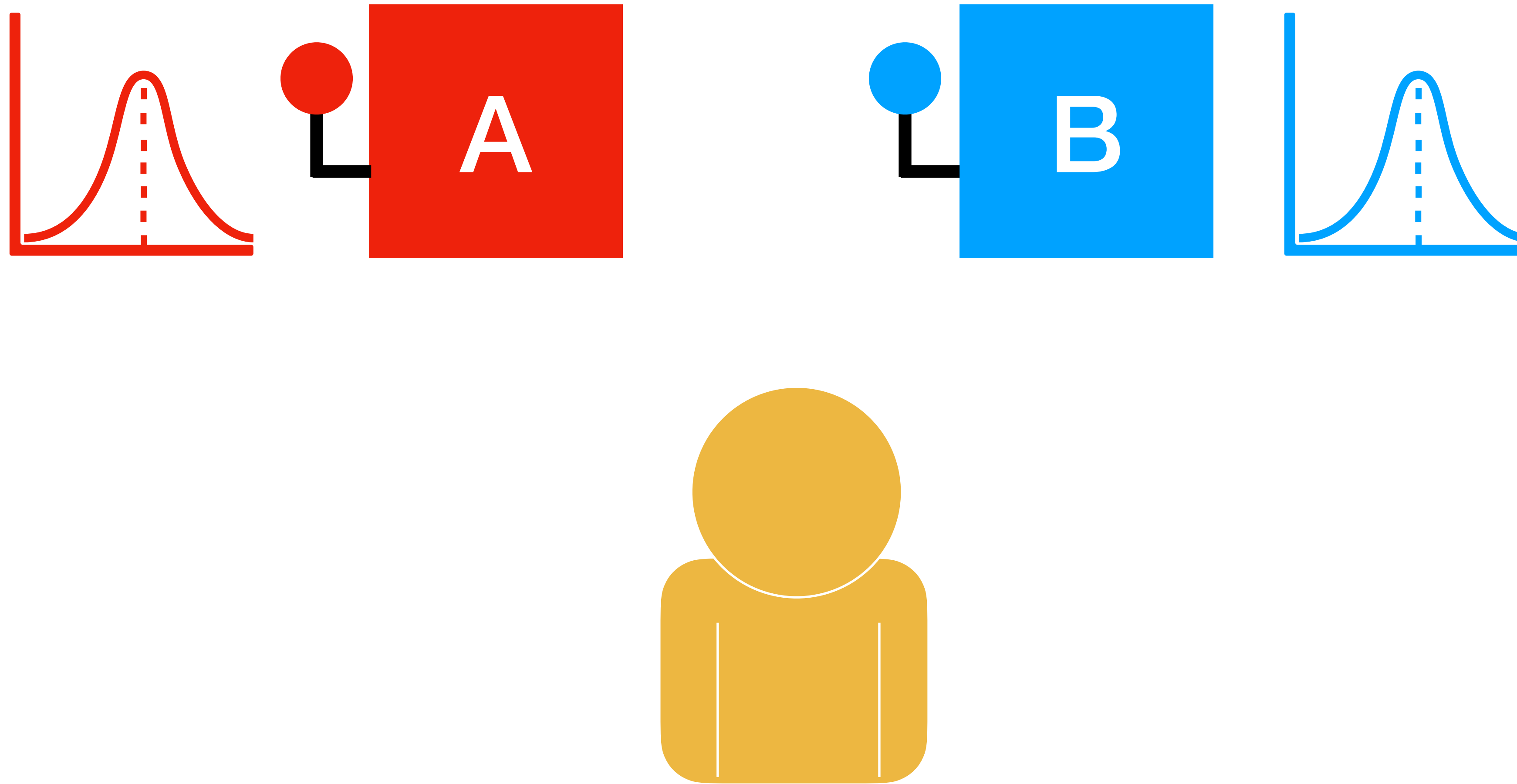
Human learning in the lab



Human learning in the lab

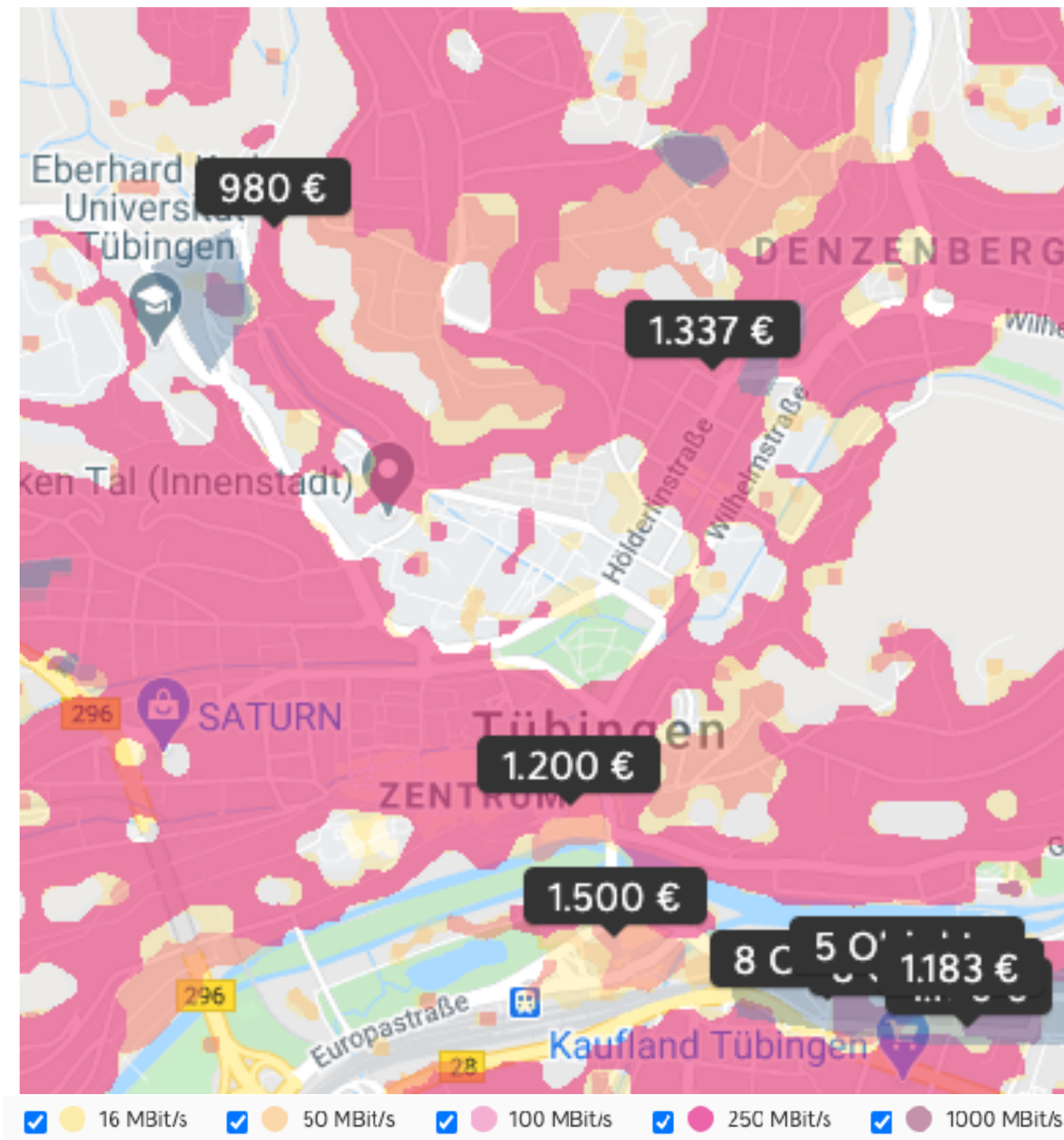


Human learning in the lab



Real life problems

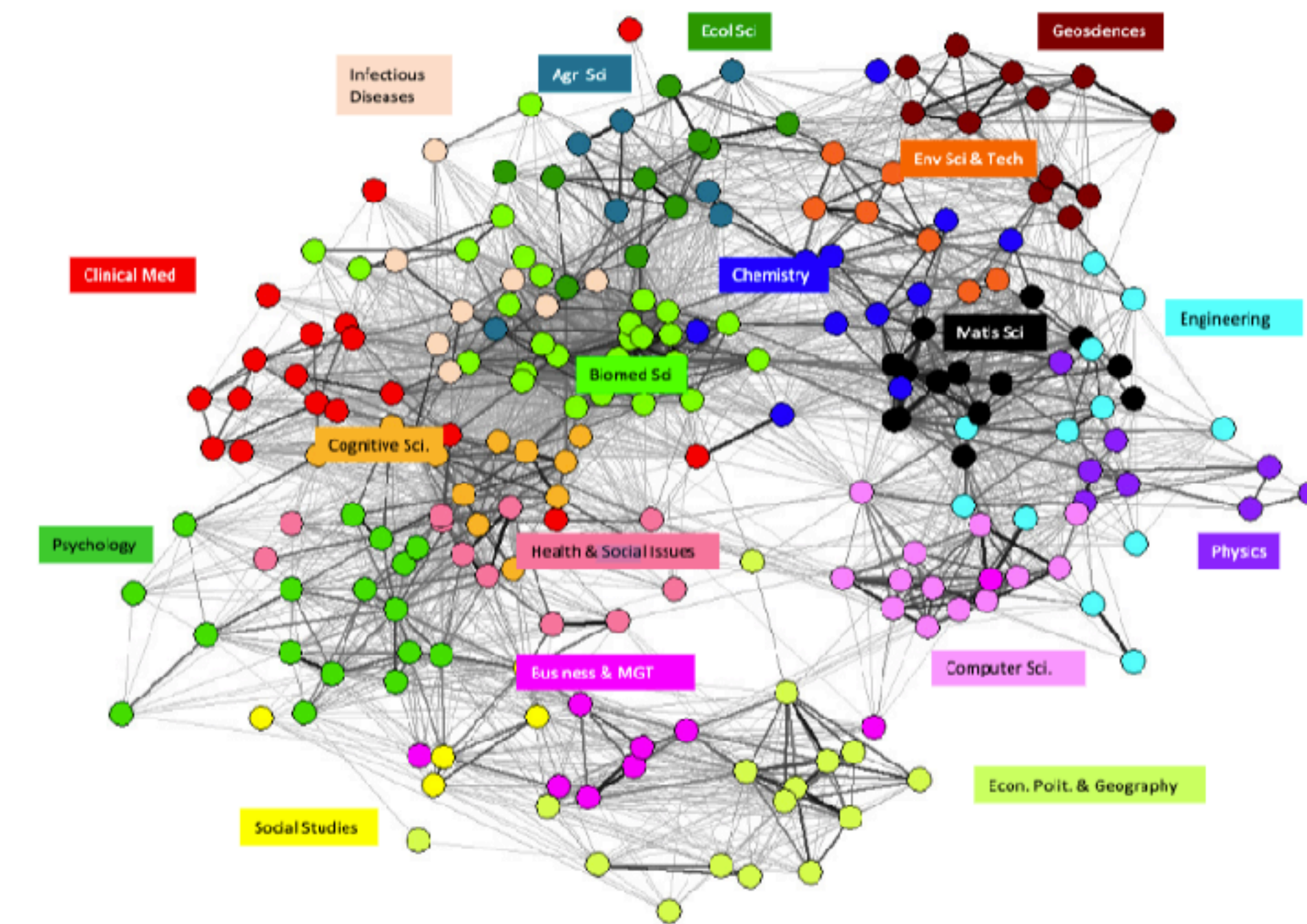
Finding a place to live



Picking what to eat



Choosing a research topic



Exploration-Exploitation Dilemma



Exploration



Exploitation

A cartoon illustration of Calvin and Hobbes from the comic strip 'Calvin and Hobbes'. They are standing on a dark blue, textured ground, looking up at a vast, dark night sky filled with numerous white stars of varying sizes. Calvin, a small boy with spiky blonde hair, is on the left, wearing a green shirt and blue pants. He is looking up with an open mouth, as if in awe. Hobbes, a large tiger with orange and black stripes and a white belly, is on the right, standing on his hind legs and looking up at the sky. Both characters have speech bubbles above them.

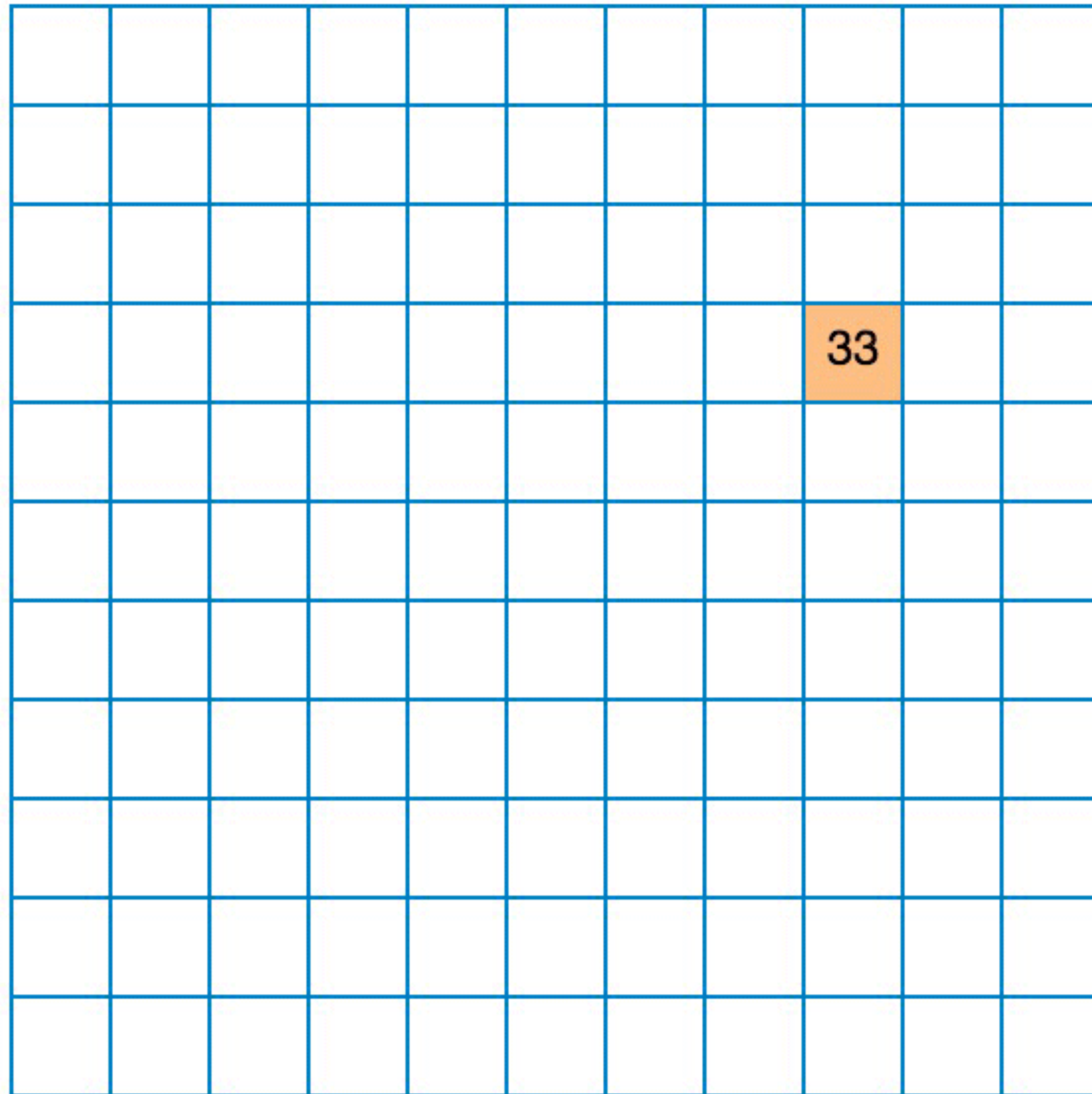
Let's
explore!

But where?

How do people navigate vast environments when we cannot explore all possibilities?



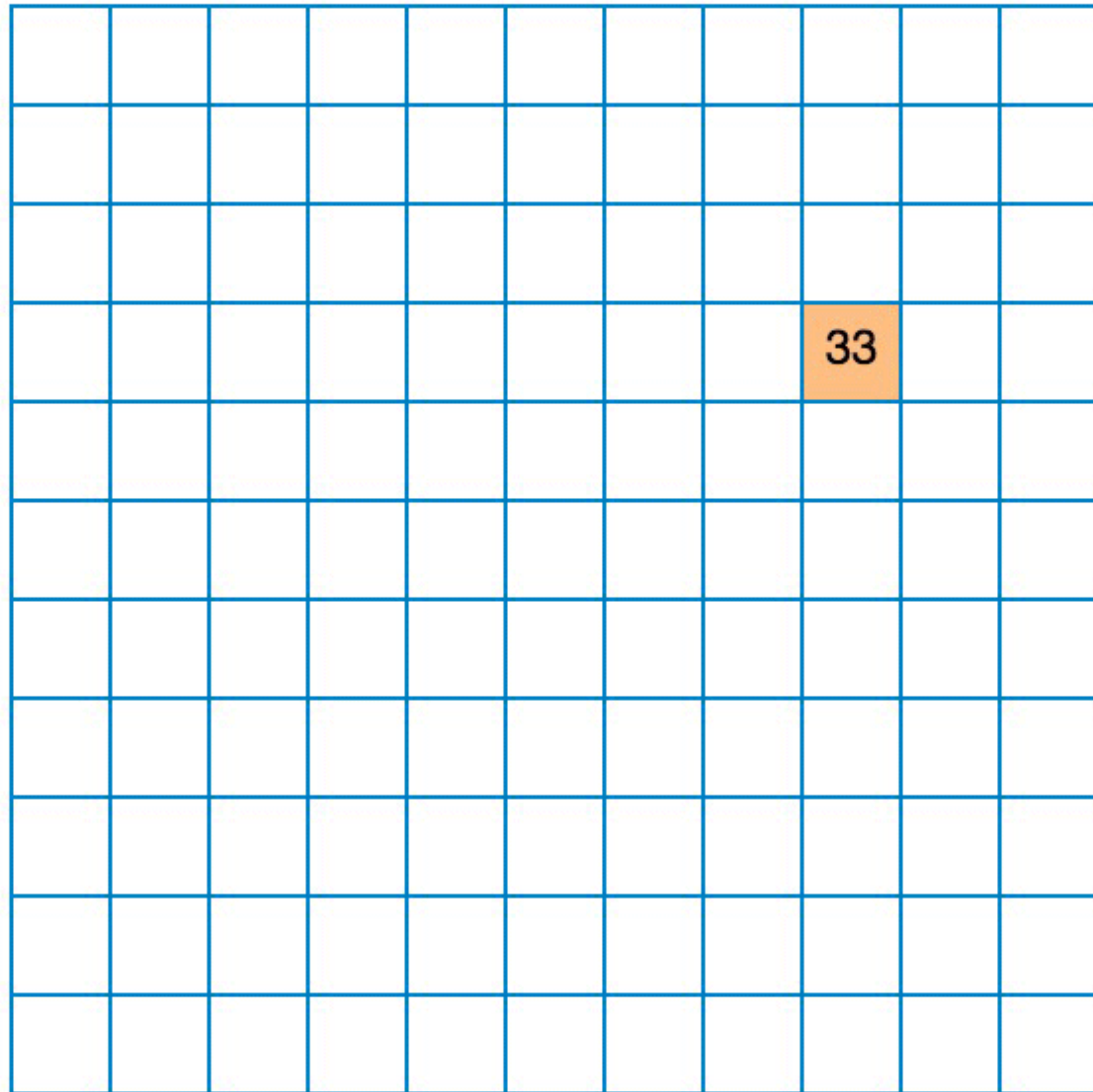
Spatially Correlated Bandit



Wu et al., (*Nature Human Behaviour* 2018)

-  click tiles on the grid
-  maximize reward
-  each tile has normally distributed rewards
-  nearby tiles have similar rewards
-  limited search horizon privileges good generalization & efficient exploration

Spatially Correlated Bandit



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Spatially Correlated Bandit

| | | | | | | | | | | |
|----|----|----|----|----|----|----|----|----|----|----|
| 7 | 5 | 10 | 22 | 32 | 32 | 28 | 24 | 22 | 26 | 33 |
| 6 | 11 | 19 | 29 | 38 | 41 | 42 | 40 | 37 | 36 | 40 |
| 22 | 27 | 30 | 35 | 43 | 50 | 53 | 53 | 51 | 49 | 46 |
| 45 | 44 | 38 | 36 | 40 | 46 | 47 | 49 | 54 | 55 | 48 |
| 61 | 55 | 46 | 40 | 37 | 32 | 27 | 31 | 44 | 52 | 44 |
| 62 | 59 | 57 | 54 | 44 | 27 | 14 | 17 | 33 | 46 | 45 |
| 53 | 59 | 68 | 71 | 59 | 36 | 17 | 15 | 28 | 45 | 51 |
| 46 | 57 | 71 | 77 | 67 | 47 | 26 | 18 | 27 | 45 | 56 |
| 45 | 56 | 65 | 67 | 60 | 46 | 29 | 20 | 27 | 42 | 55 |
| 51 | 57 | 58 | 53 | 47 | 40 | 30 | 23 | 28 | 40 | 49 |
| 60 | 62 | 58 | 47 | 39 | 38 | 35 | 31 | 35 | 41 | 46 |

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Experiment 1

30-Armed Bandit (Univariate)



Experiment 2

121-Armed Bandit (Bivariate)



Experiment 3

121-Armed Bandit (Natural)



Number of grids left: 6
Number of clicks left: 40



Participants acquired rewards by clicking
on new or previously revealed tiles

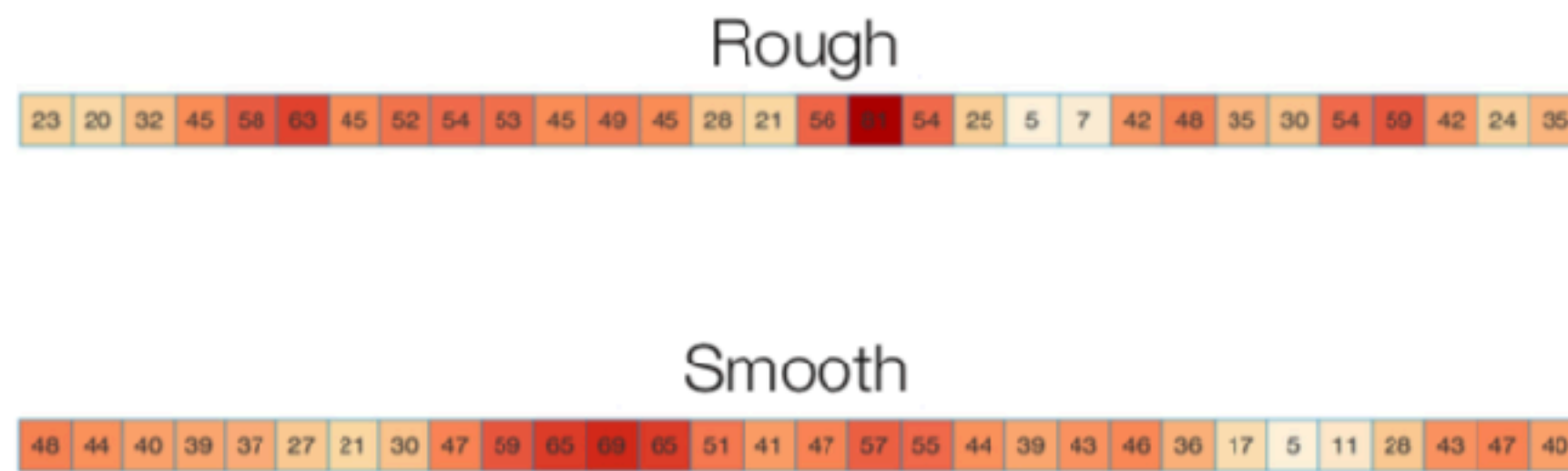


Number of grids left: 6
Number of clicks left: 1



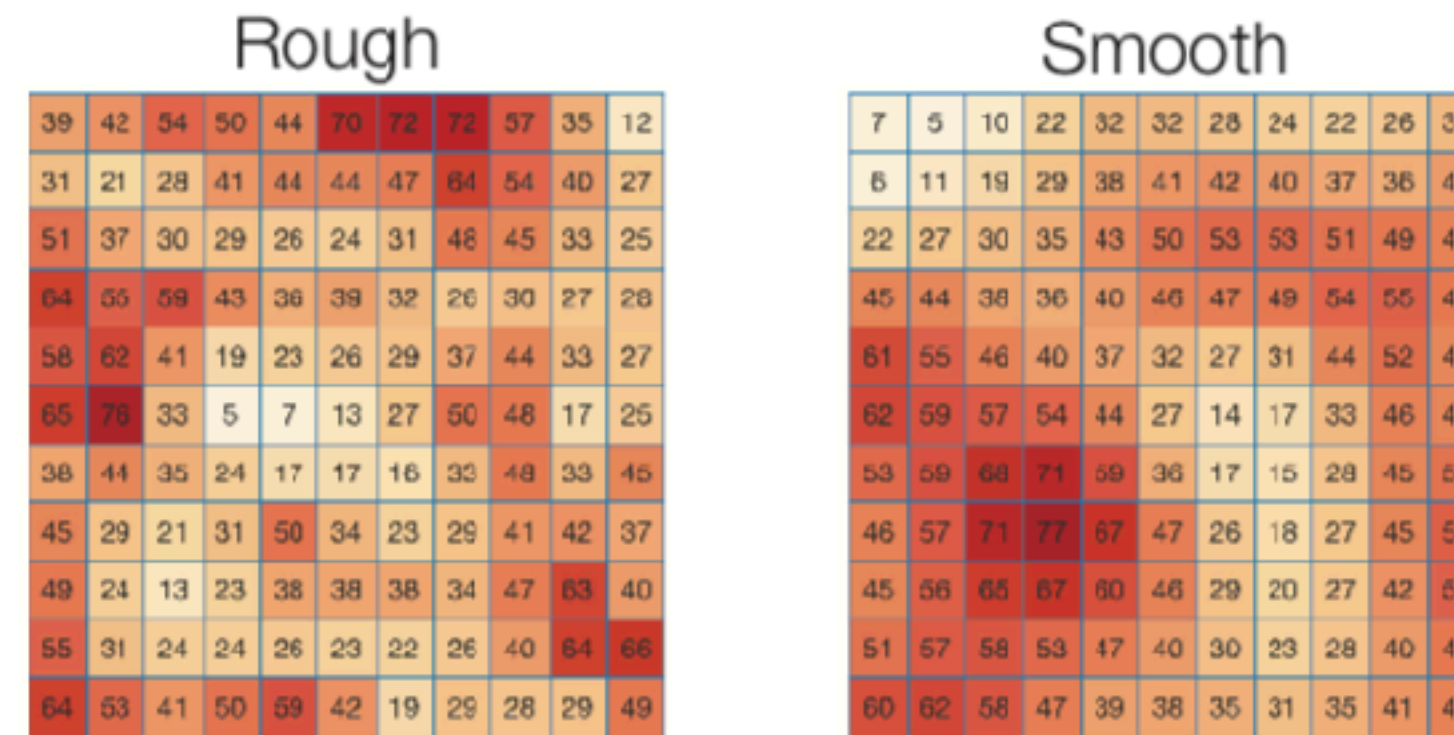
Experiment 1

30-Armed Bandit (Univariate)



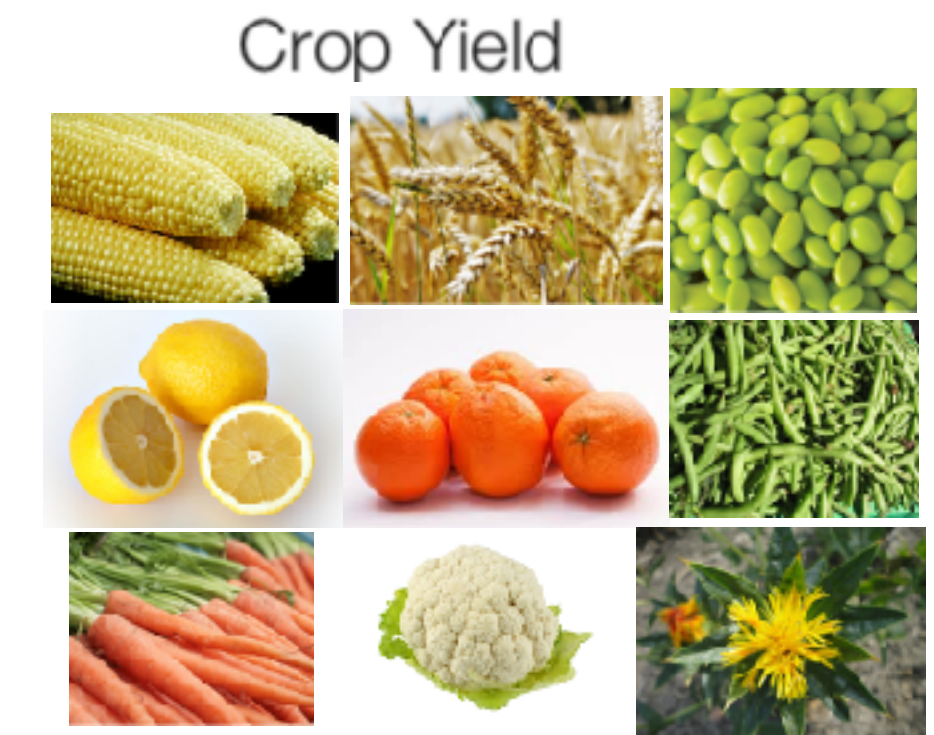
Experiment 2

121-Armed Bandit (Bivariate)

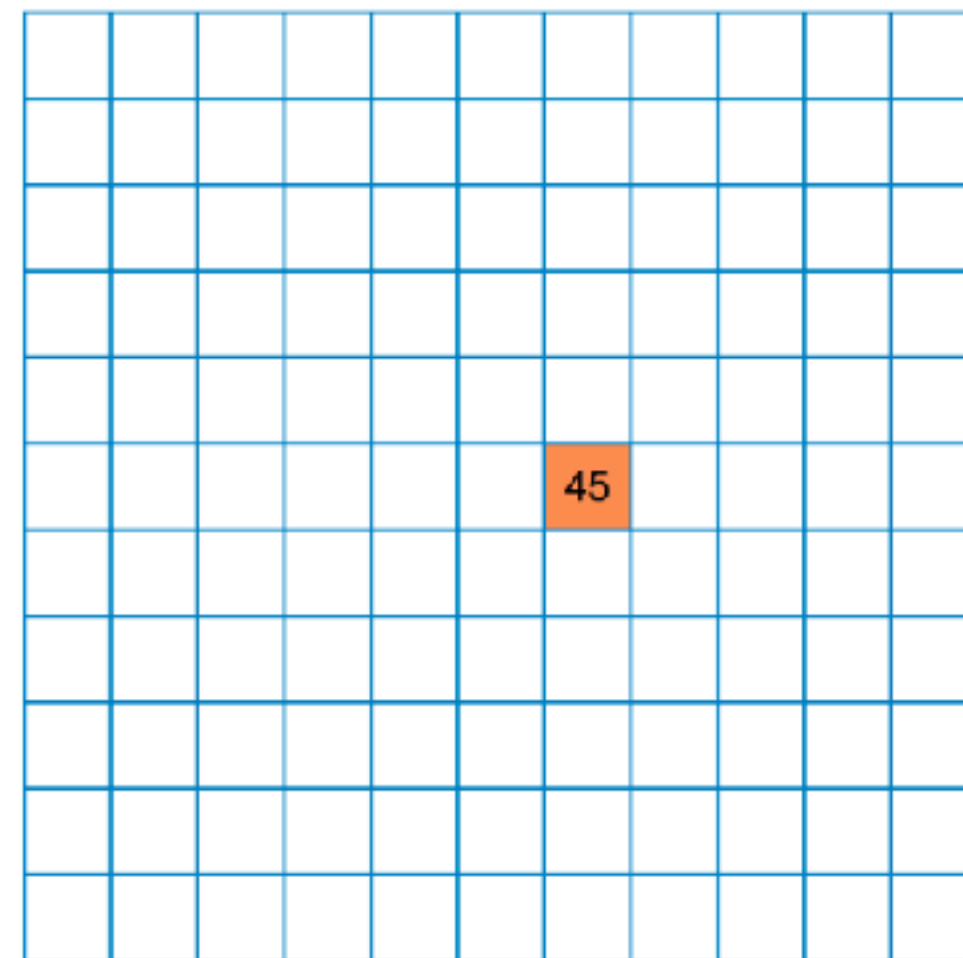


Experiment 3

121-Armed Bandit (Natural)



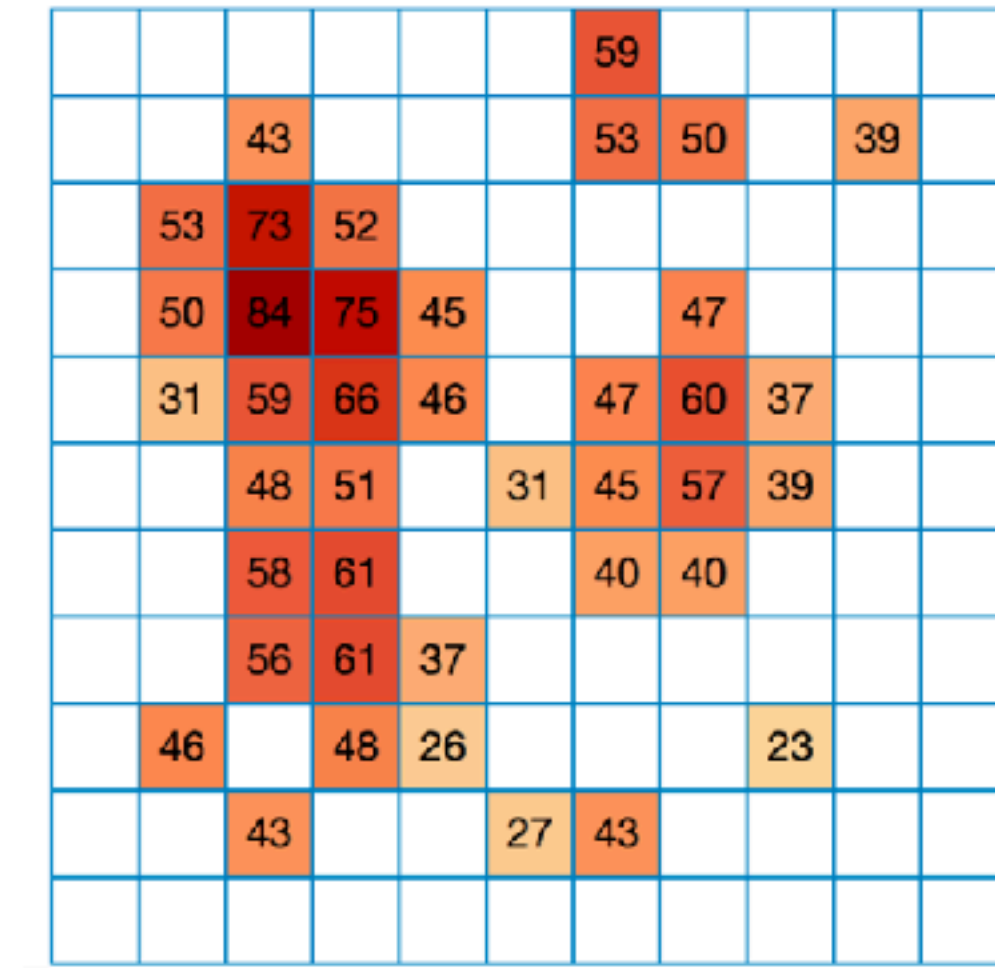
Number of grids left: 6
Number of clicks left: 40



Participants acquired rewards by clicking
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Number of grids left: 6
Number of clicks left: 1



Modeling Human Search

Modeling Human Search

- Exploration is not performed blindly



Modeling Human Search

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- Search is guided by generalization



Modeling Human Search

- Exploration is not performed blindly
- Search is guided by generalization
- Generalization as Bayesian inference about novel options:
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 - Uncertainty



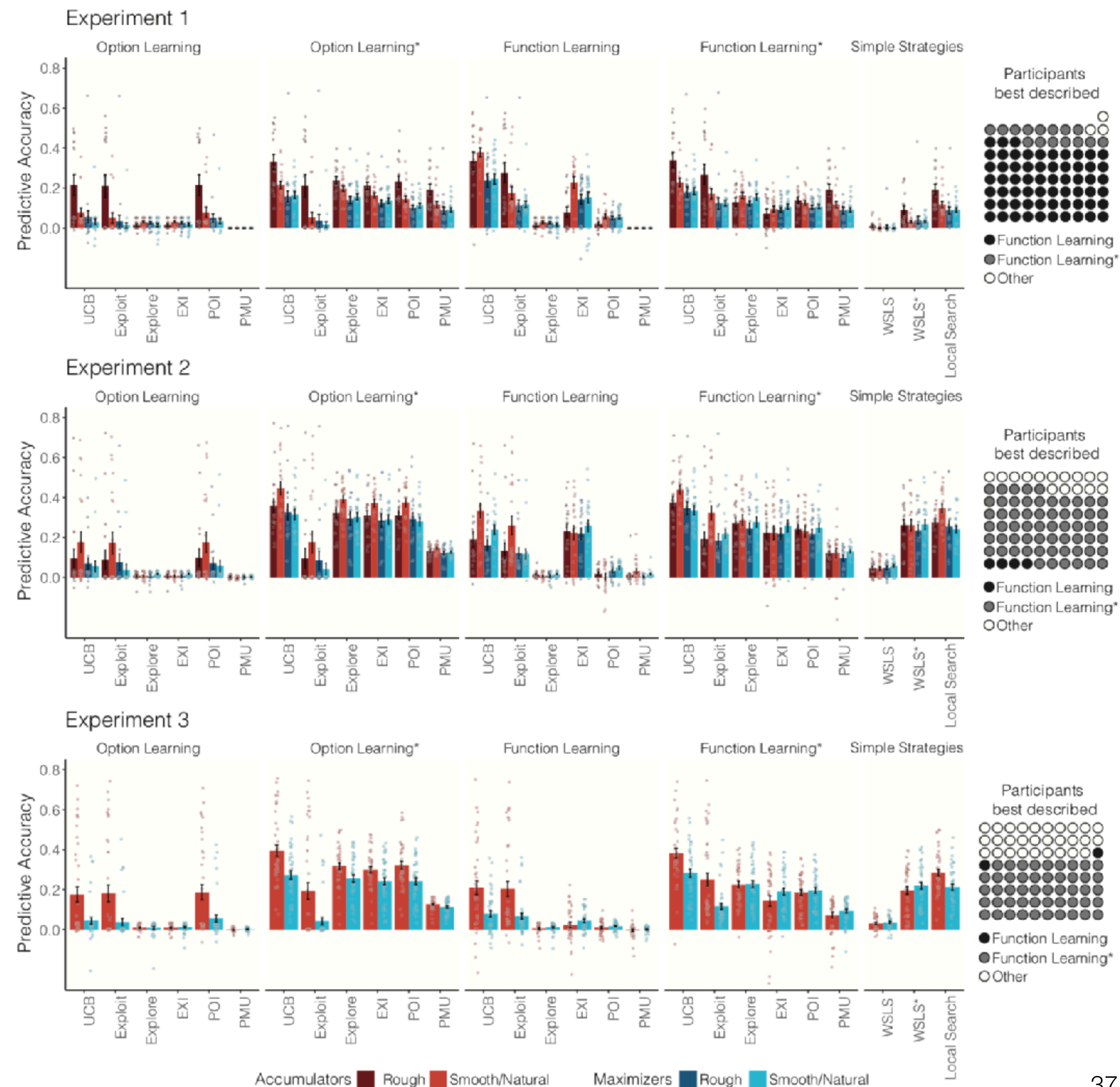
Modeling Human Search

- Exploration is not performed blindly
- Search is guided by generalization
- Generalization as Bayesian inference about novel options:
 - Expected reward
 - Uncertainty
- Human search is directed towards both ingredients



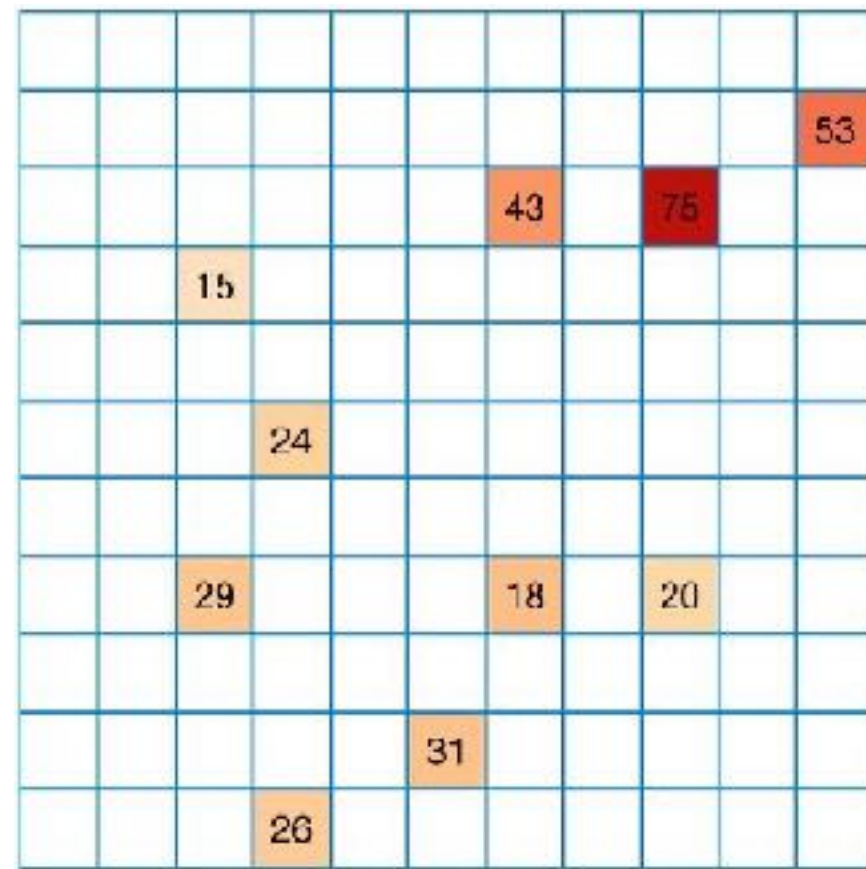
Model comparison

- We performed a large-scale comparison of 27 different models using cross-validated (out-of-sample) predictions
- Some heuristic models but mostly reinforcement learning models * sampling strategies
- ... here, I focus on the best model, which consistently outperformed all others across a variety of manipulation checks

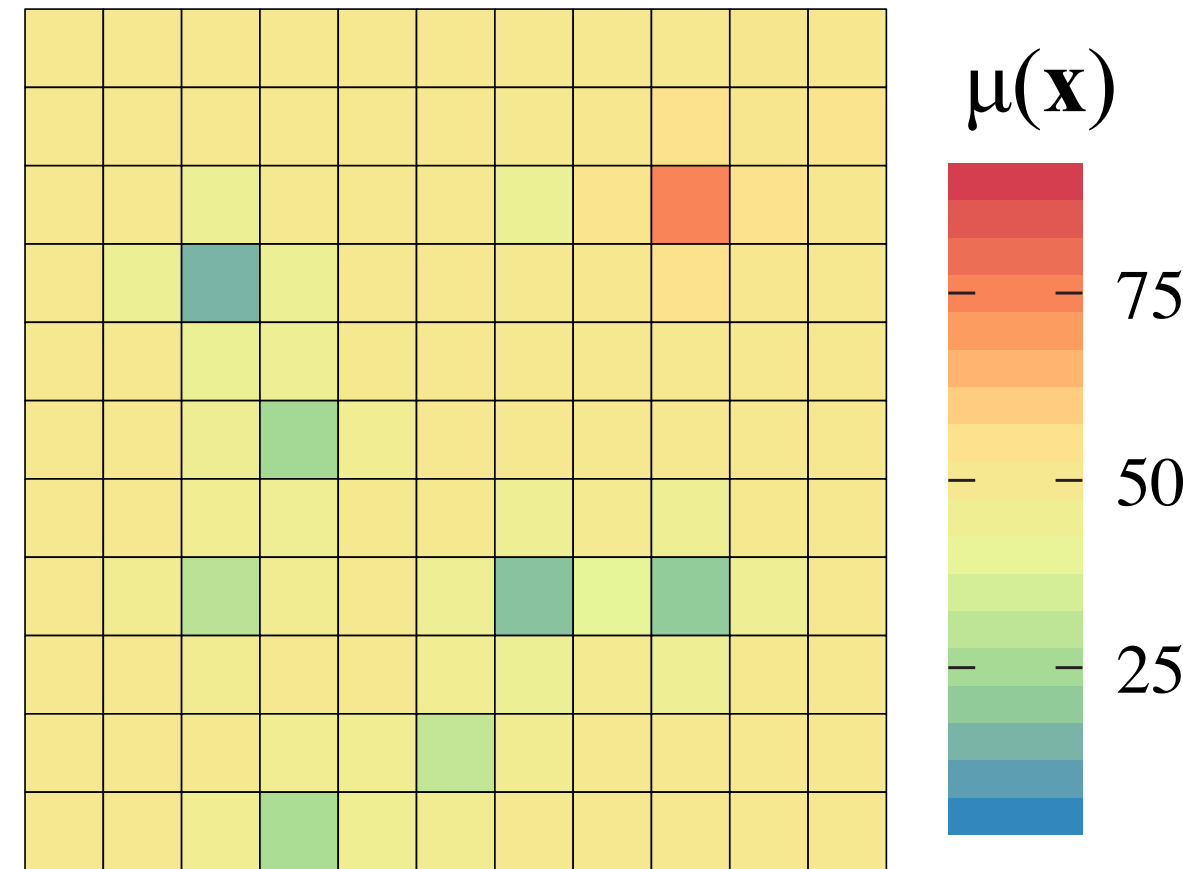


GP-UCB Model

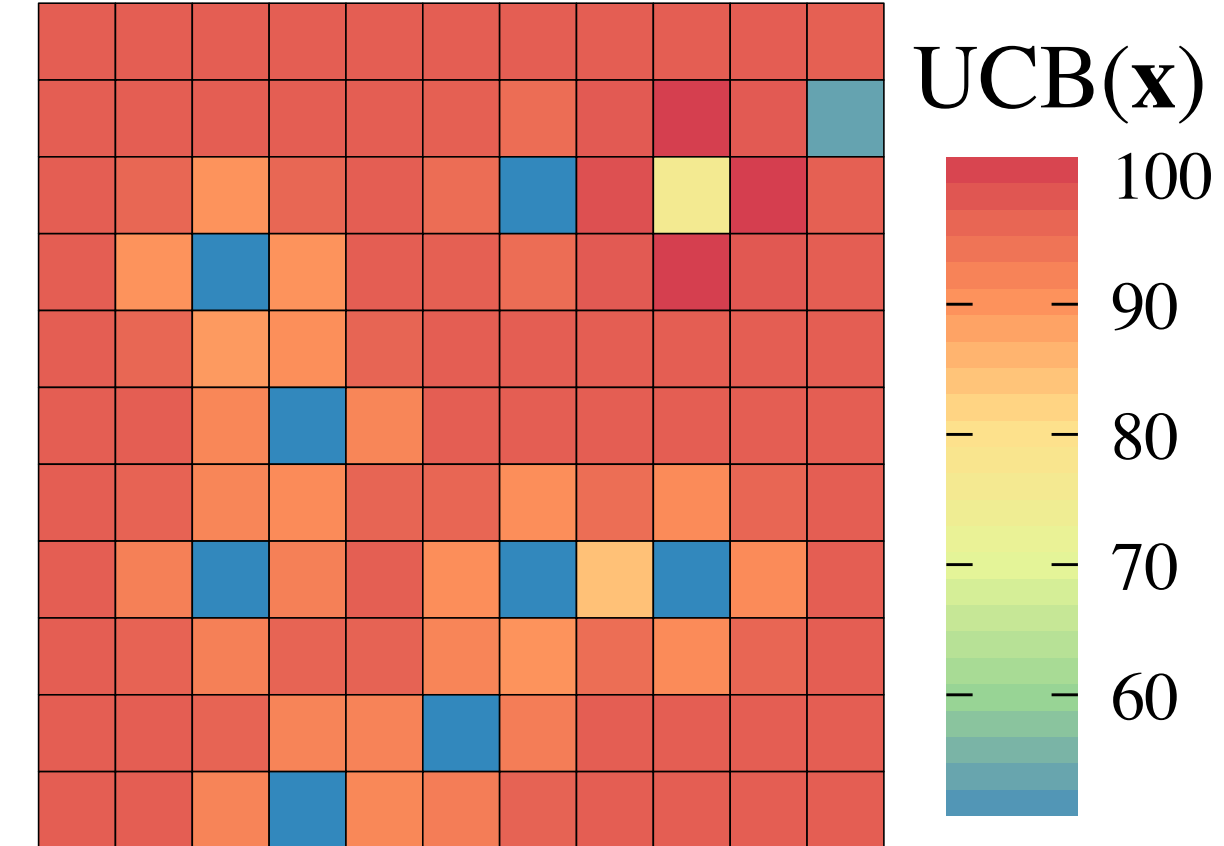
Observations



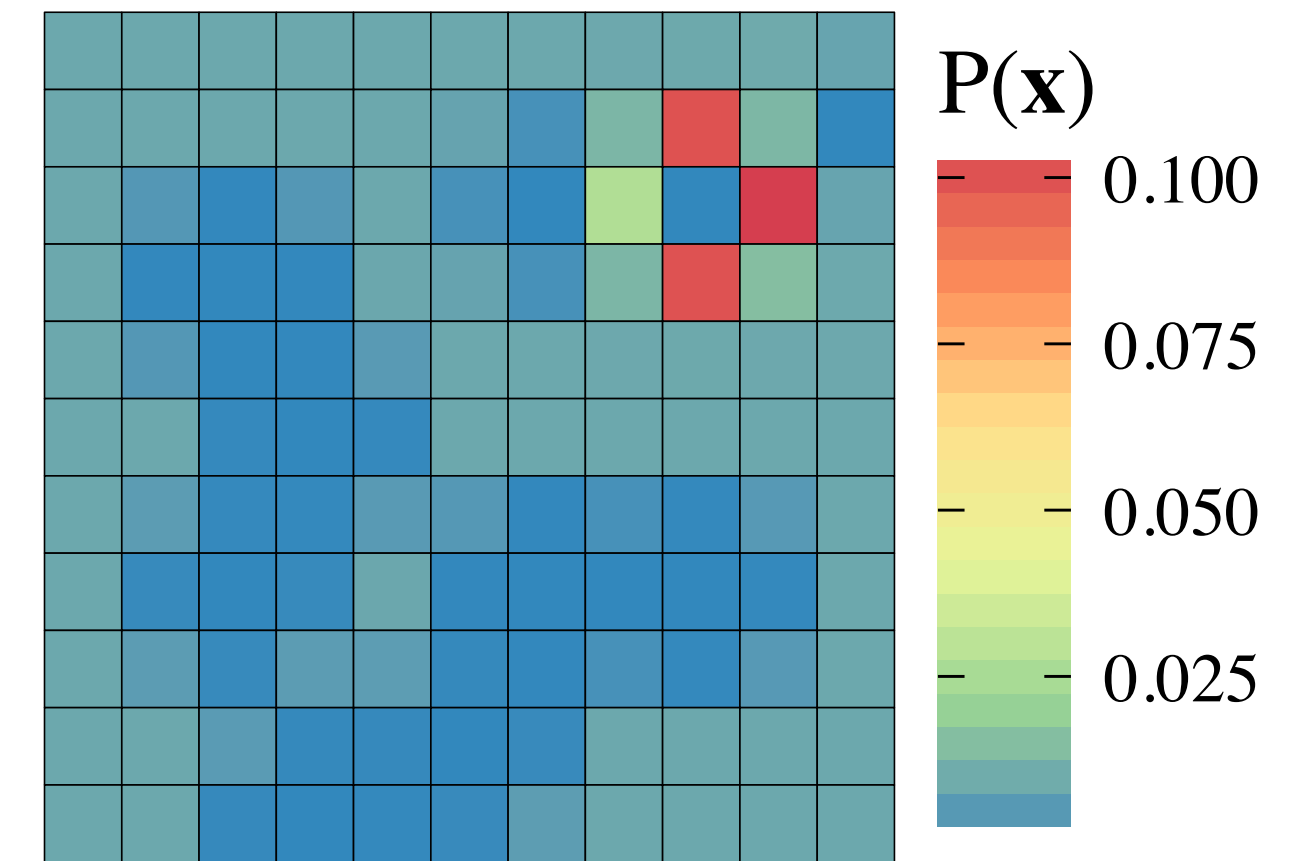
Gaussian Process (GP)



Upper Confidence Bound (UCB) Sampling

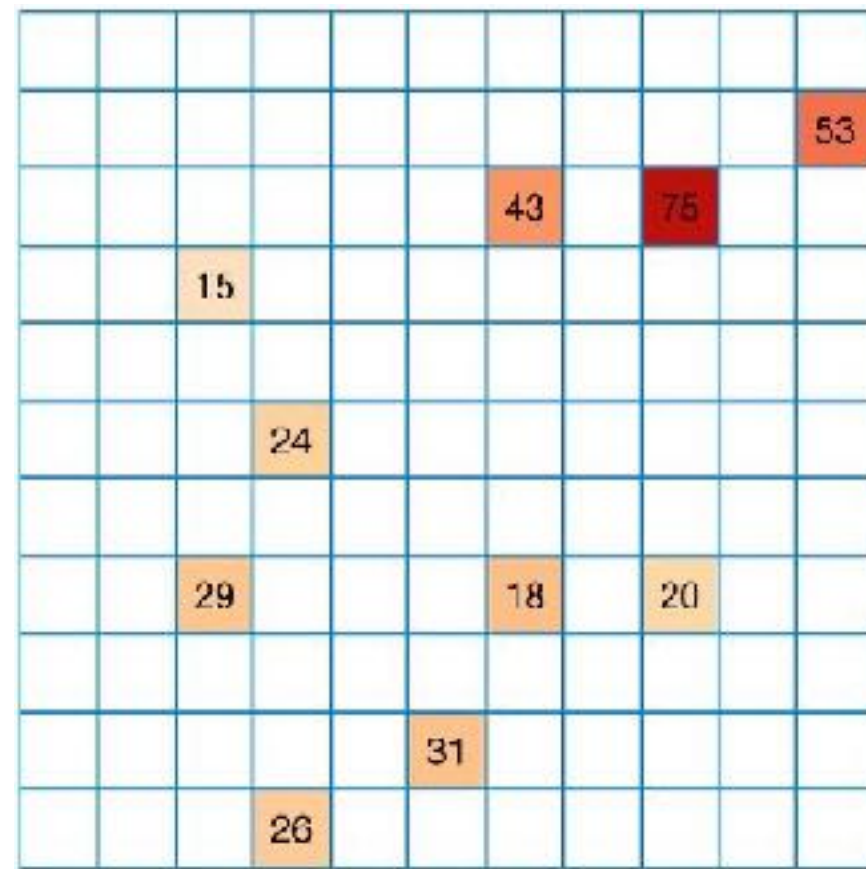


Softmax Choice Rule

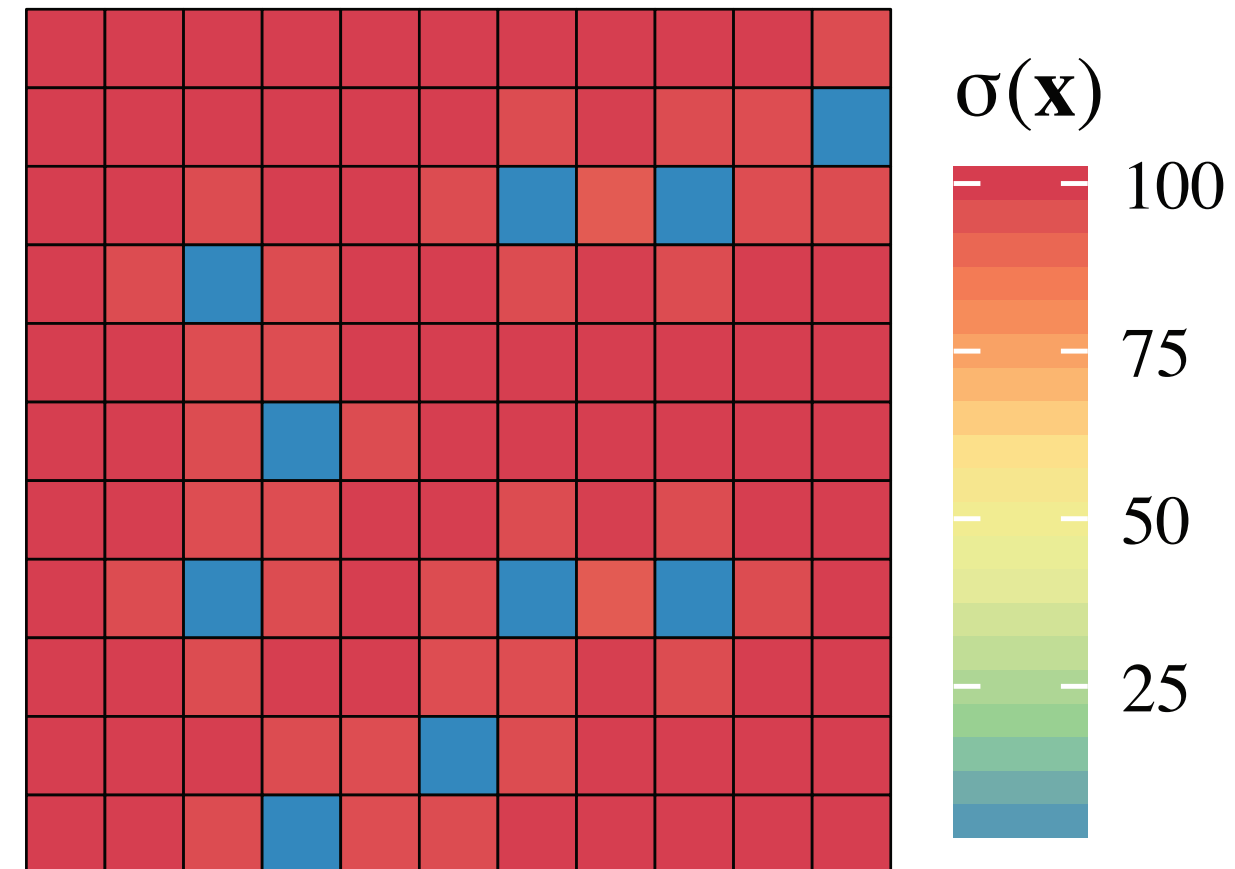


GP-UCB Model

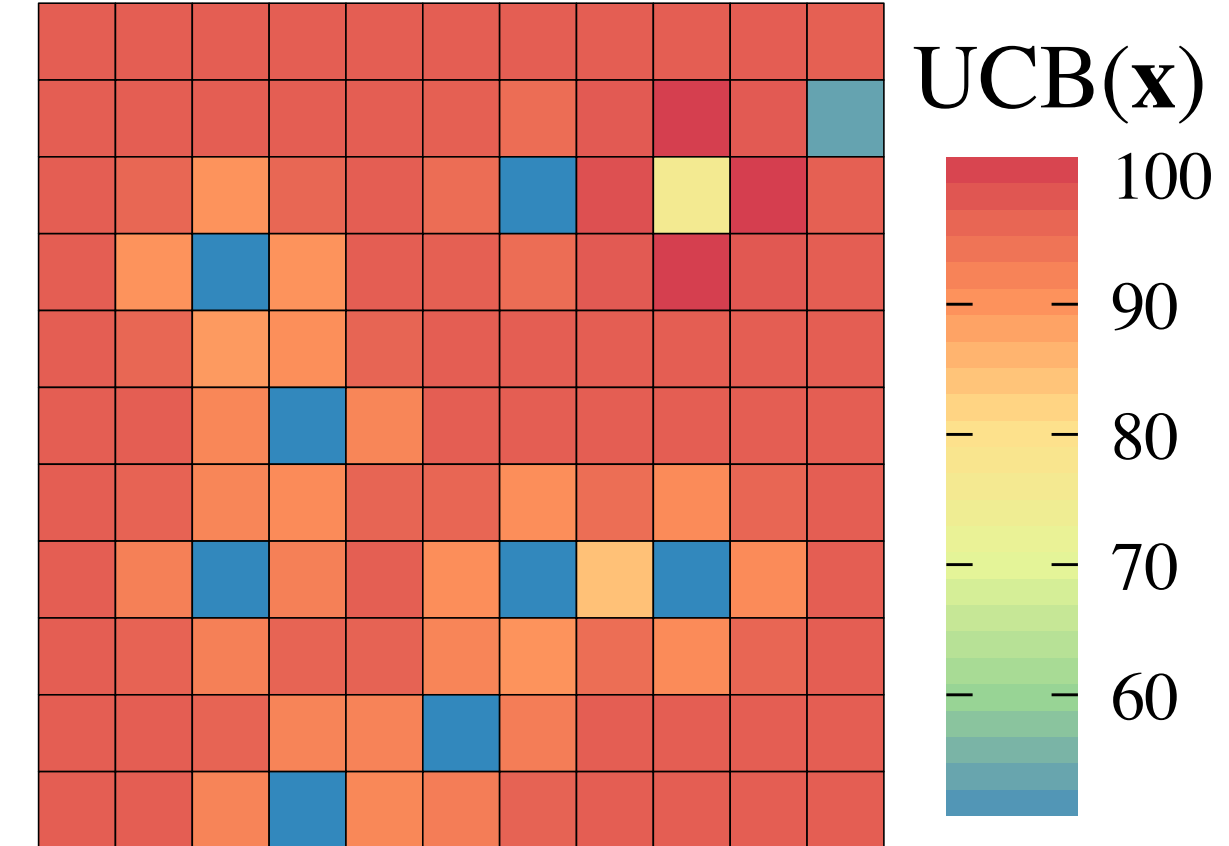
Observations



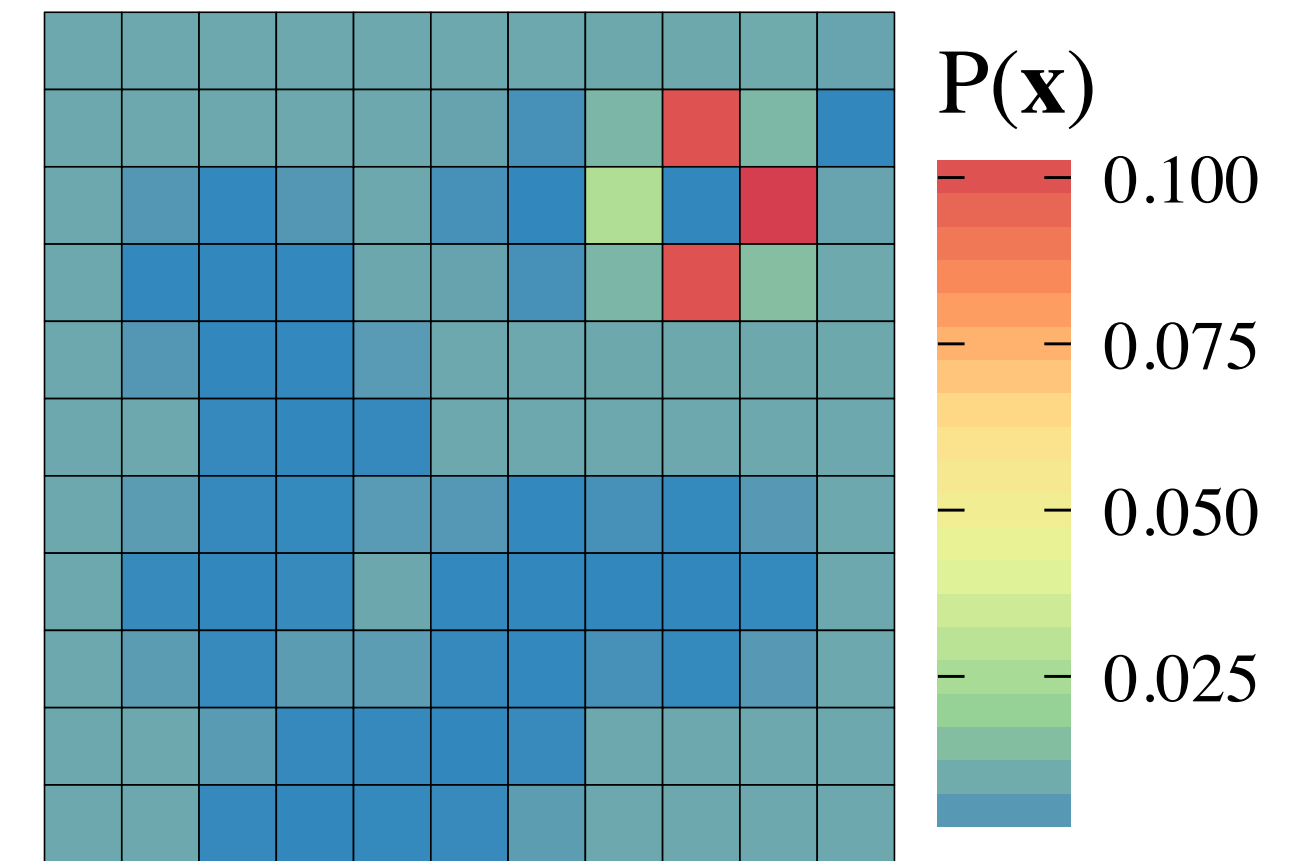
Gaussian Process (GP)



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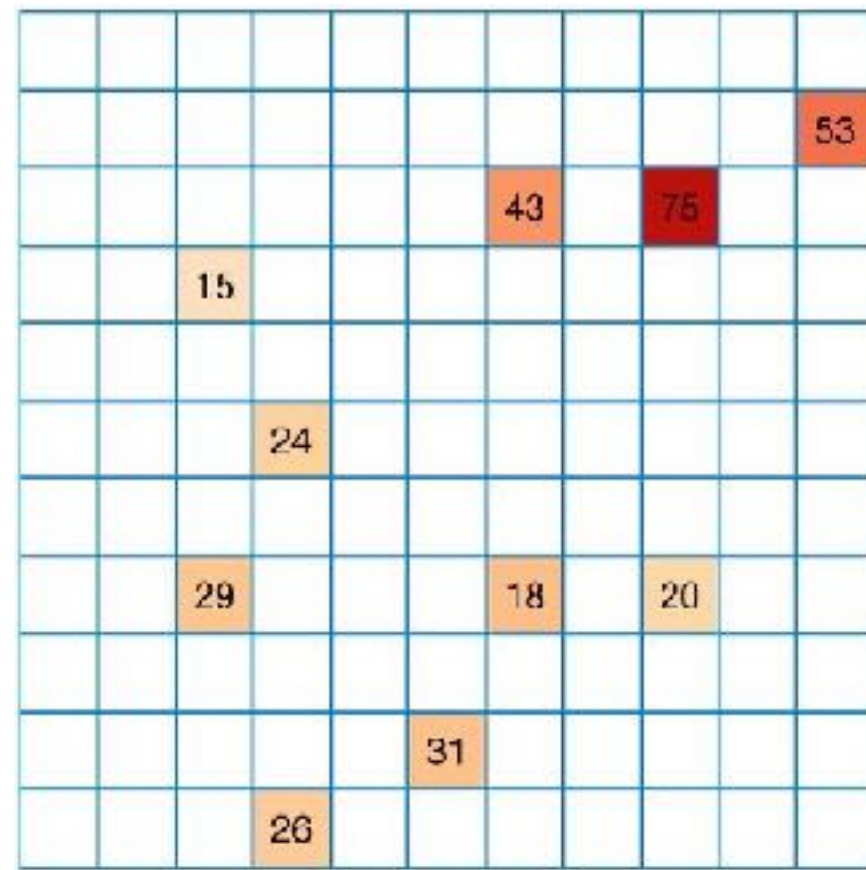


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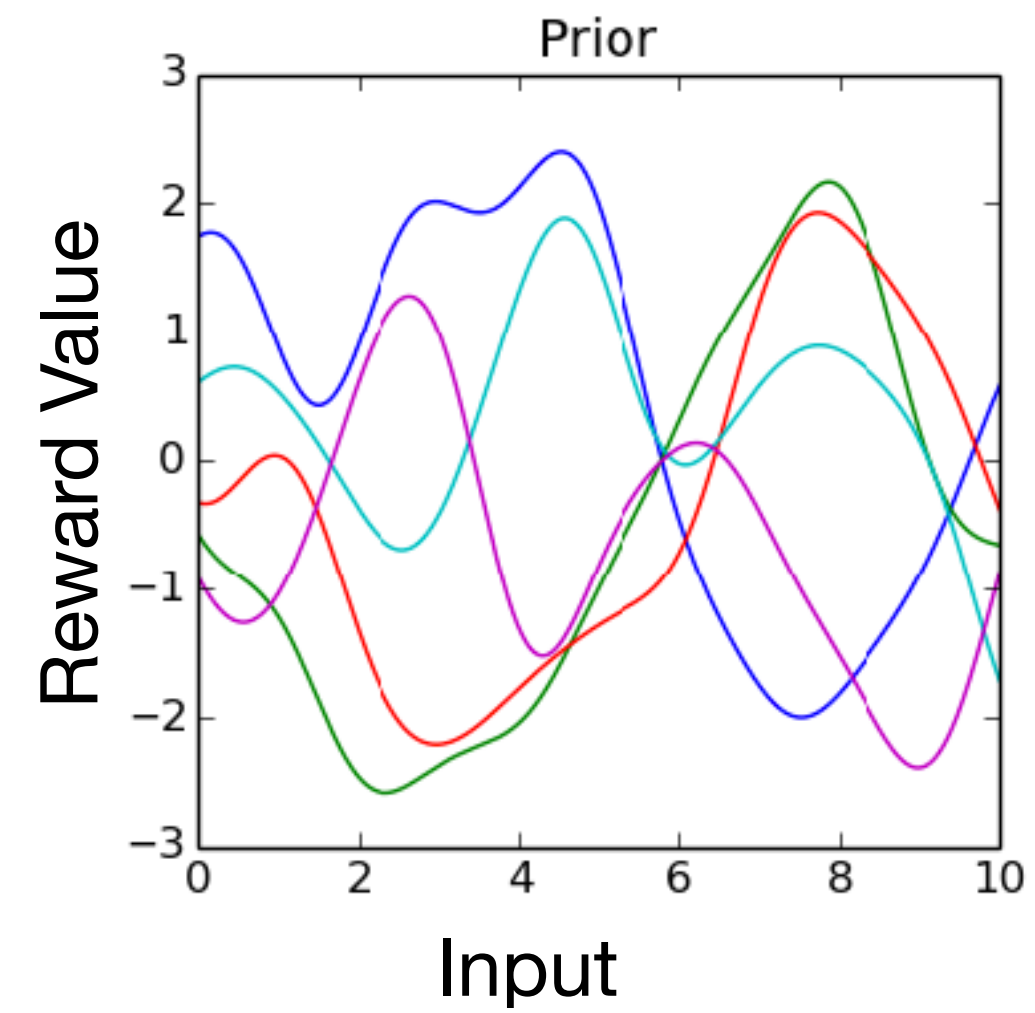


GP-UCB Model

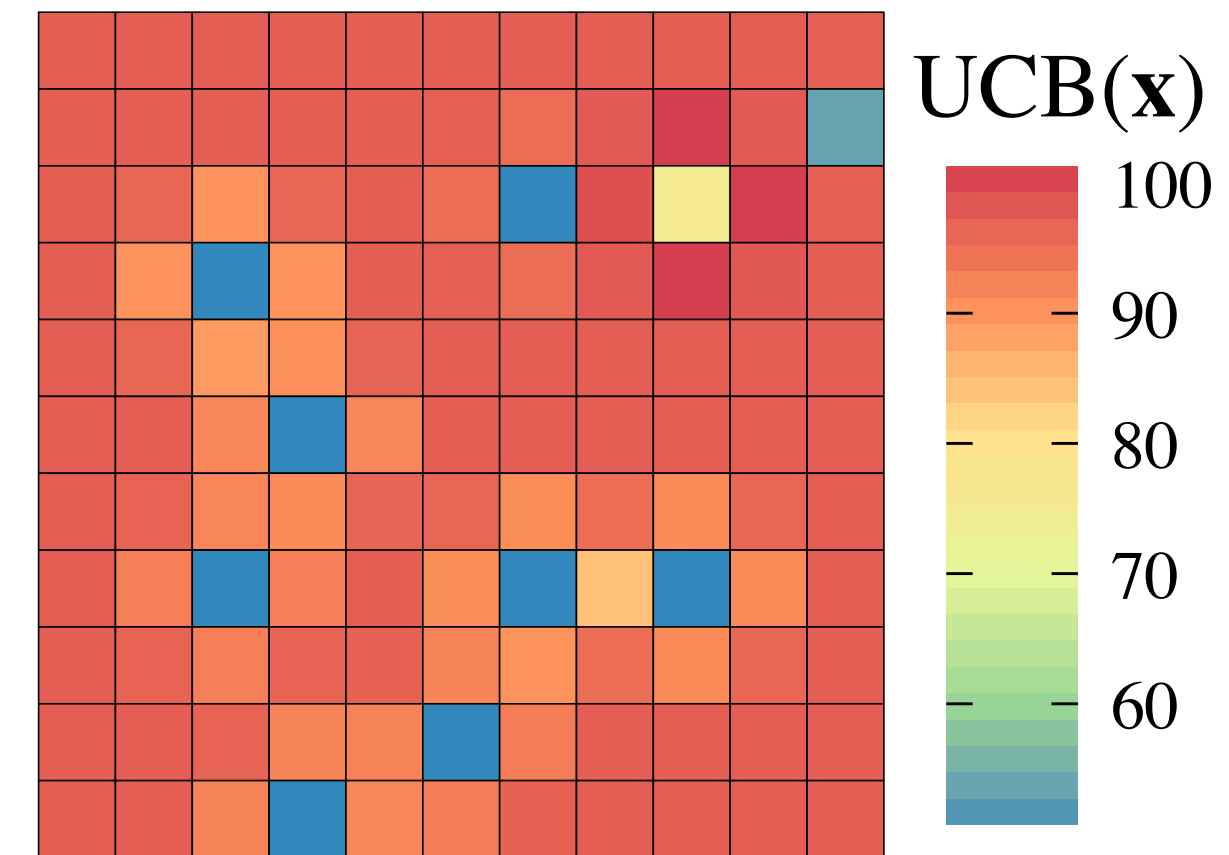
Observations



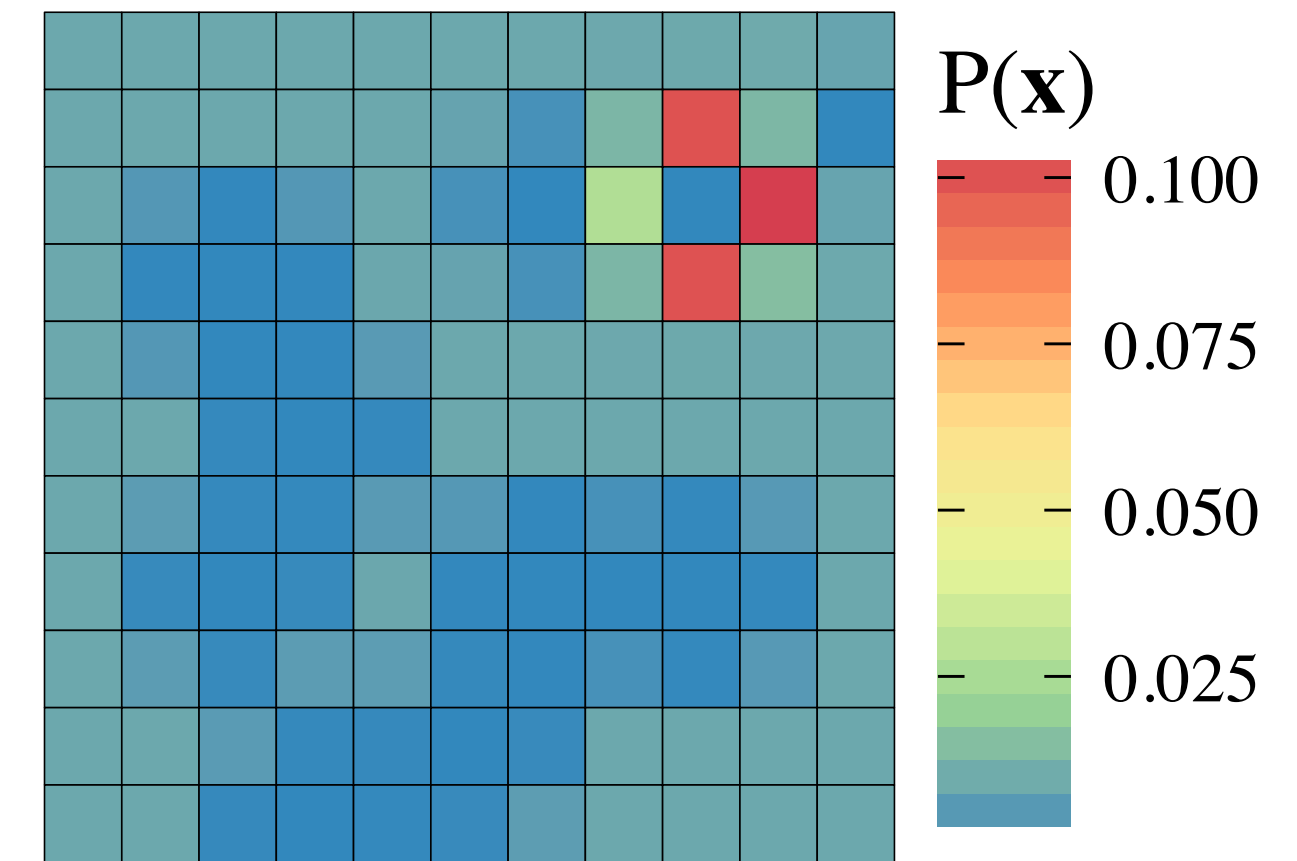
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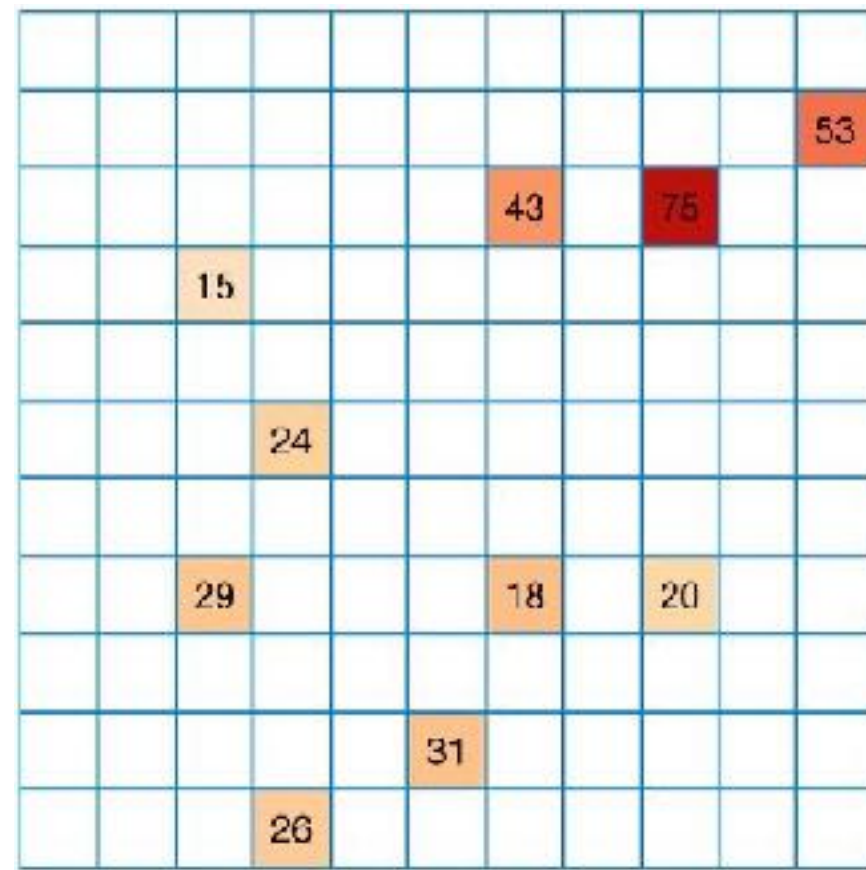


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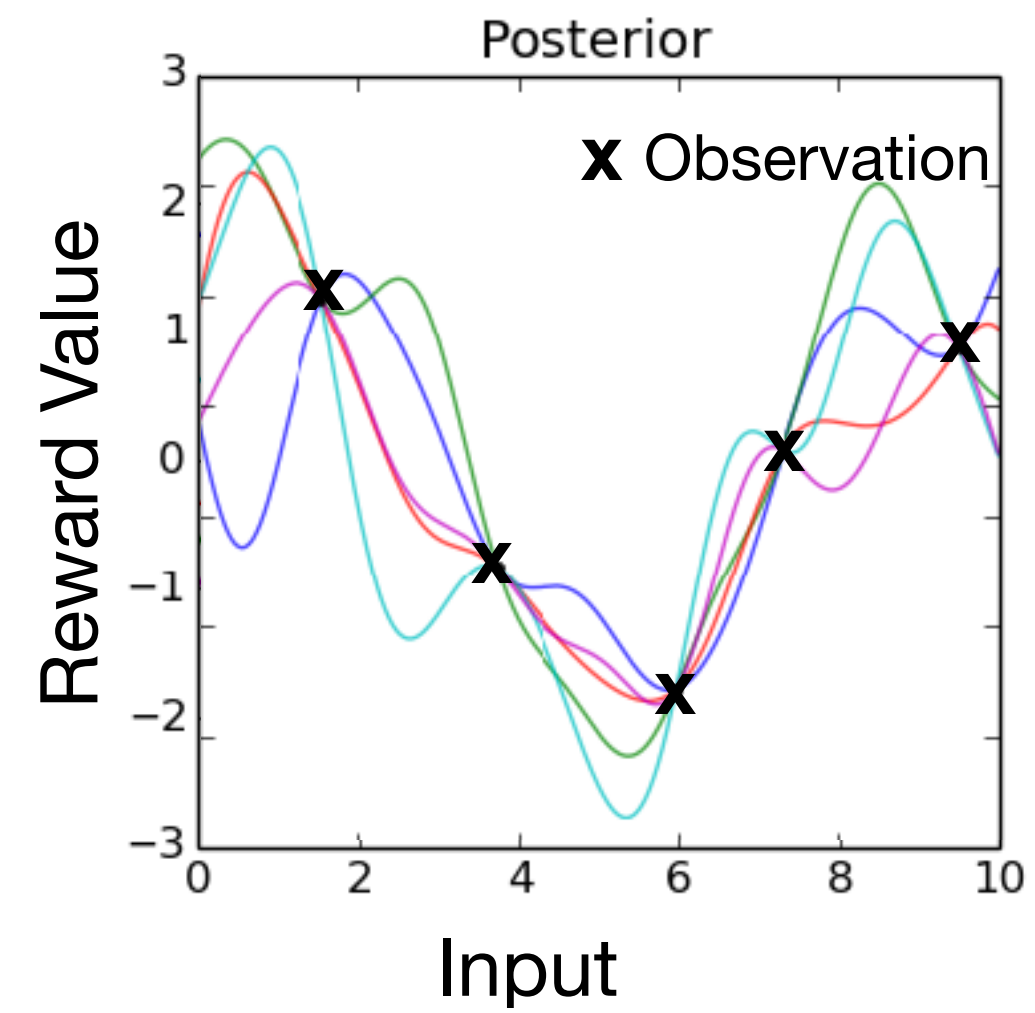


GP-UCB Model

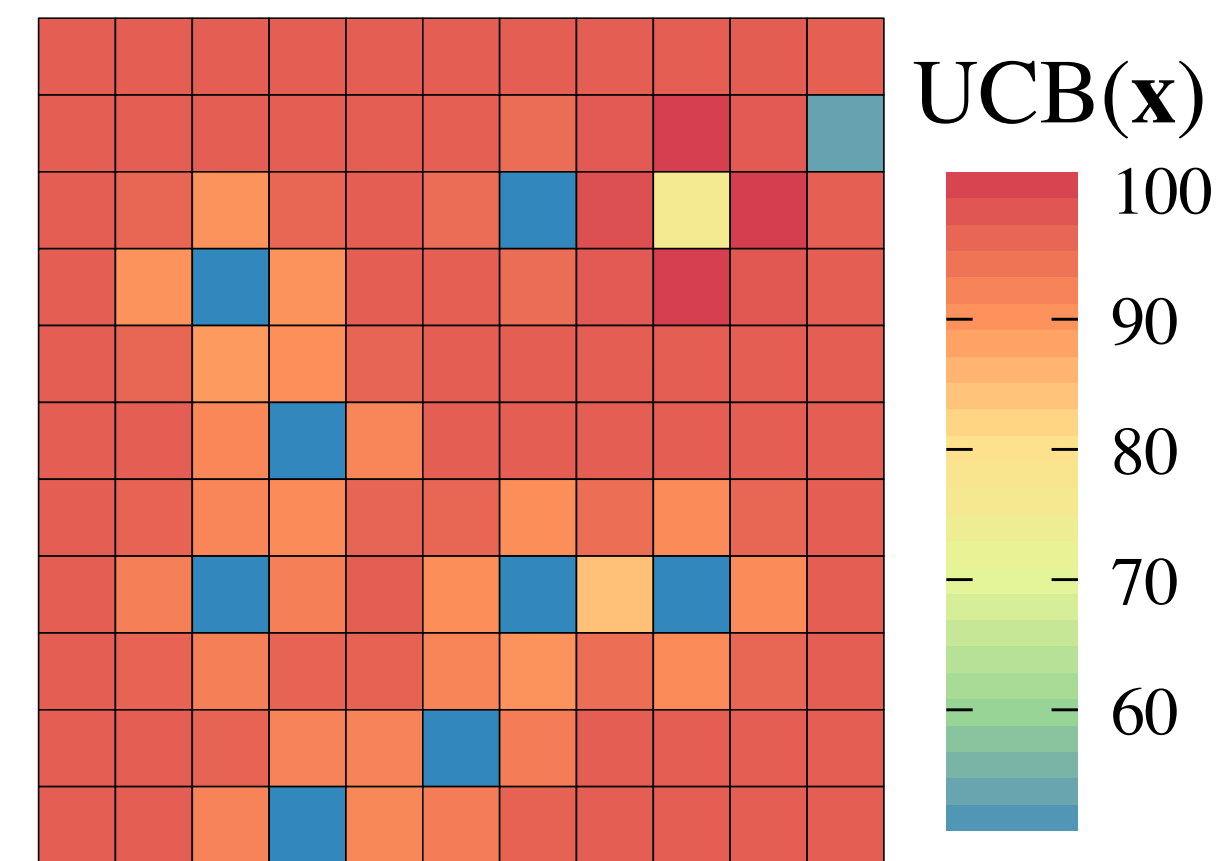
Observations



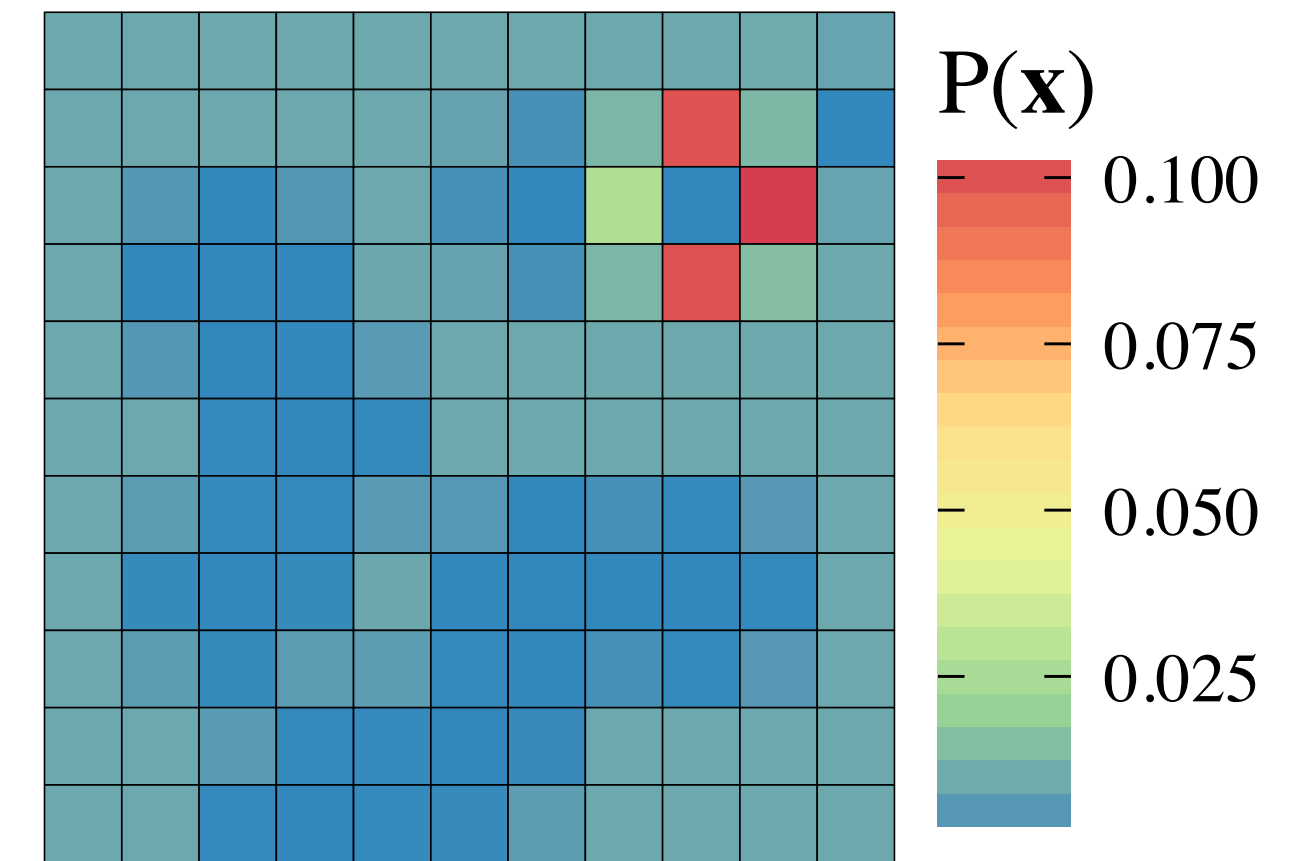
Gaussian Process (GP)



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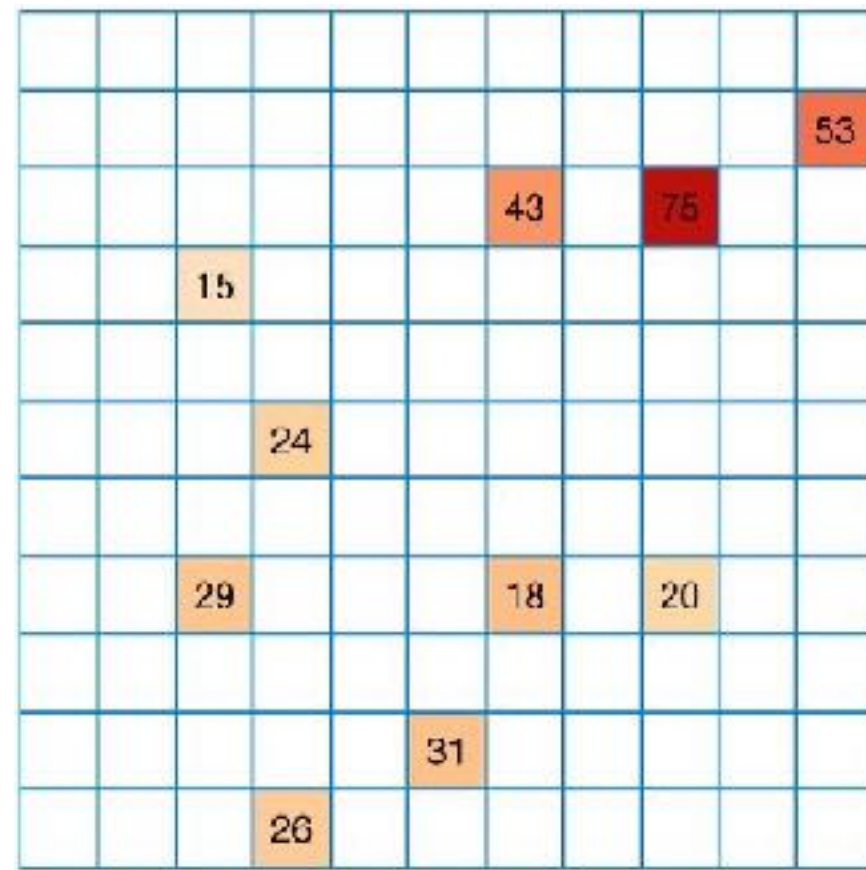


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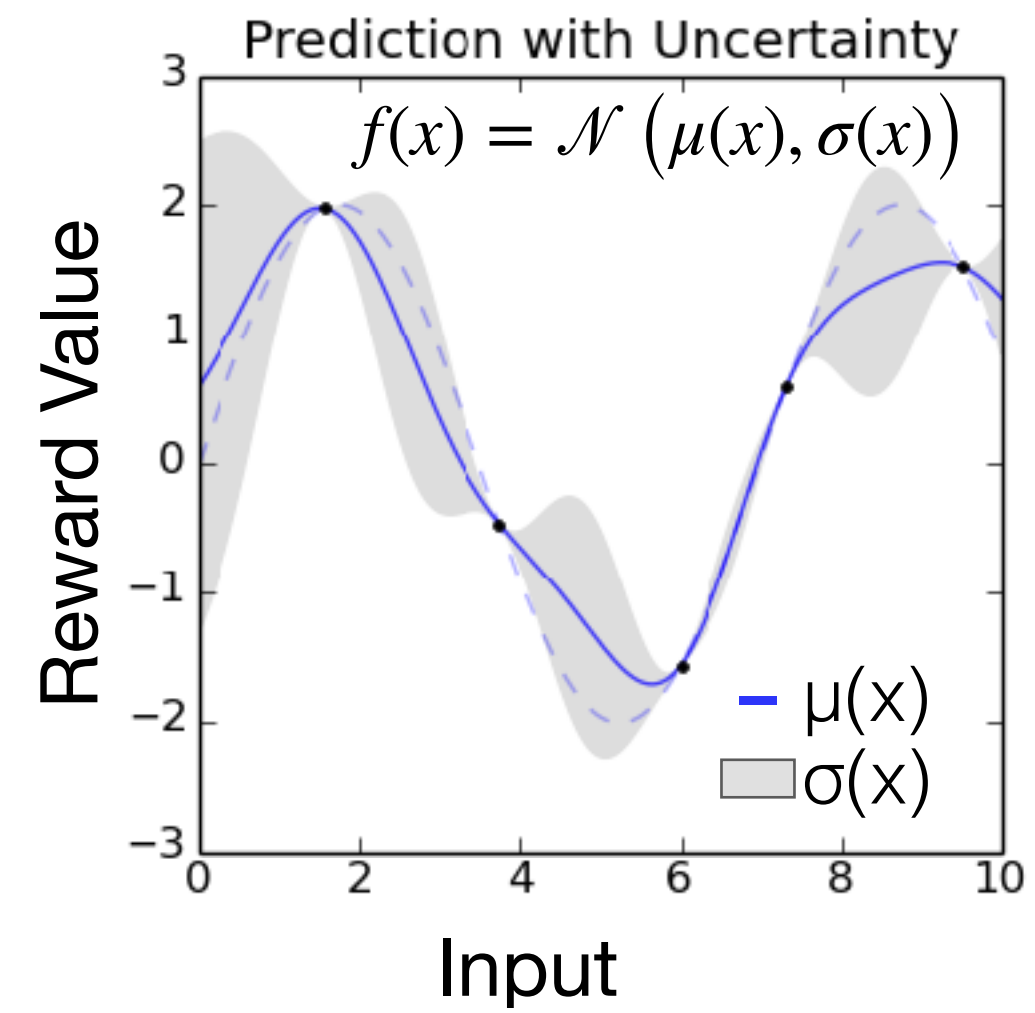


GP-UCB Model

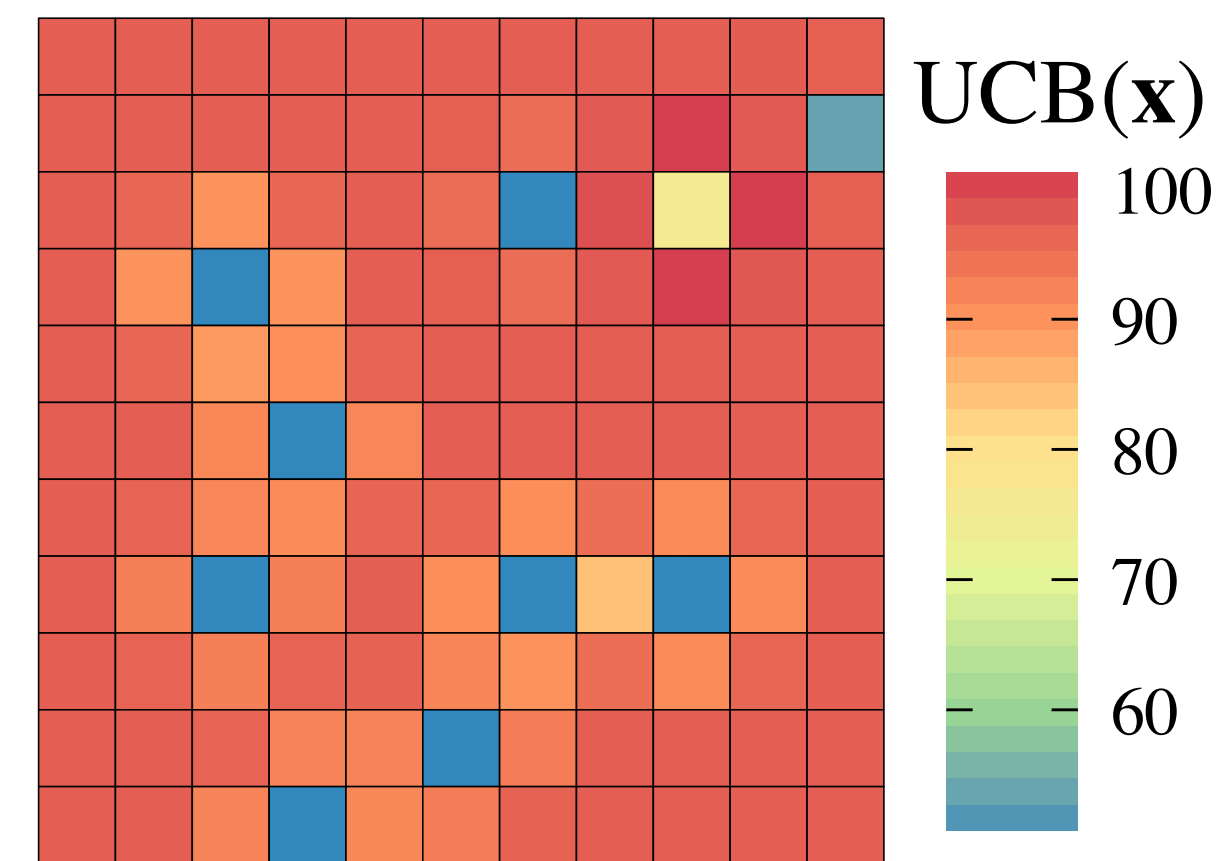
Observations



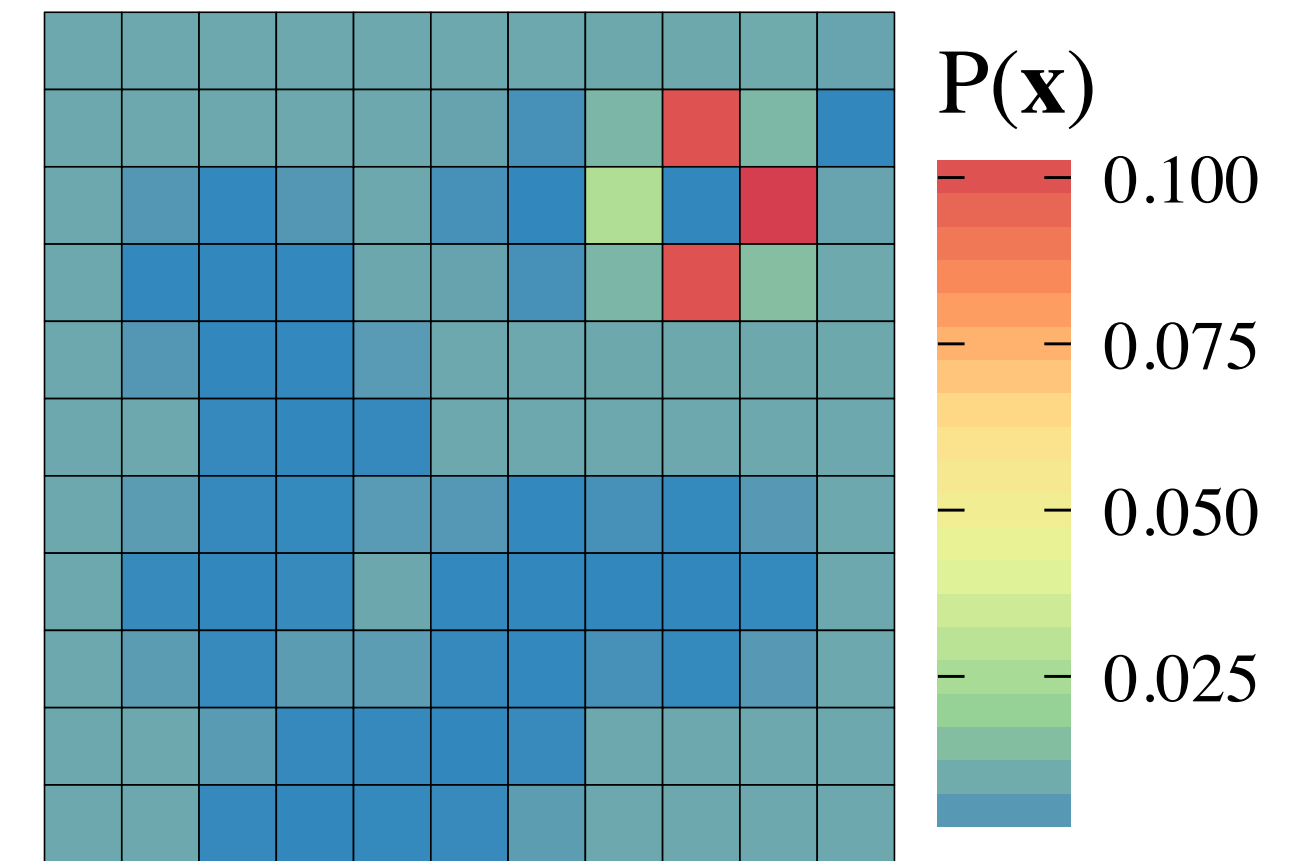
Gaussian Process (GP)



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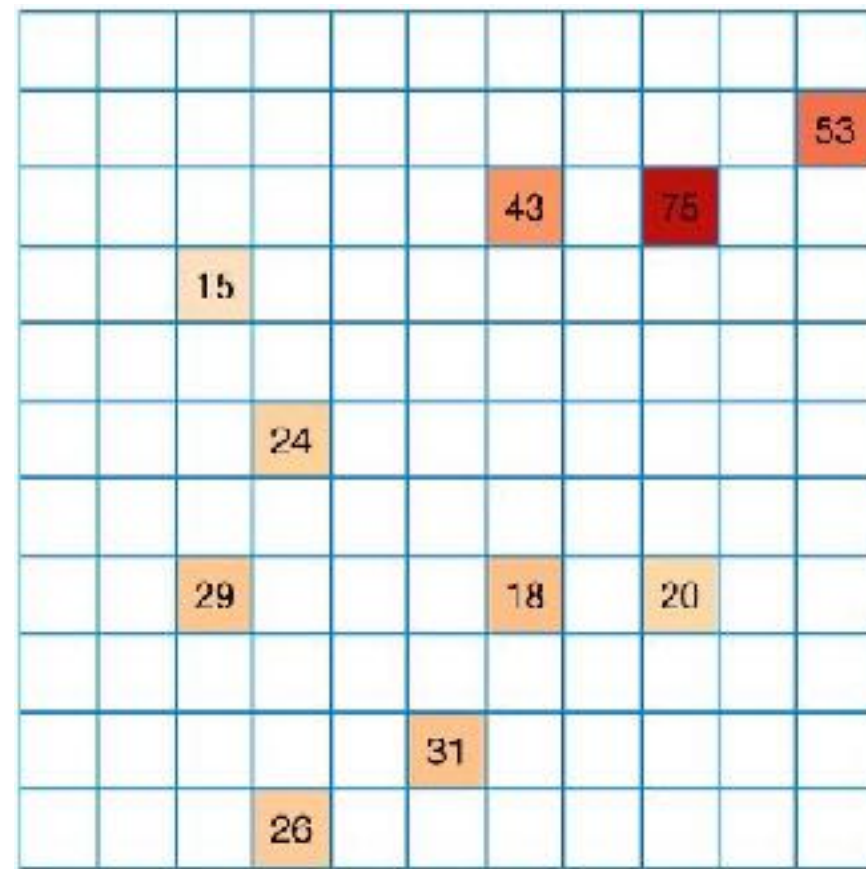


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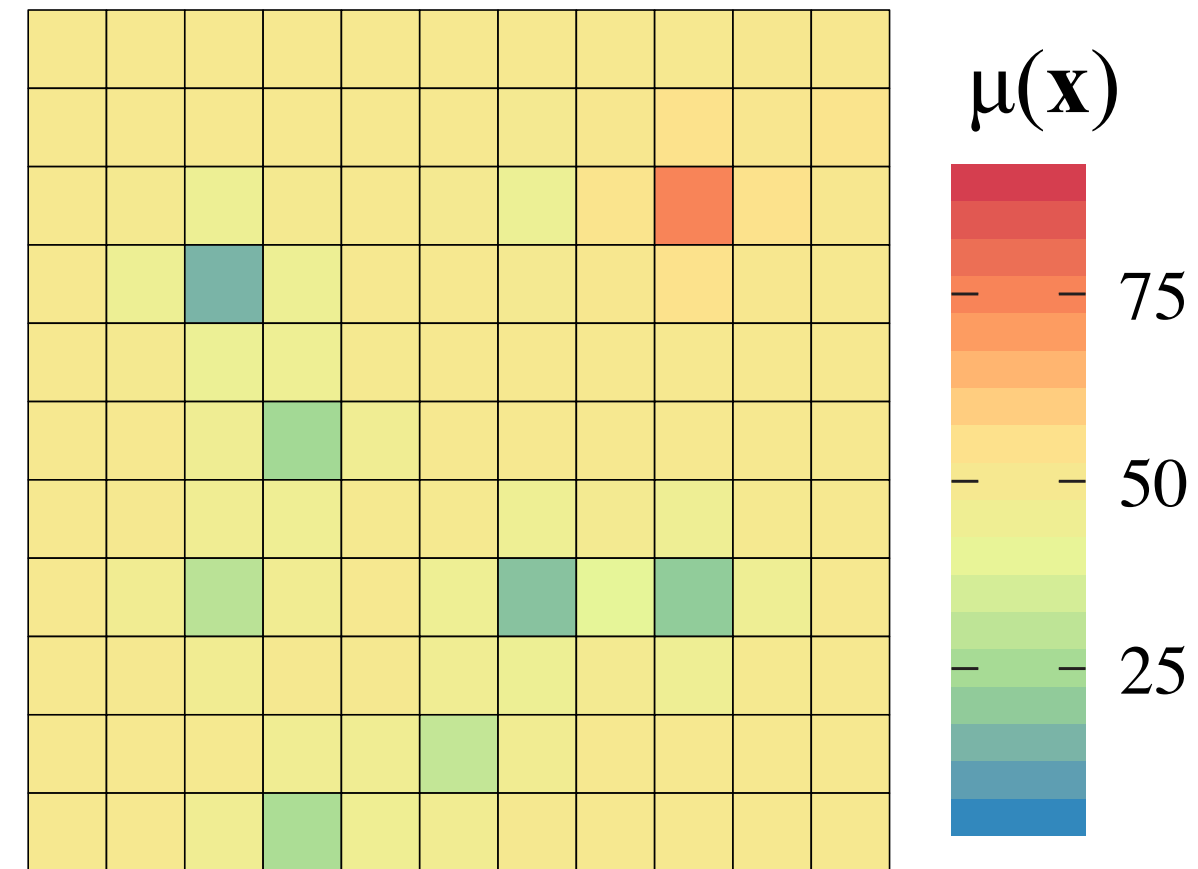


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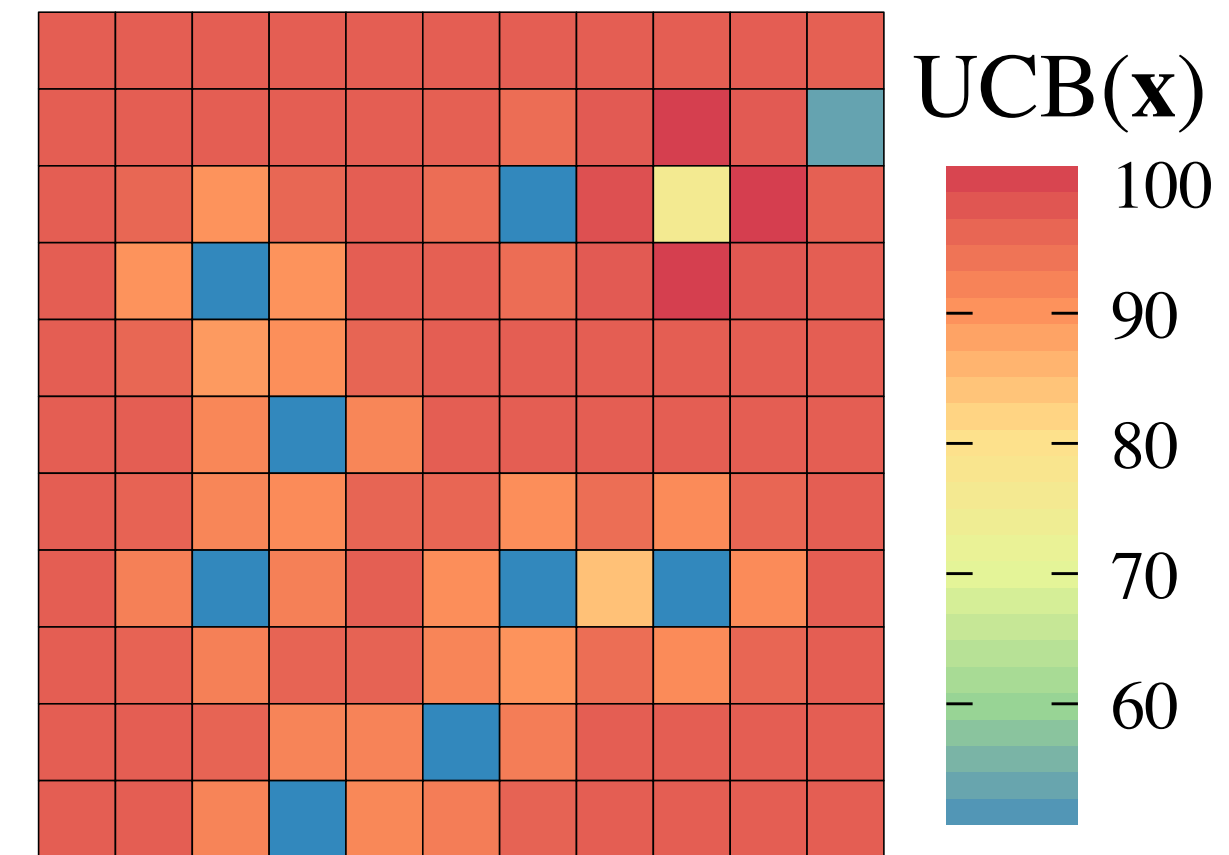
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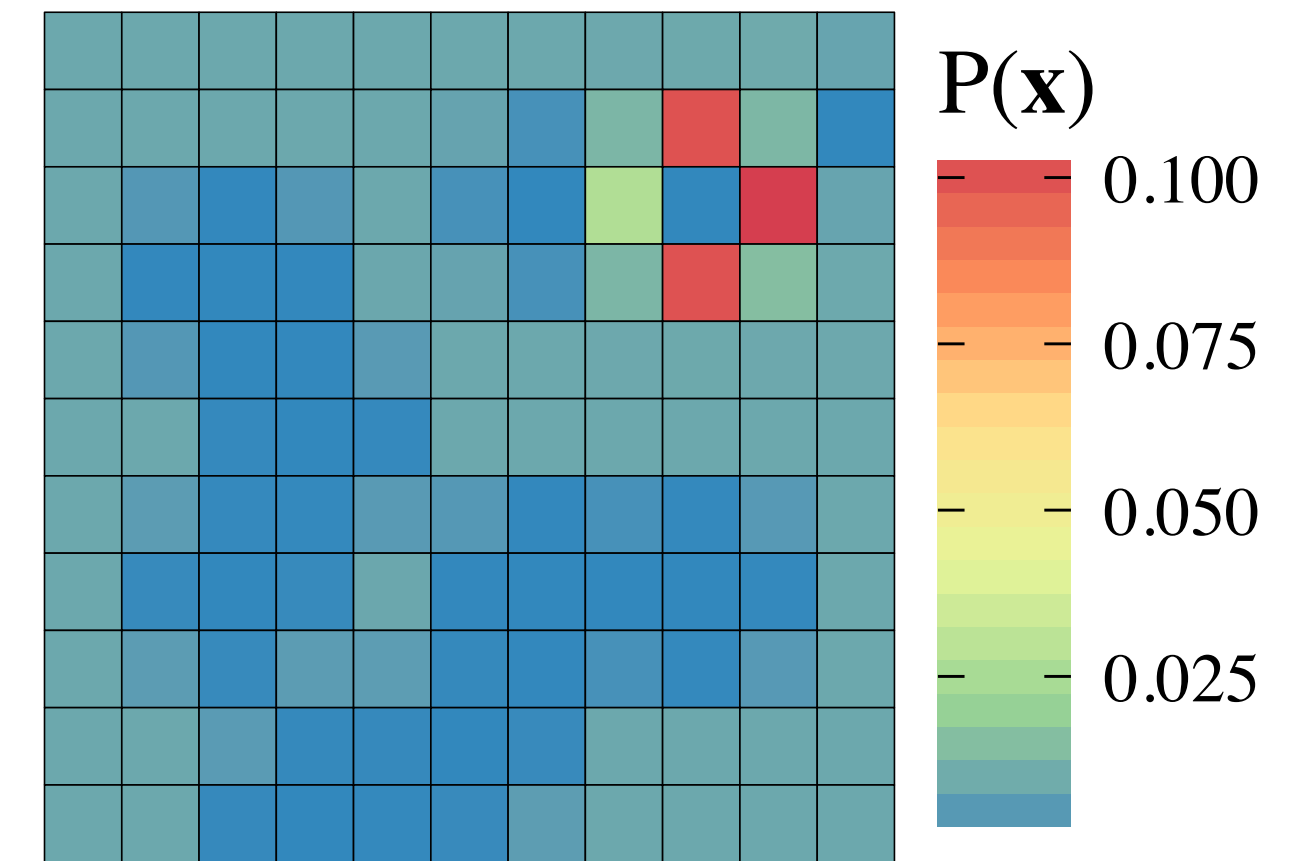
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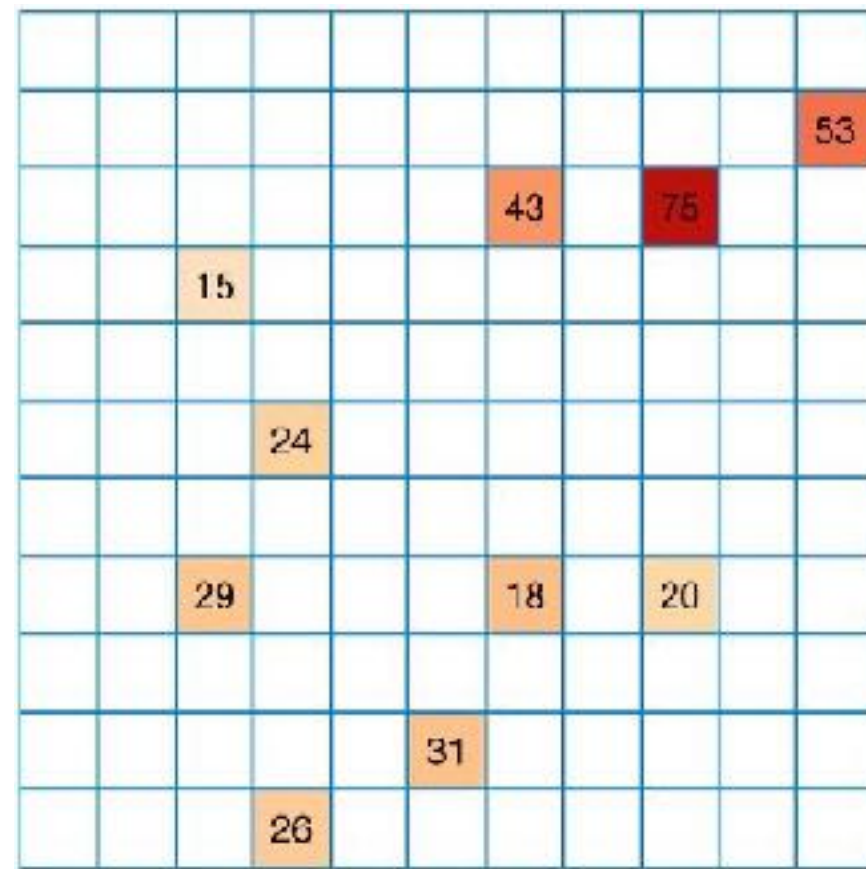


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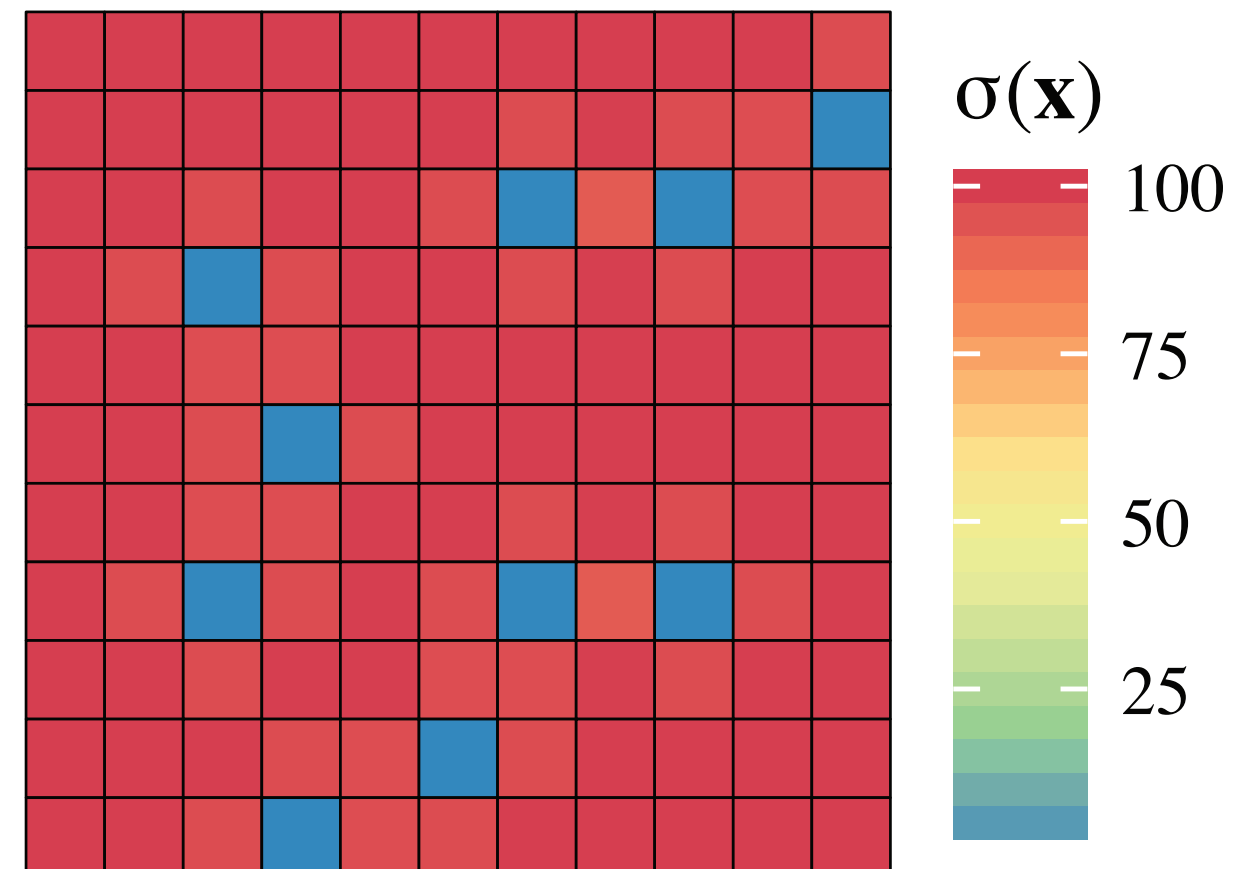


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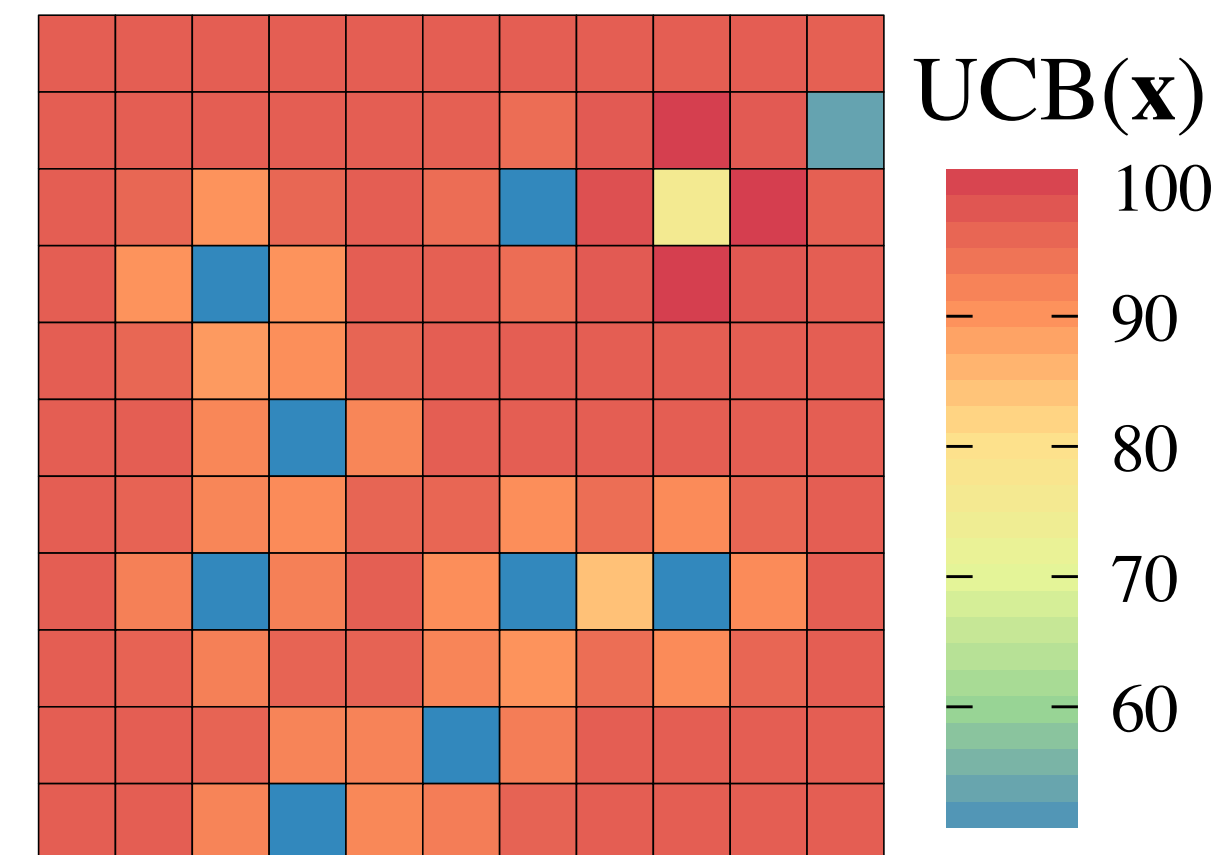
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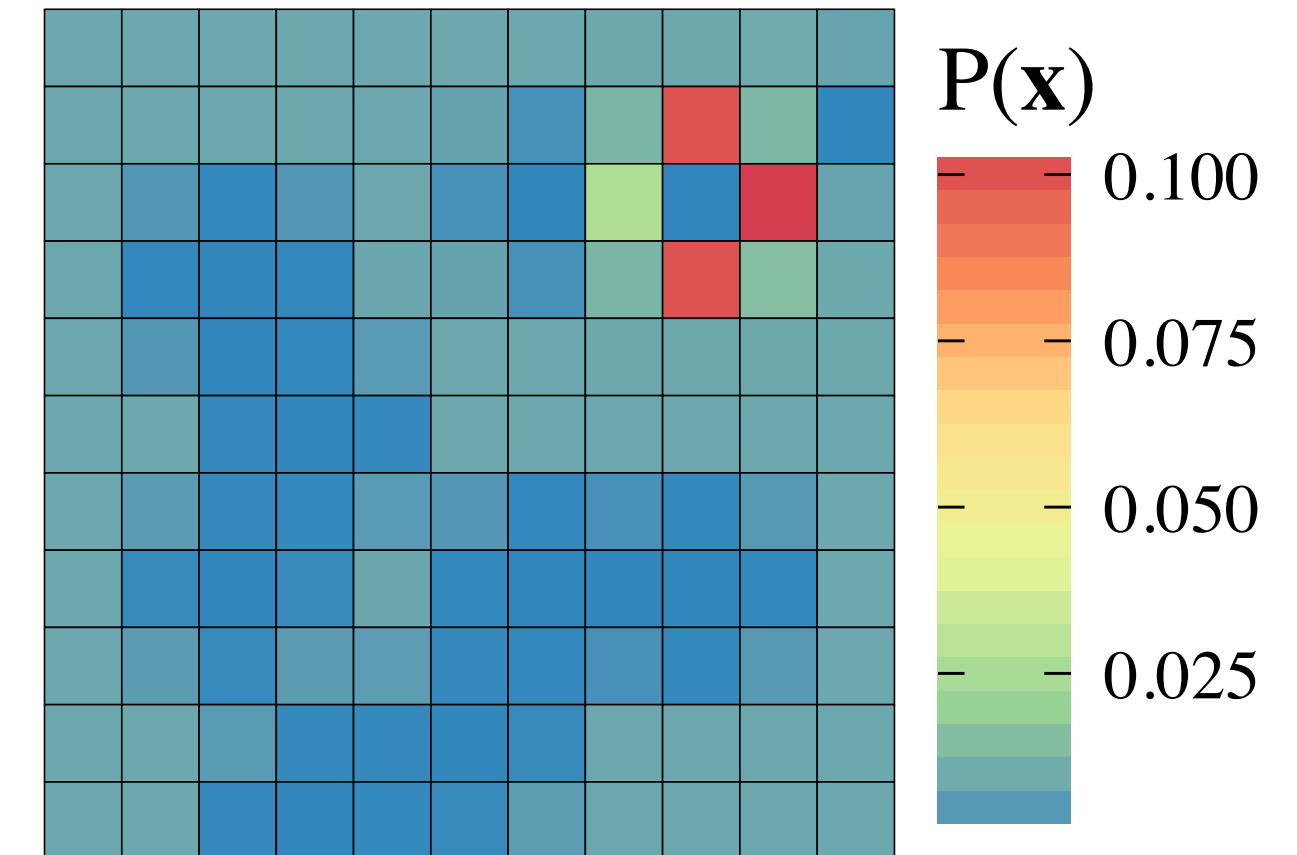
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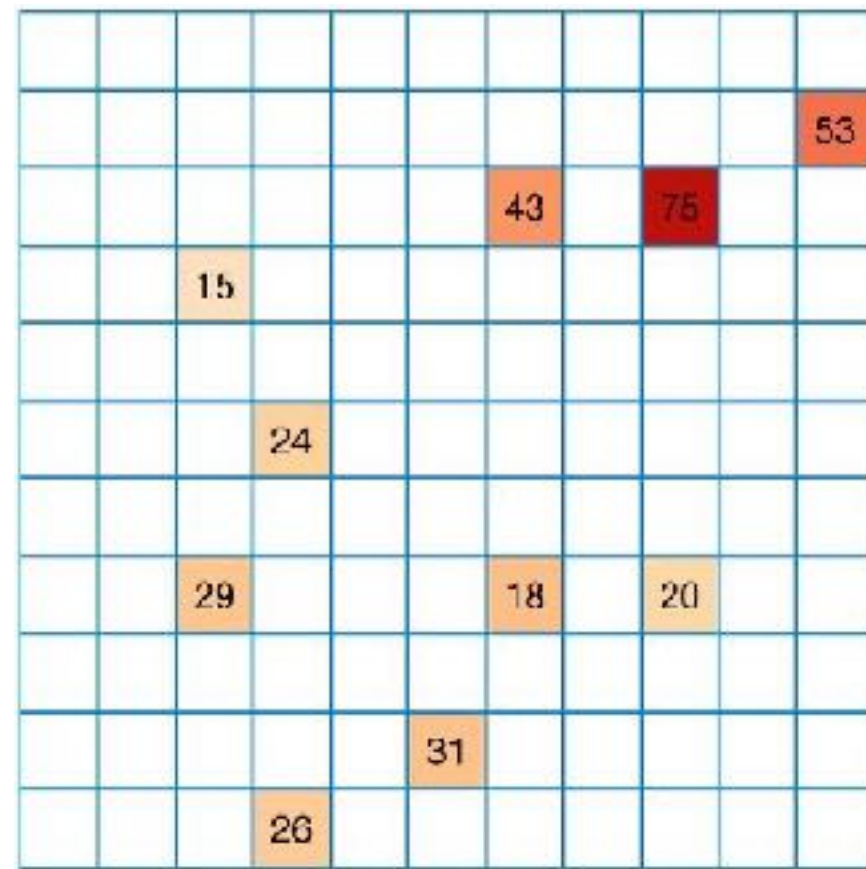


Softmax Choice Rule

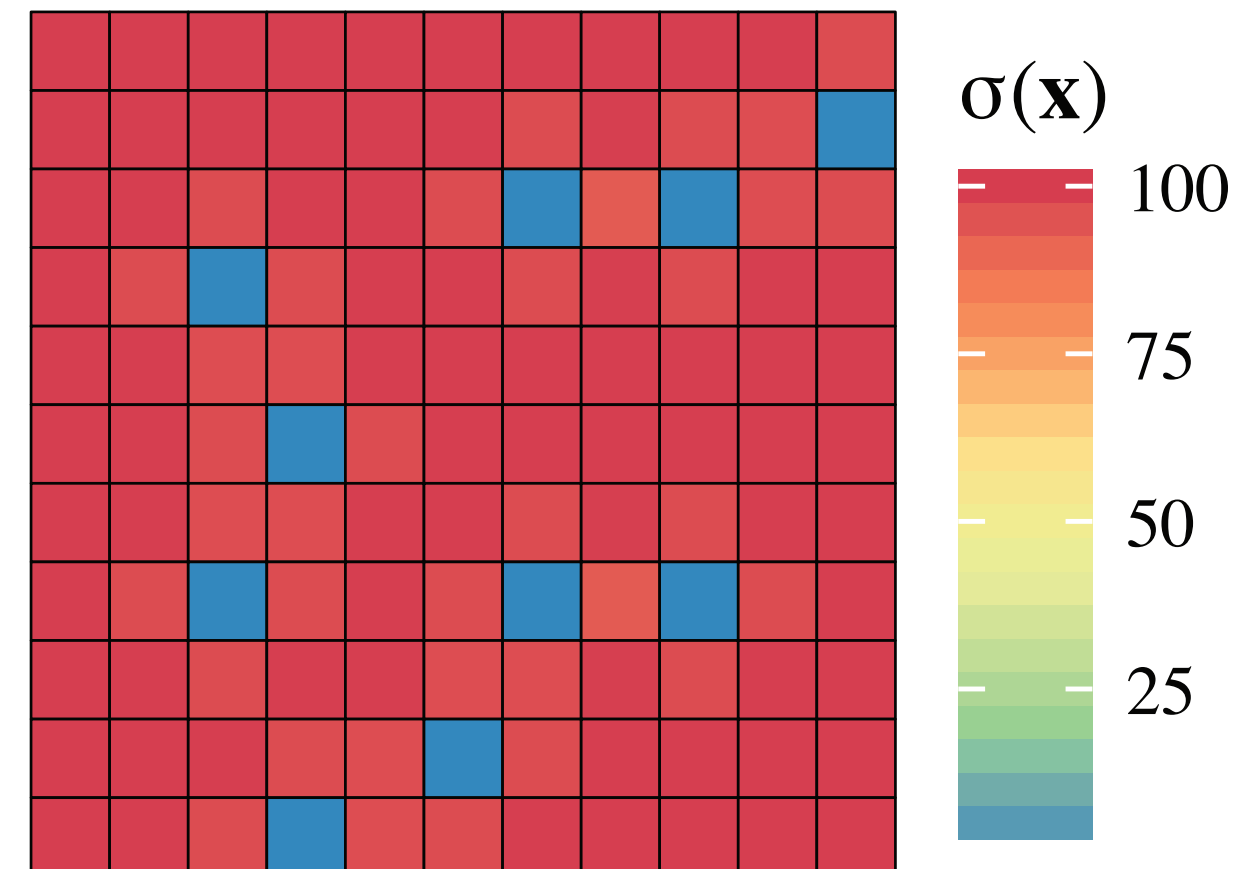


GP-UCB Model

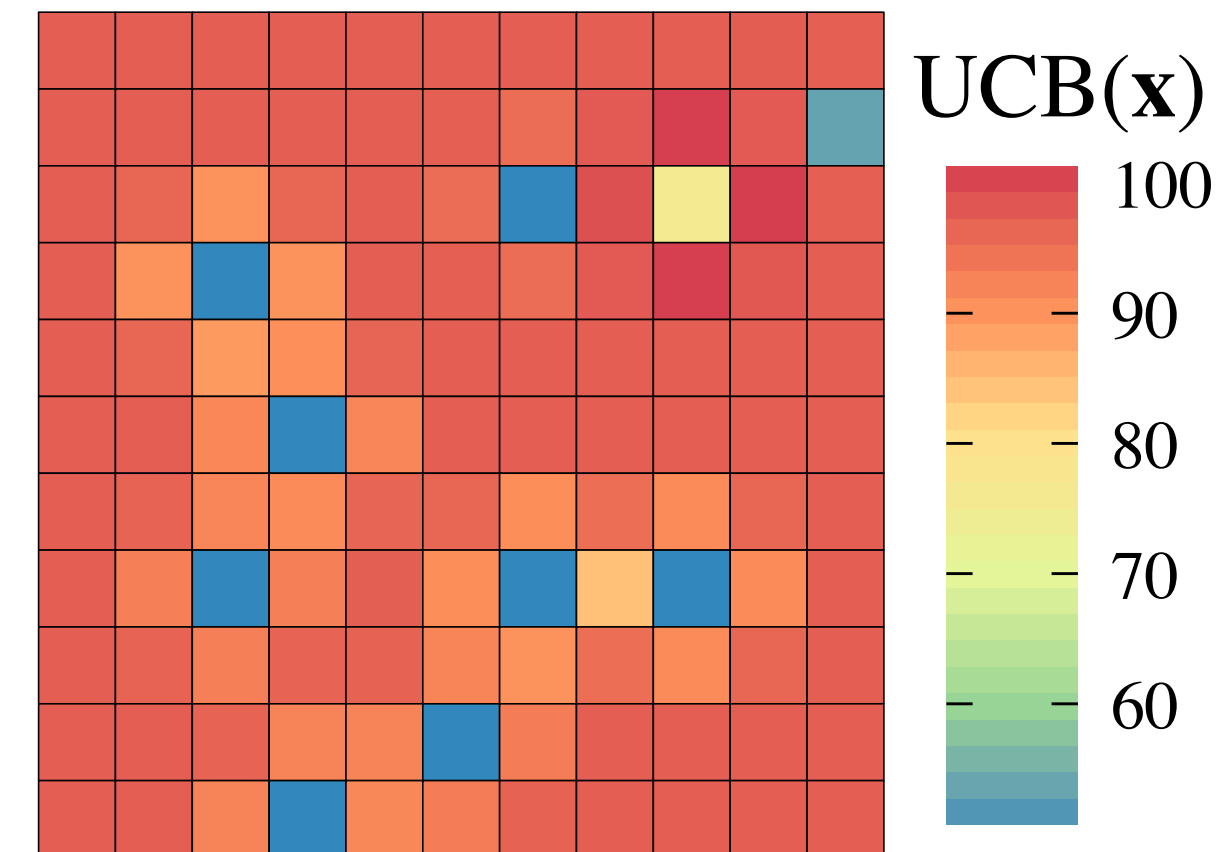
Observations



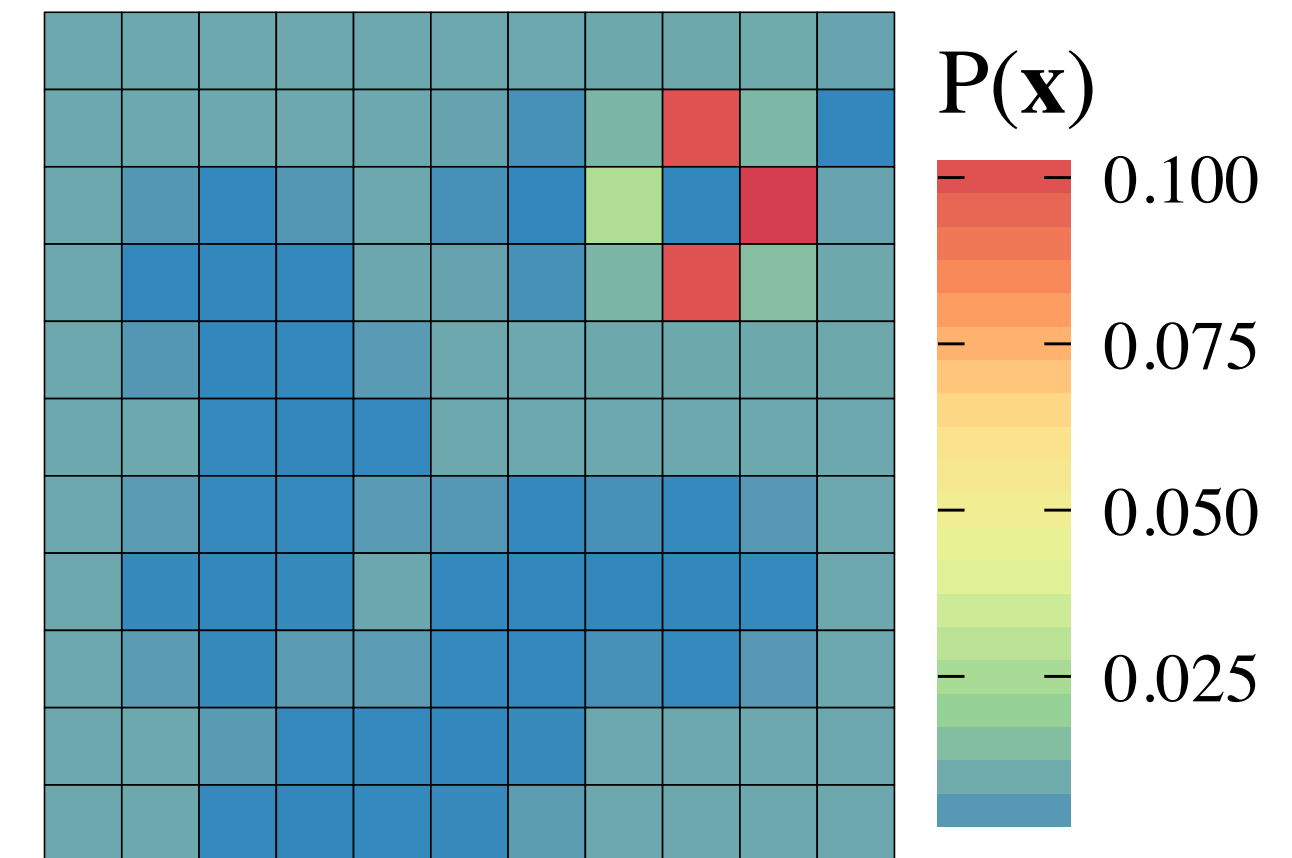
Gaussian Process (GP)



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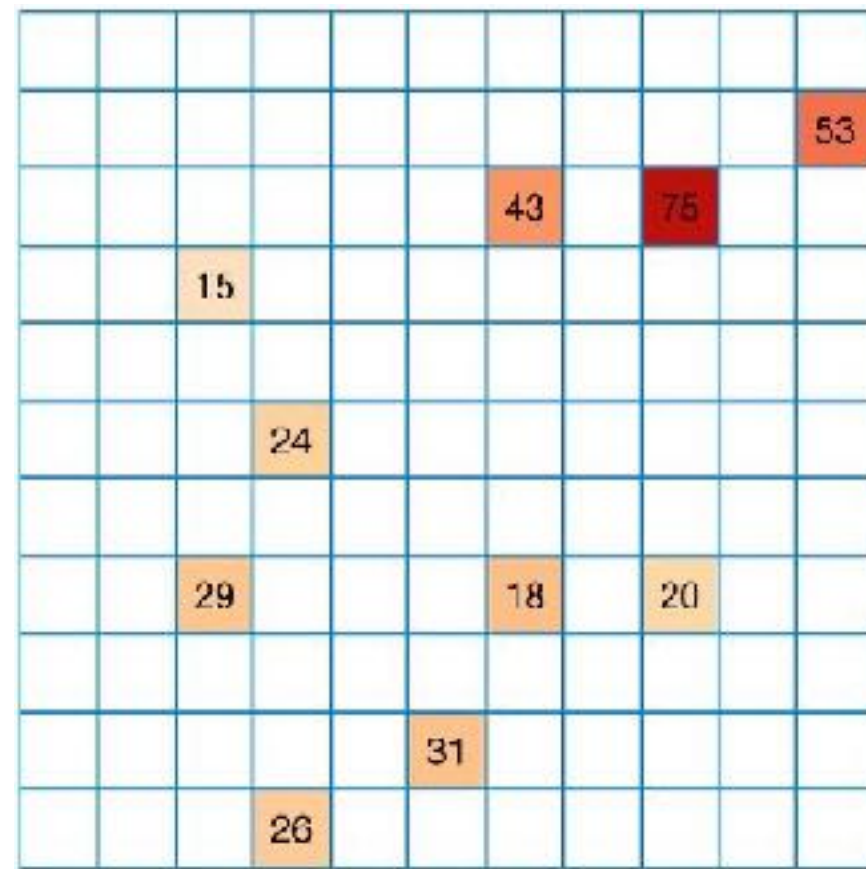
Softmax Choice Rule



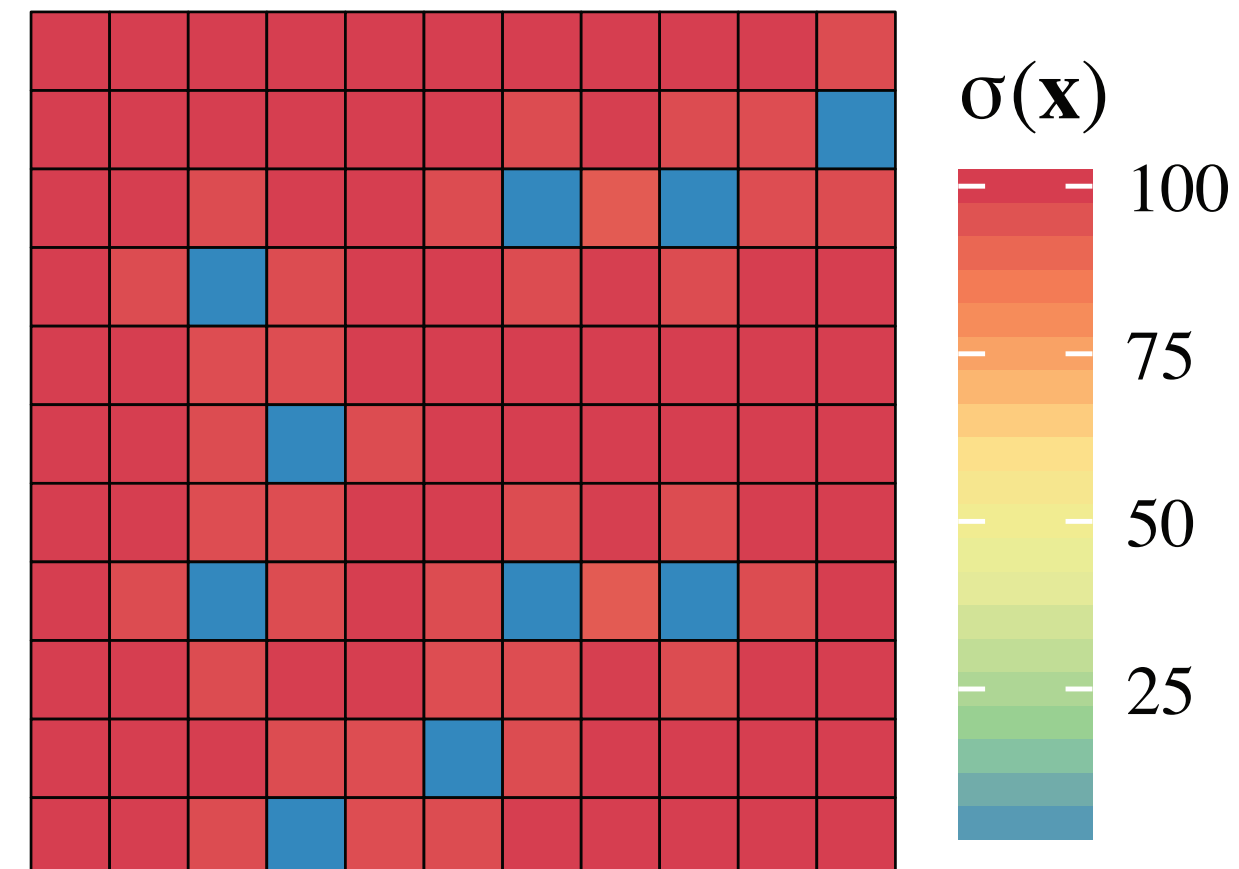
$$k_{RBF}(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{||\mathbf{x} - \mathbf{x}'||^2}{2\lambda^2}\right)$$

GP-UCB Model

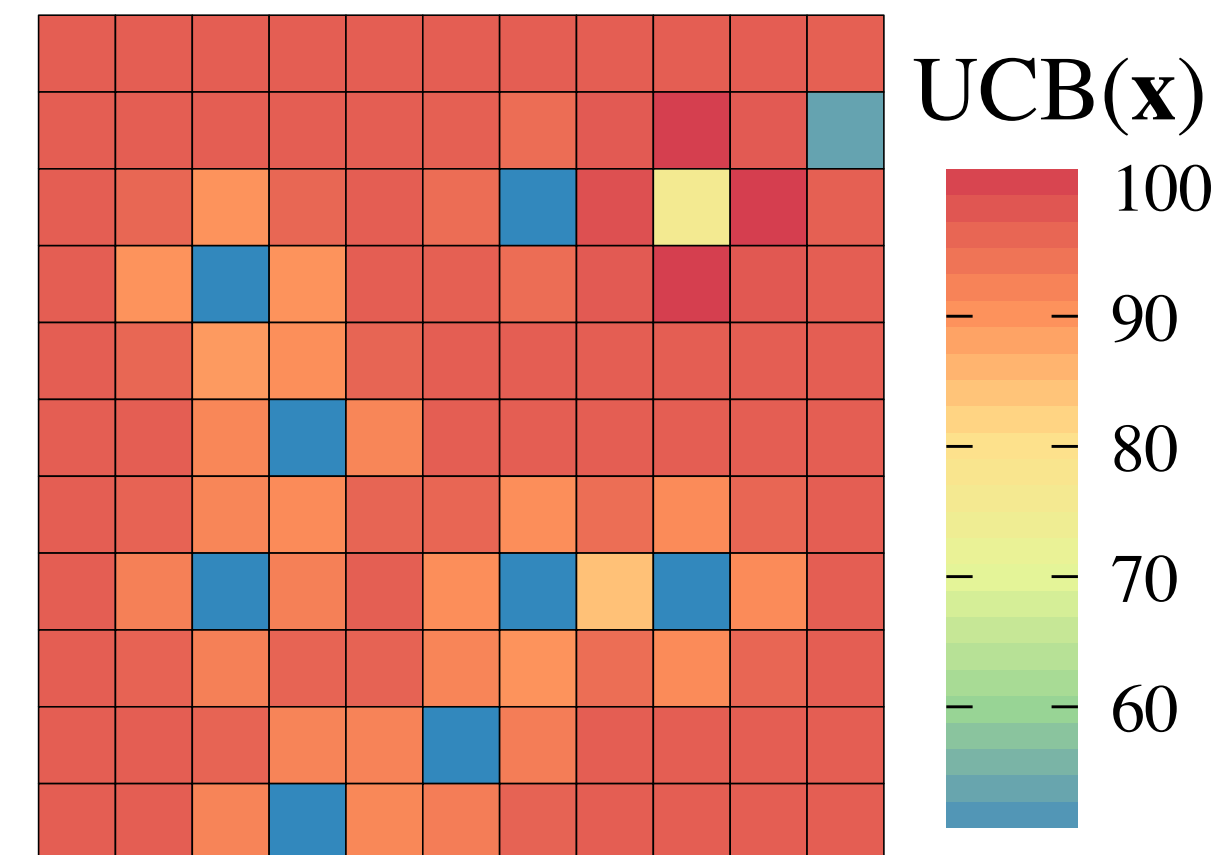
Observations



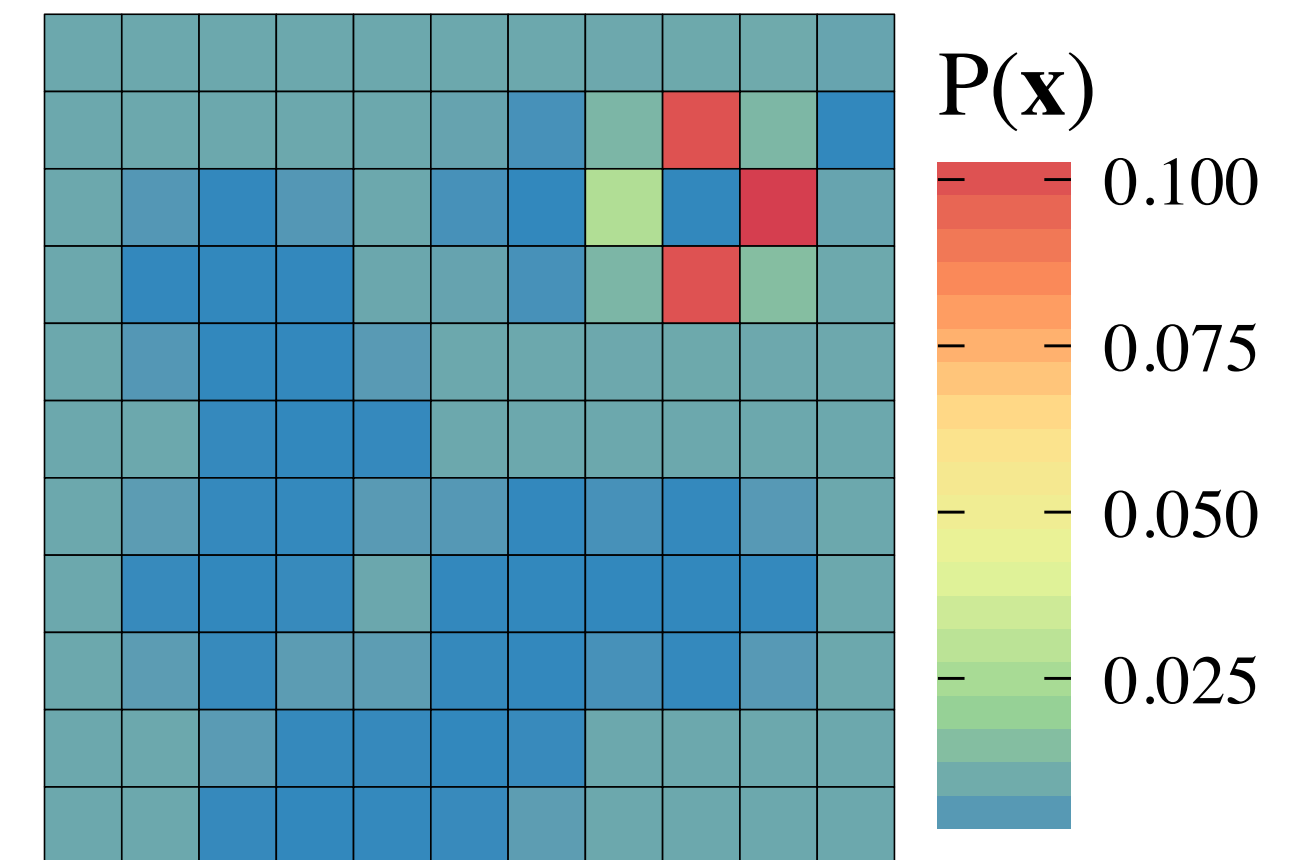
Gaussian Process (GP)



Upper Confidence Bound (UCB) Sampling

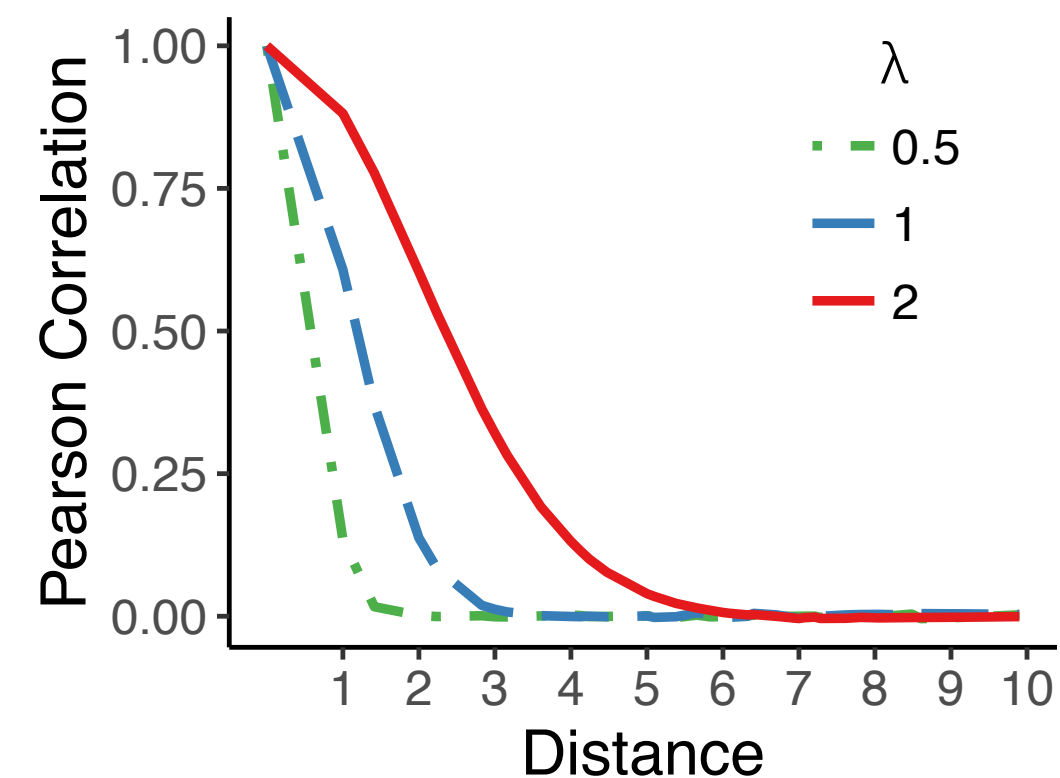


Softmax Choice Rule



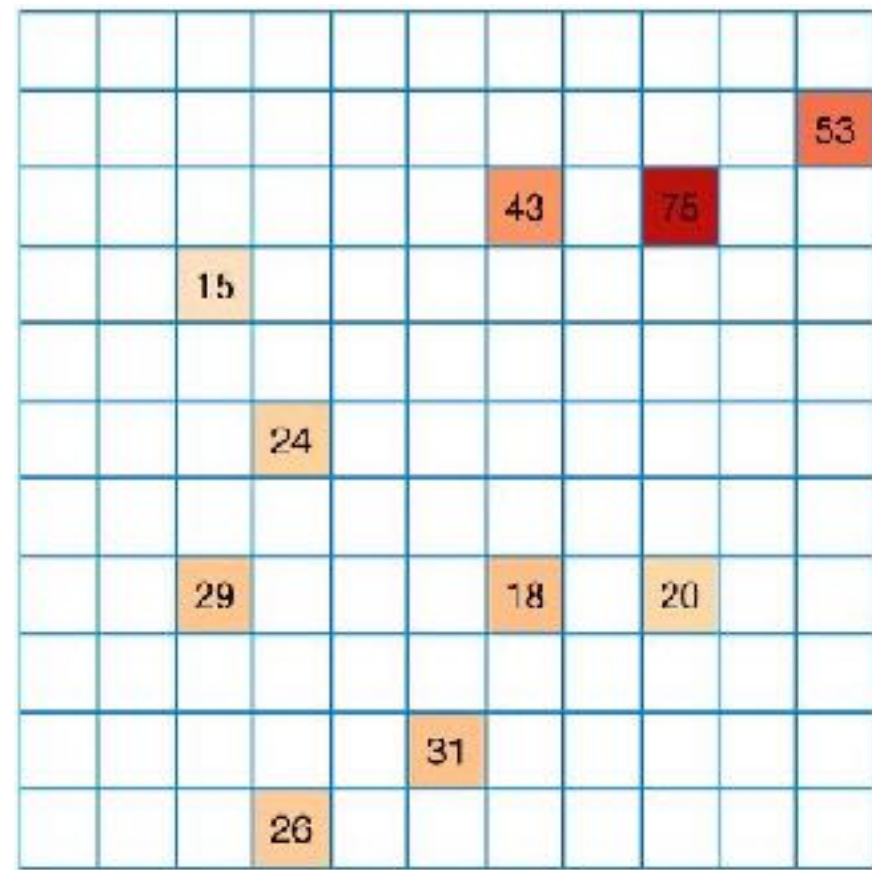
$$k_{RBF}(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{||\mathbf{x} - \mathbf{x}'||^2}{2\lambda^2}\right)$$

Generalization λ

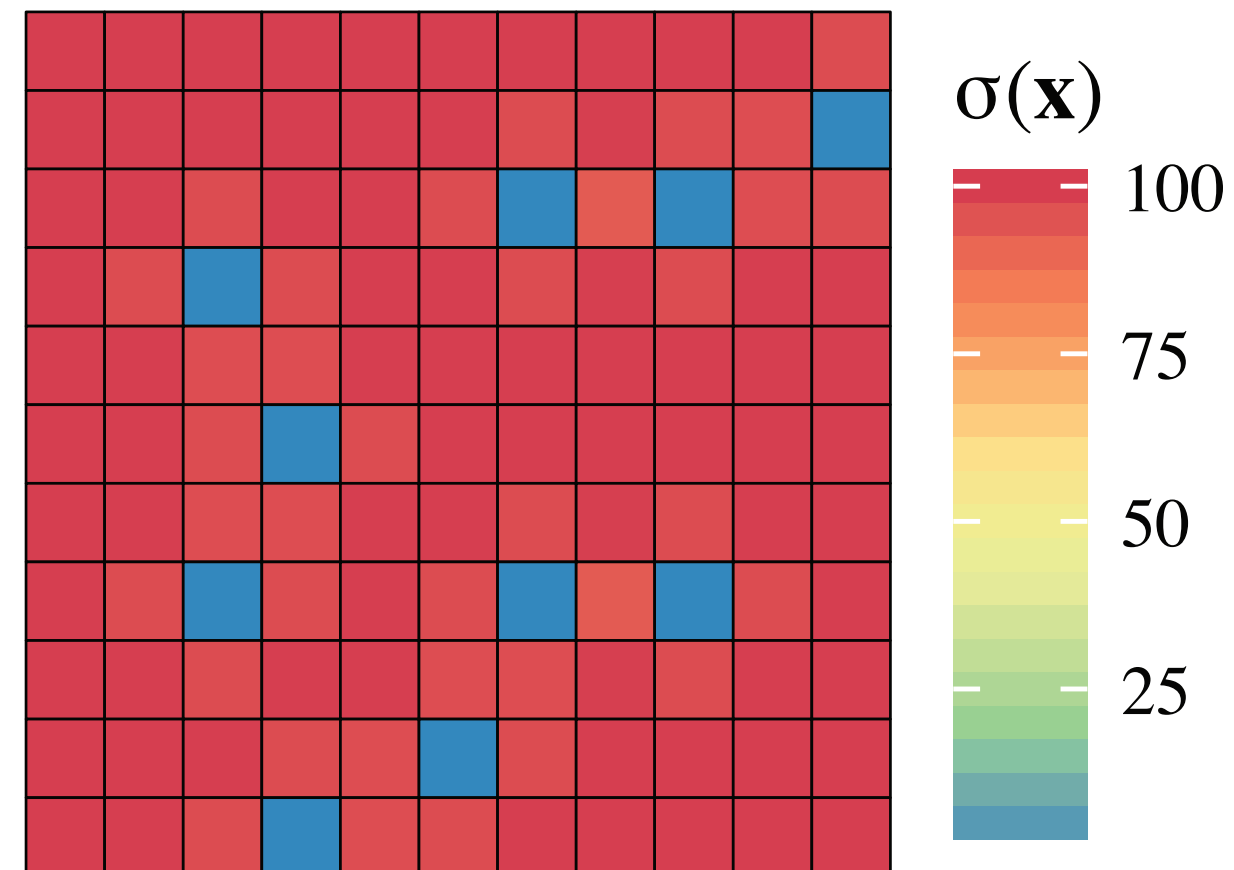


GP-UCB Model

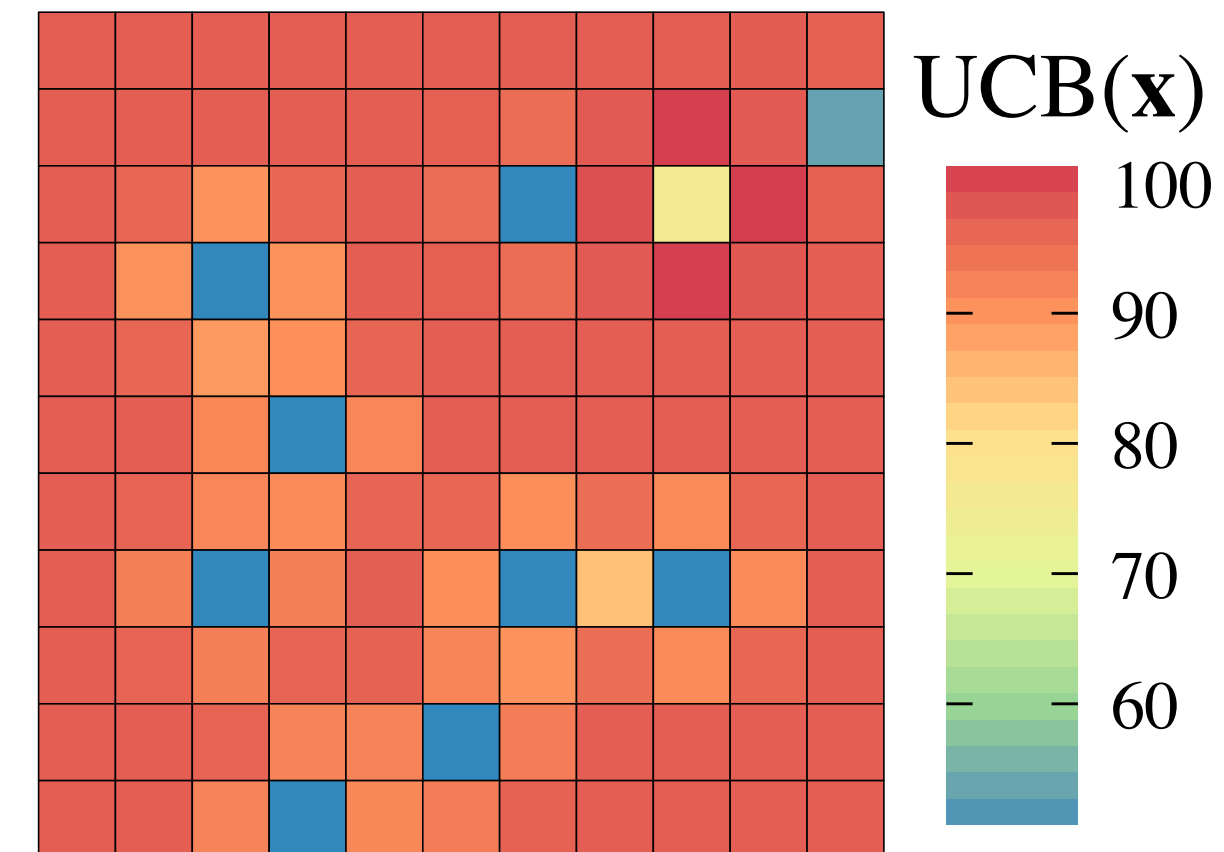
Observations



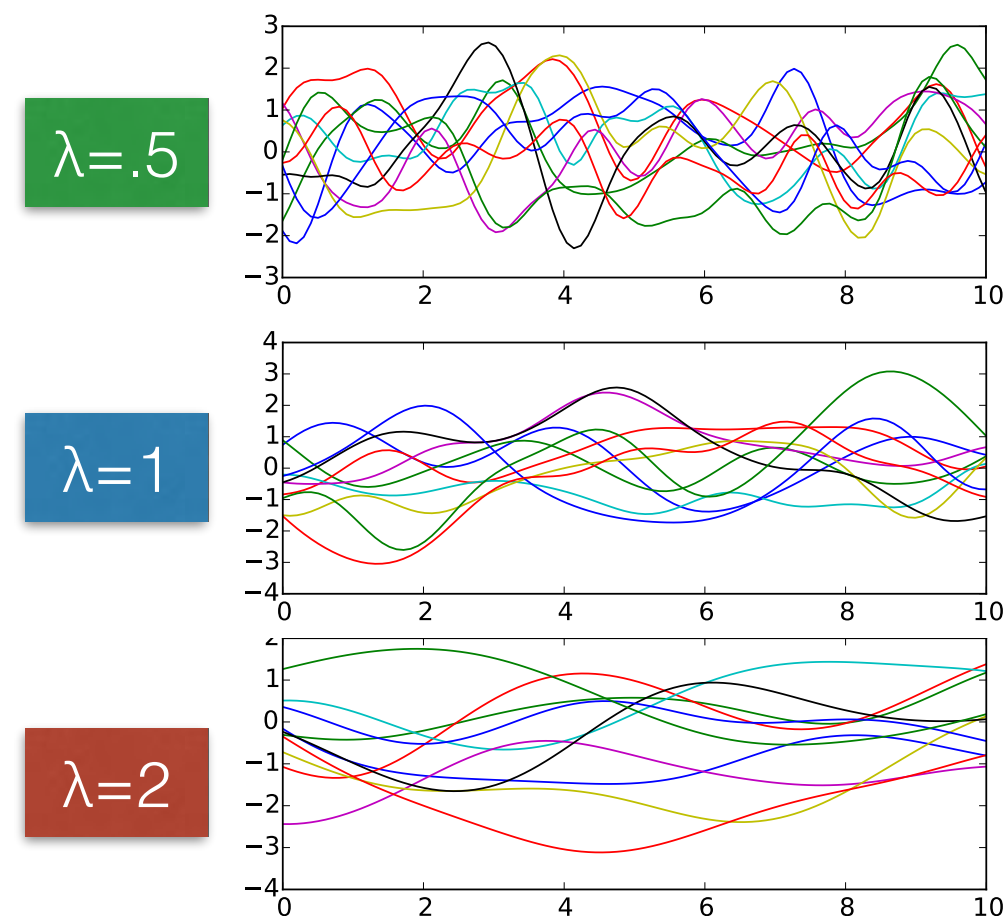
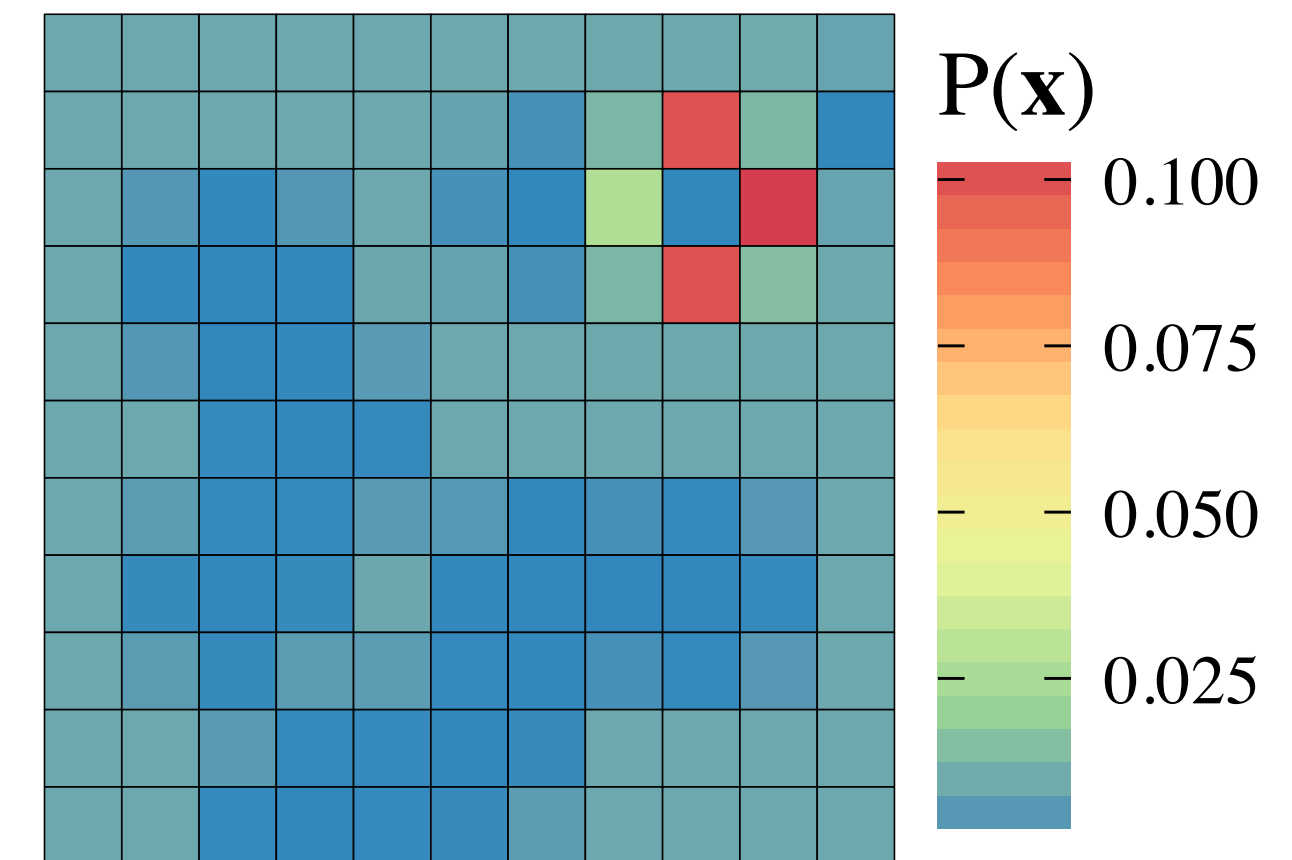
Gaussian Process (GP)



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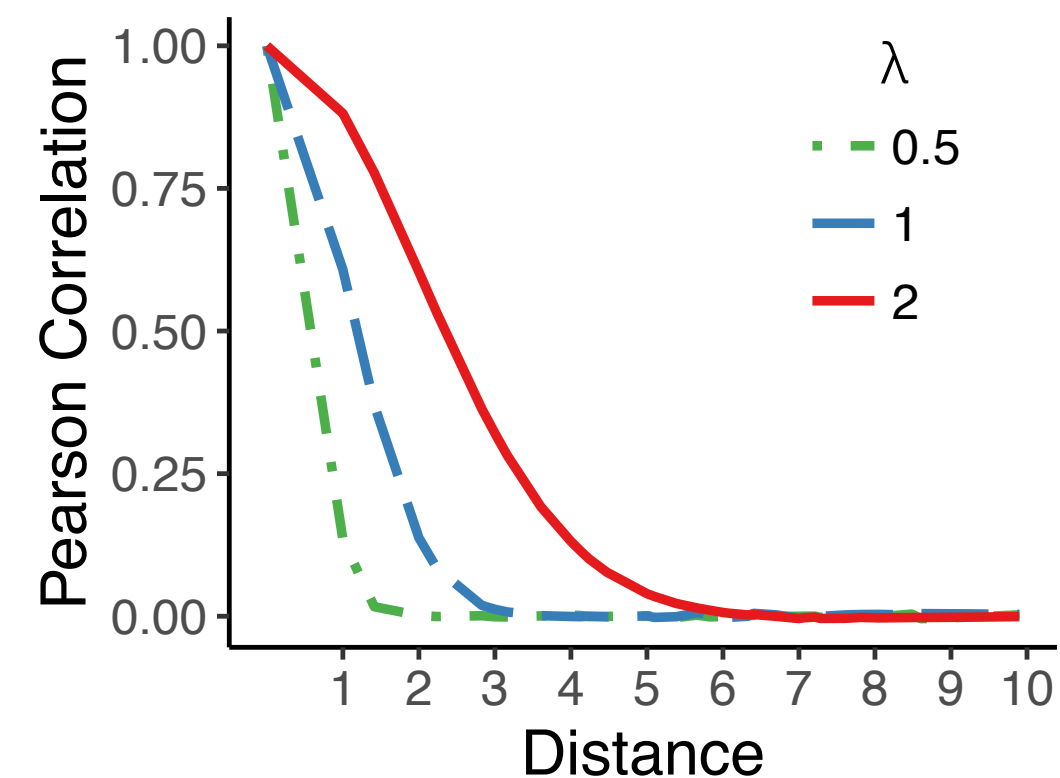


Softmax Choice Rule



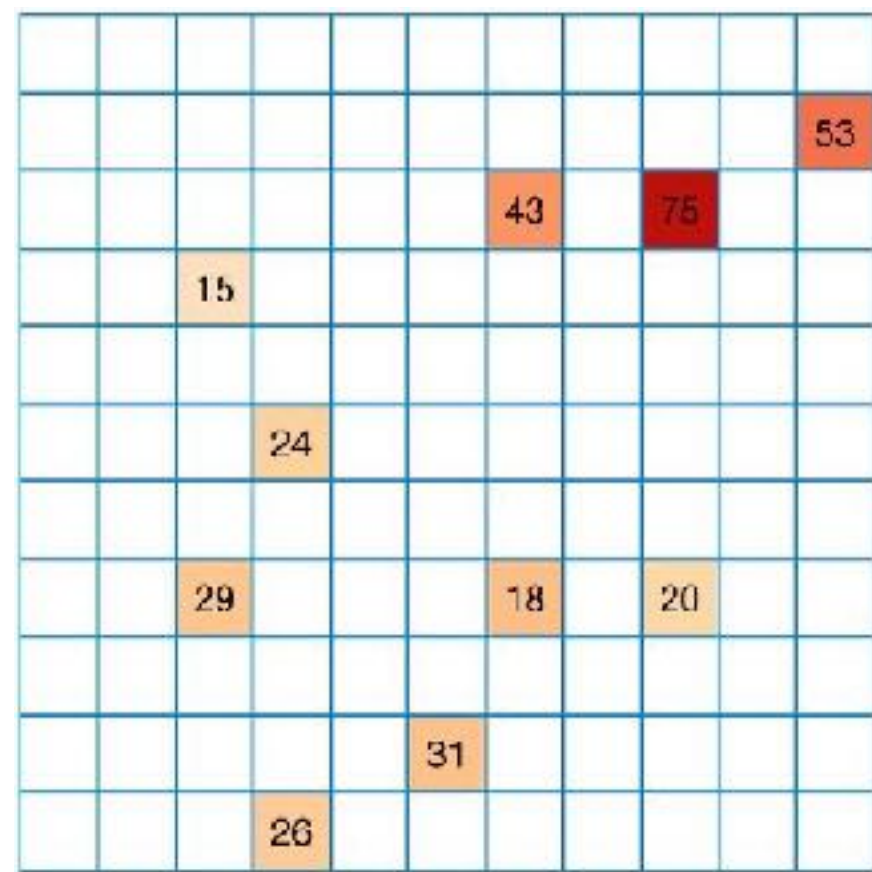
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Generalization λ

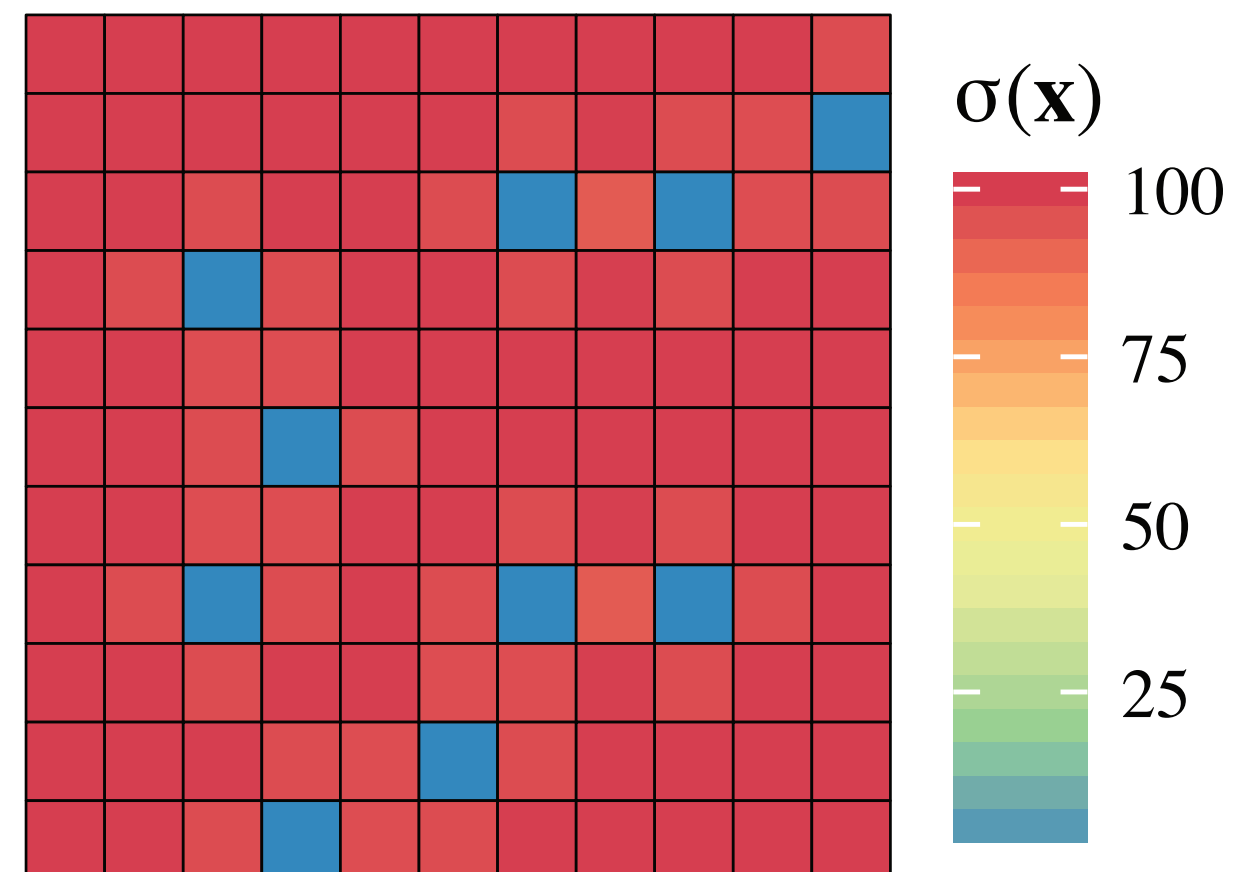


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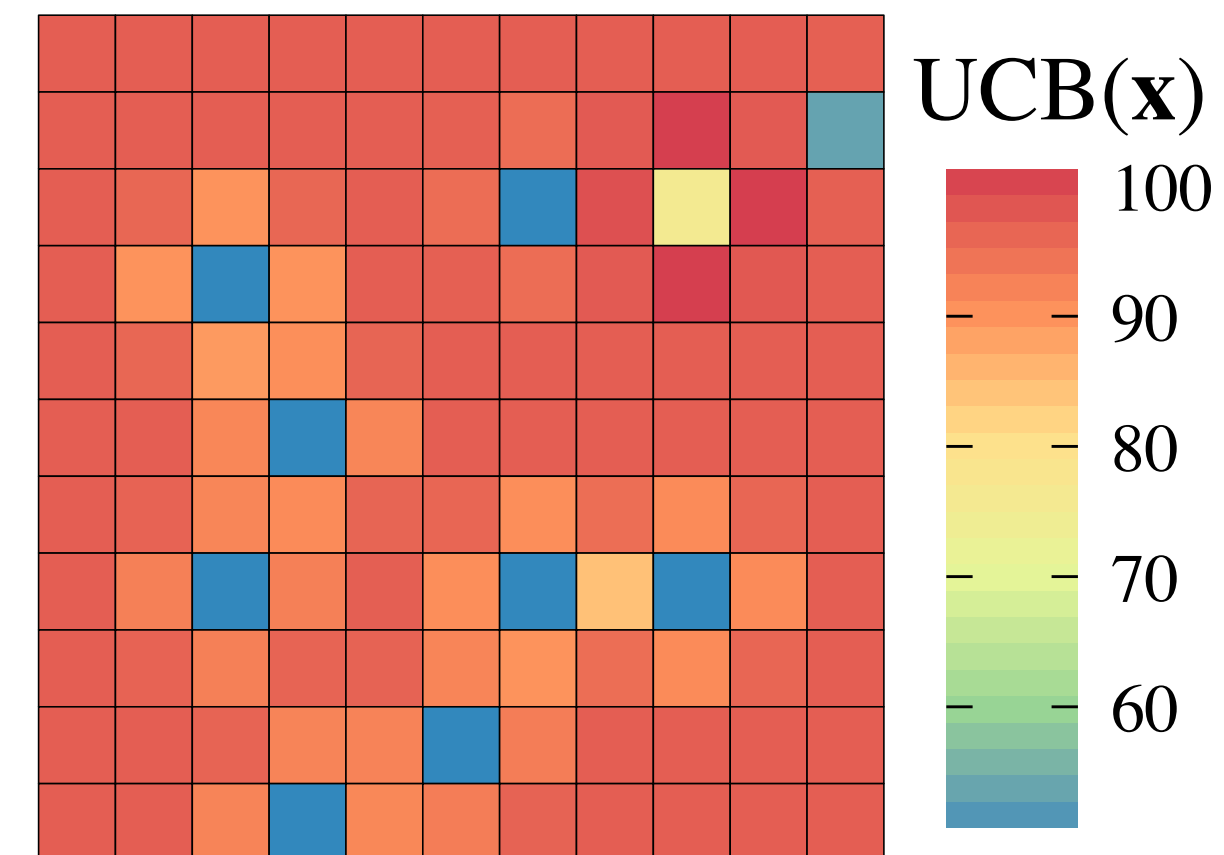
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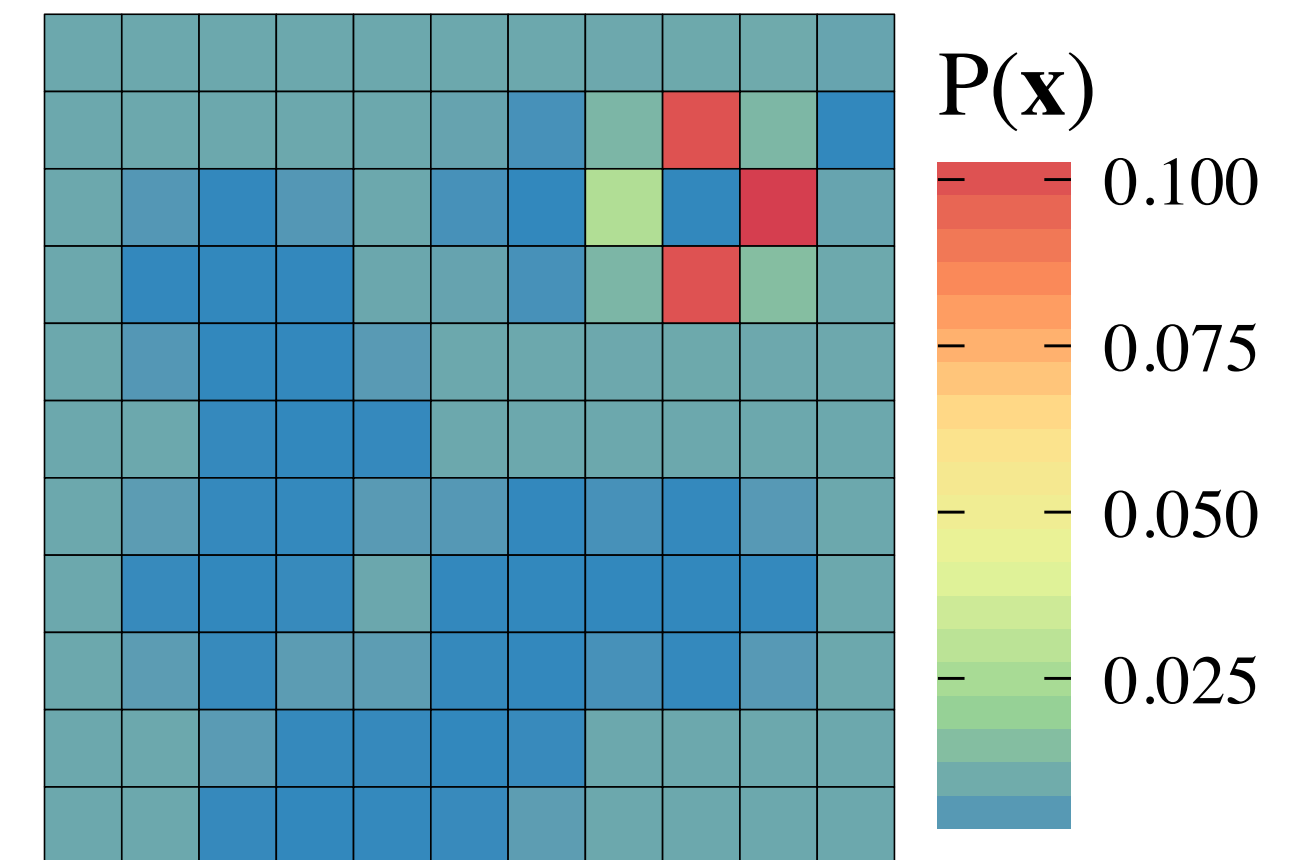
Gaussian Process (GP)



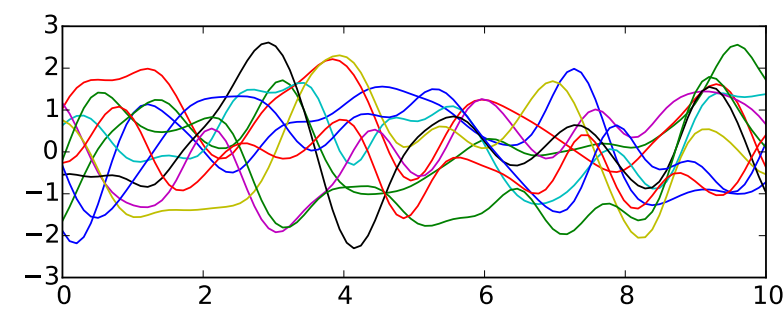
Upper Confidence Bound (UCB) Sampling



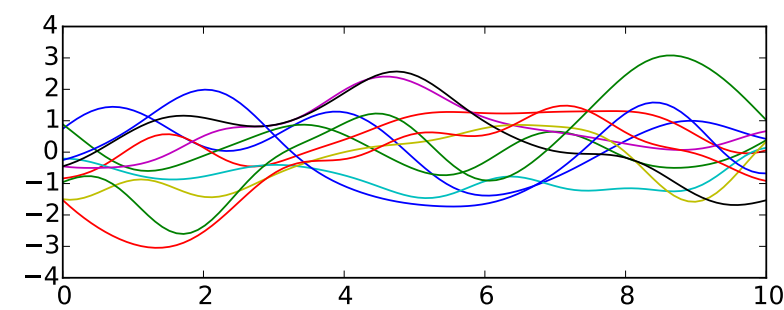
Softmax Choice Rule



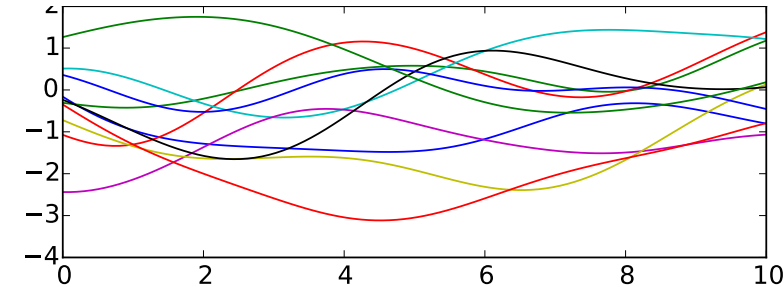
$\lambda=.5$



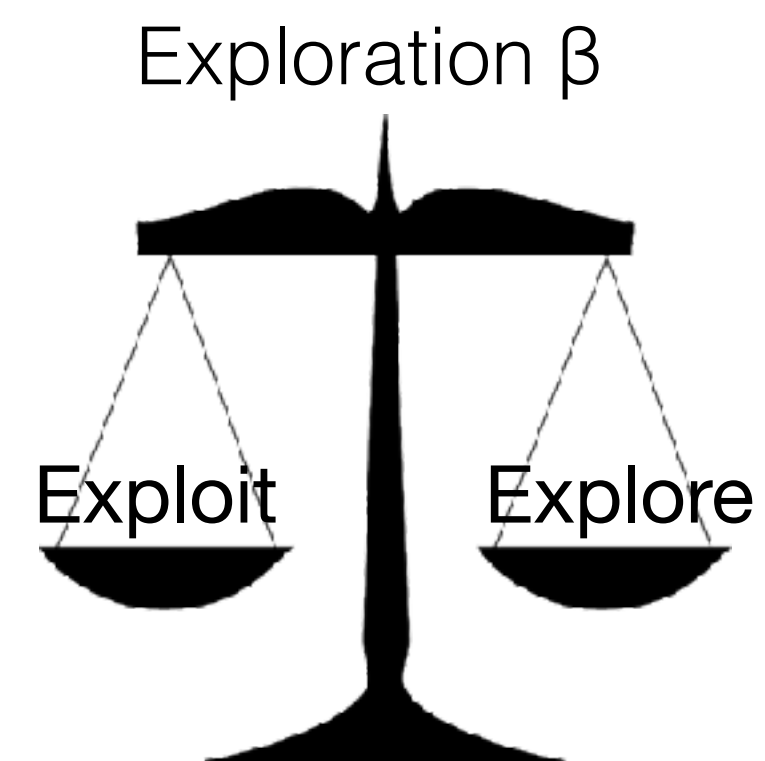
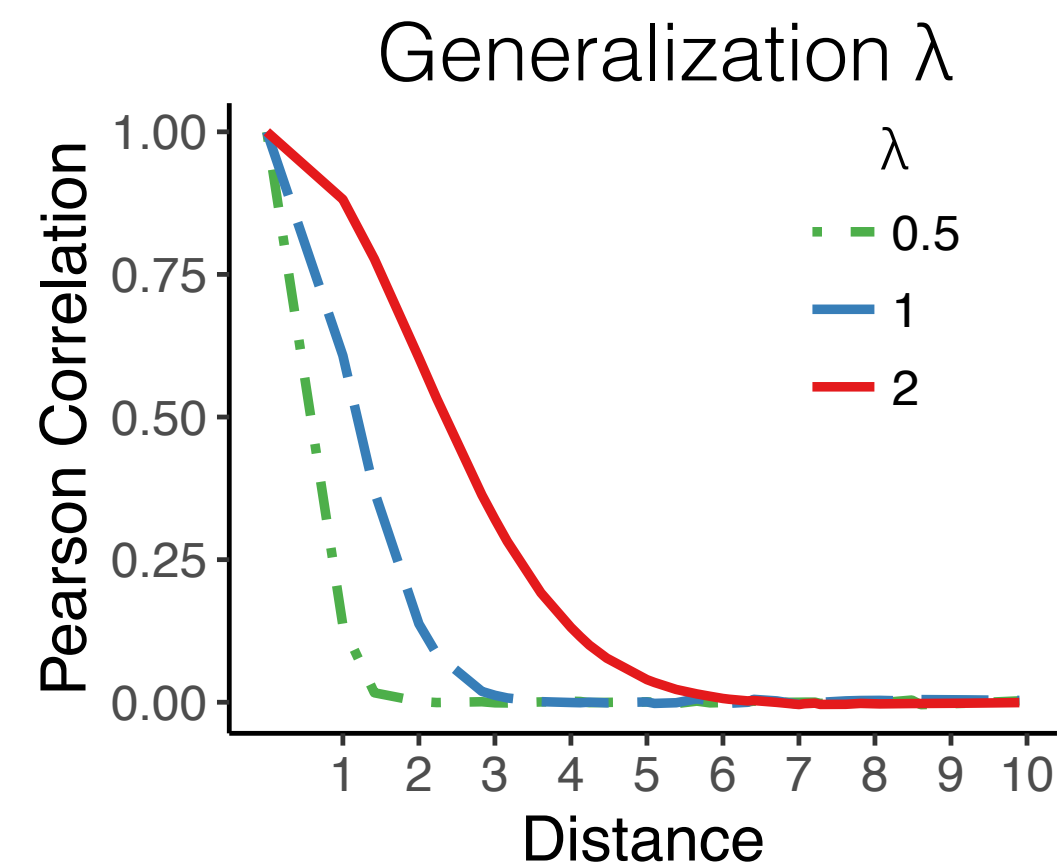
$\lambda=1$



$\lambda=2$

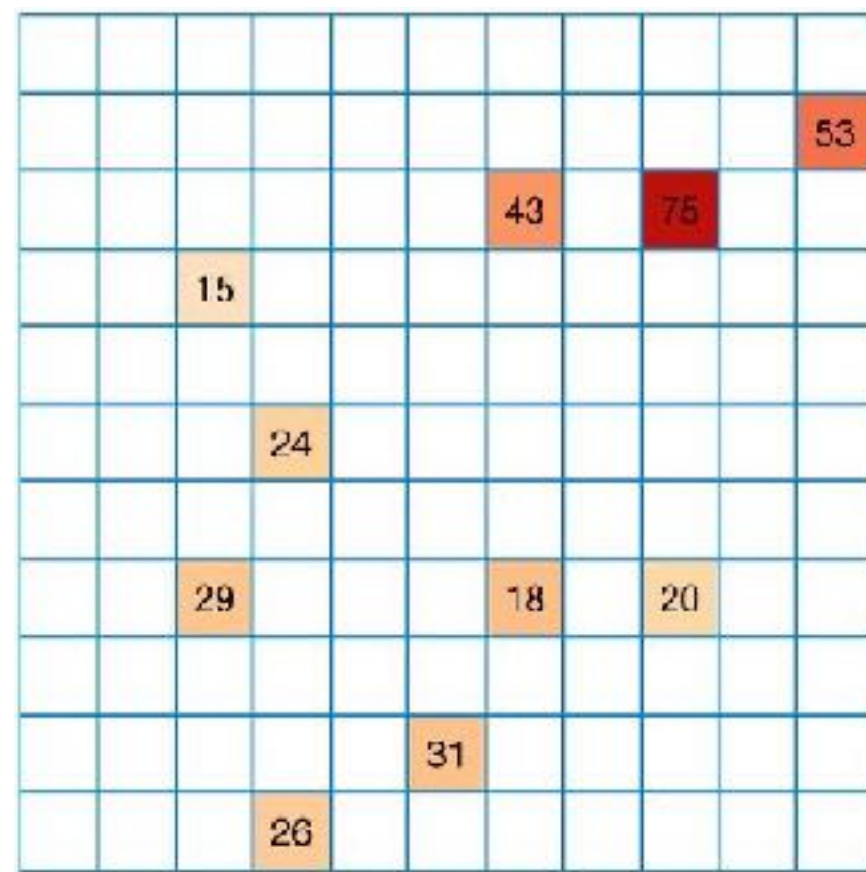


$$k_{RBF}(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{||\mathbf{x} - \mathbf{x}'||^2}{2\lambda^2}\right) \quad UCB(\mathbf{x}_i) = \mu(\mathbf{x}_i) + \beta\sigma(\mathbf{x}_i)$$

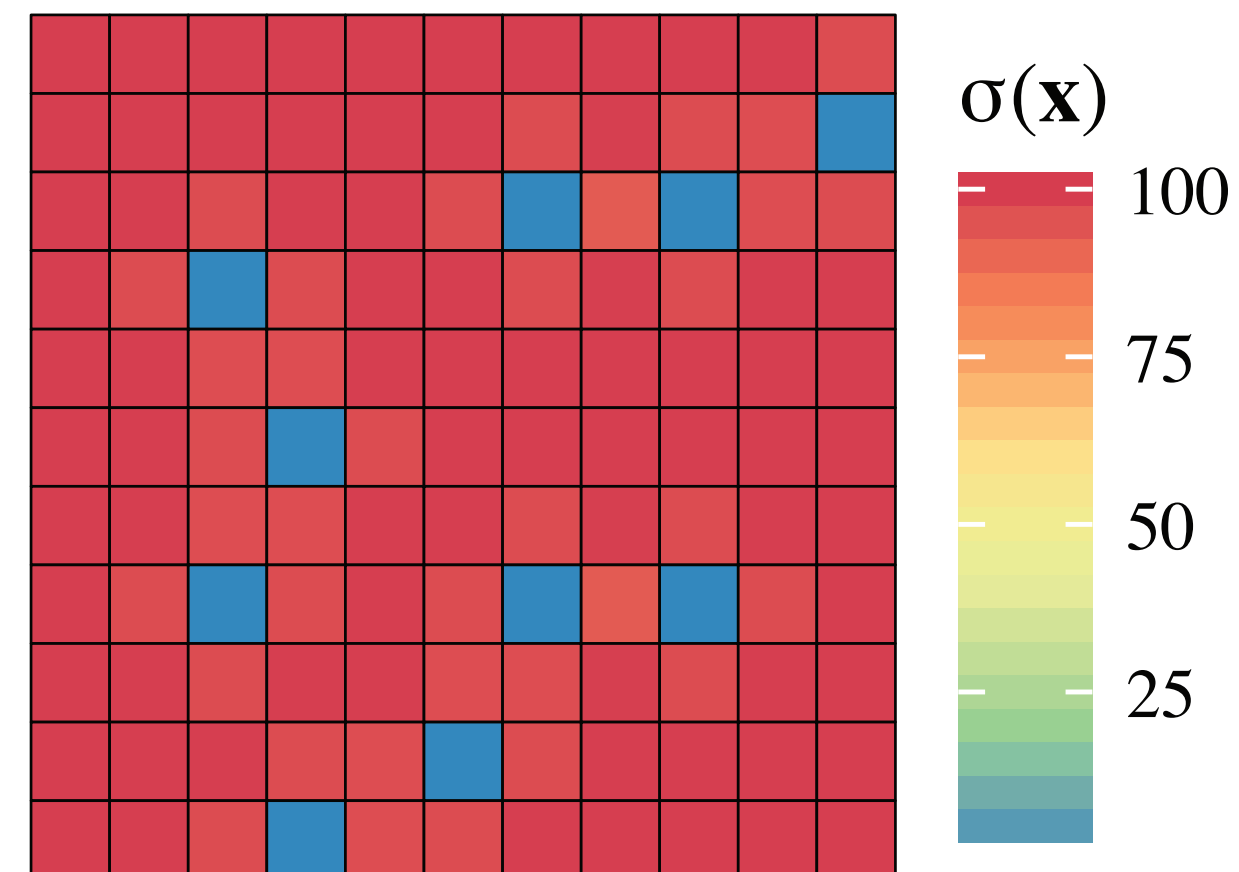


GP-UCB Model

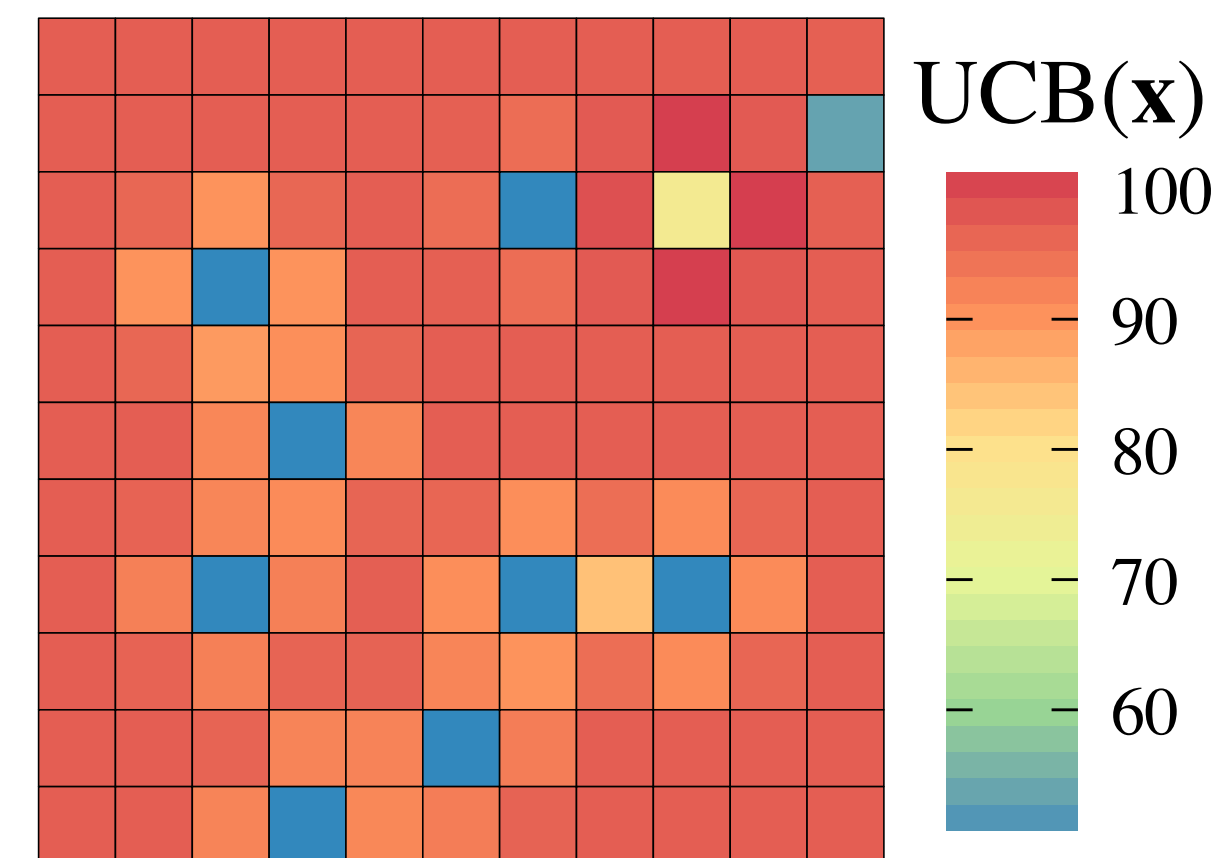
Observations



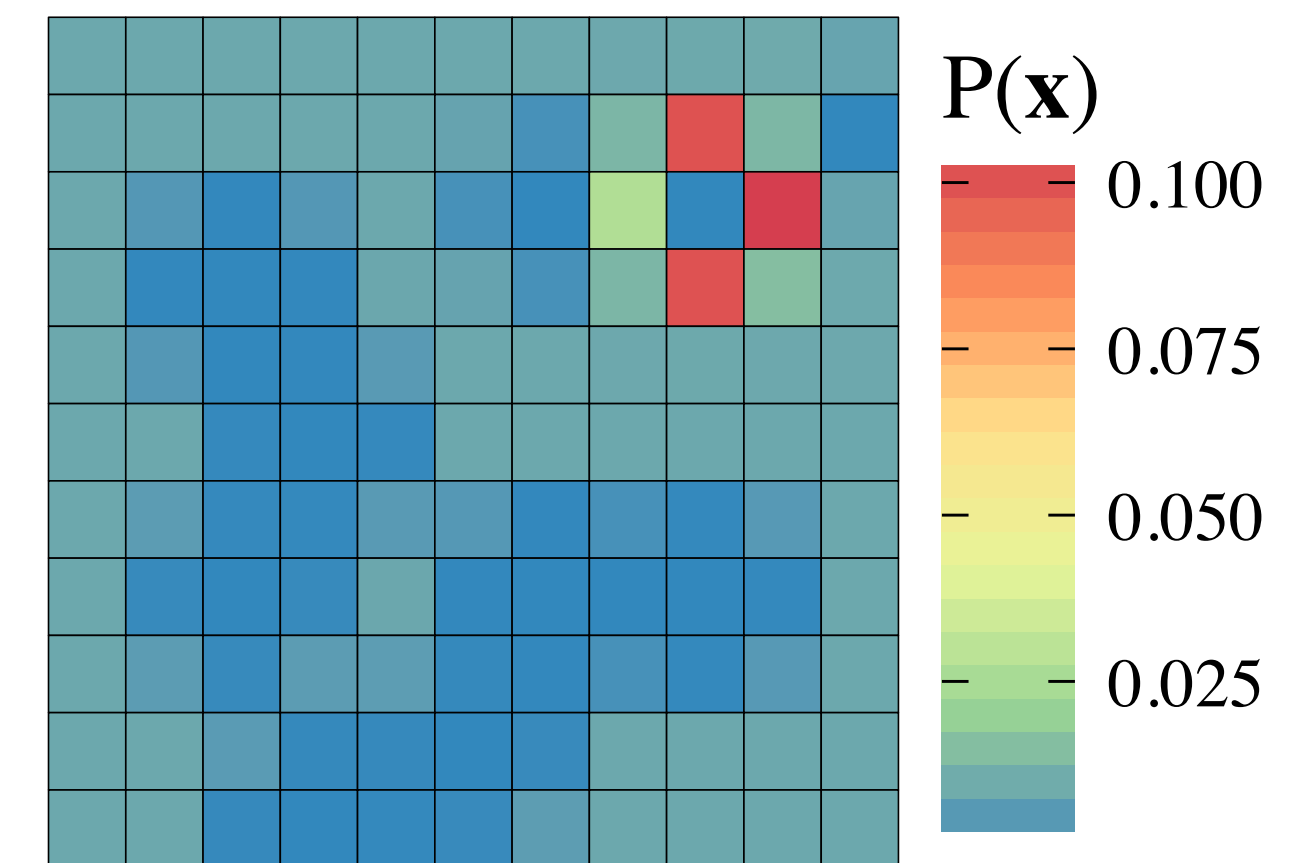
Gaussian Process (GP)



Upper Confidence Bound (UCB) Sampling



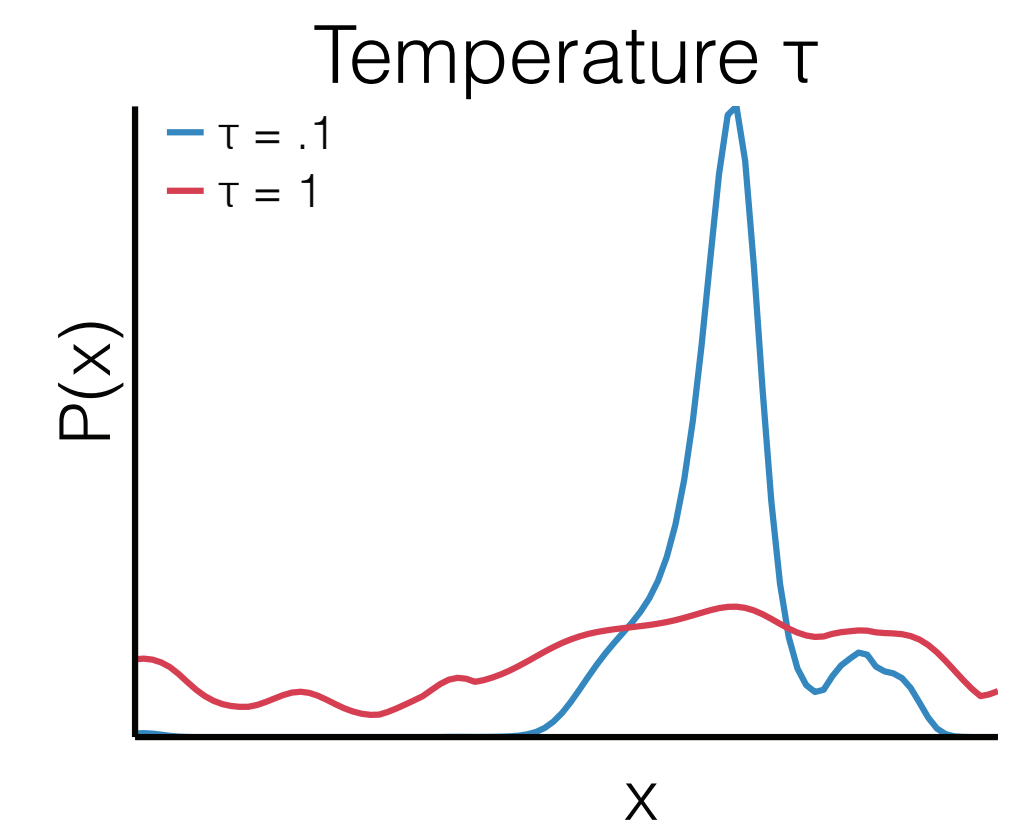
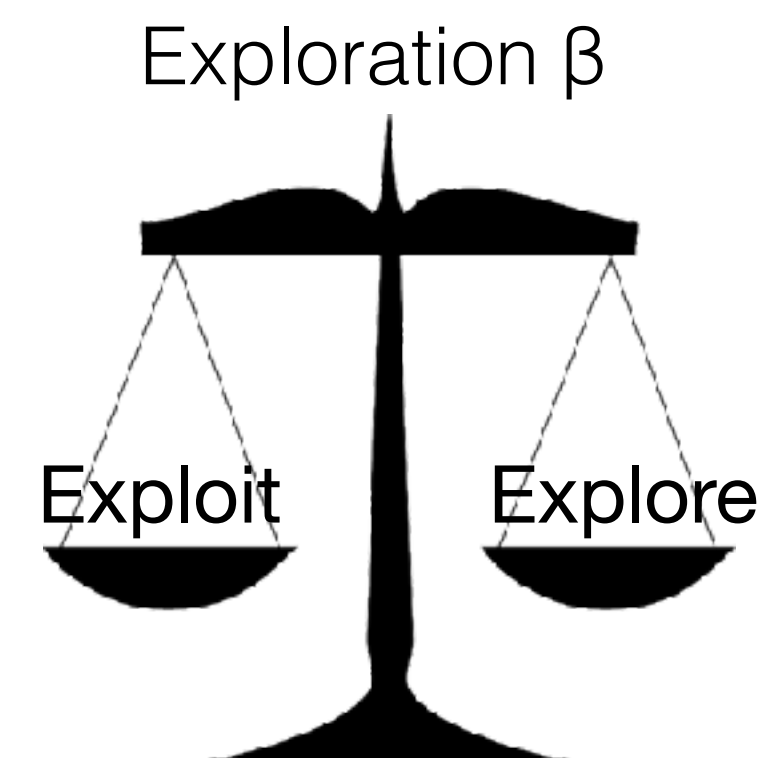
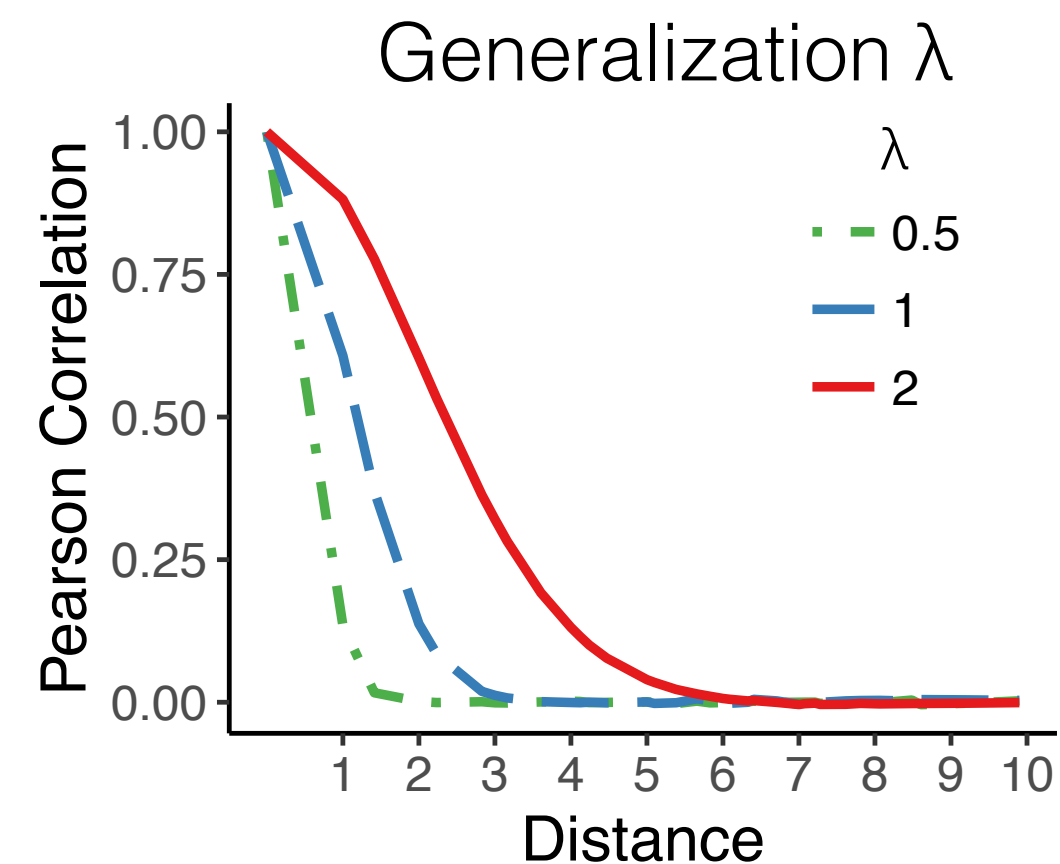
Softmax Choice Rule



$$k_{RBF}(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{||\mathbf{x} - \mathbf{x}'||^2}{2\lambda^2}\right)$$

$$UCB(\mathbf{x}_i) = \mu(\mathbf{x}_i) + \beta\sigma(\mathbf{x}_i)$$

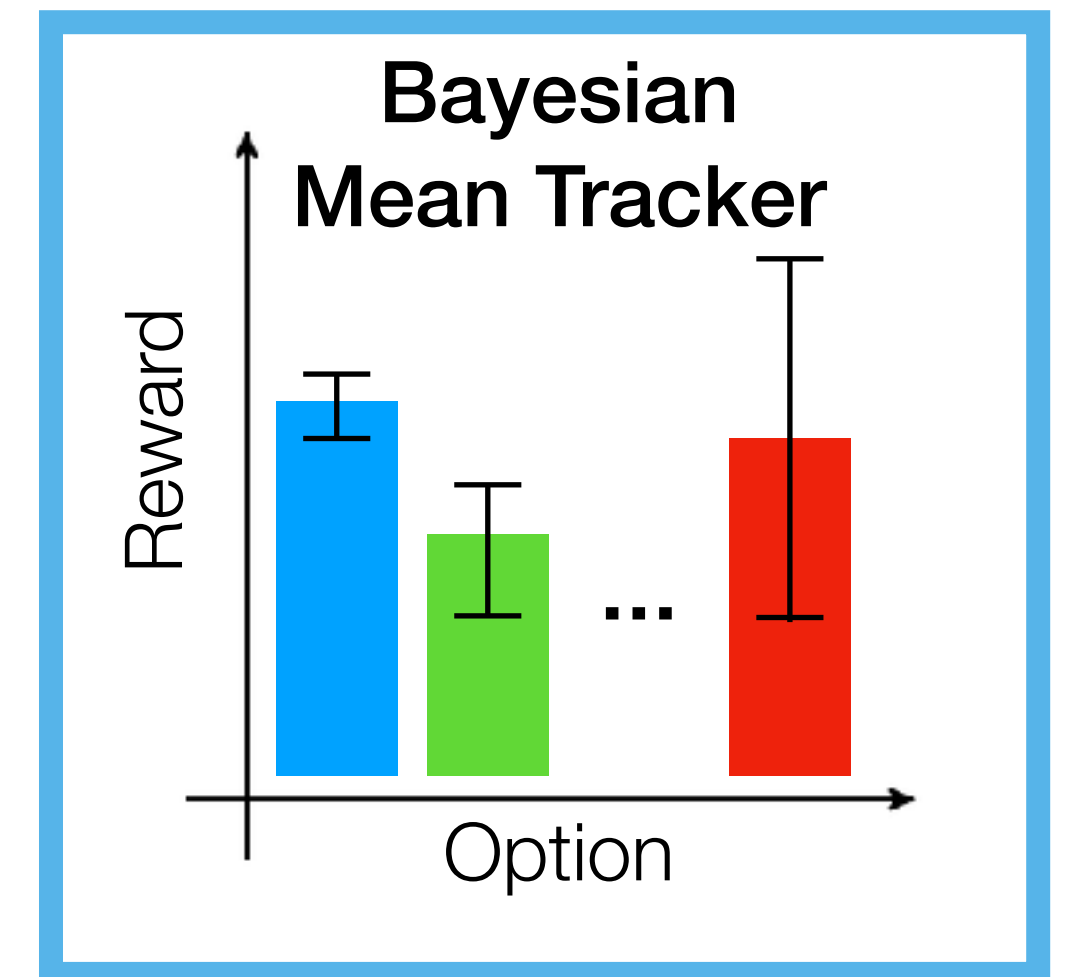
$$P(\mathbf{x}_i) \propto \exp(UCB(\mathbf{x}_i)/\tau)$$



Model Comparison

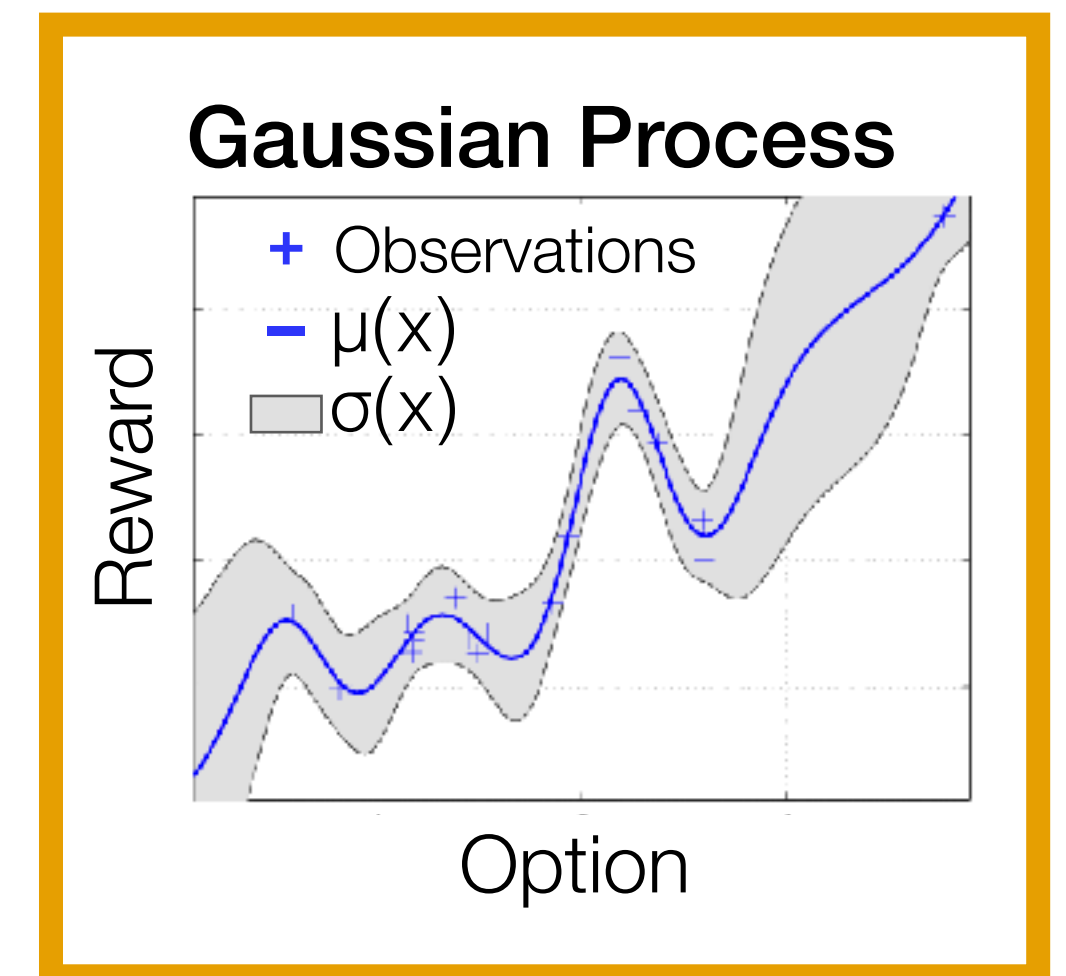
- **Traditional RL model:**

- Learns the value of each option independently
 - e.g., Rescorla-Wagner, Q-learning, Kalman Filter, *Bayesian Mean Tracker* (BMT), etc...
- Can balance explore-exploit dilemma using a variety of sampling strategies, but offers limited guidance about *where to explore*

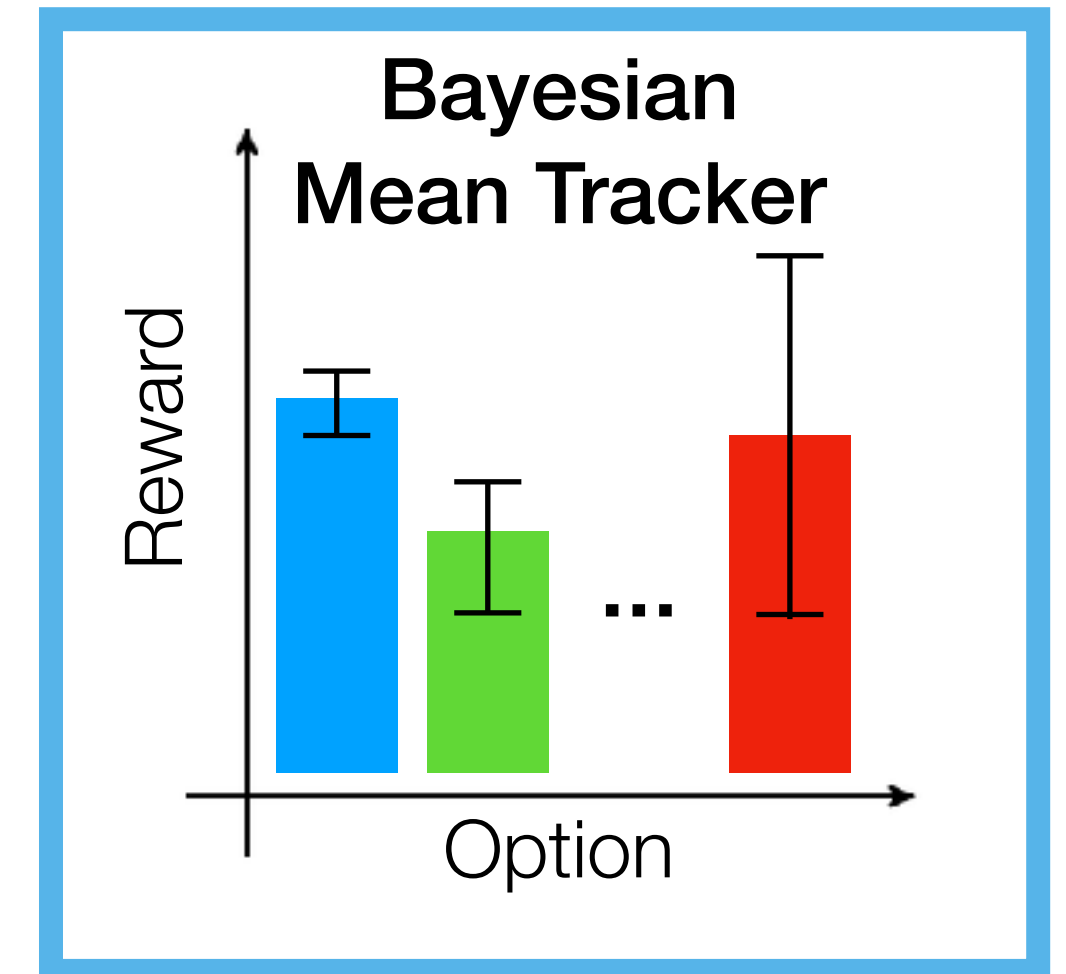


- **Function learning model:**

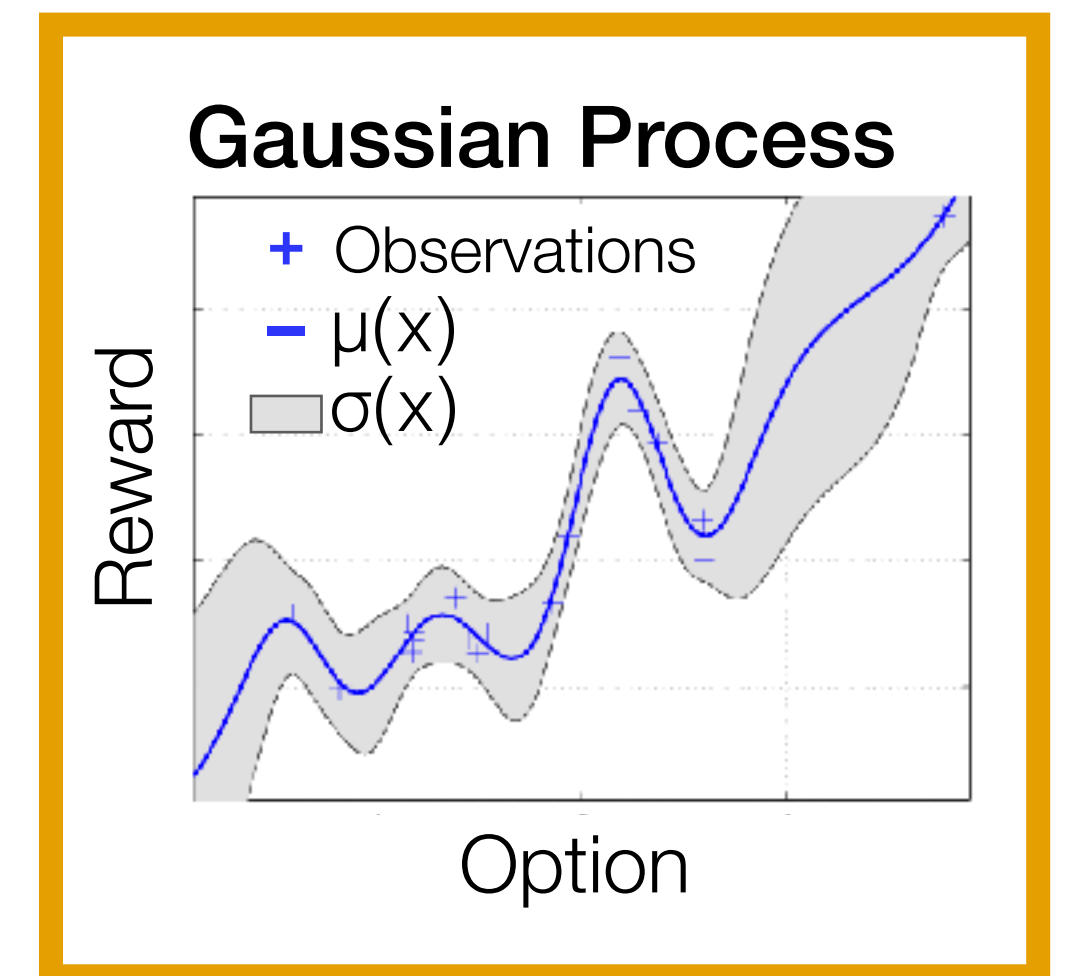
- Uses function approximation to generalize about novel option
 - e.g., Neural Network function approximators, *Gaussian Process* (GP) model, etc...
- Balances explore-exploit using the same sampling strategies as option learning models, but also makes predictions about *where to explore* through generalization



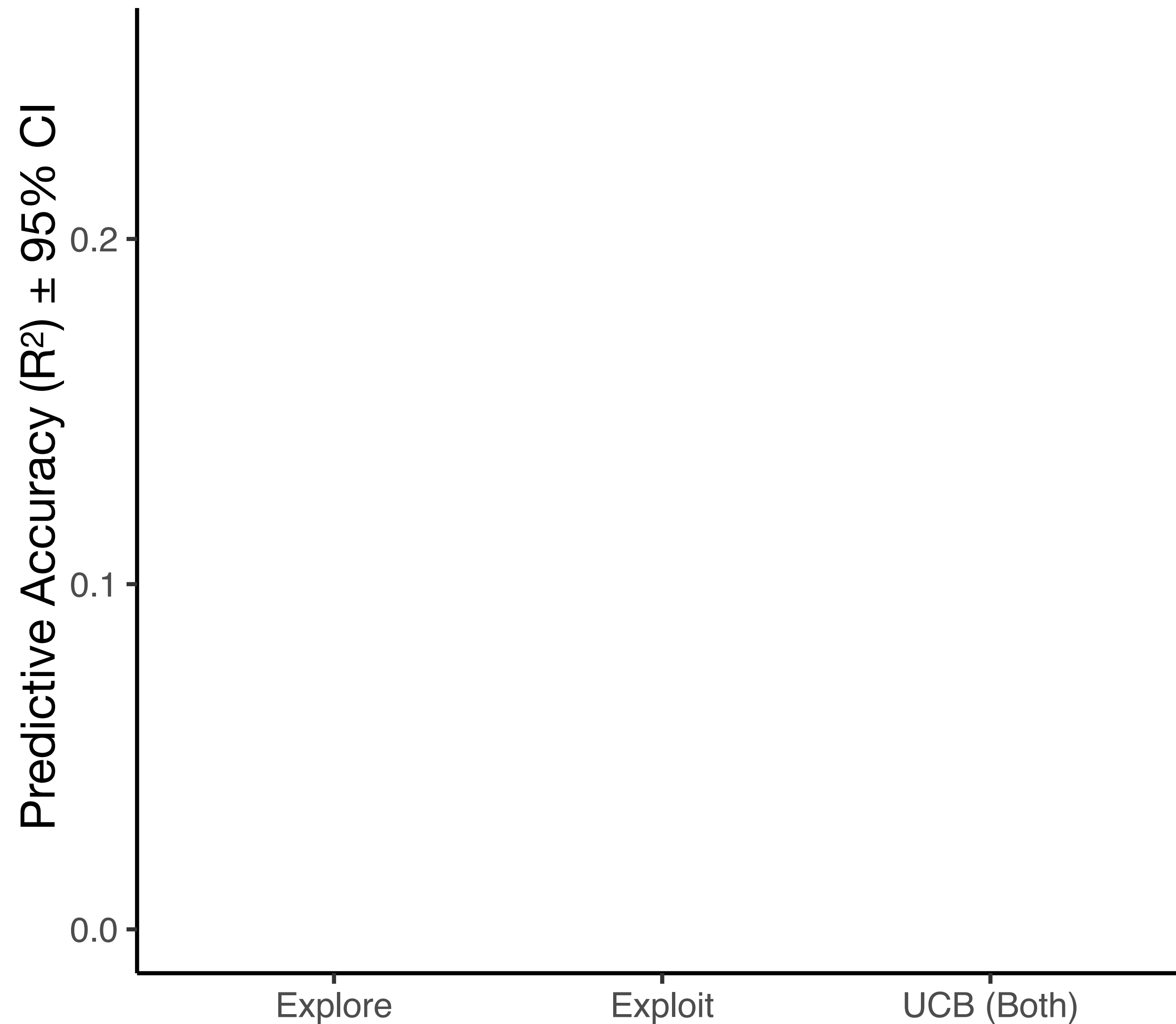
Model Comparison



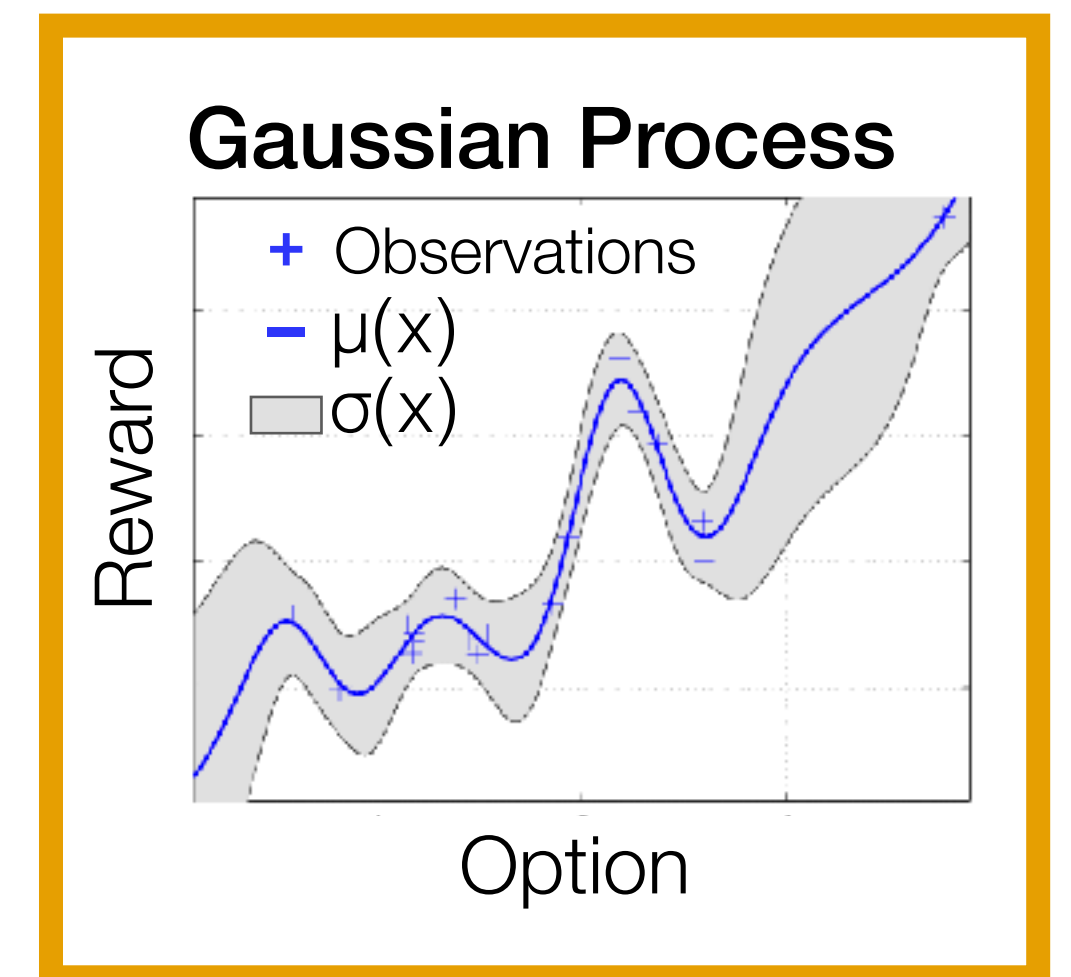
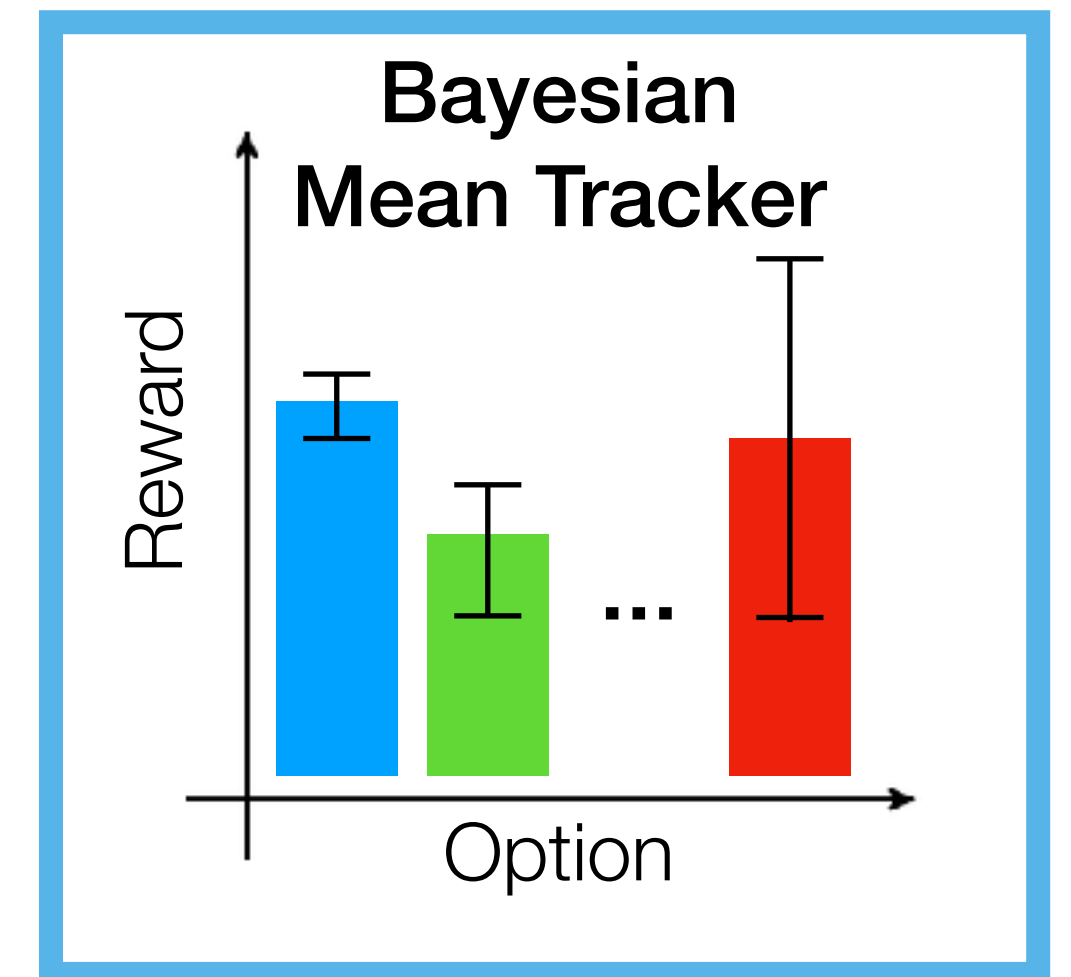
$$R^2 = 1 - \frac{\log \mathcal{L}(\mathcal{M}_k)}{\log \mathcal{L}(\mathcal{M}_{\text{rand}})}$$



Model Comparison

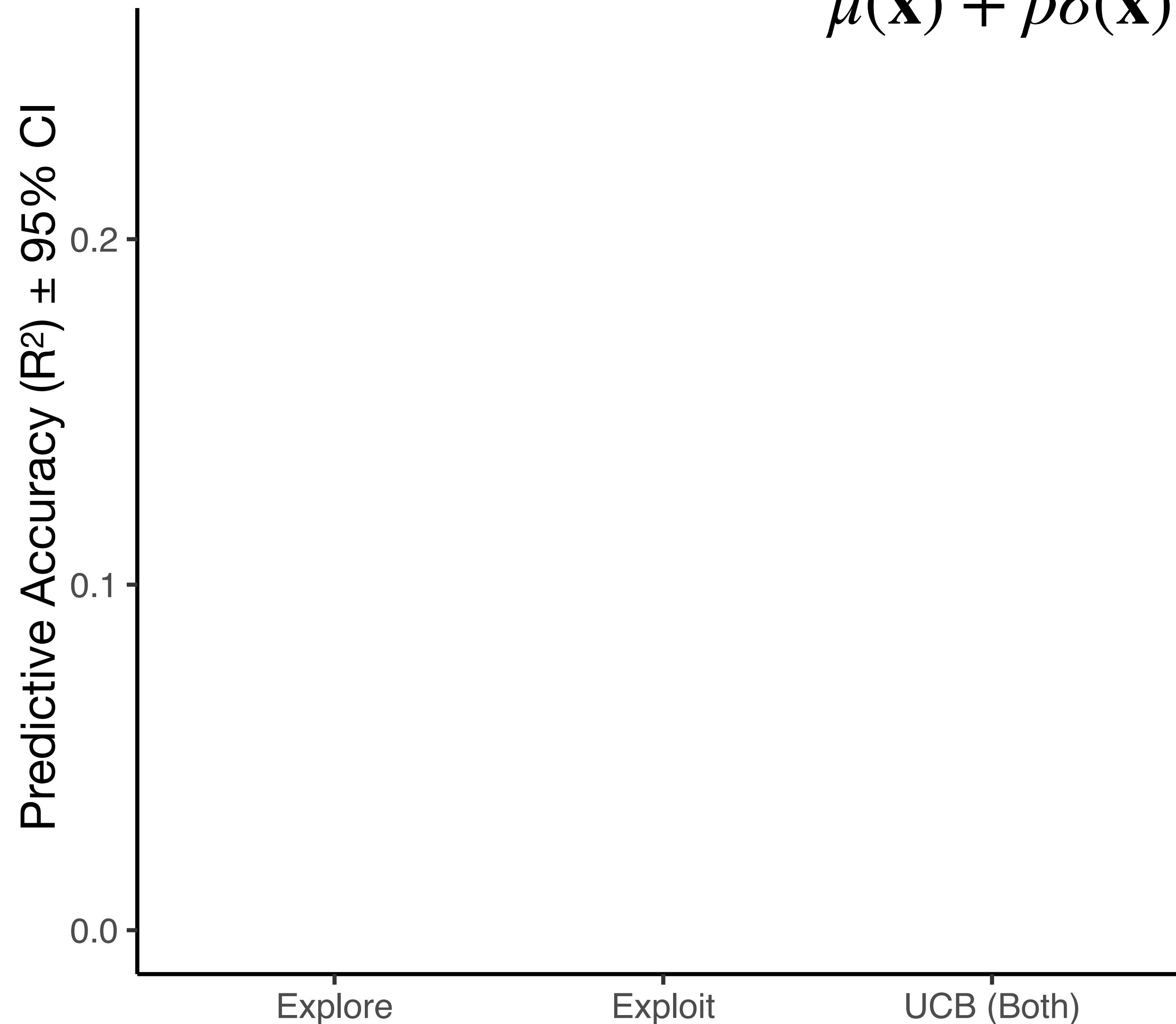


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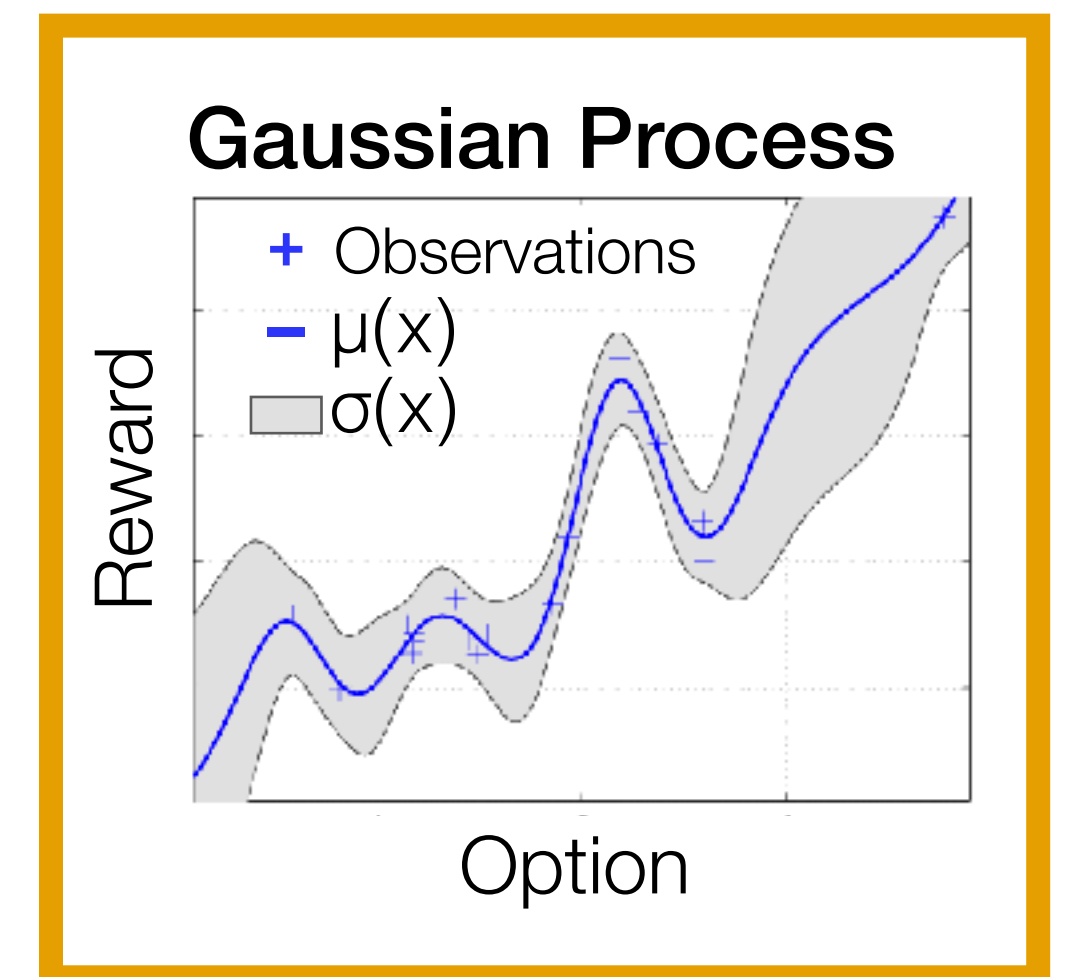
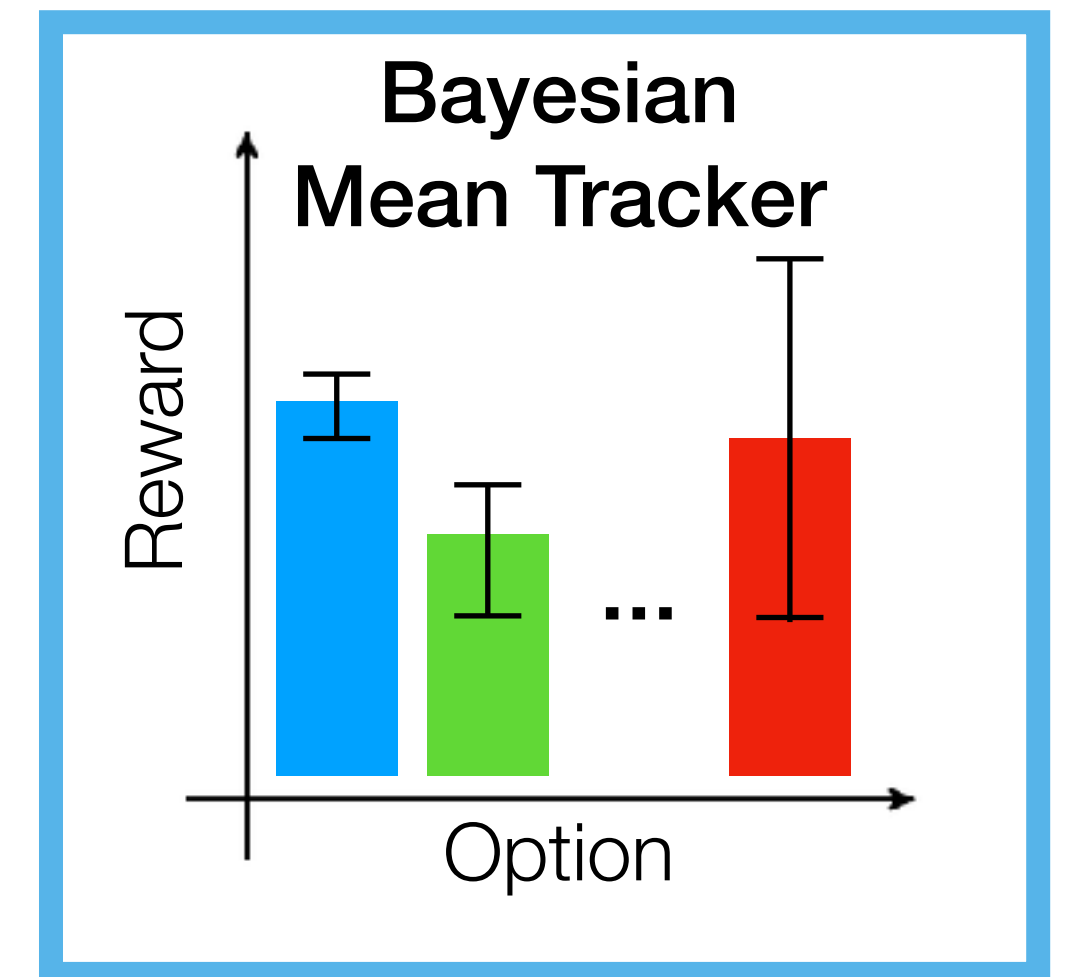


Model Comparison

$$\mu(\mathbf{x}) + \beta\sigma(\mathbf{x})$$

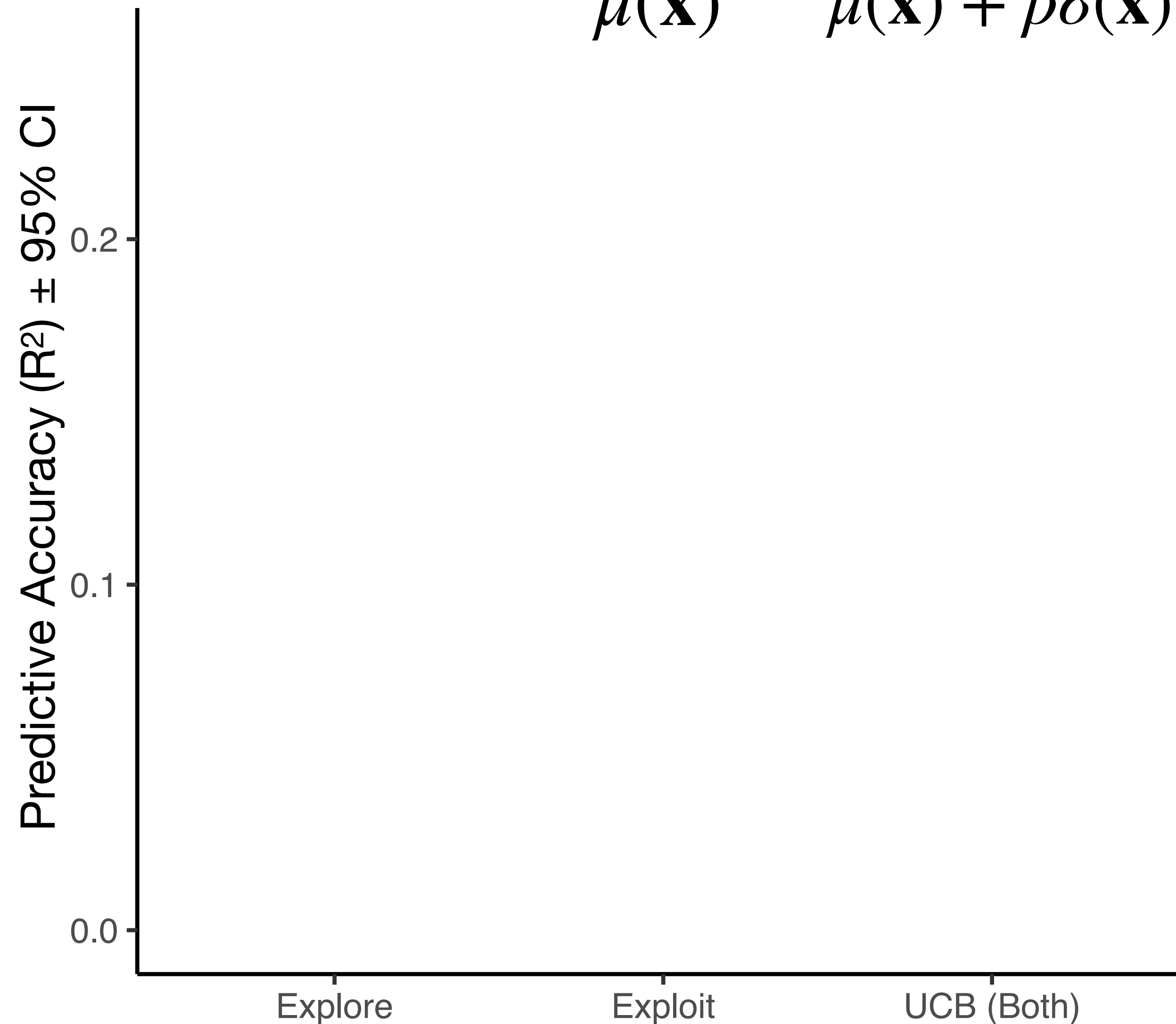


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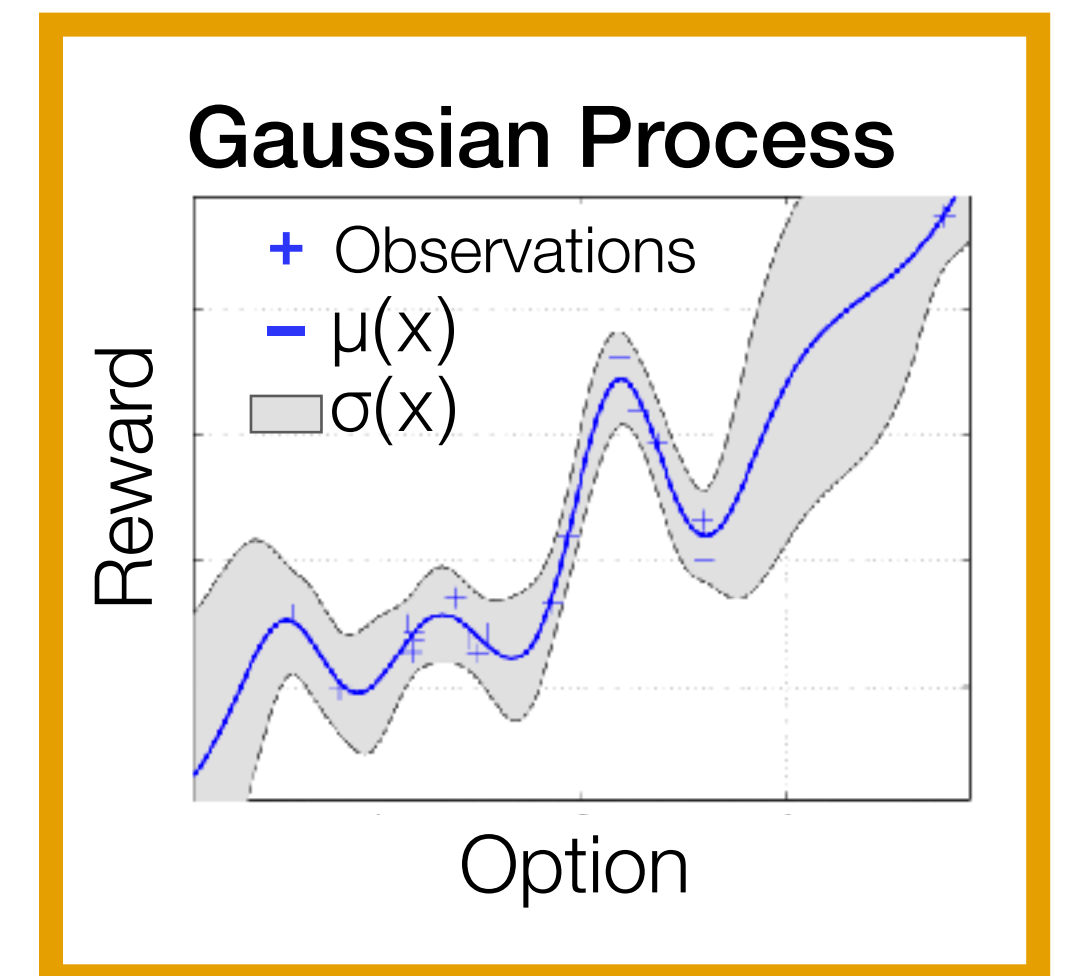
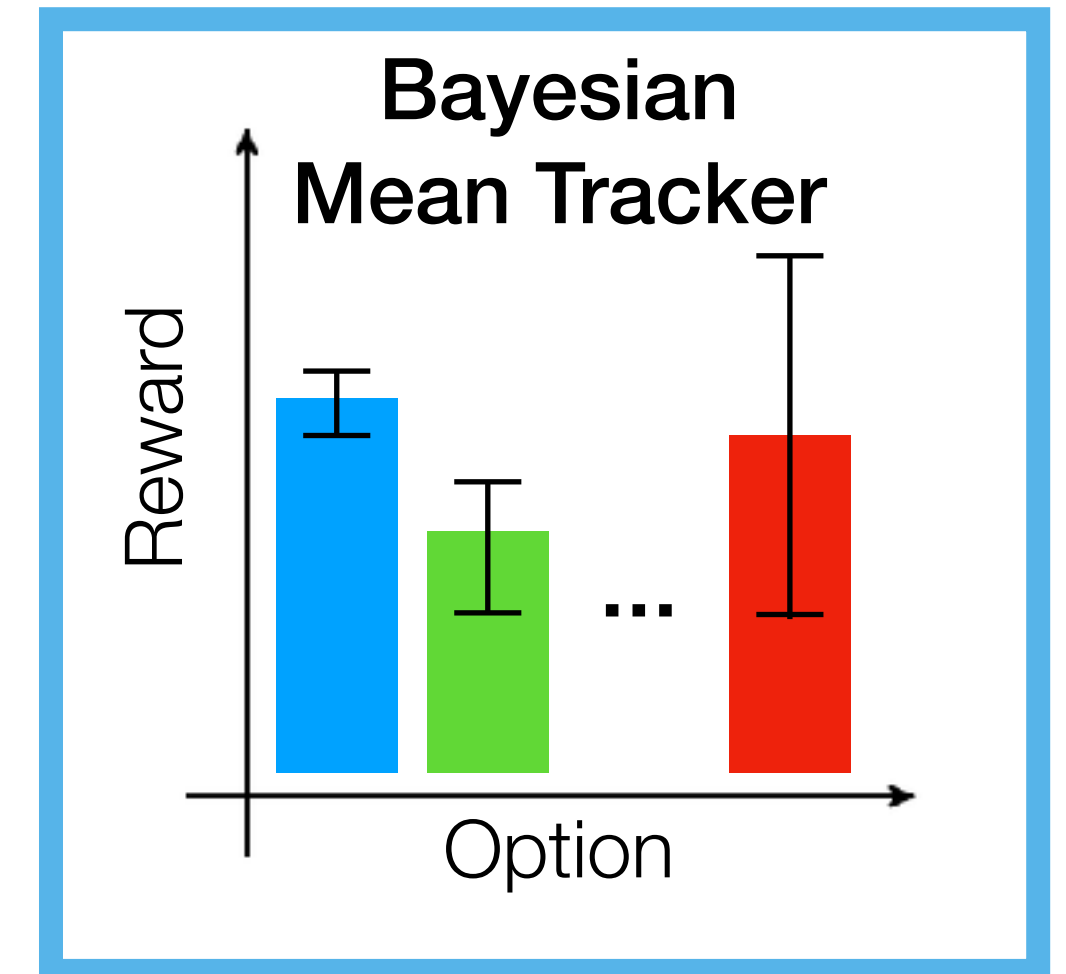


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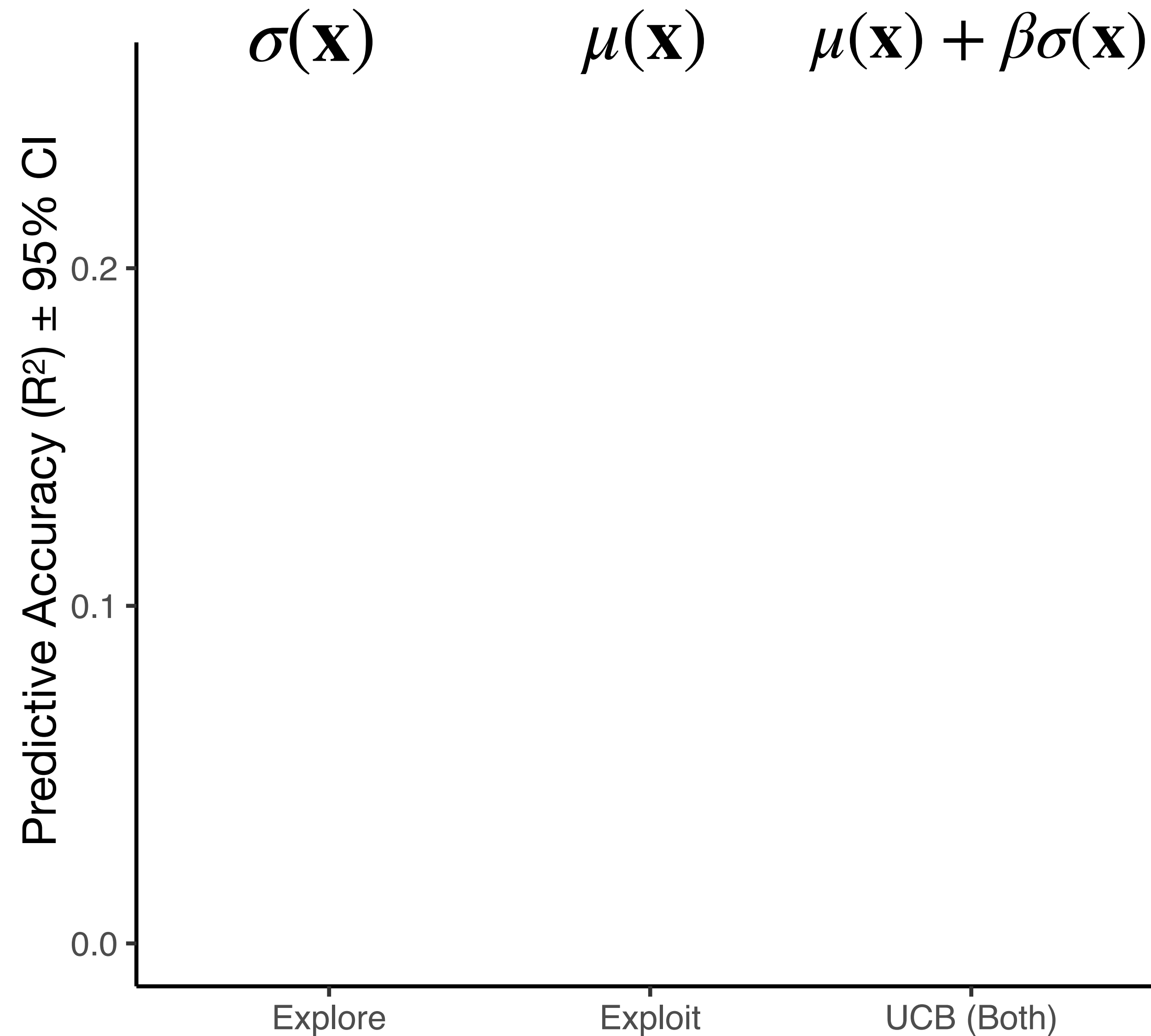
$$\mu(\mathbf{x}) \quad \mu(\mathbf{x}) + \beta\sigma(\mathbf{x})$$



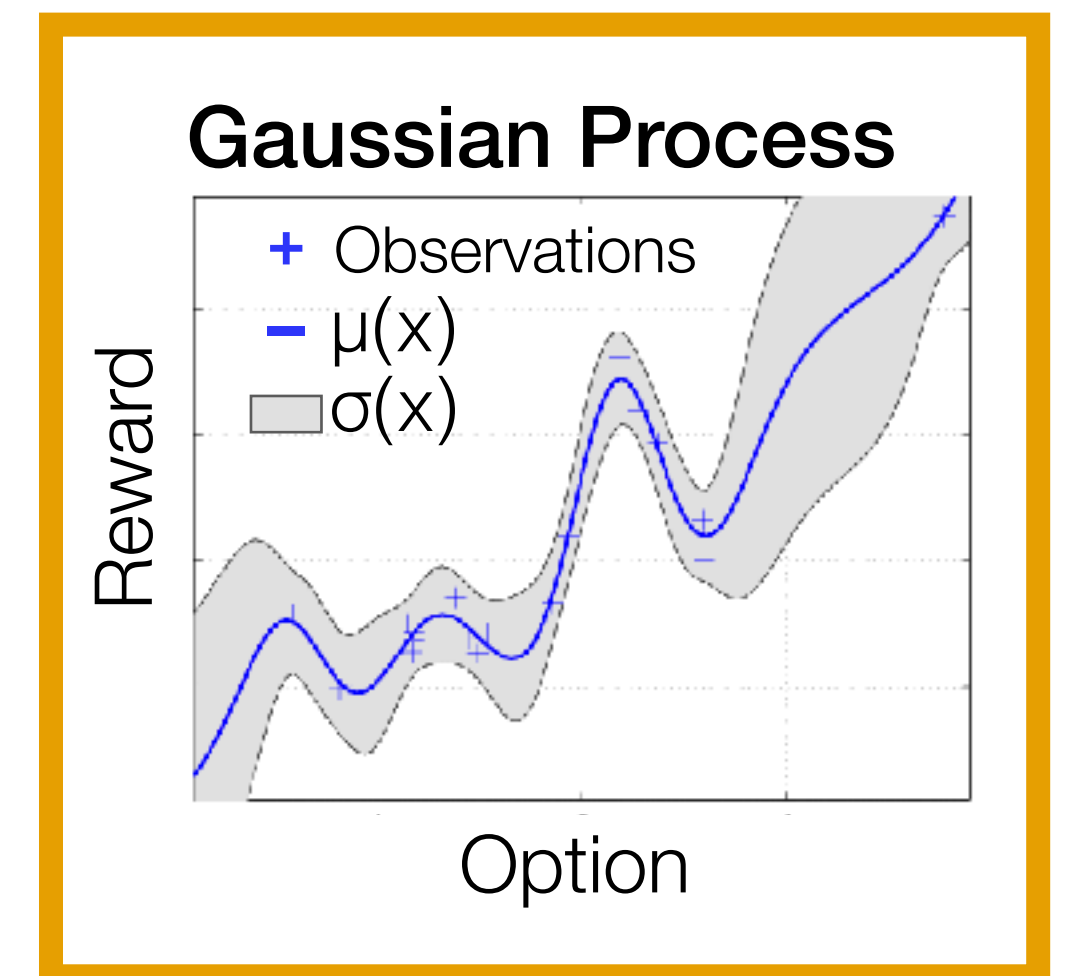
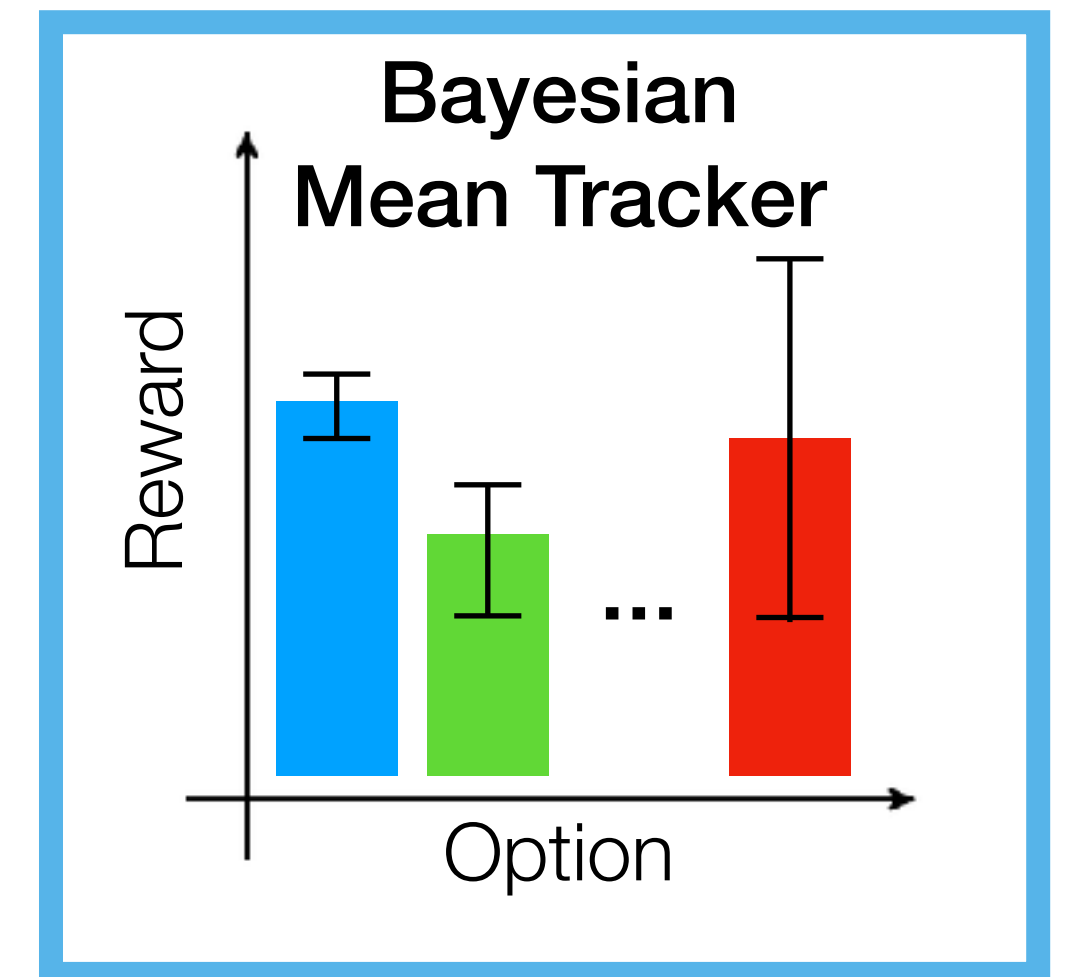
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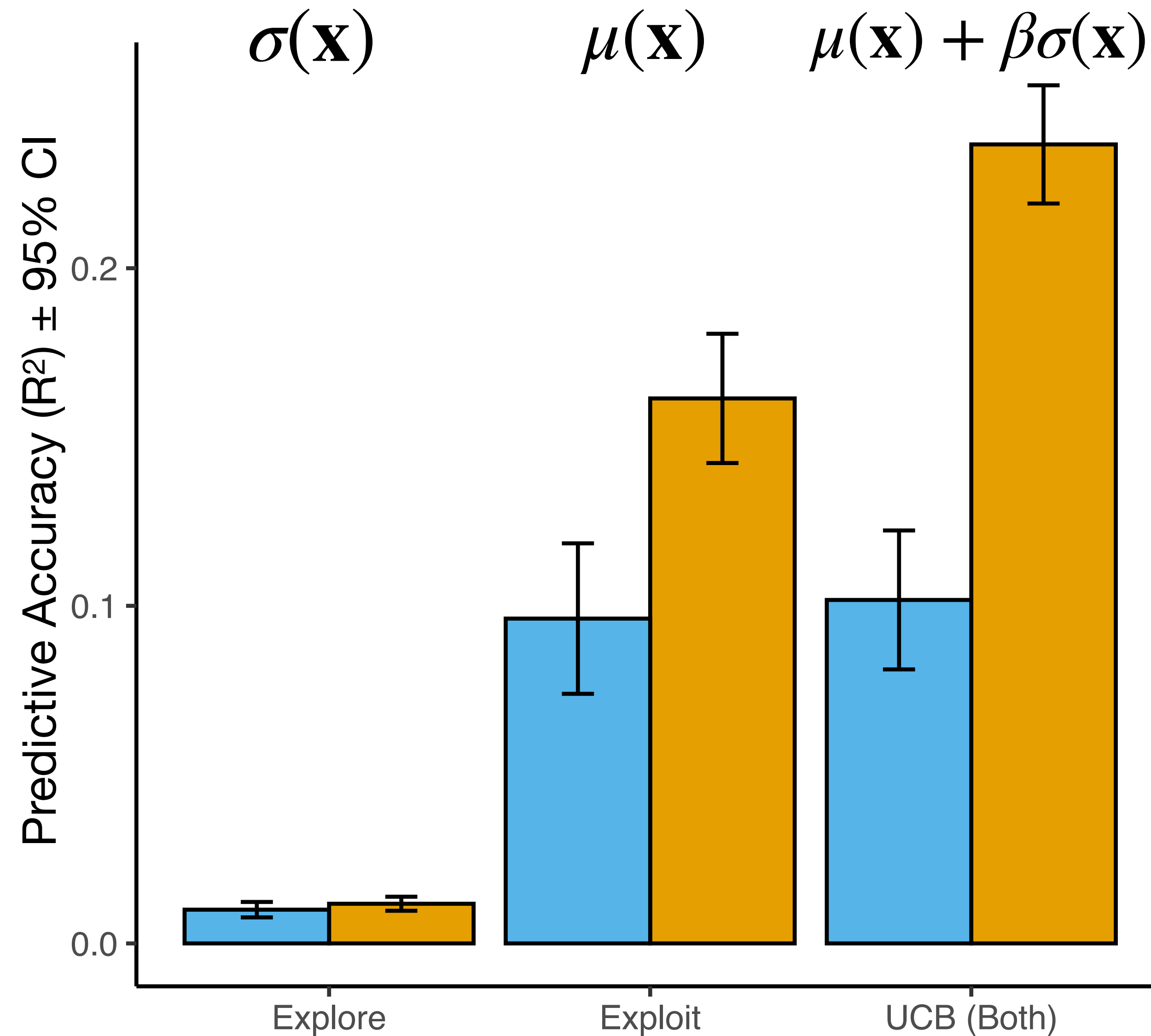
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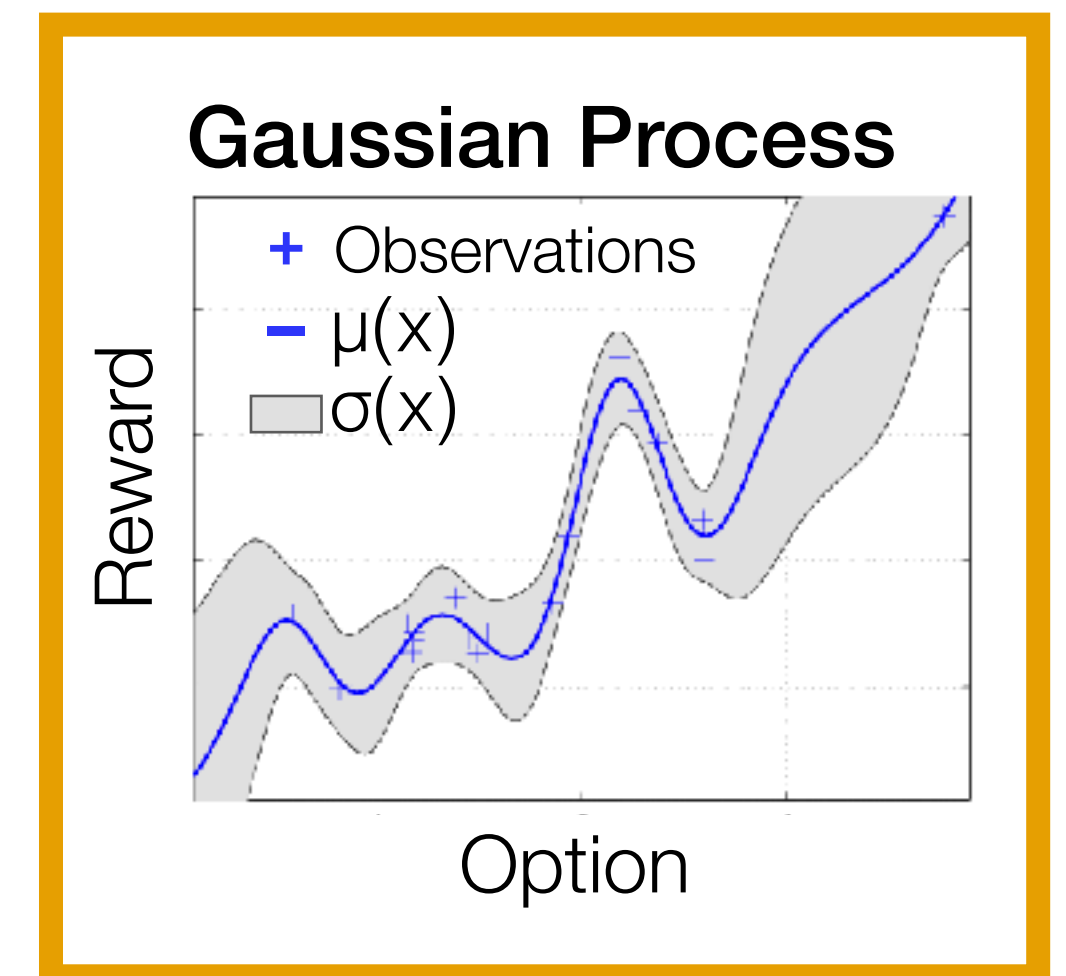
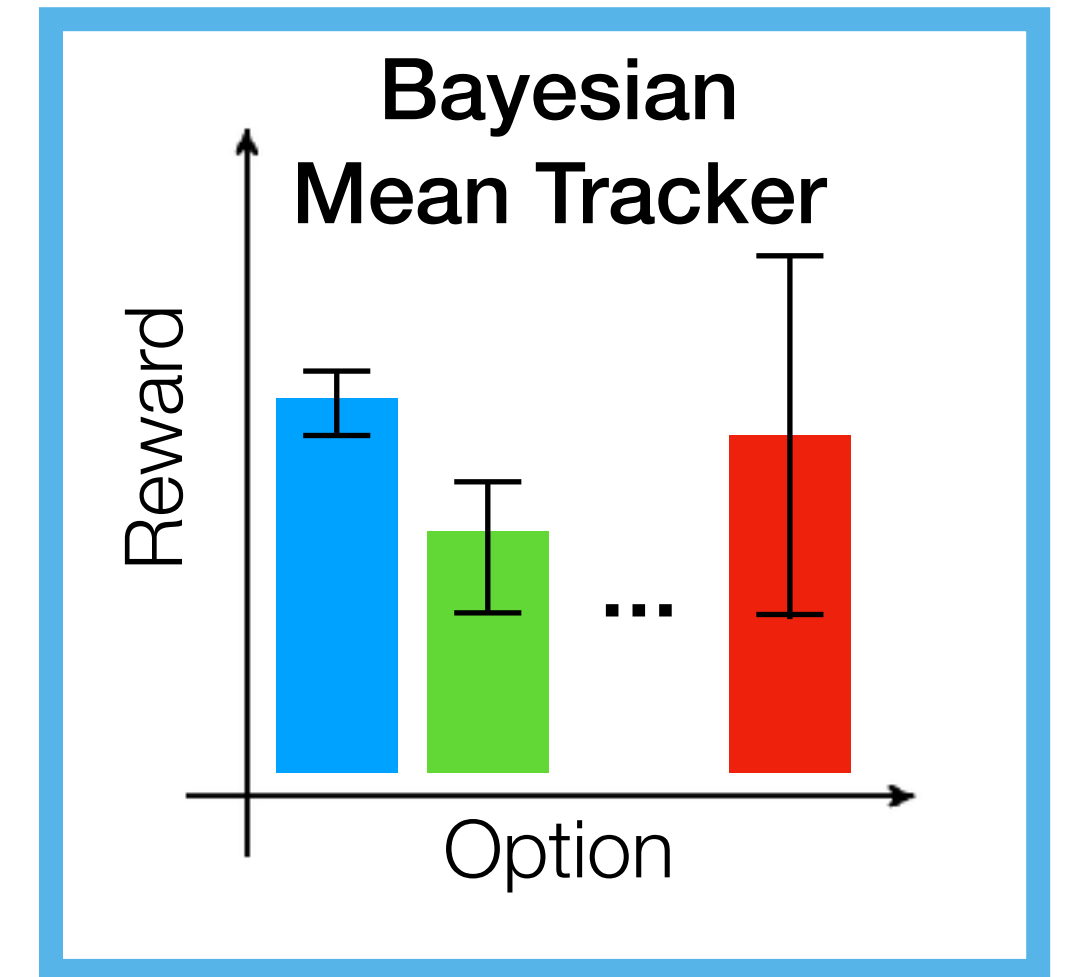
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$$R^2 = 1 - \frac{\log \mathcal{L}(\mathcal{M}_k)}{\log \mathcal{L}(\mathcal{M}_{\text{rand}})}$$



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Wu, Schulz, Nelson, Speekenbrink & Meder (*Nature Human Behaviour* 2018)

2. Learning like a child

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Meder, Wu, Schulz & Ruggeri (*Dev Sci* in press)

3. Graph-structured Generalization

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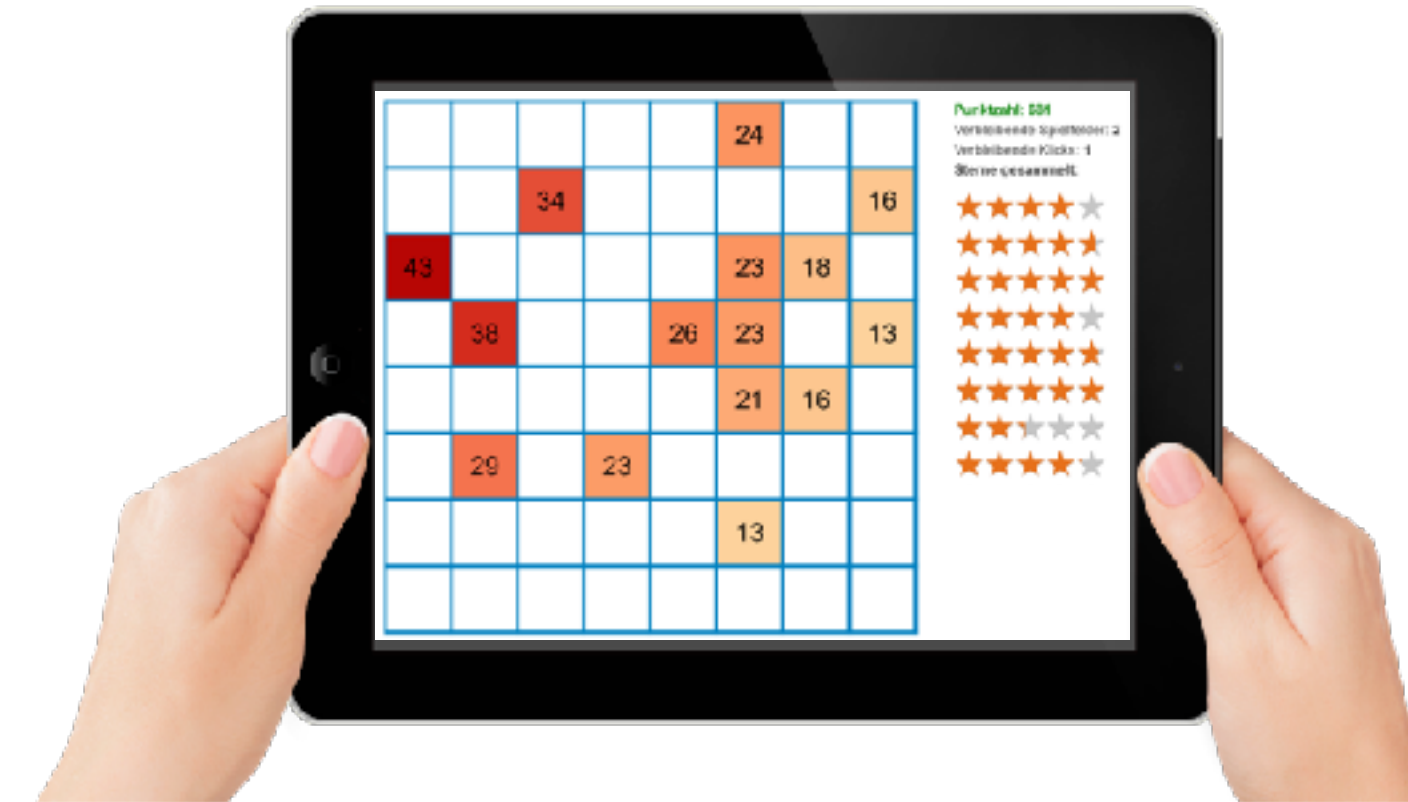
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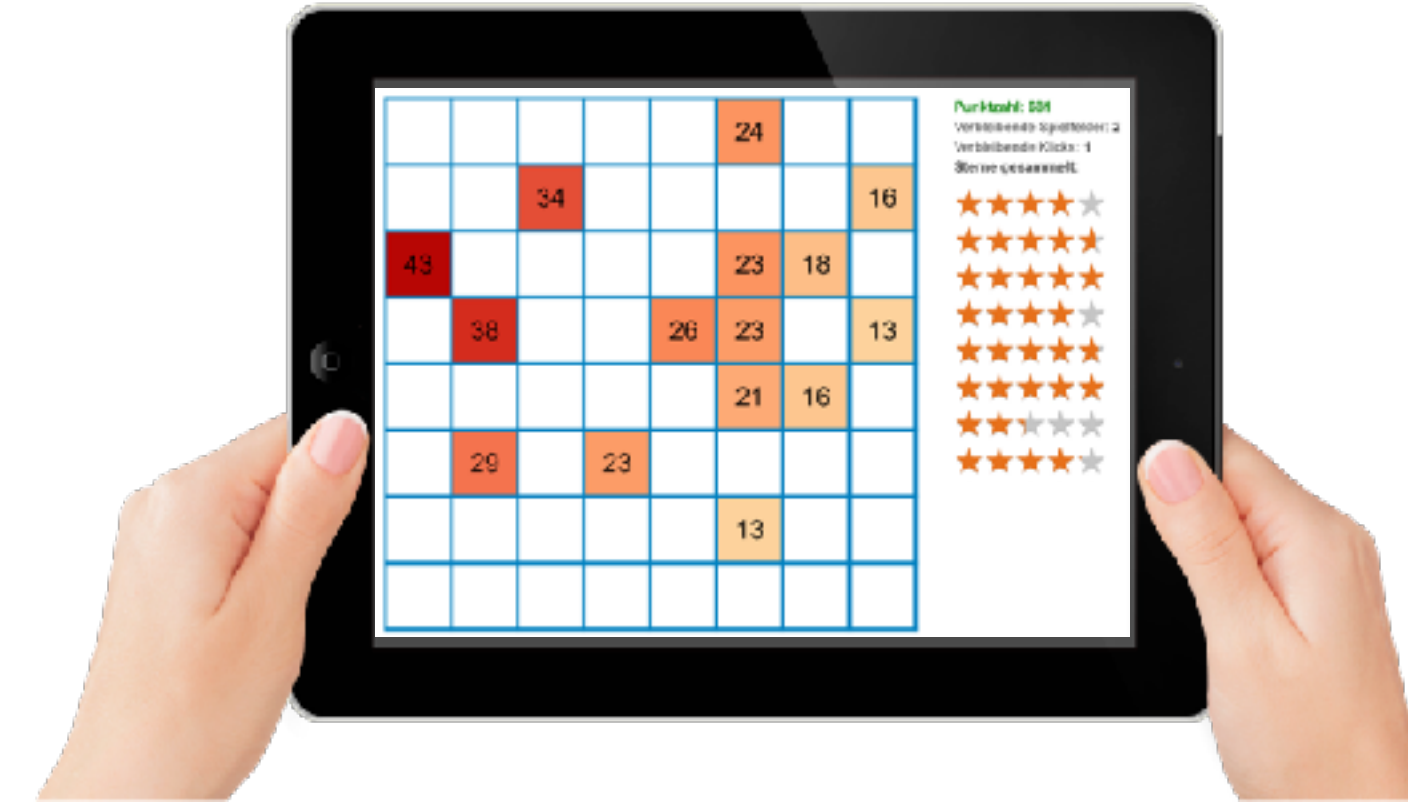
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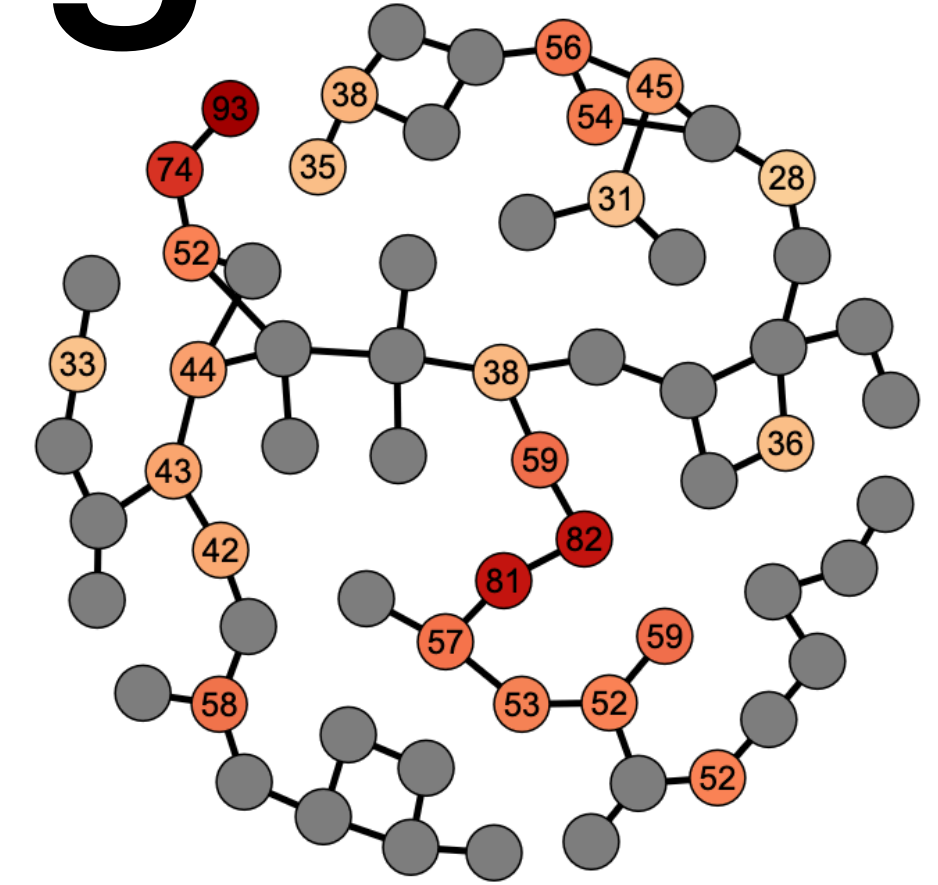
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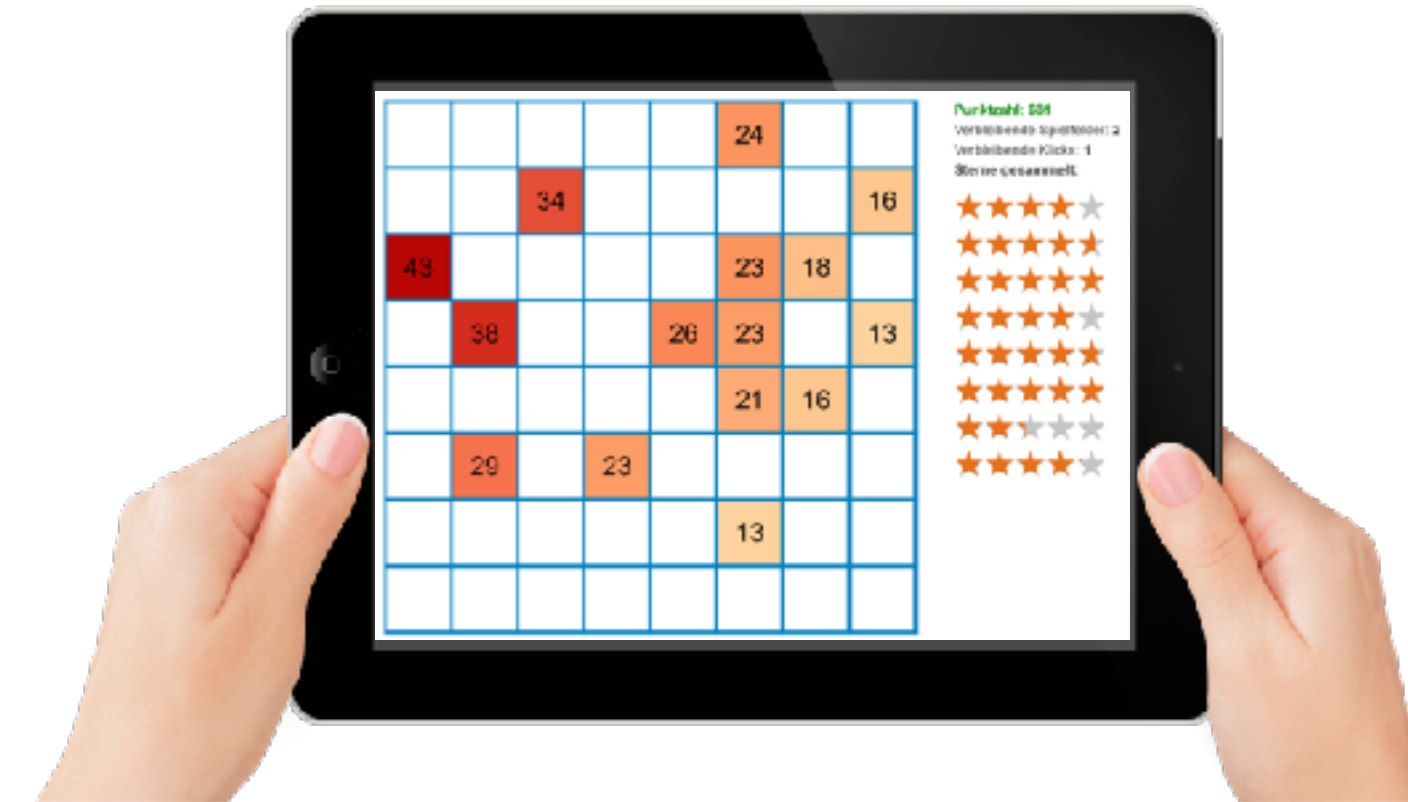
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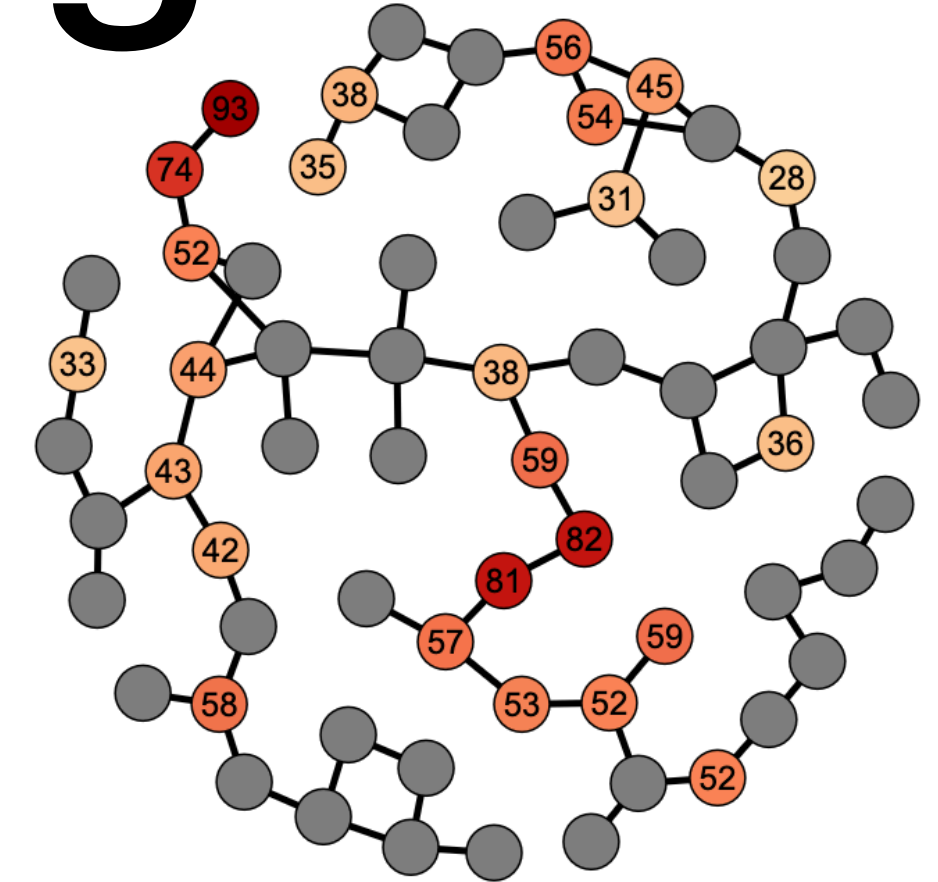
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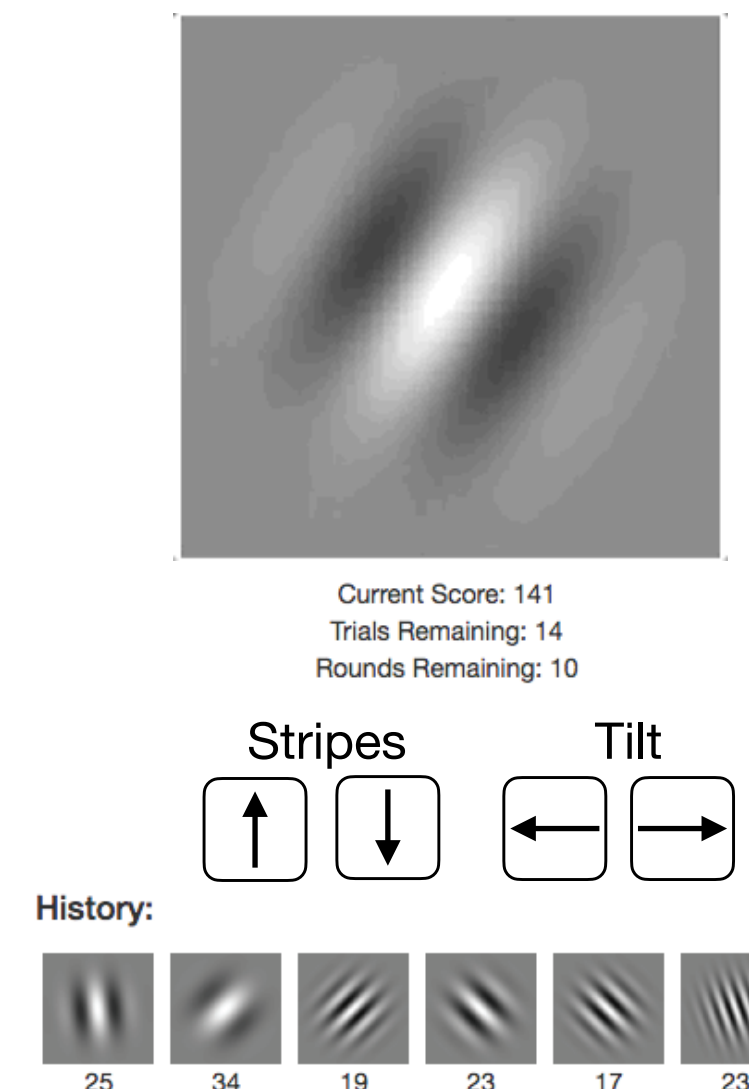
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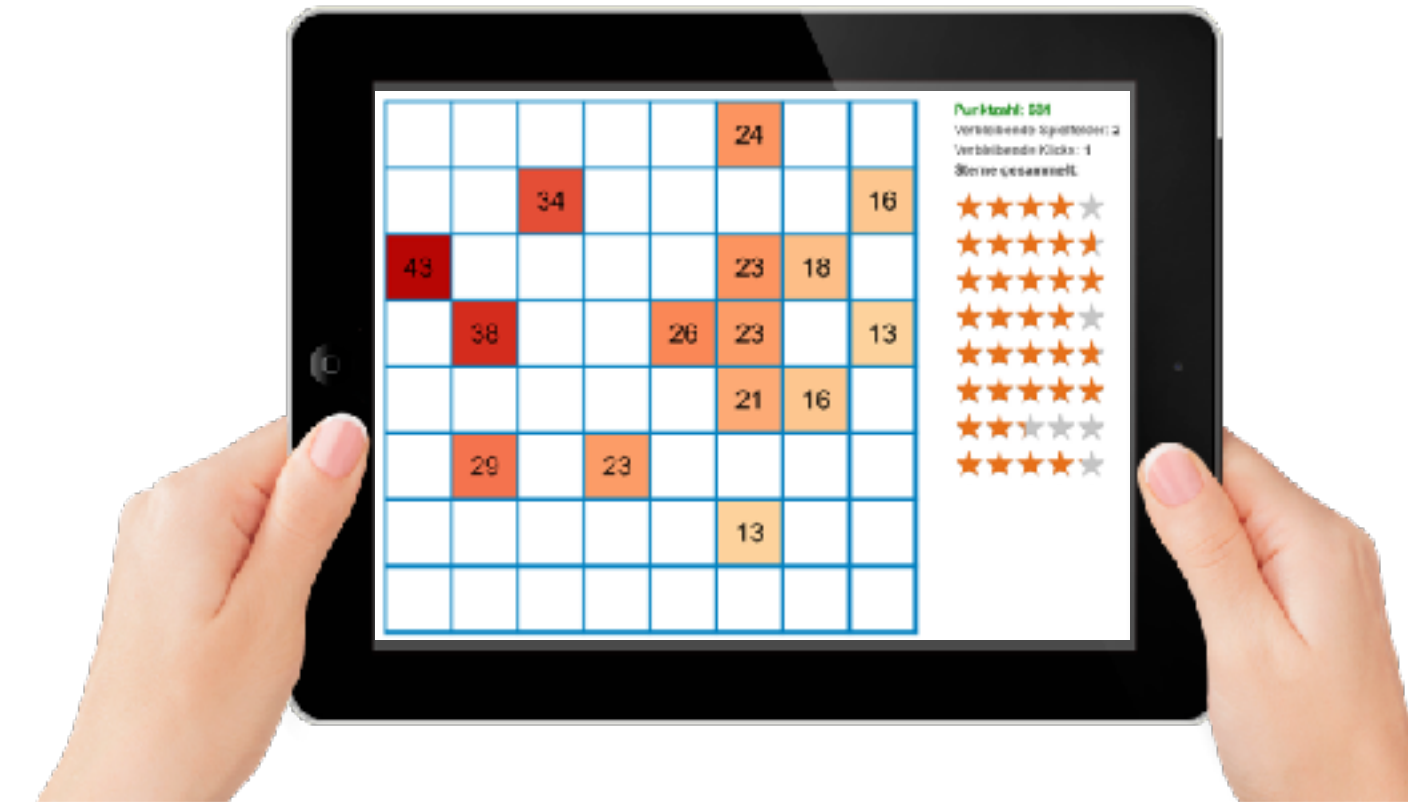
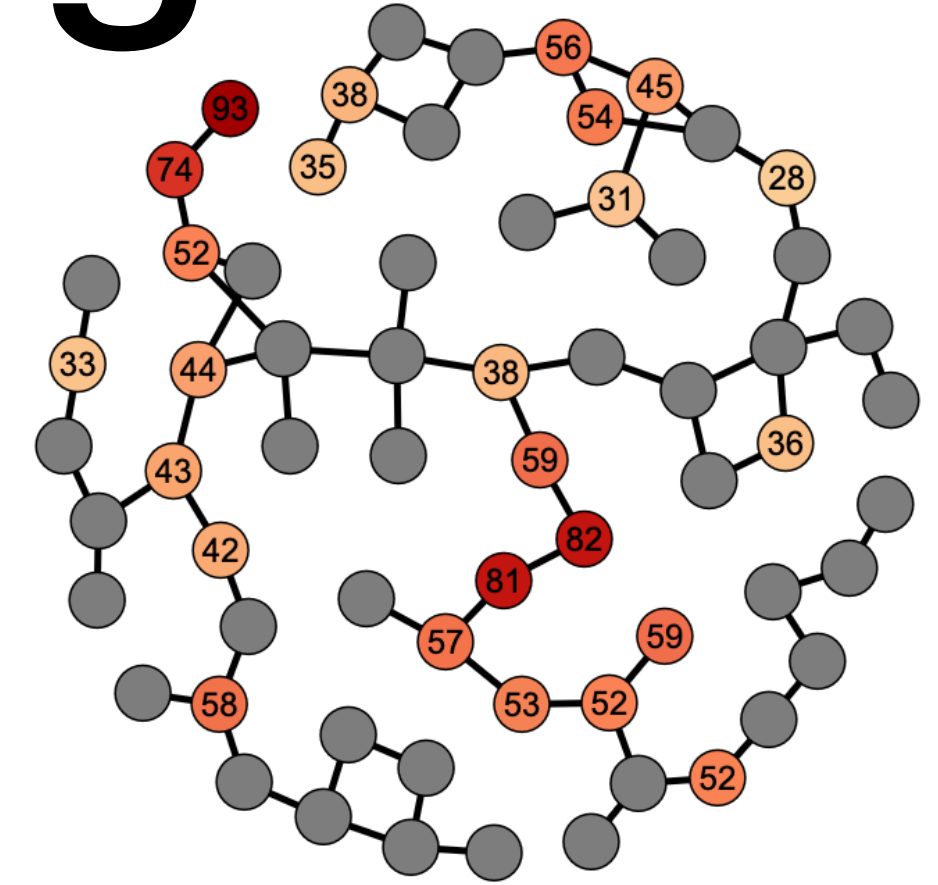
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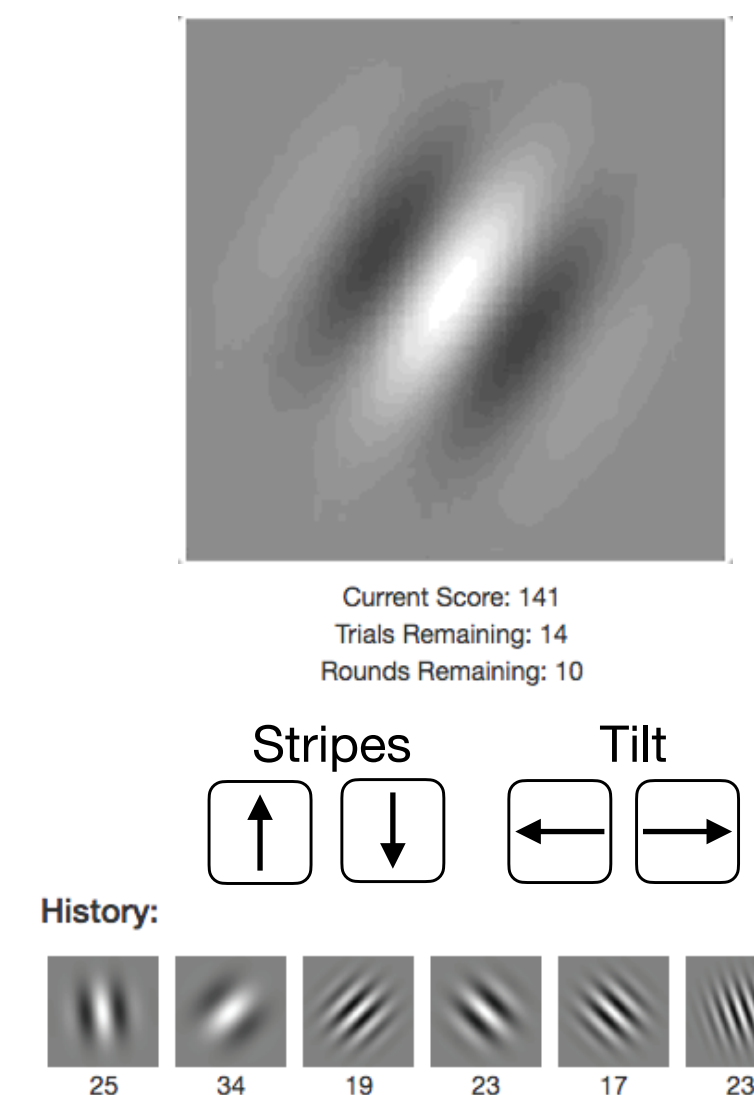
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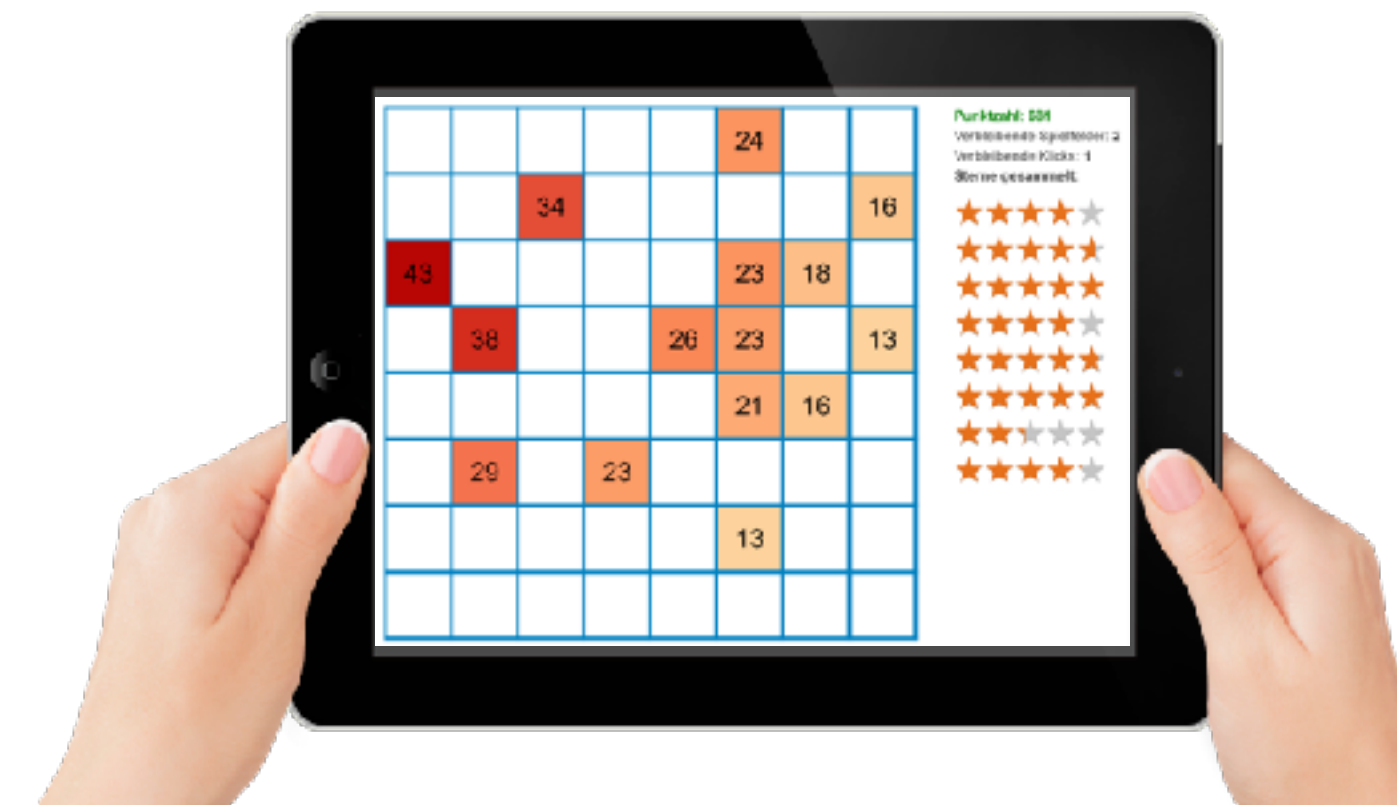
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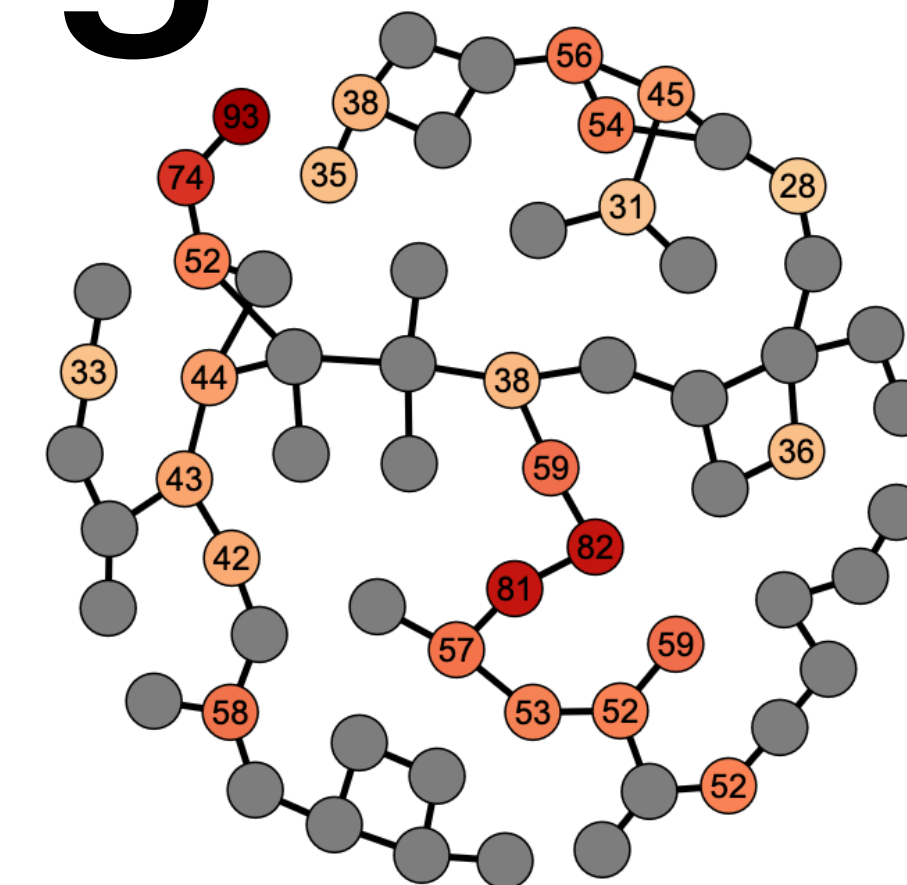
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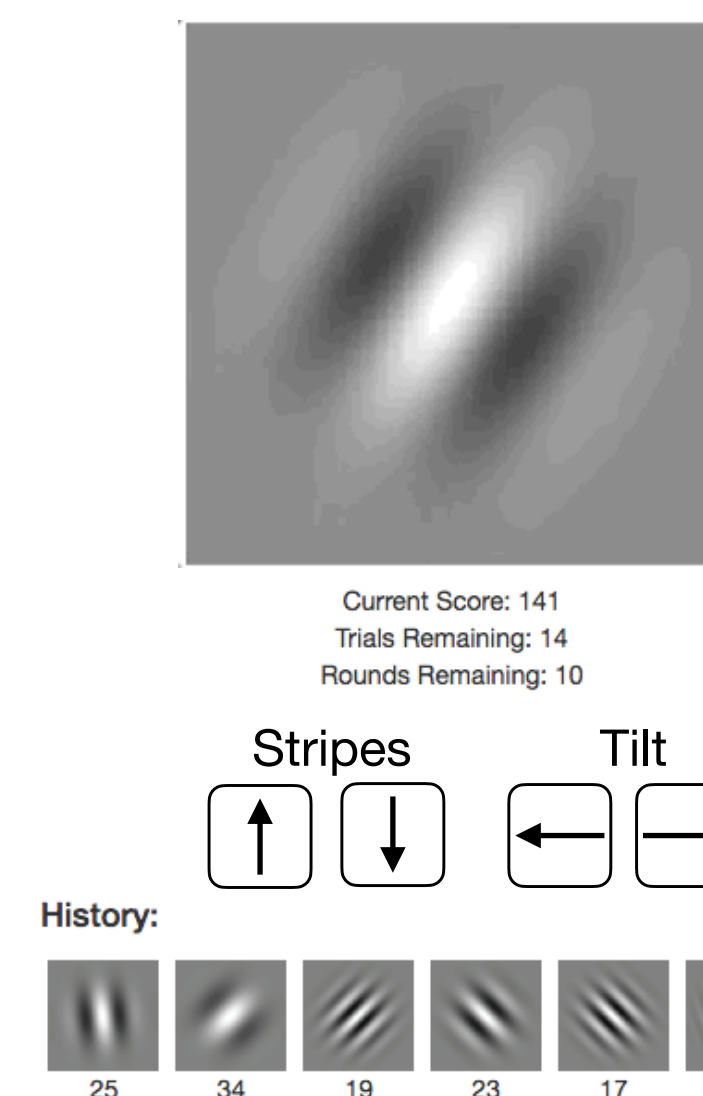
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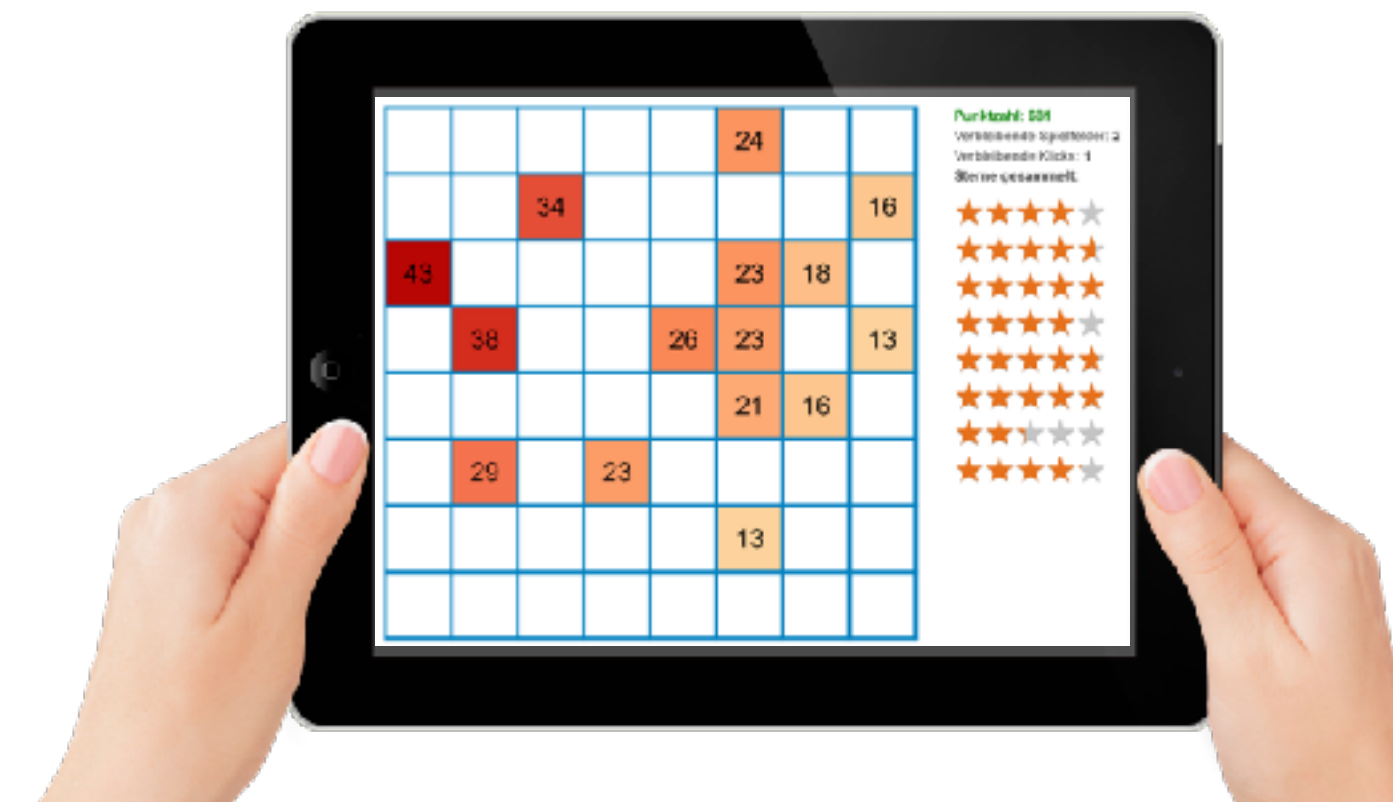
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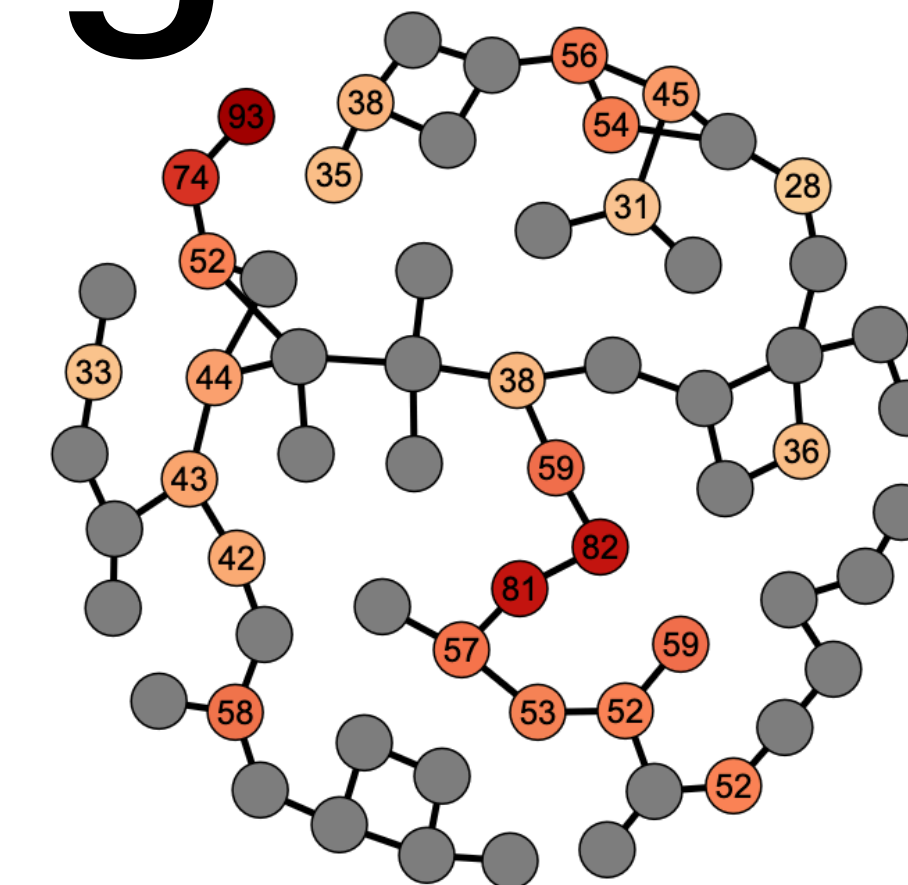
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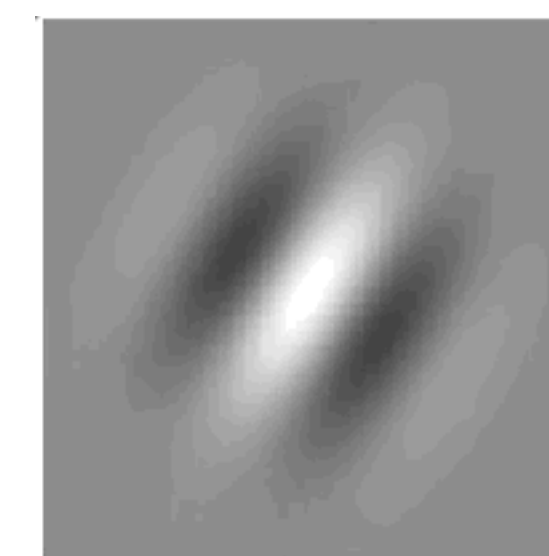
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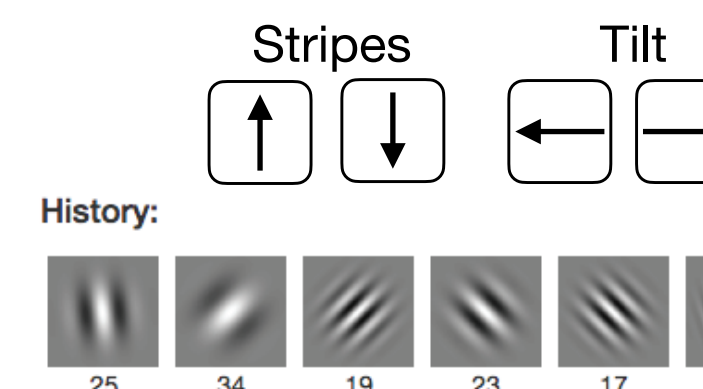
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Current Score: 141
Trials Remaining: 14
Rounds Remaining: 10



Wu, Schulz, Garvert, Meder & Schuck
(*PLOS Comp Bio* 2020)



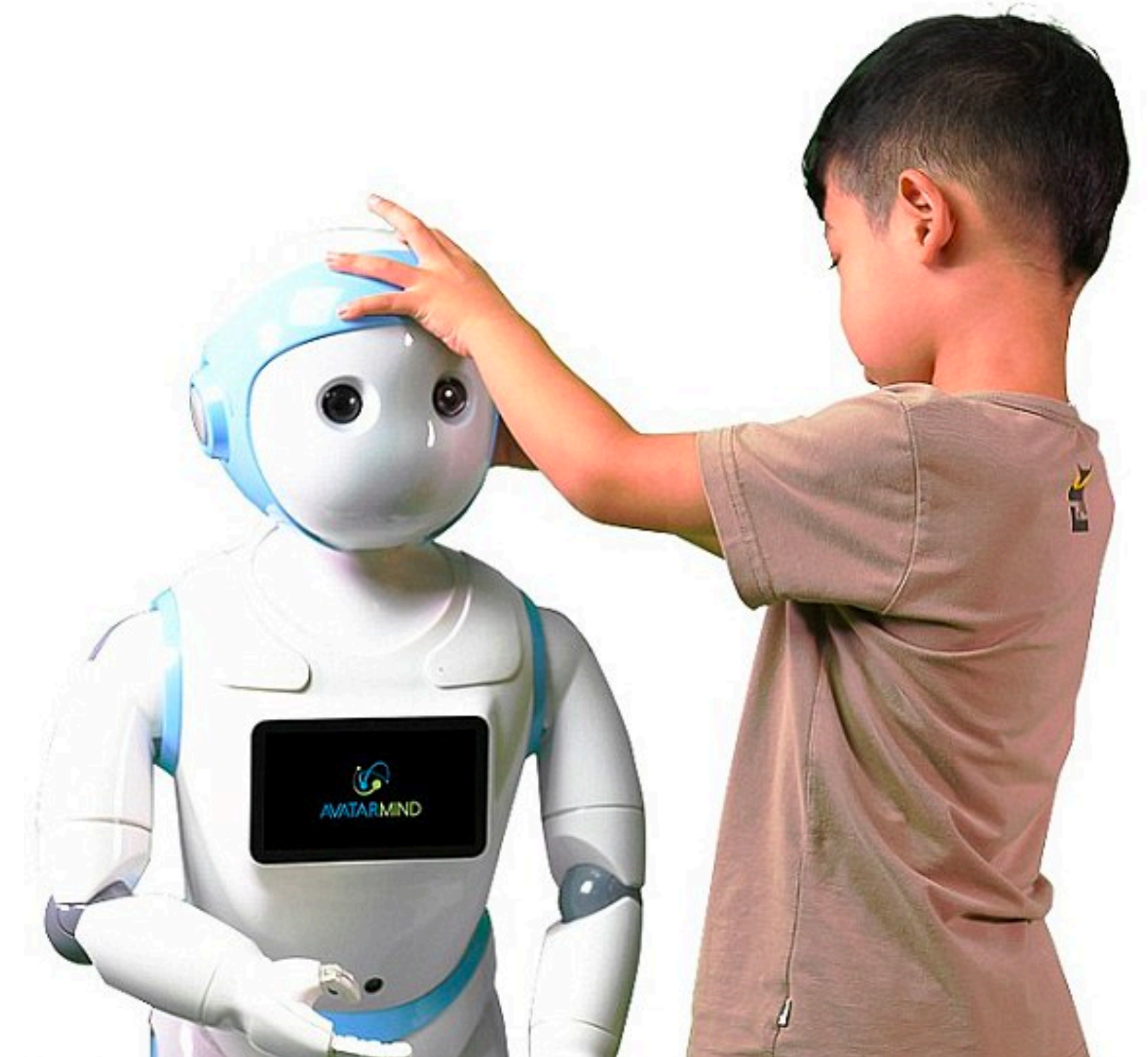
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Part 2

How to learn like a child

What AI can learn from Children

- Josh Tenenbaum (MIT): Children are the only known information processing system that demonstrably and reproducibly develop into intelligent systems
- Turing (1950) suggested we should build AI that learns like a child
- How do children learn differently from adults?



What AI can learn from Children

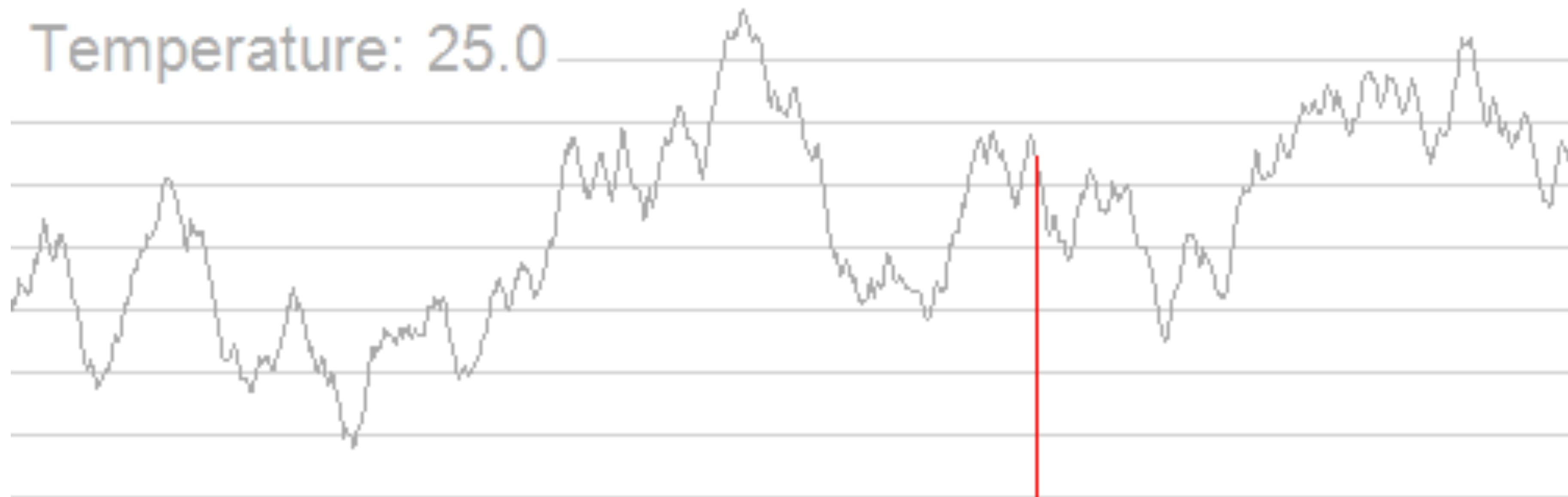
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- Turing (1950) suggested we should build AI that learns like a child
- How do children learn differently from adults?
- One robust finding is they are highly variable!



video by Francis Vachon

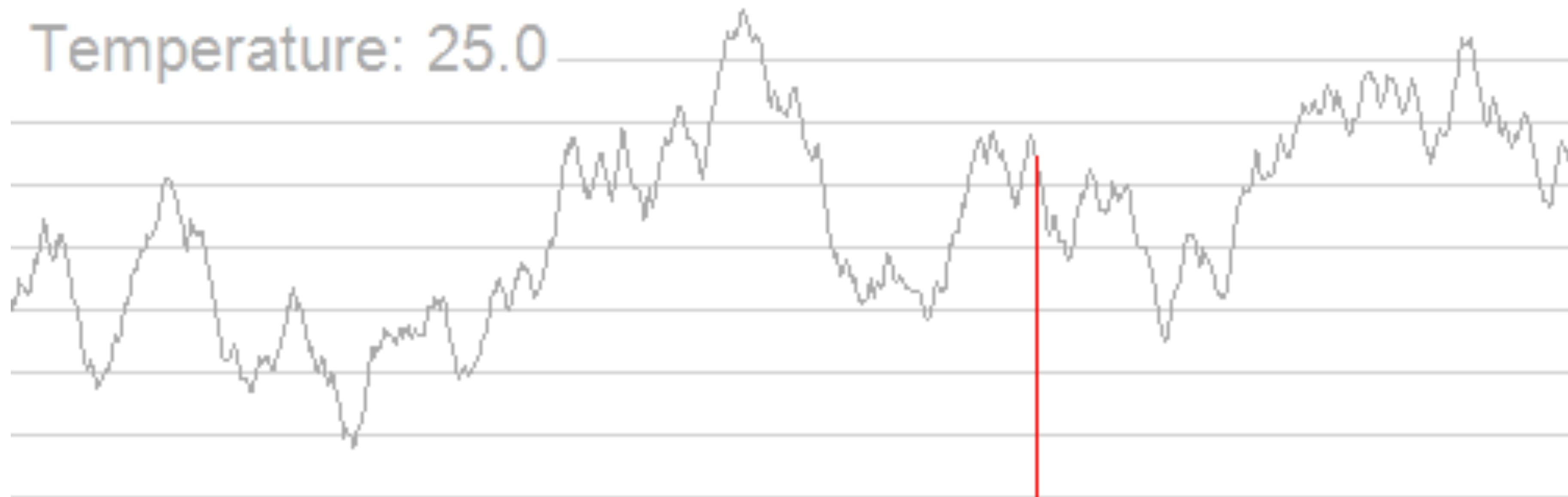
What explains the extensive variability found in children's search behavior?

- High temperature sampling hypothesis:
 - Children initially perform high-temperature search, which gradually “cool offs” as they grow older (Gopnik et al., *Curr Dir Psych Sci* 2017)



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Sources of Developmental Differences

- Higher **temperature** sampling that cools off over age? (Gopnik et al., 2017)



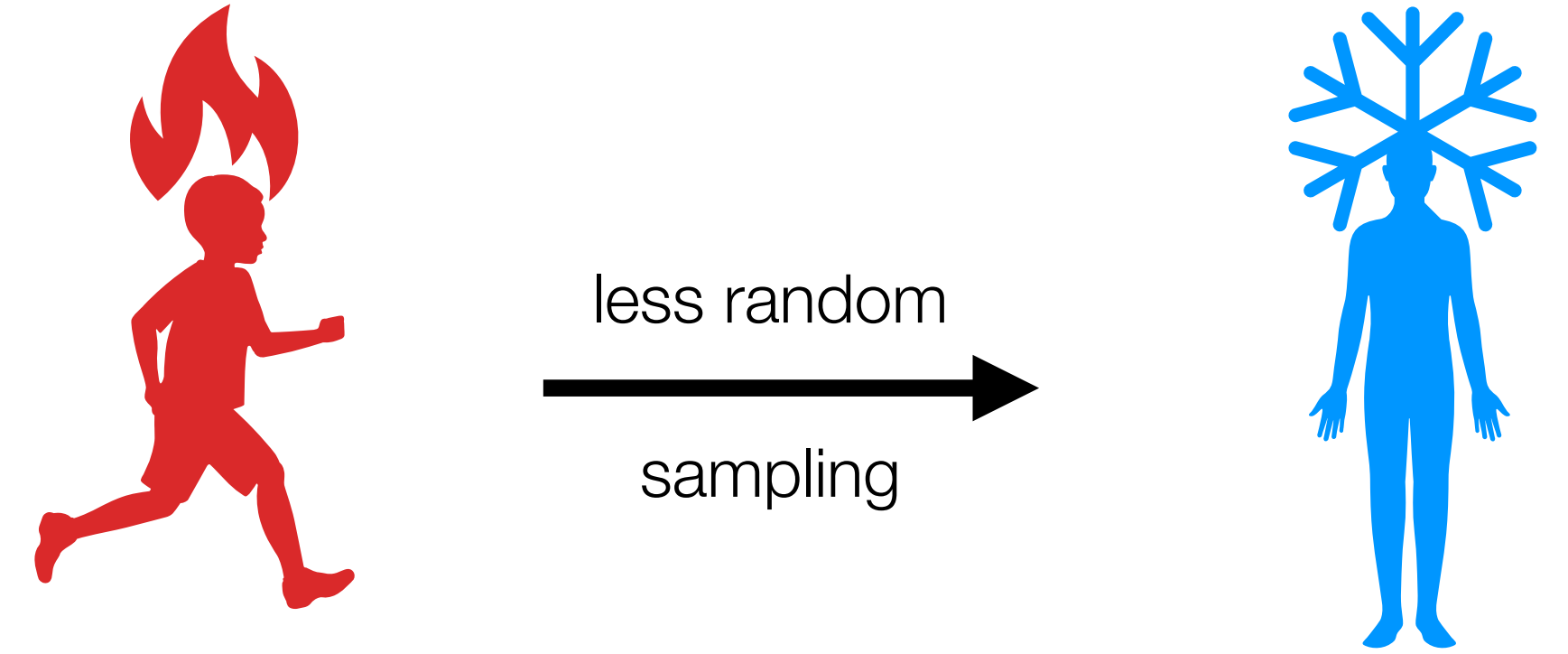
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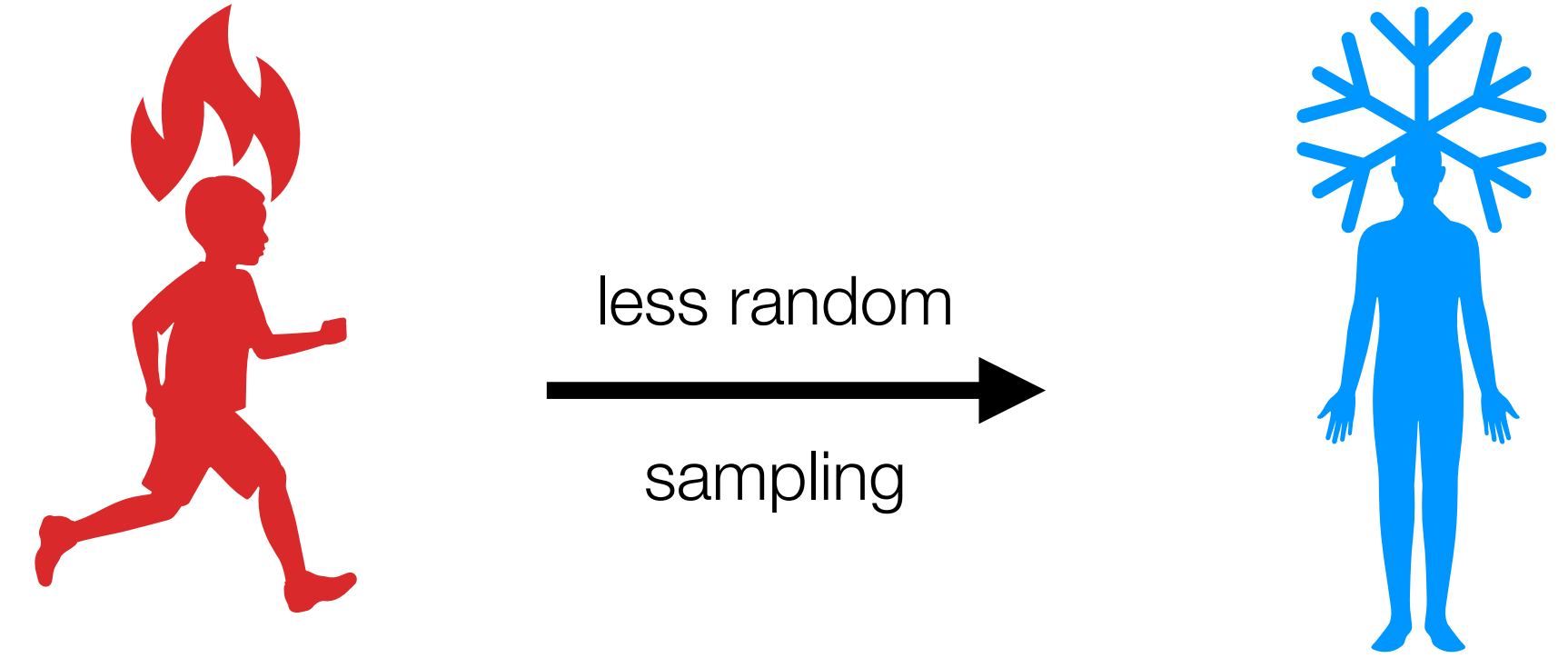
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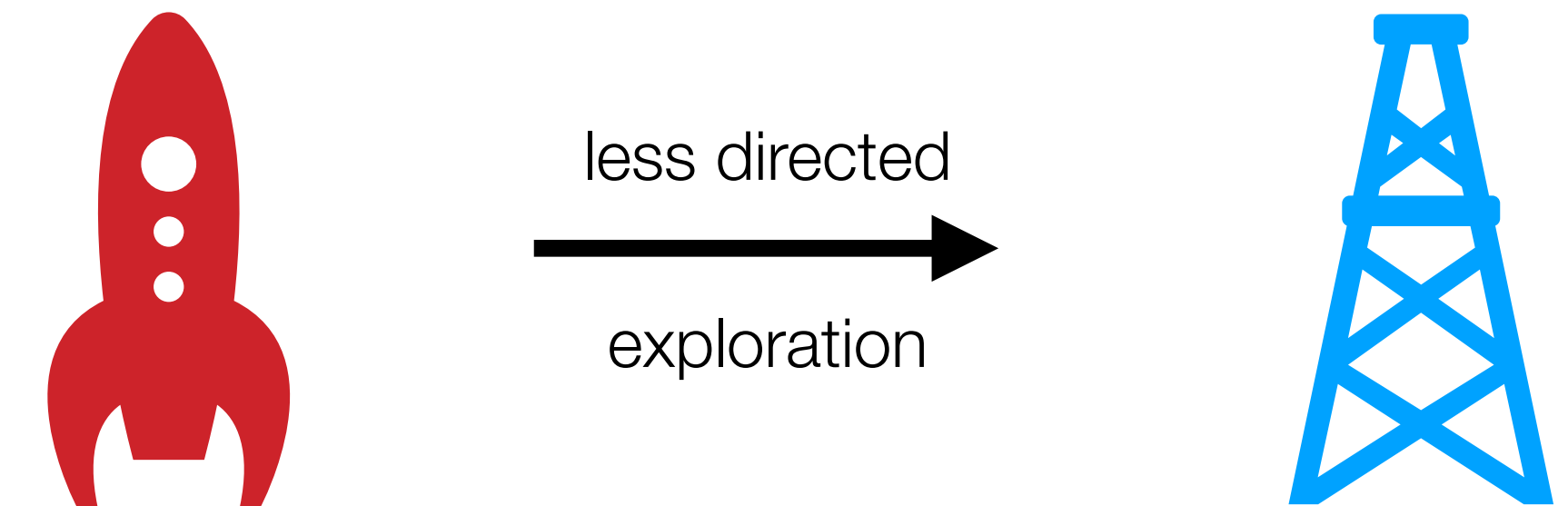


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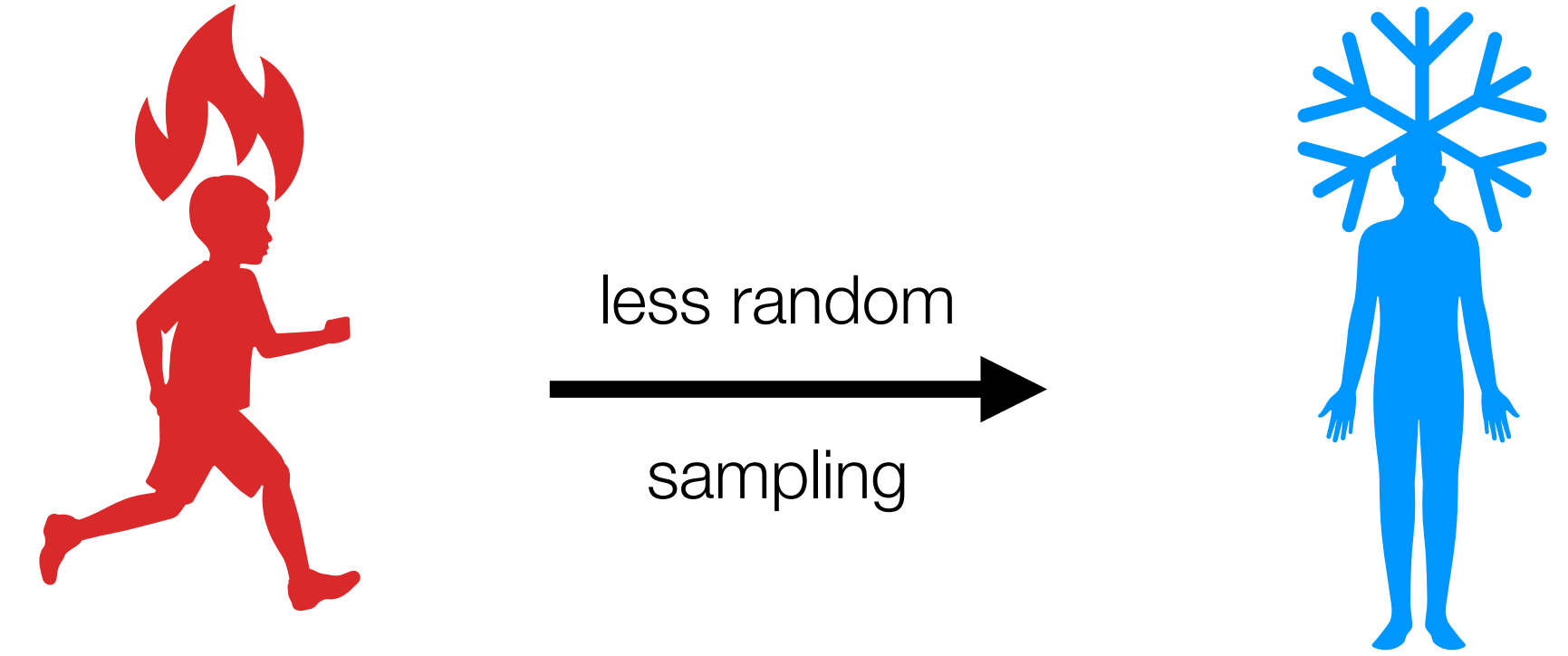


- Changes in **directed exploration** rather than random exploration? (Wilson et al., 2014)

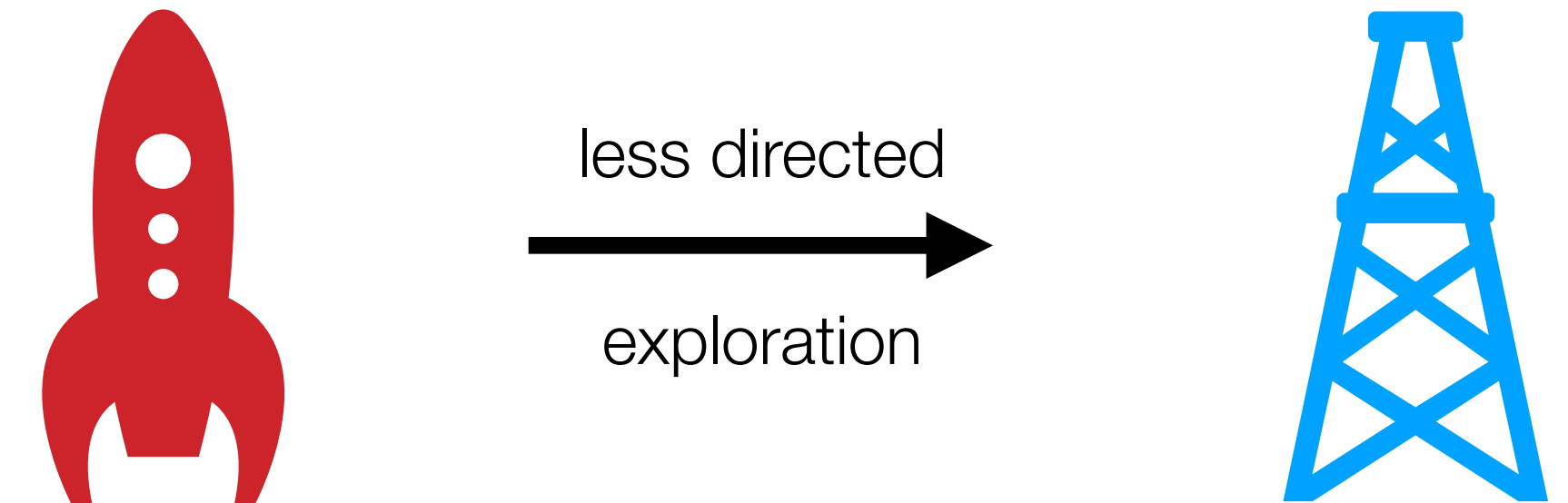


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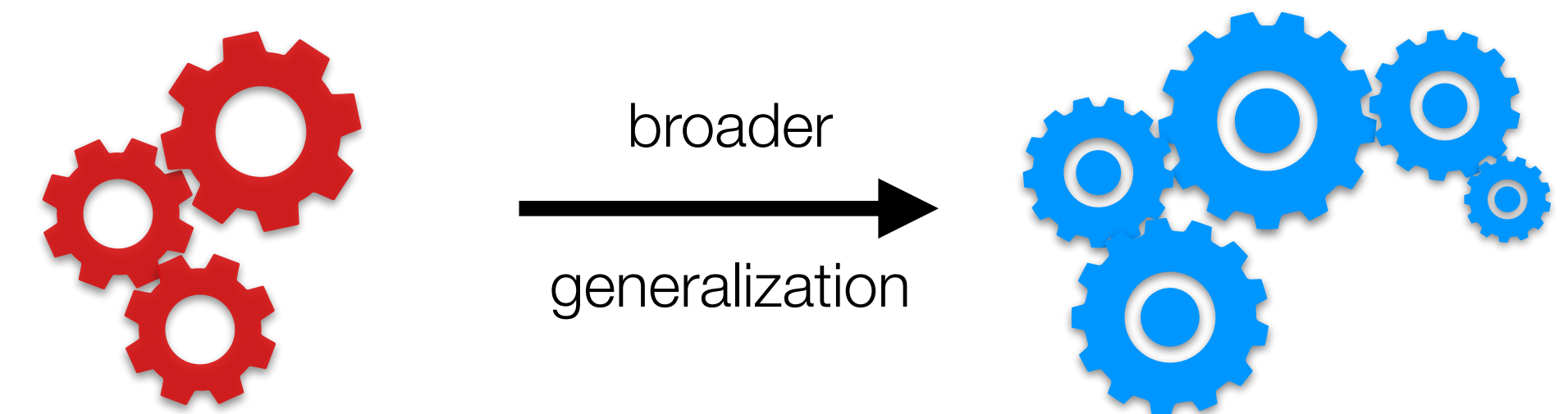
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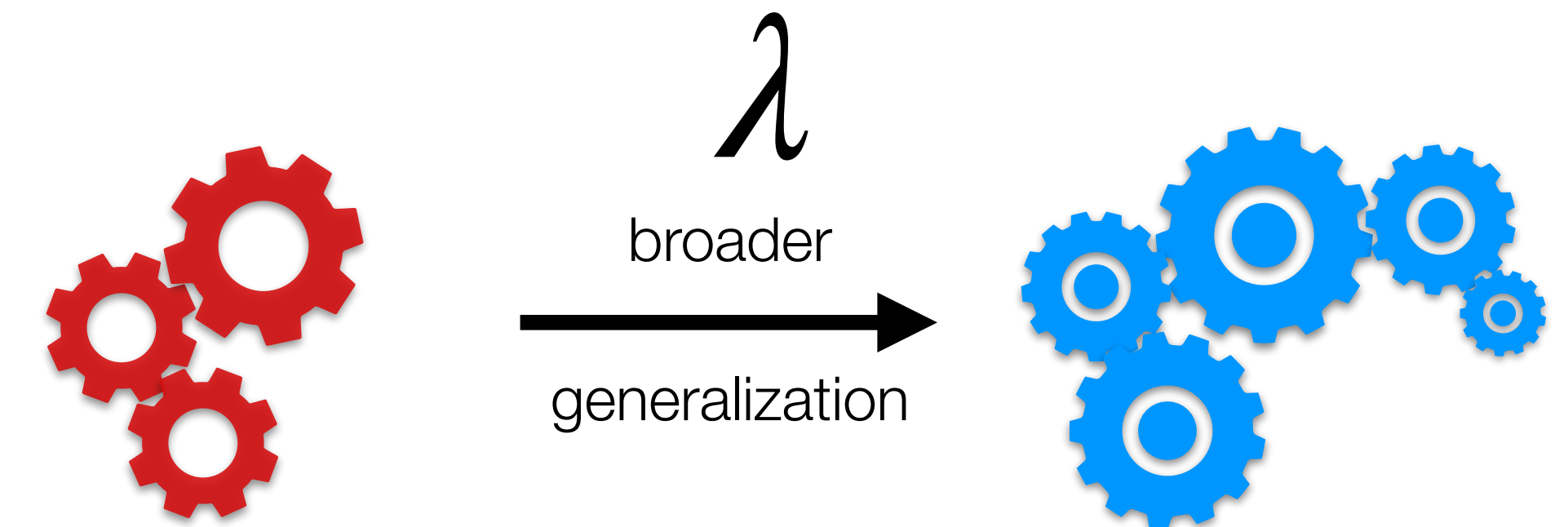
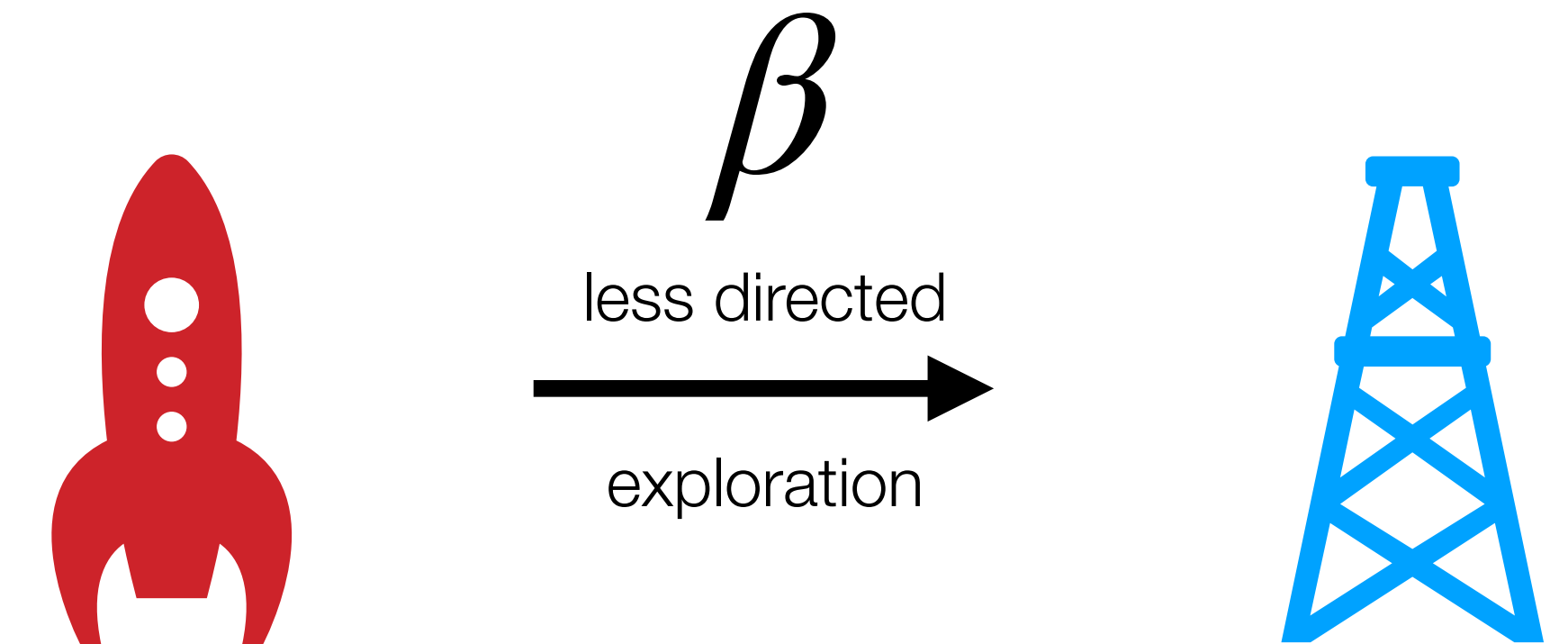
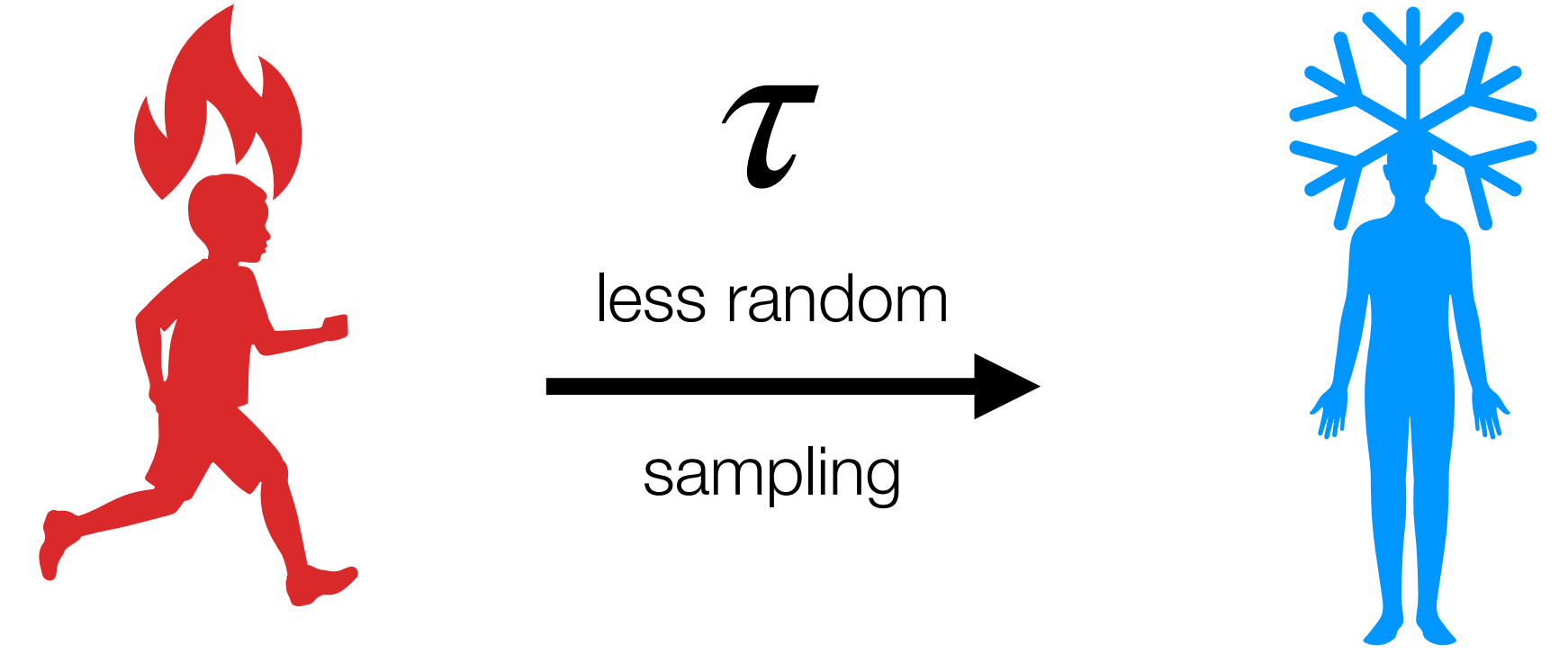


- Refinement of cognitive representations and processes supporting **generalization**? (Blanco et al., 2016)

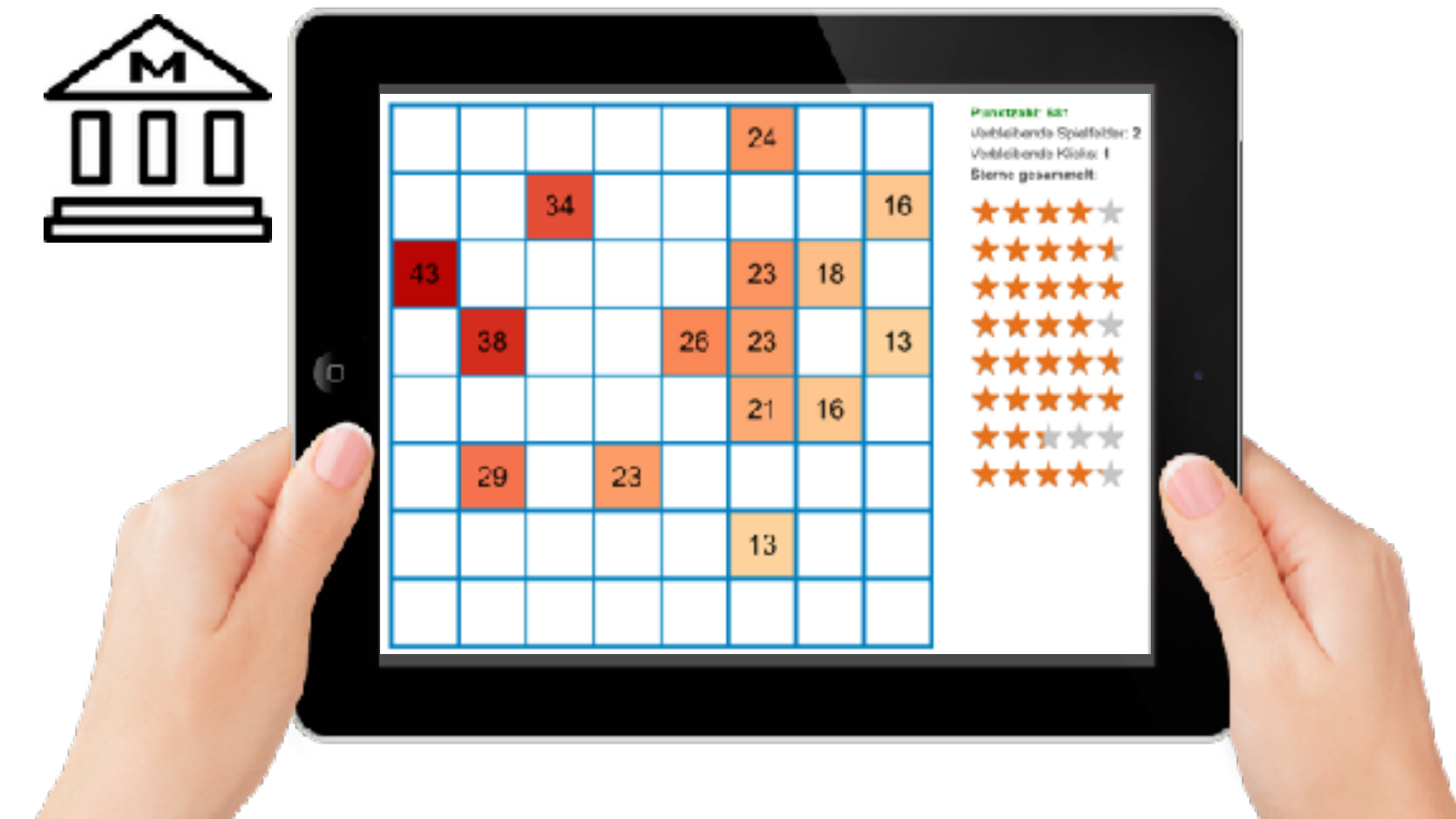


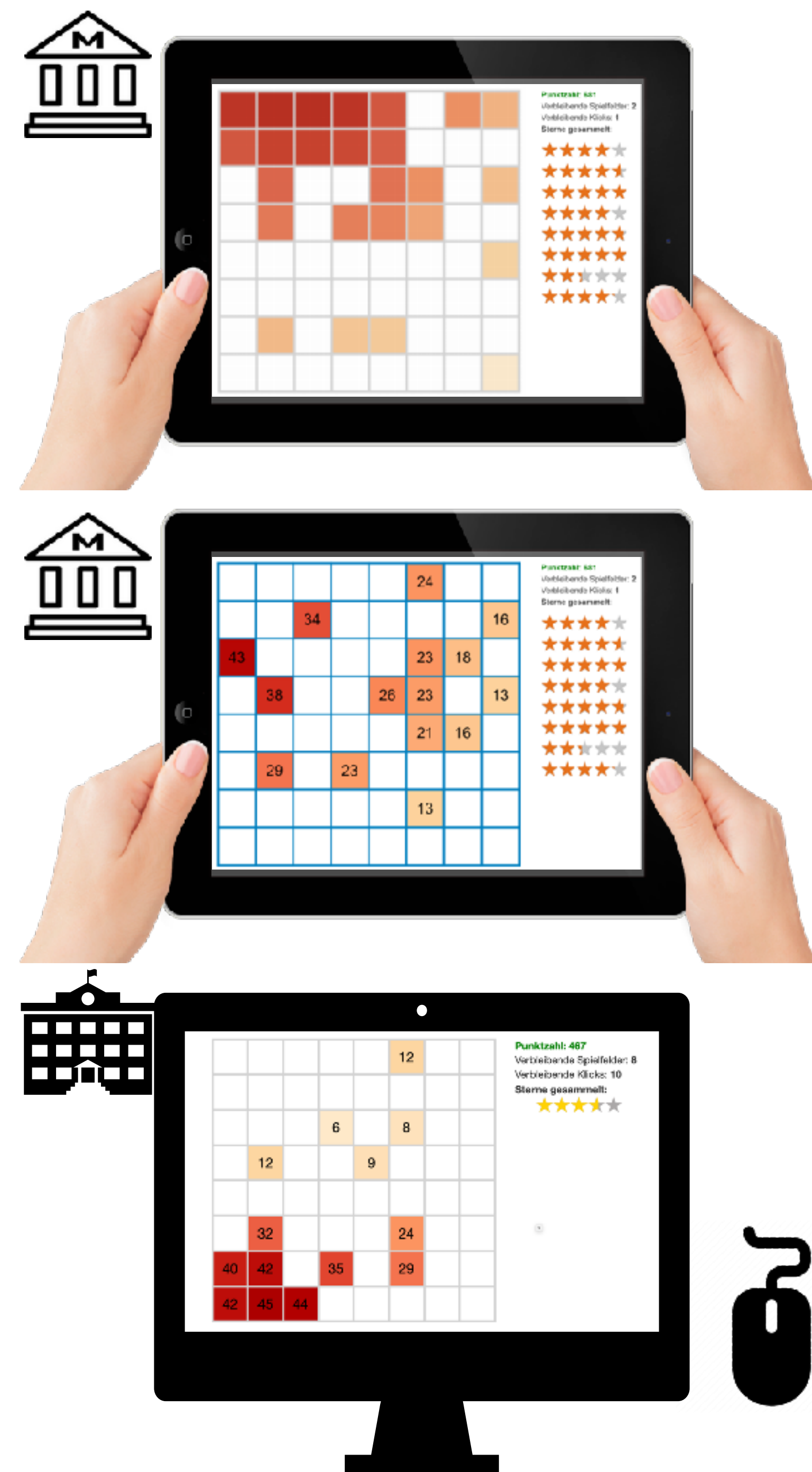
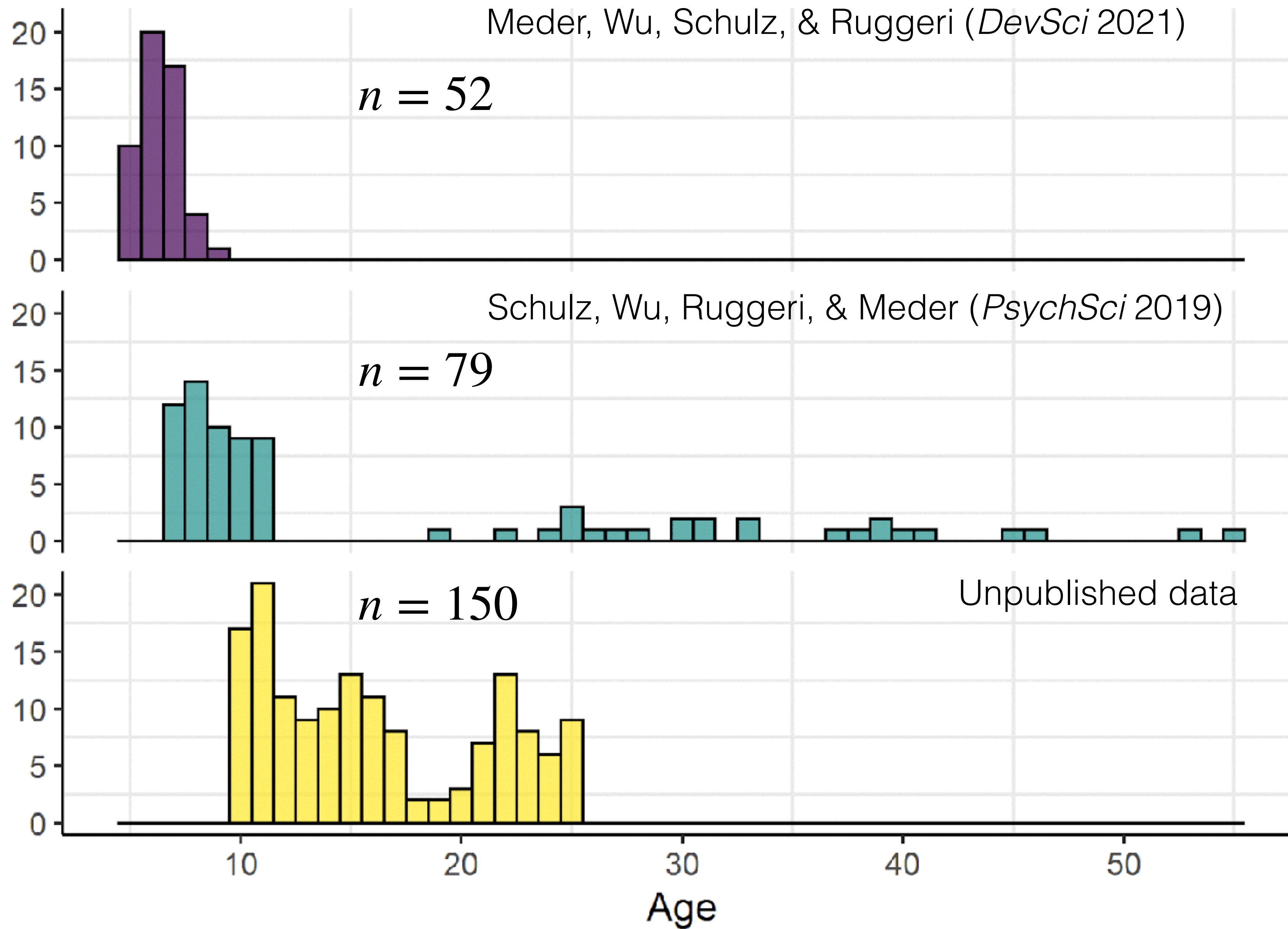
Sources of Developmental Differences

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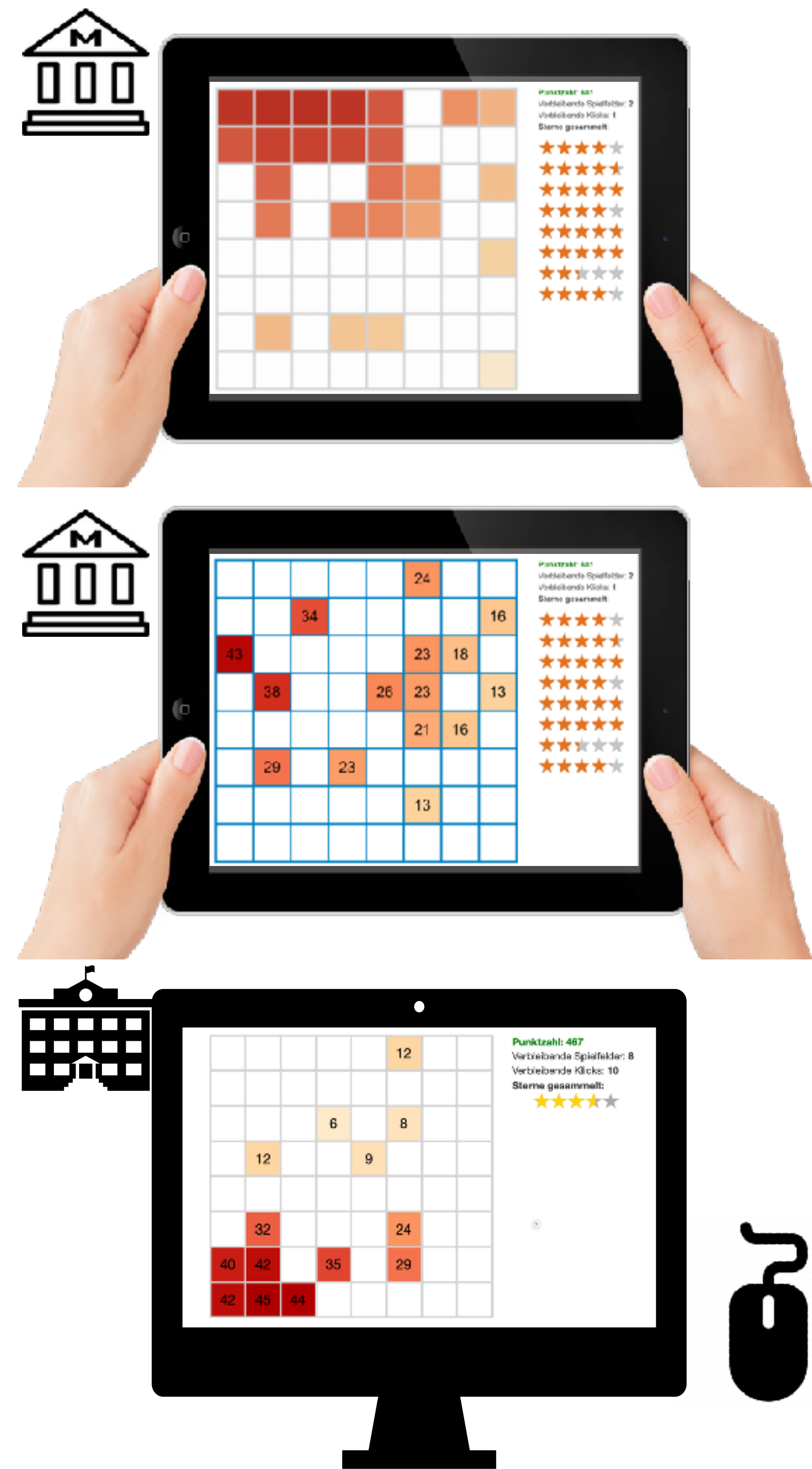
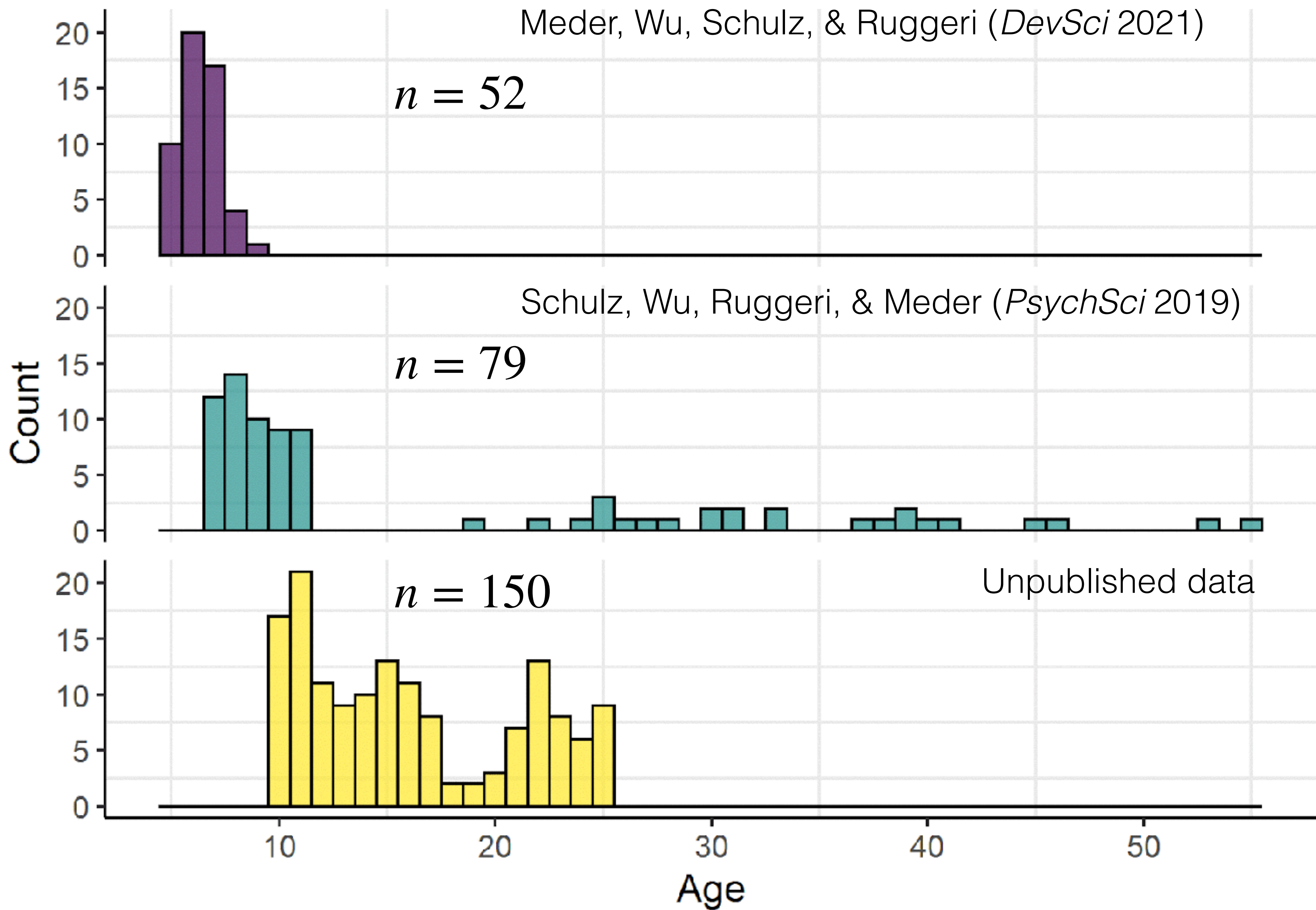


Schulz, Wu, Ruggeri, & Meder (*PsychSci* 2019)



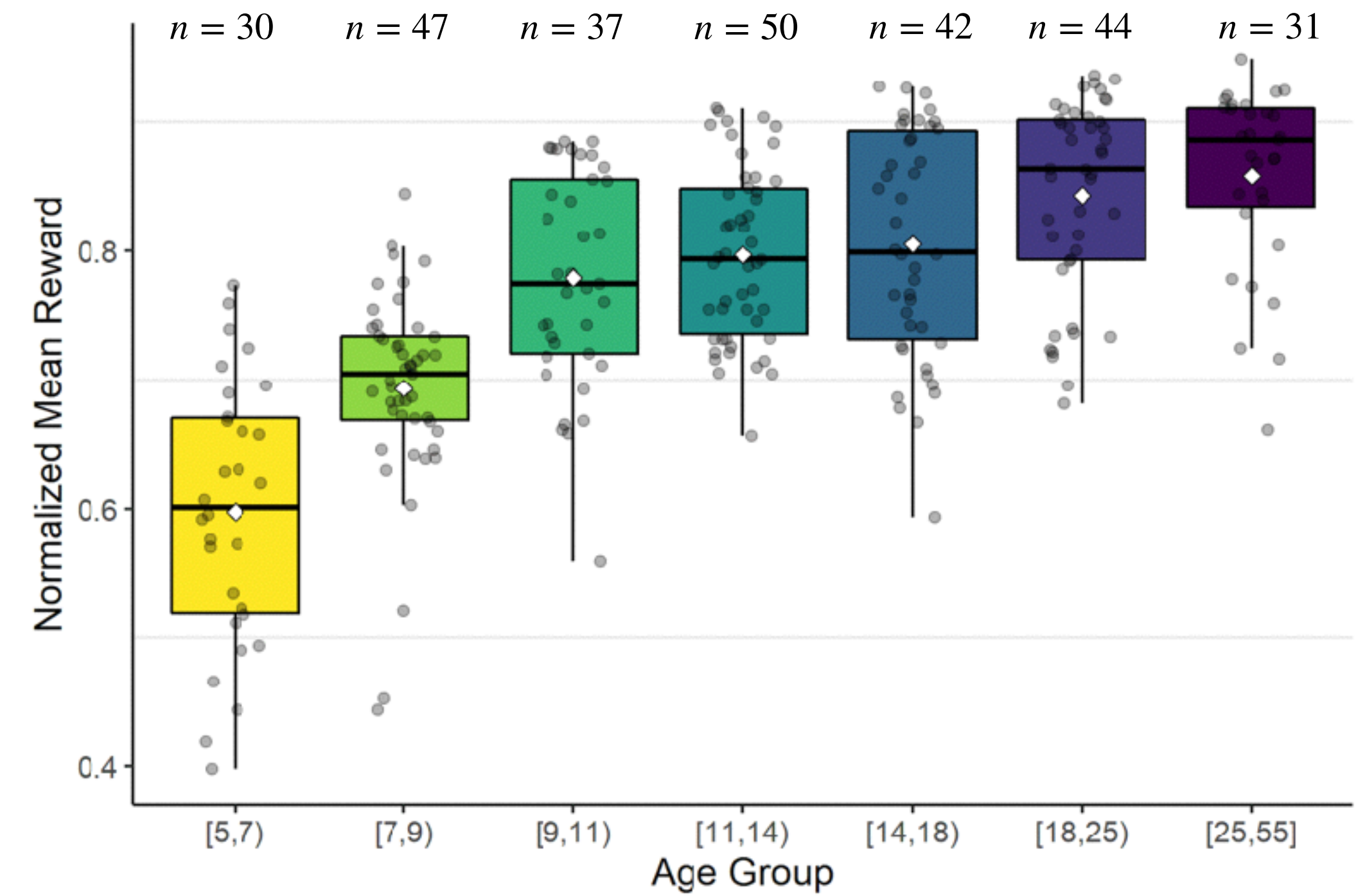


Filtered to use the same sets of environments, same grid size, and same number of trials per round



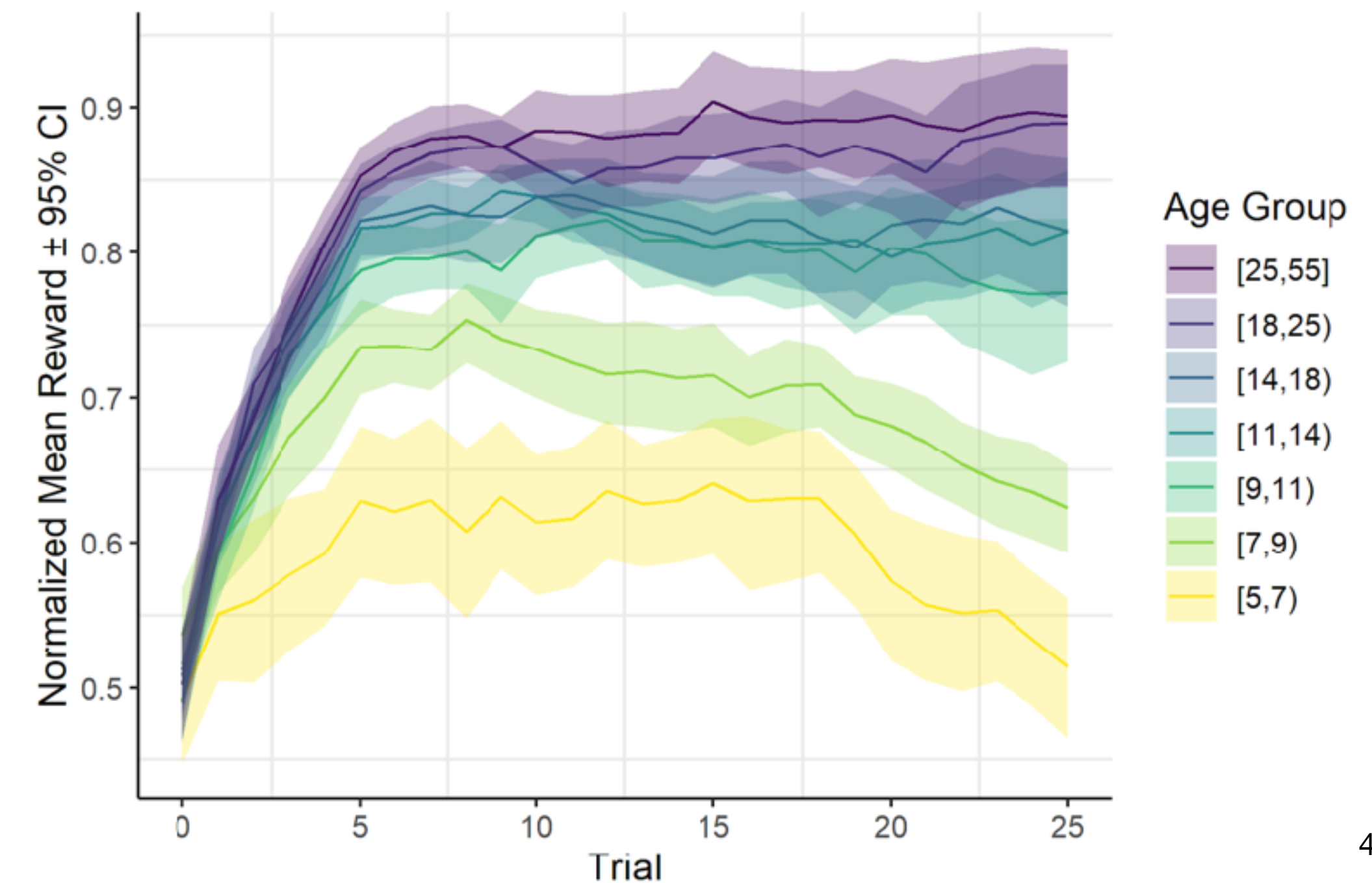
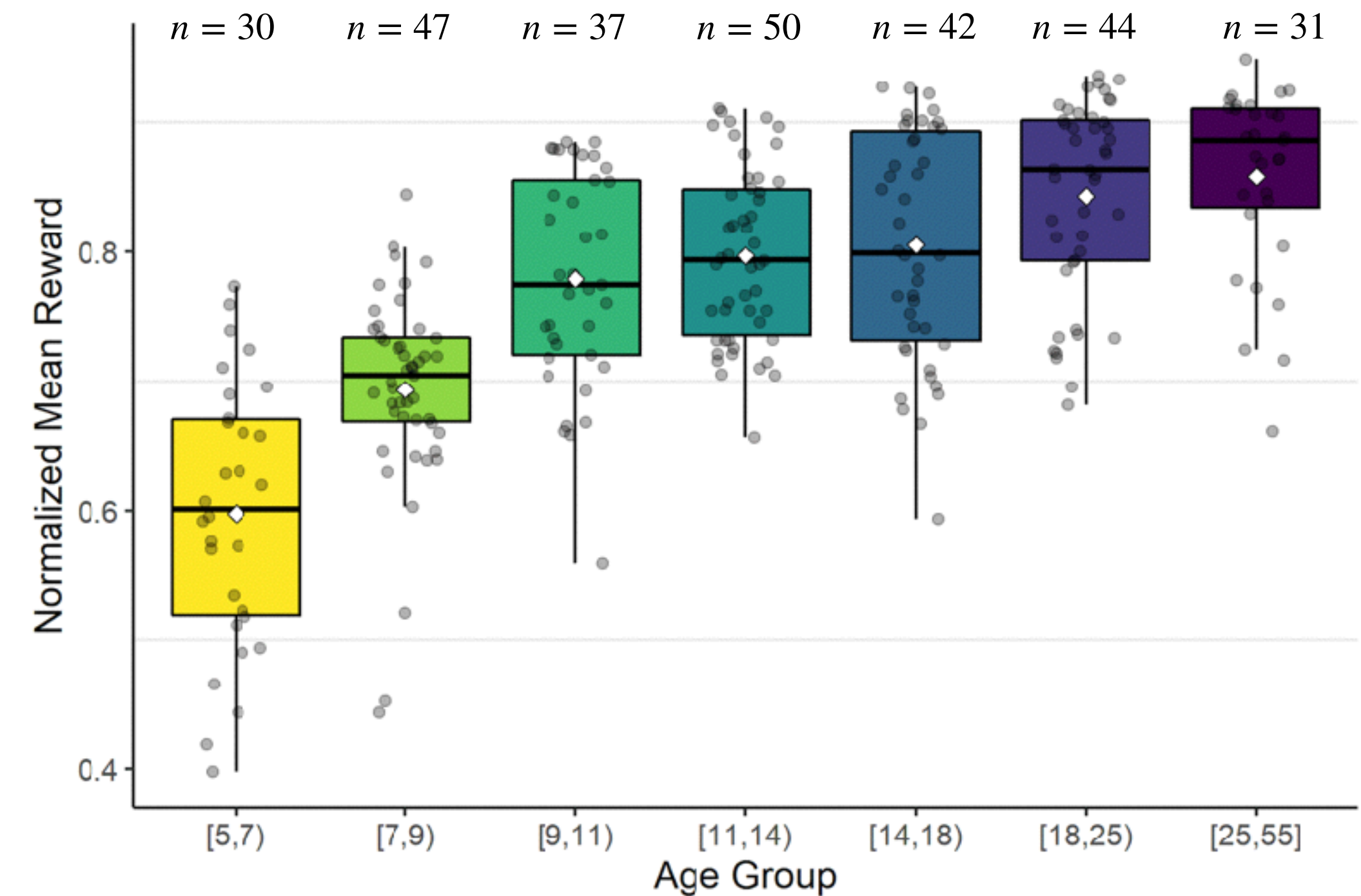
Behavioral results

- Performance increases over age



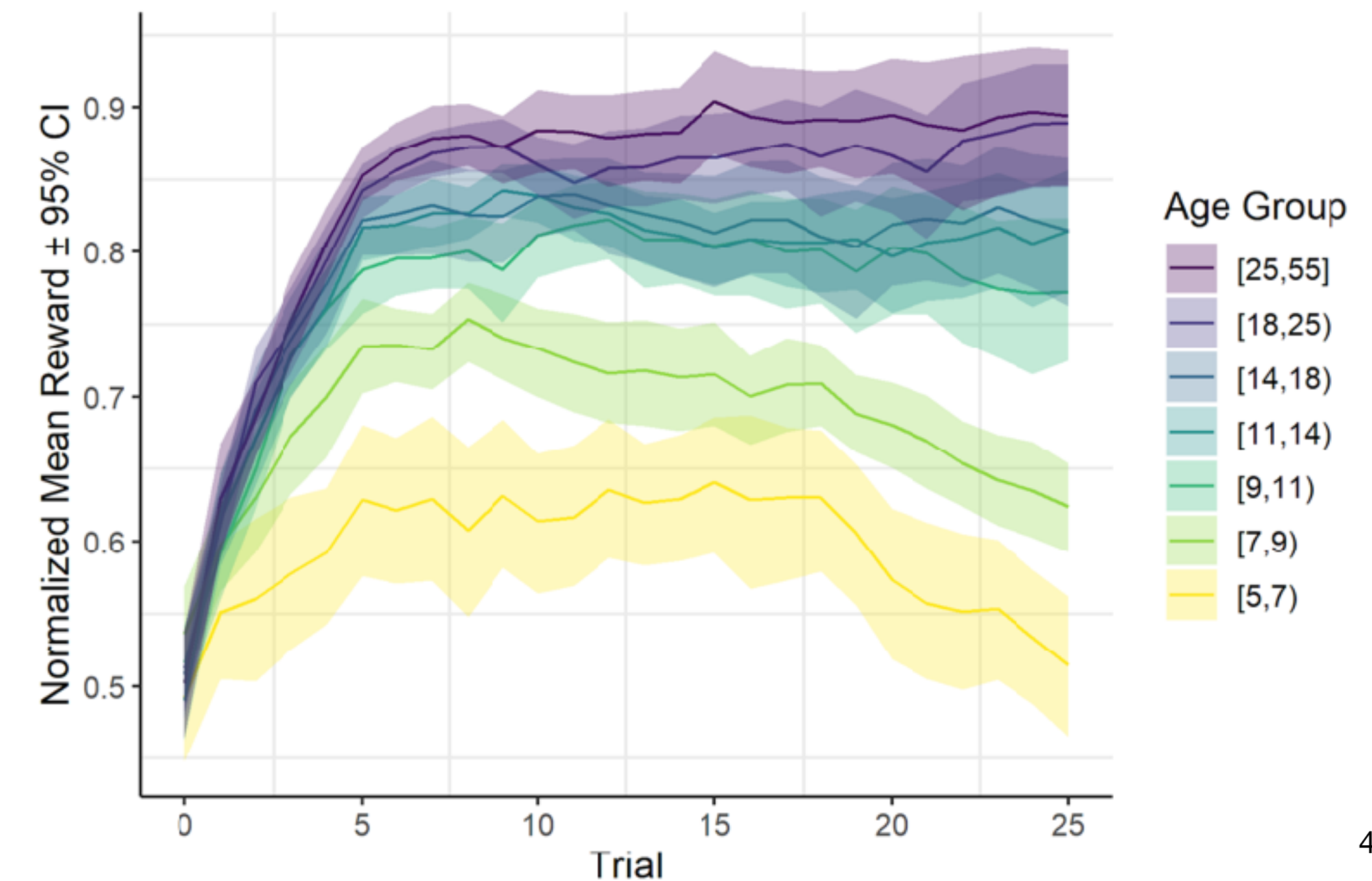
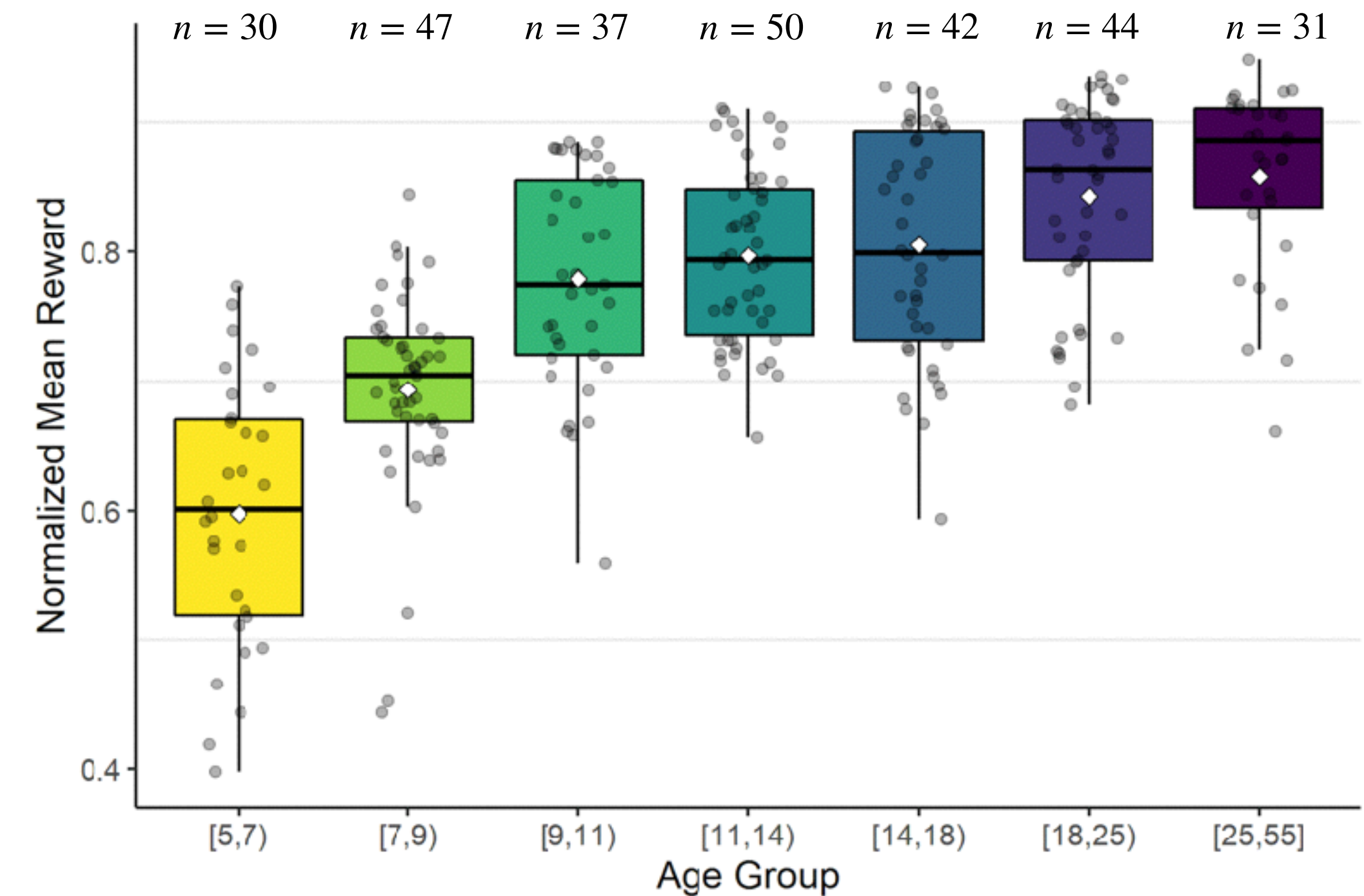
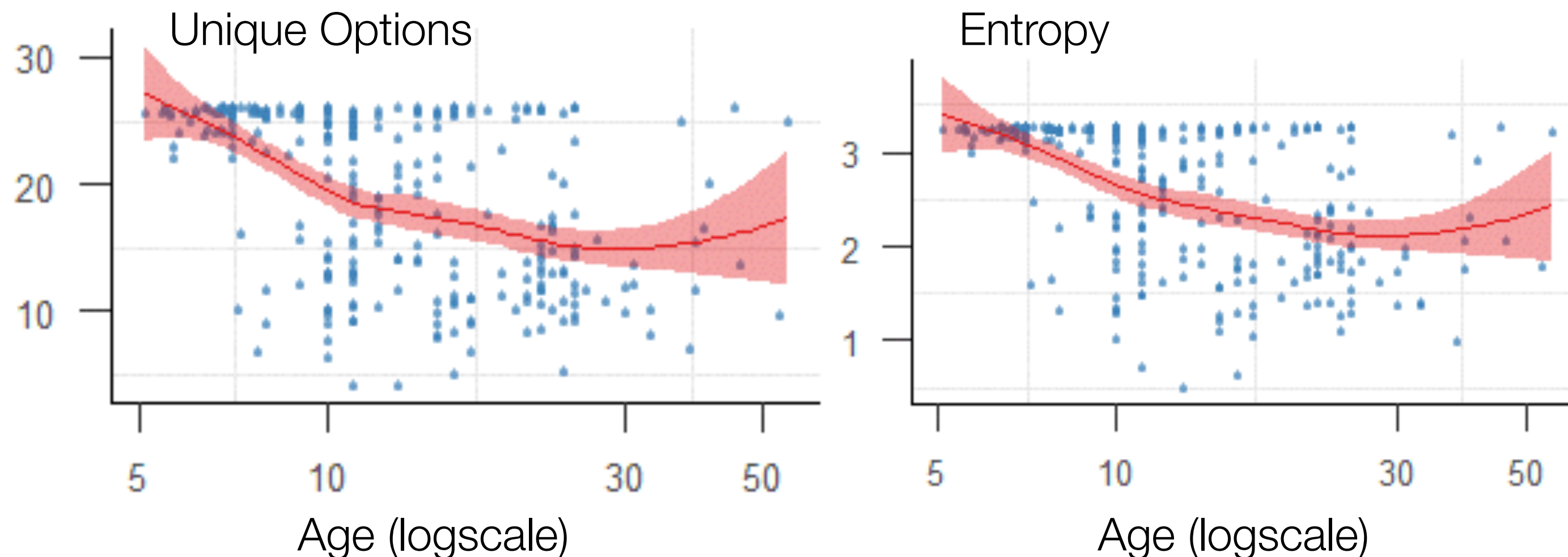
Behavioral results

- Performance increases over age
- Age-related differences are already evident in the first few trials
 - Older subjects have steeper learning curves
 - Younger children have decaying learning curves, consistent with over-exploration, i.e., more unique options and higher entropy of choices



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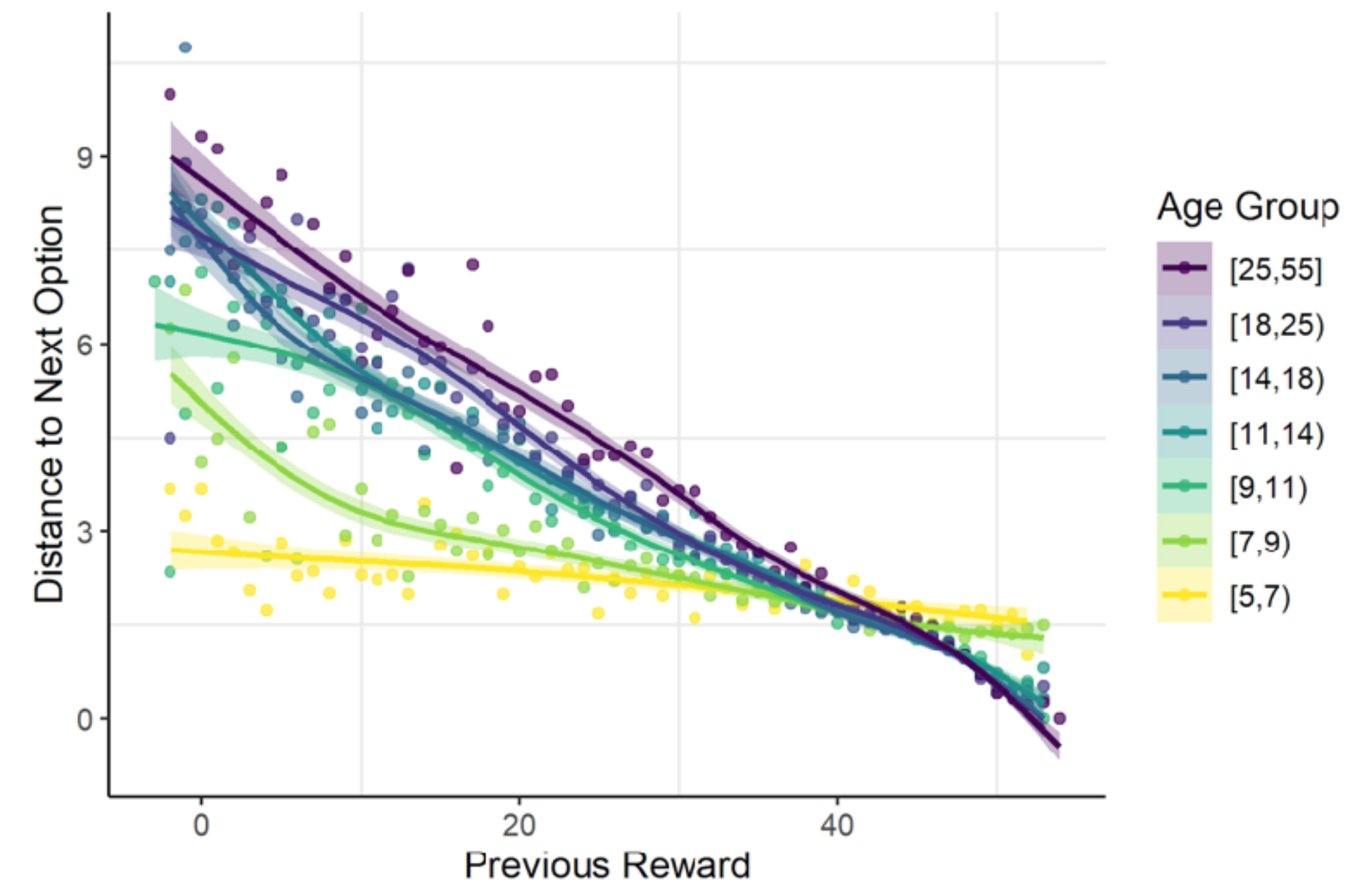
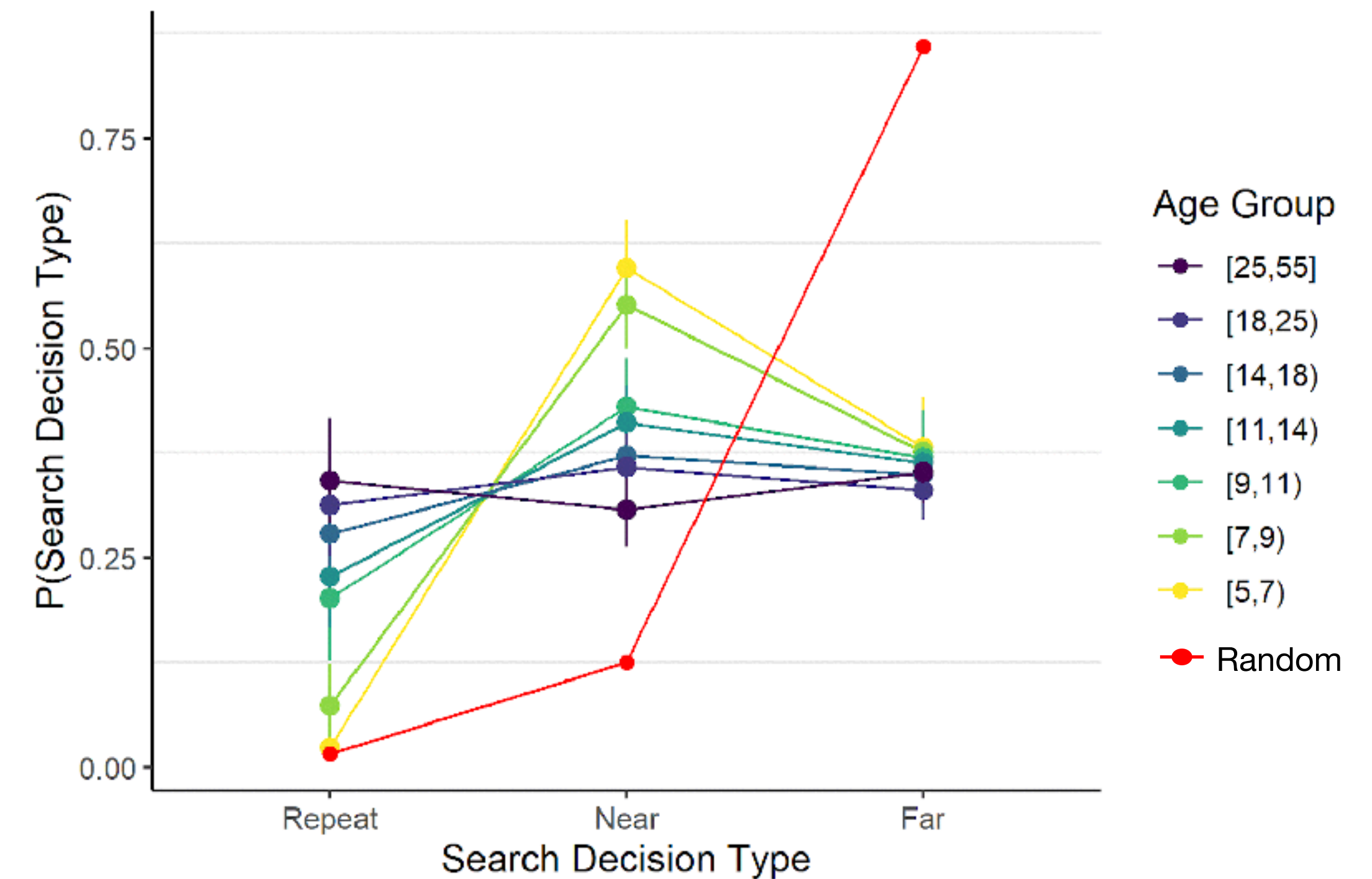
Behavioral results

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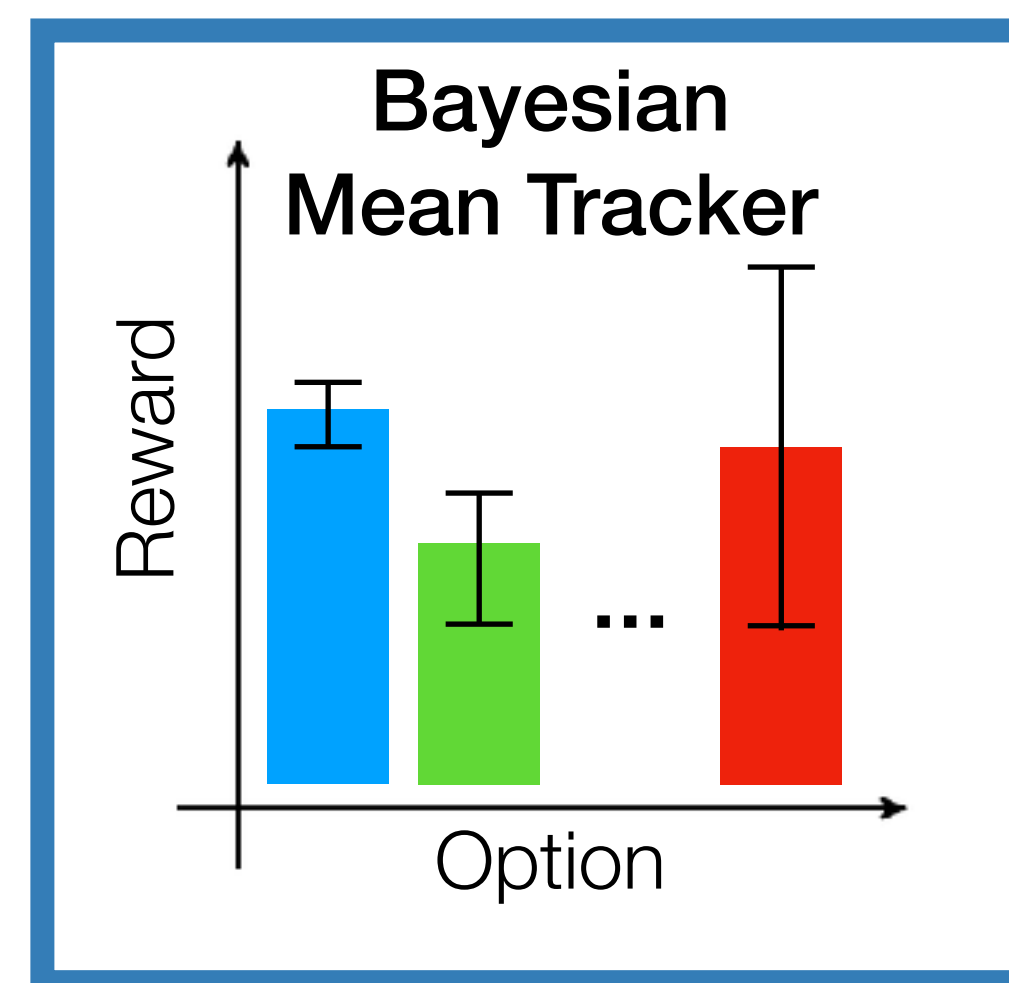
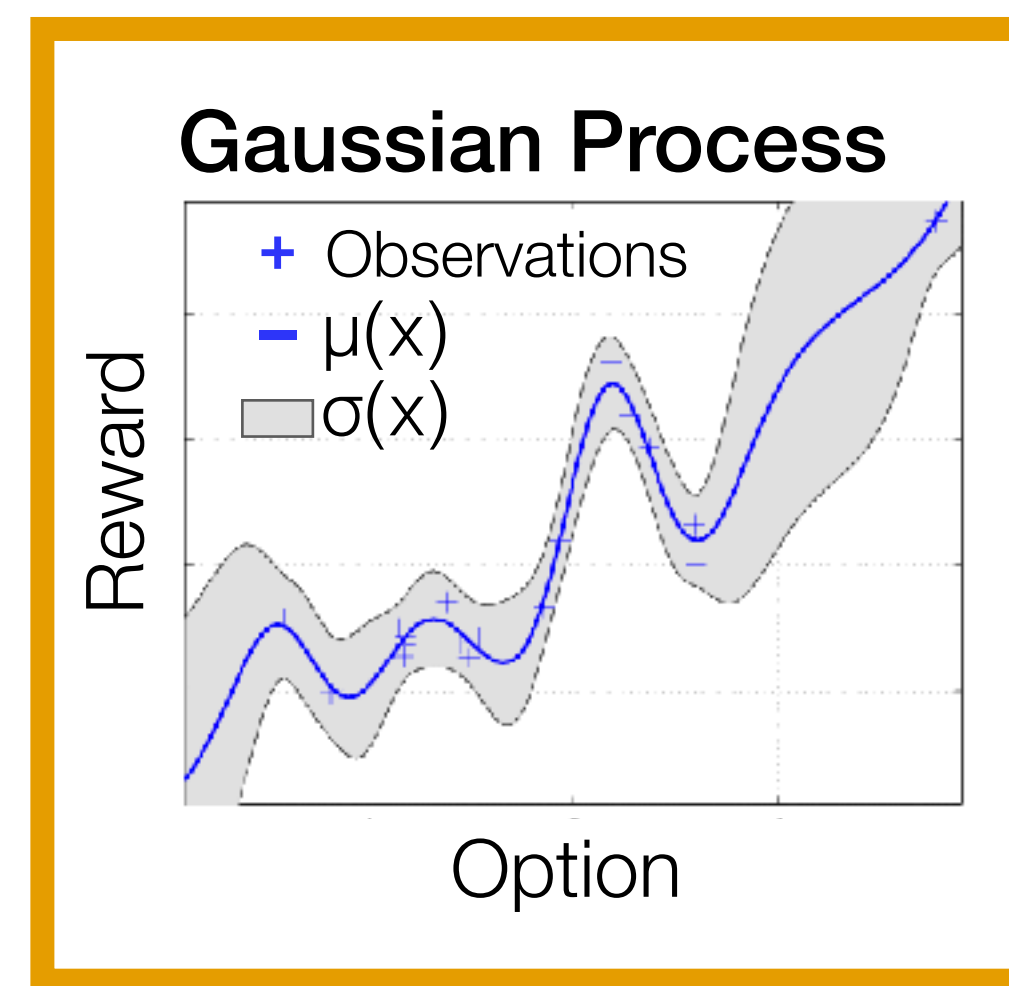
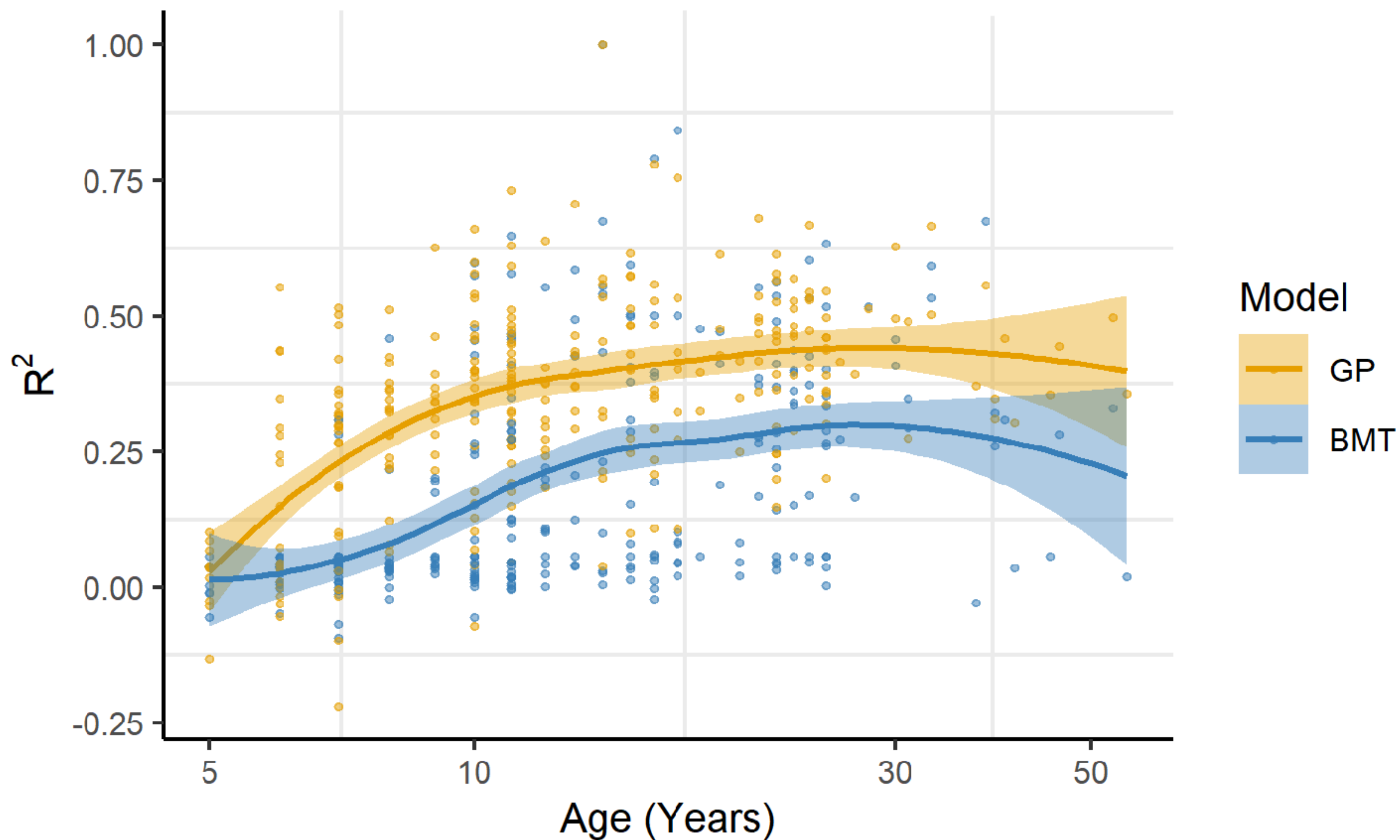
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- Younger children are also less responsive in adapting search distance to reward outcomes
 - Over the lifespan, this develops into a linear relationship, resembling a gradual form of win-stay lose-shift



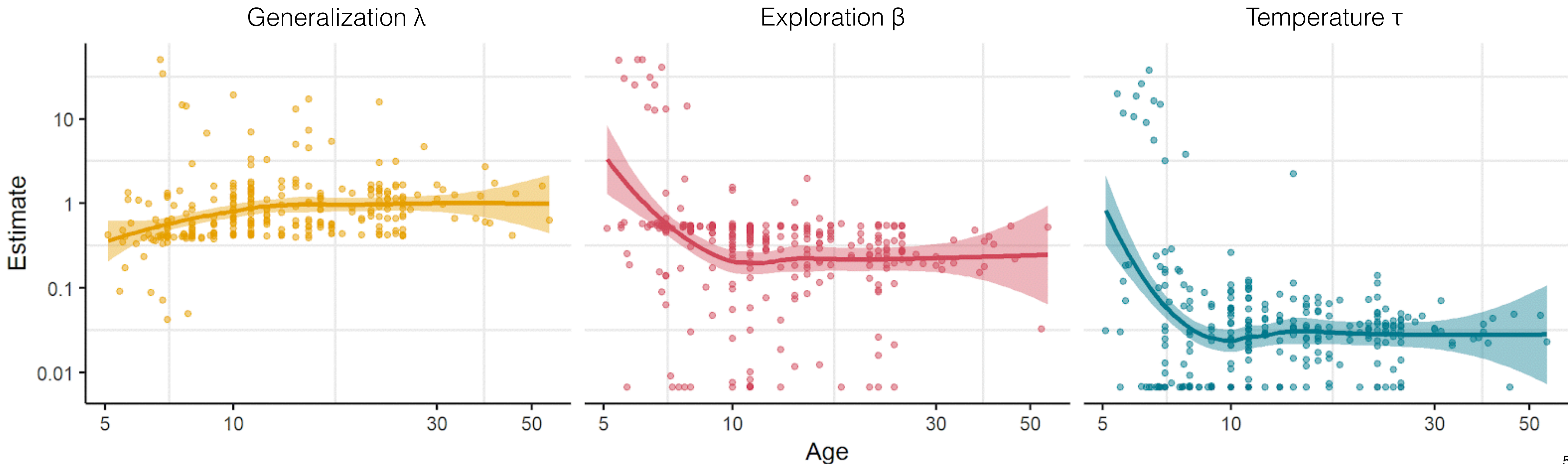
Model results

$$R^2 = 1 - \frac{\log \mathcal{L}(\mathcal{M}_k)}{\log \mathcal{L}(\mathcal{M}_{\text{rand}})}$$

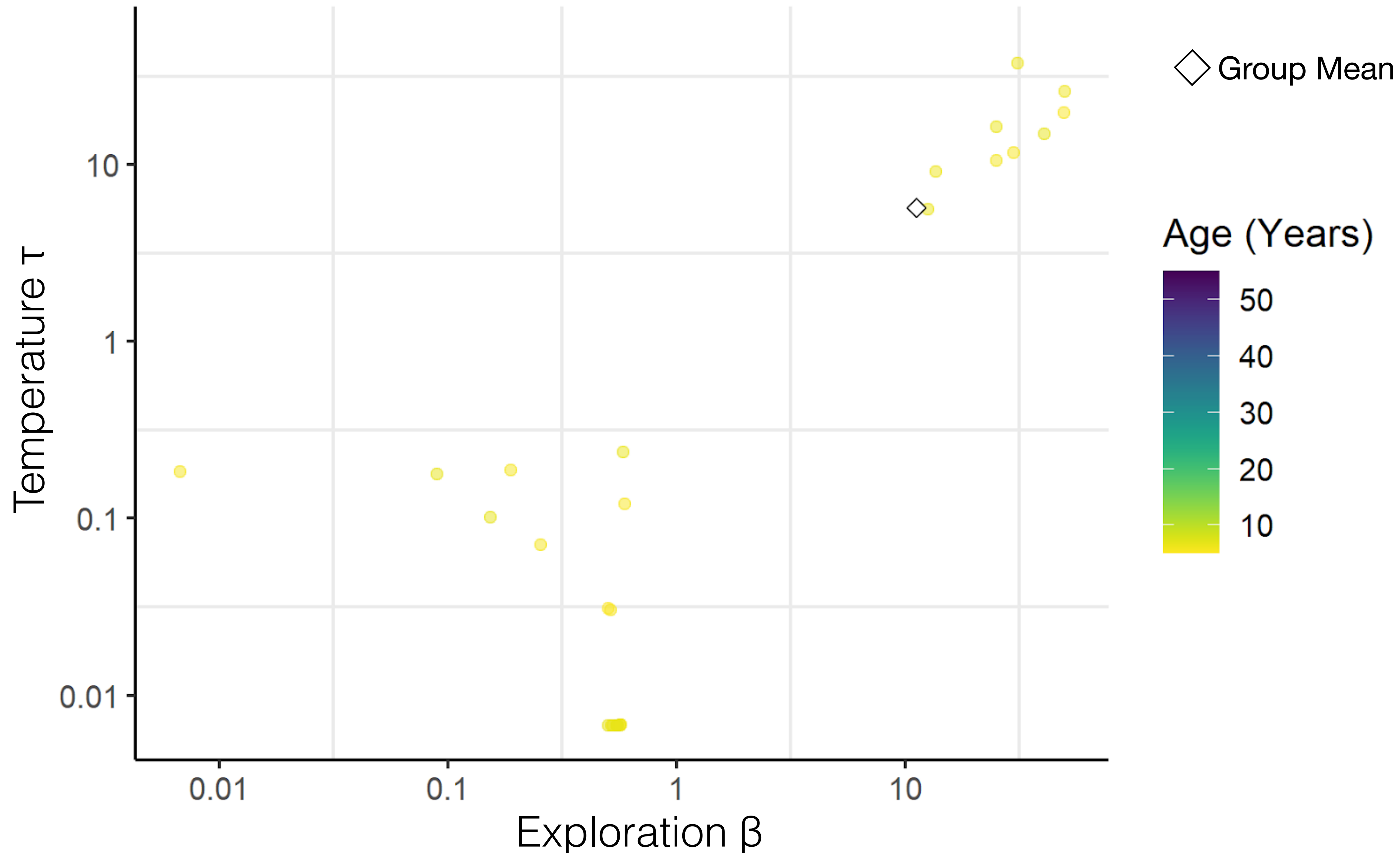


Parameter estimates

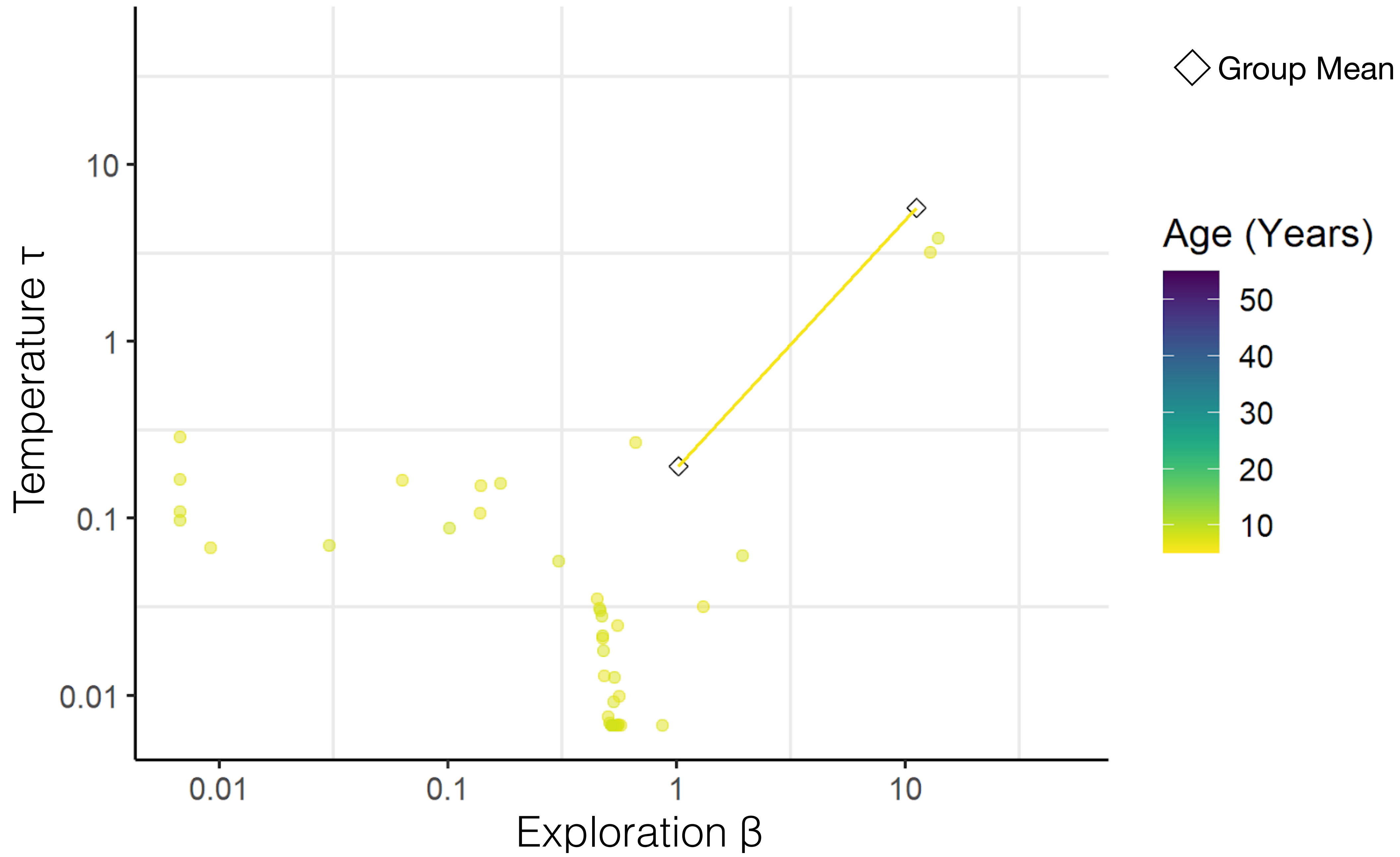
- Small uptick in generalization λ
- Large decrease in both uncertainty-directed exploration β and temperature τ



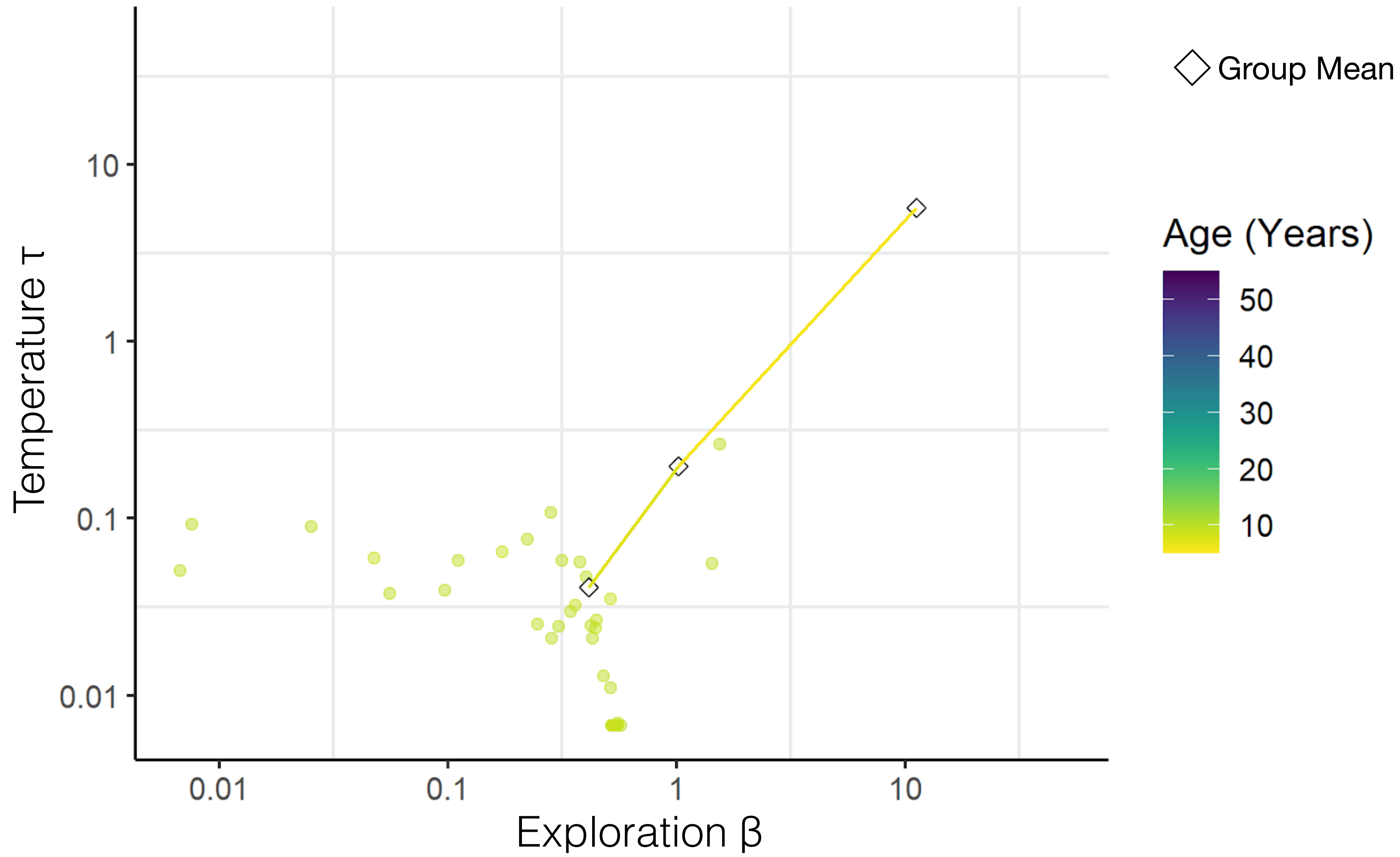
Age Group [5,7)



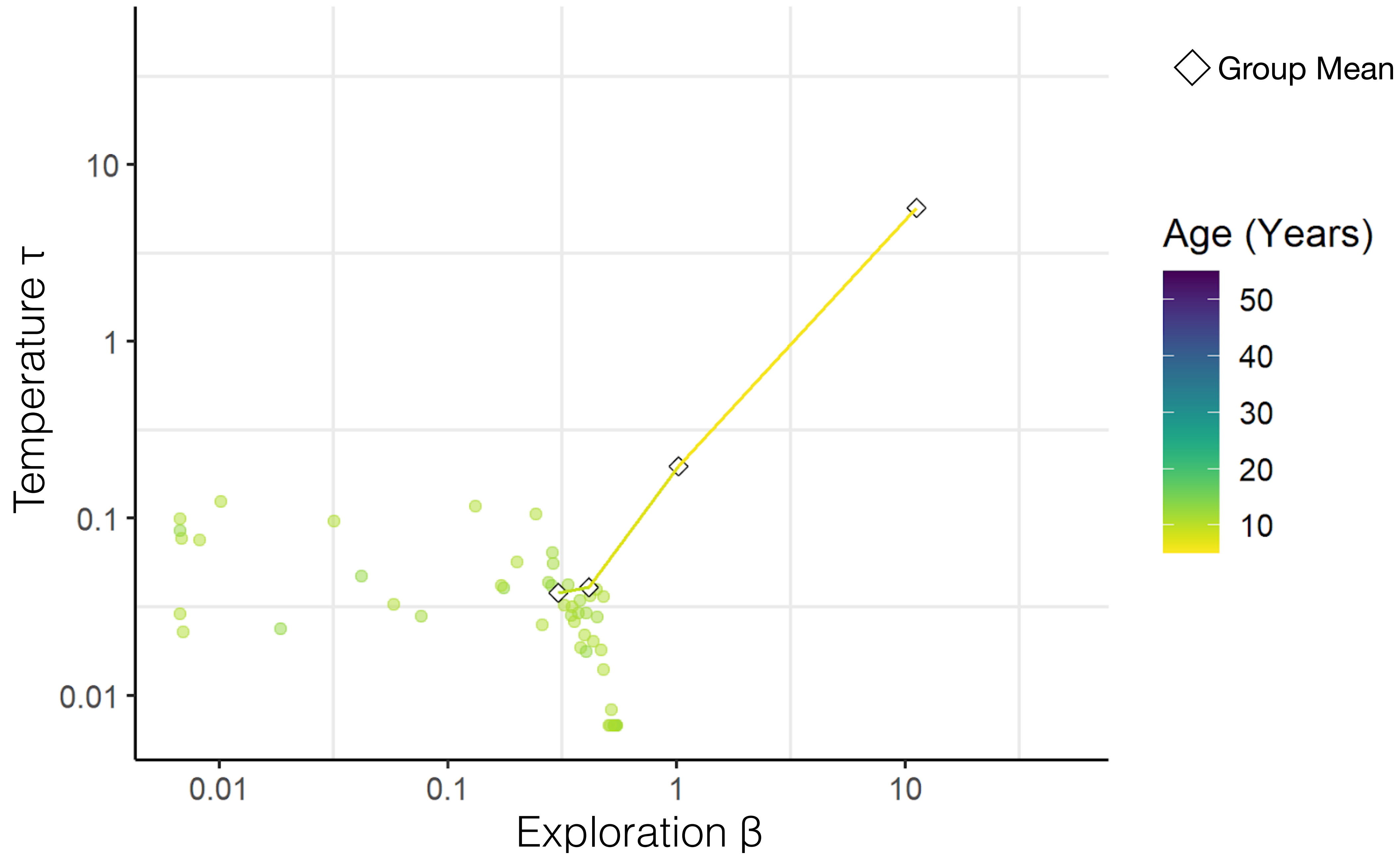
Age Group [7,9)



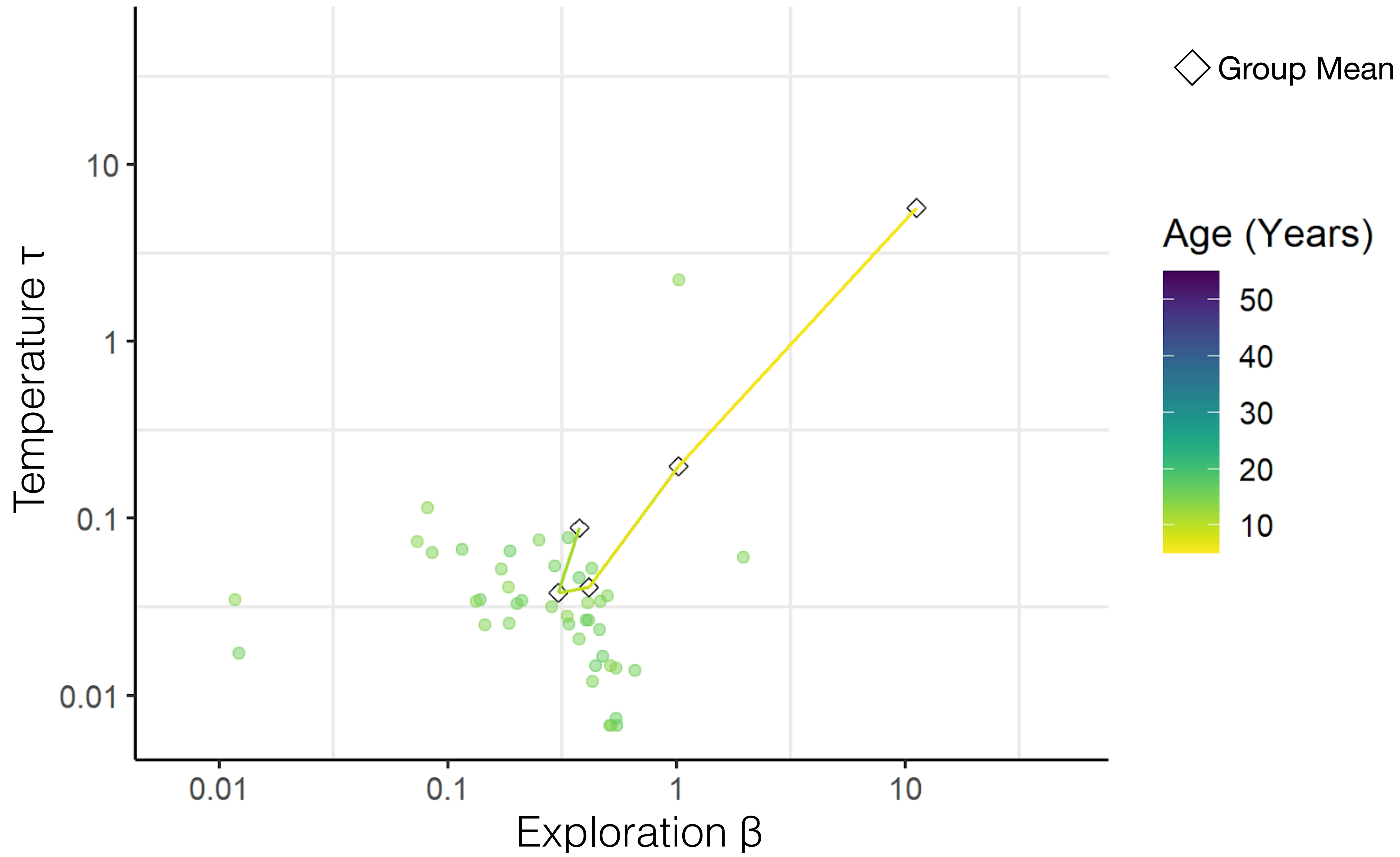
Age Group [9,11)



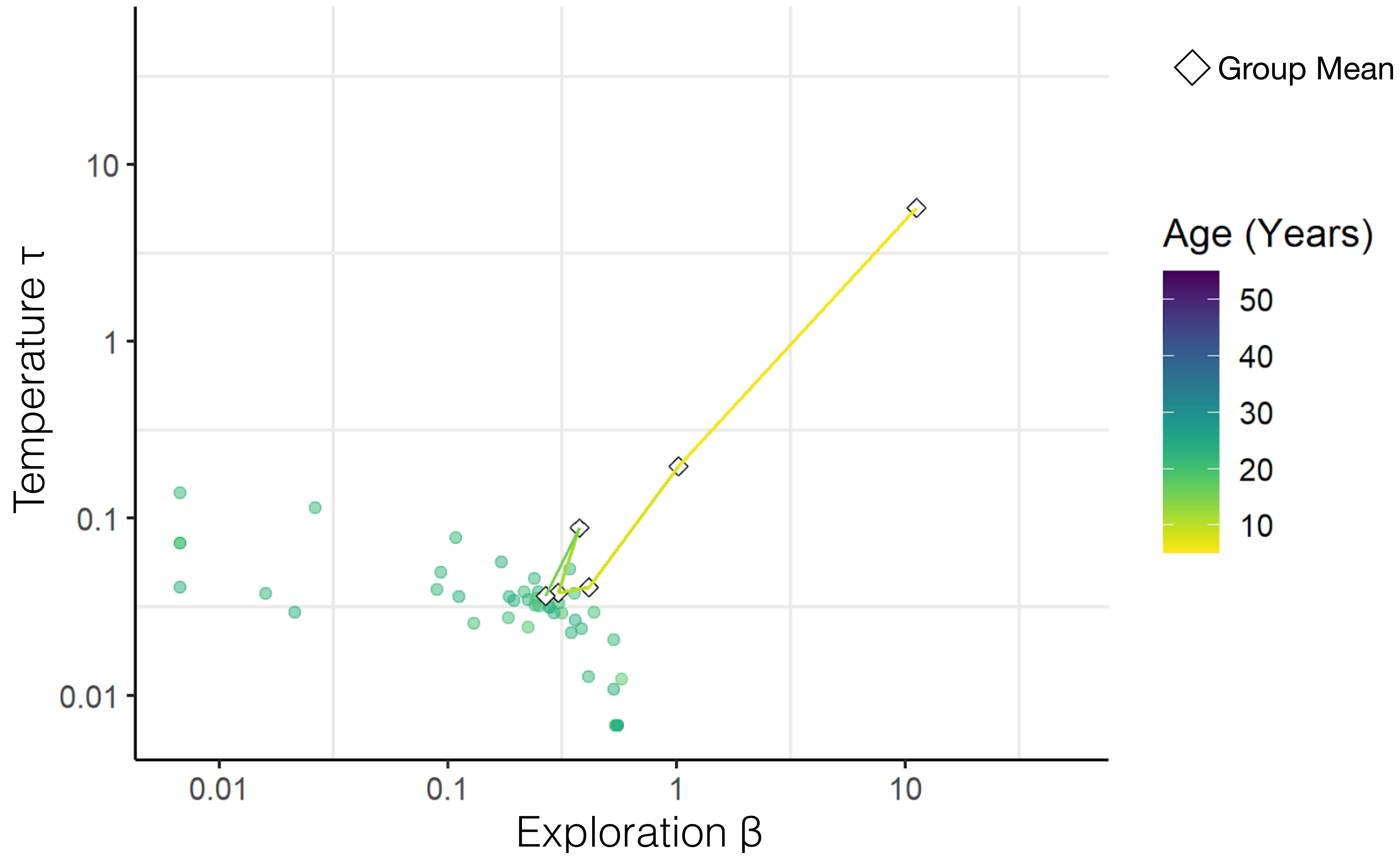
Age Group [11,14)



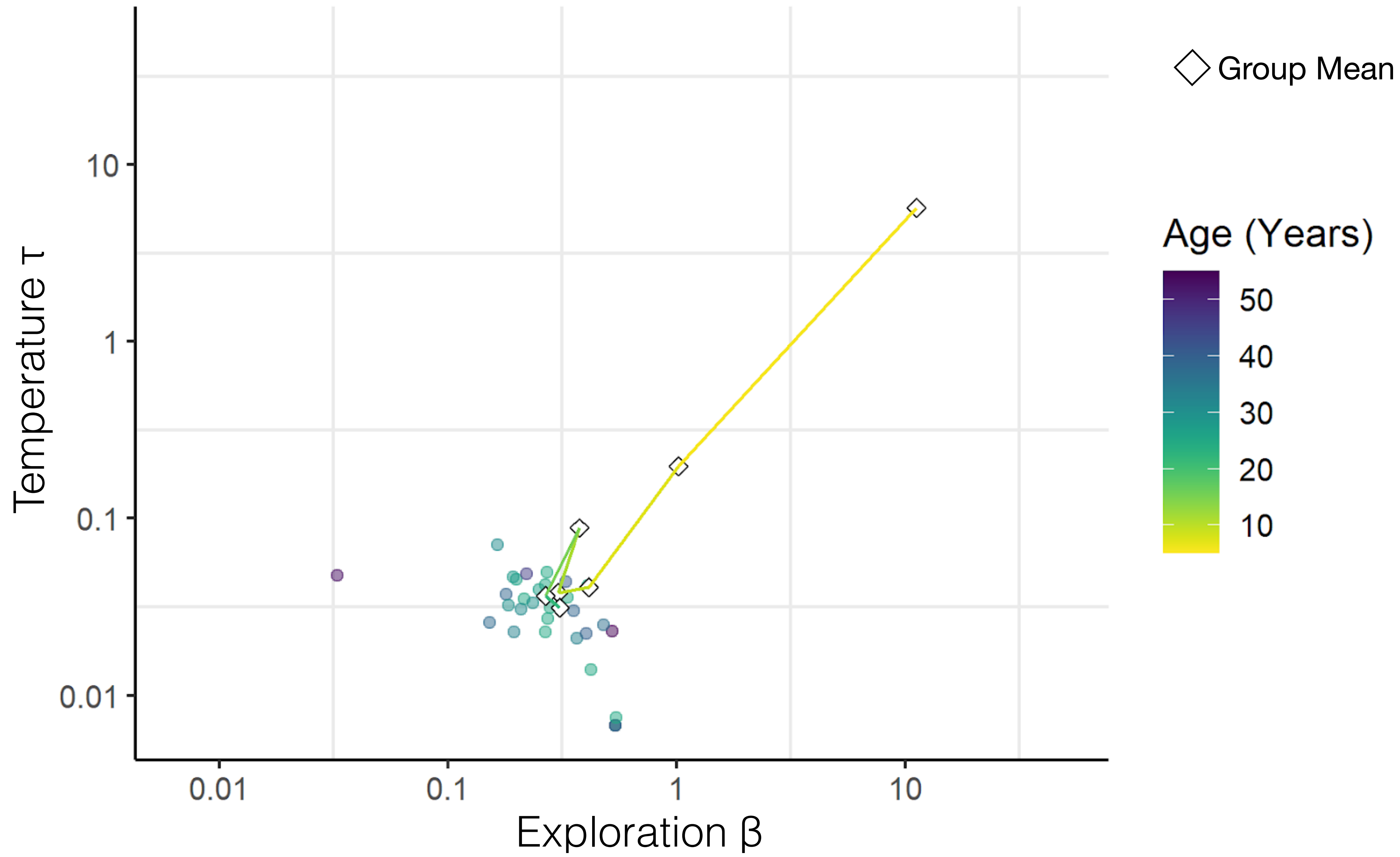
Age Group [14,18)



Age Group [18,25)



Age Group [25,55]

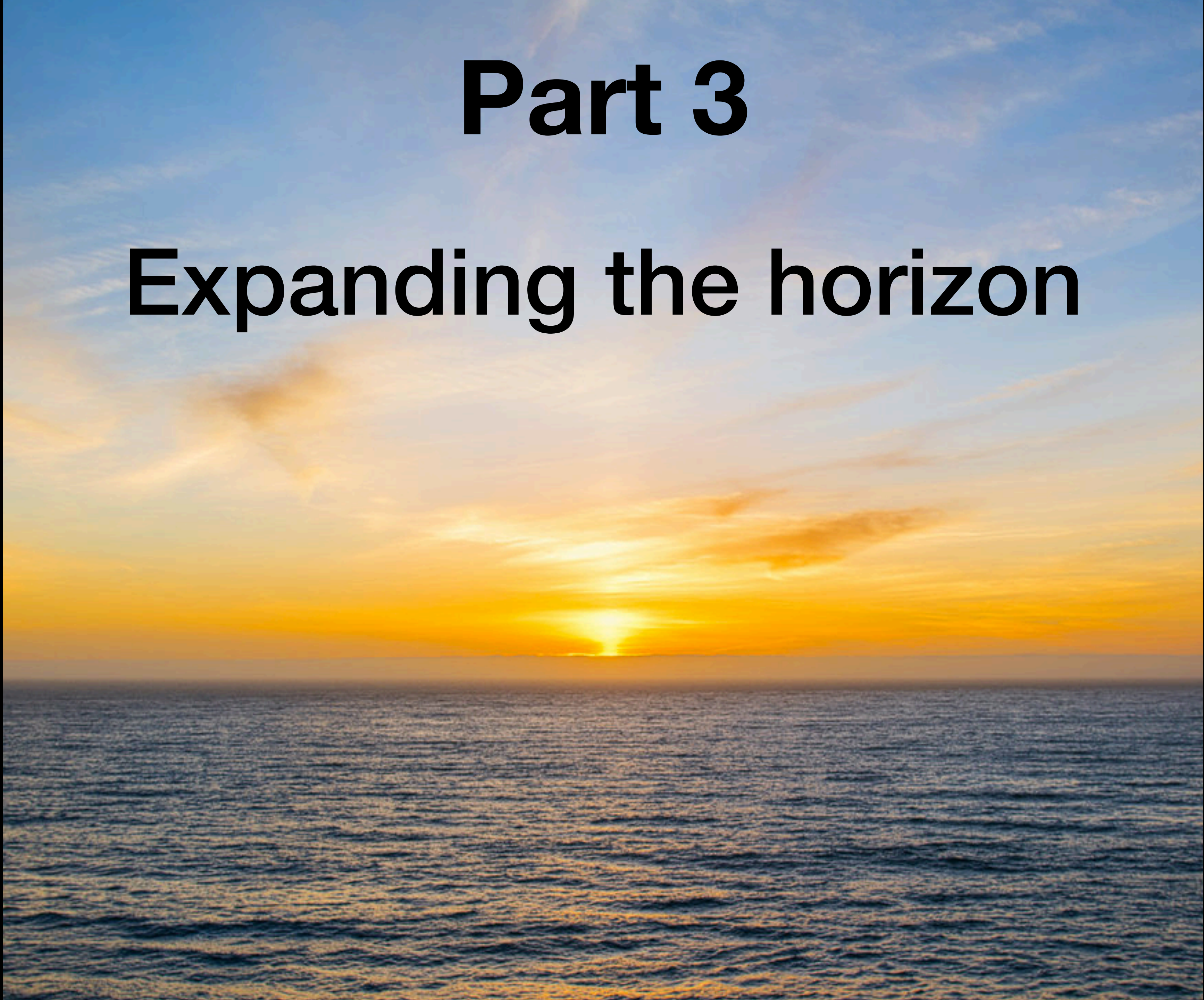


Summary and Future Directions

- The strategic use of uncertainty-directed exploration and predictive generalization comes online already at a very young age (5-7 year olds)
 - Simultaneous reduction in both directed and random exploration in early childhood
 - Children are not just more random, but also hungrier for information
- While there is an uptick in random exploration during adolescence, this is relatively minor compared to changes in childhood
 - Consistent with theories that increased exploration in adolescence is largely driven by social rather than cognitive factors
- Future work can use model simulations to examine which is the best normative developmental trajectory through model space

Part 3

Expanding the horizon



Part 3

Expanding the horizon

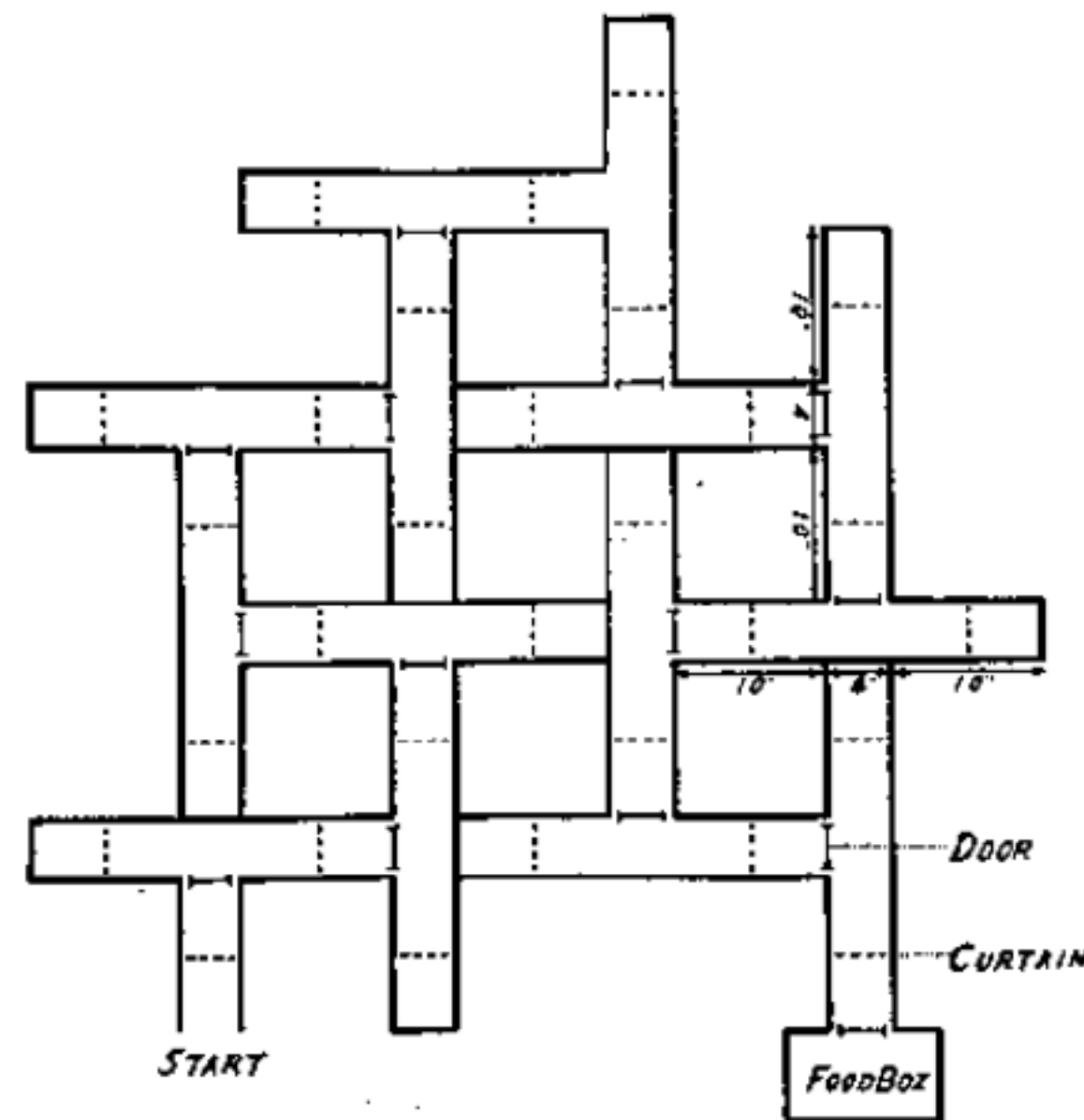
**Generalization in Conceptual and
Structured domains**

Cognitive Maps for Navigation

Cognitive Maps



Tolman (Psych Rev, 1948)



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.)

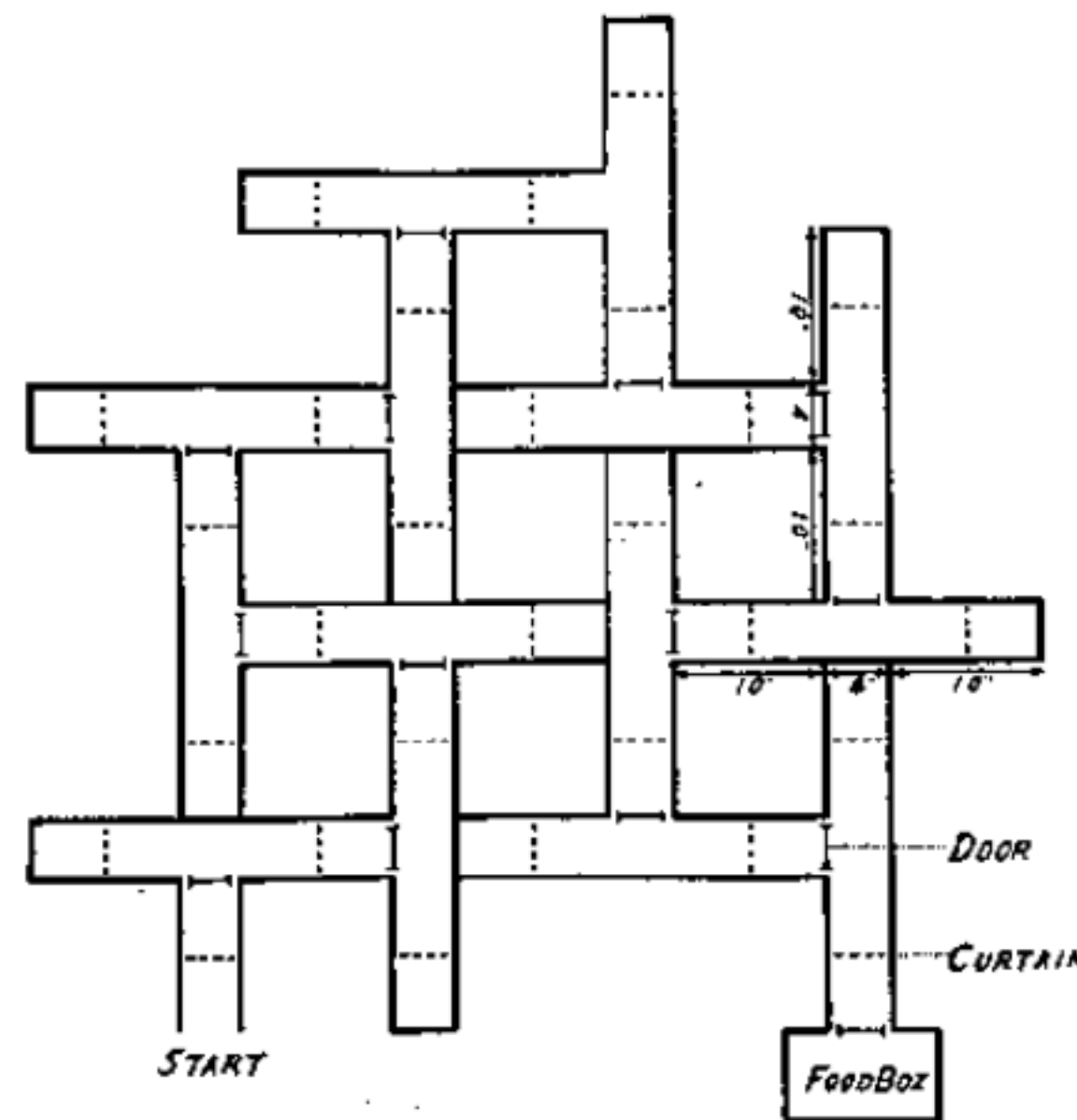
... “in the course of learning something like a field map of the environment gets established in the rat's brain”

Cognitive Maps for Navigation

Cognitive Maps



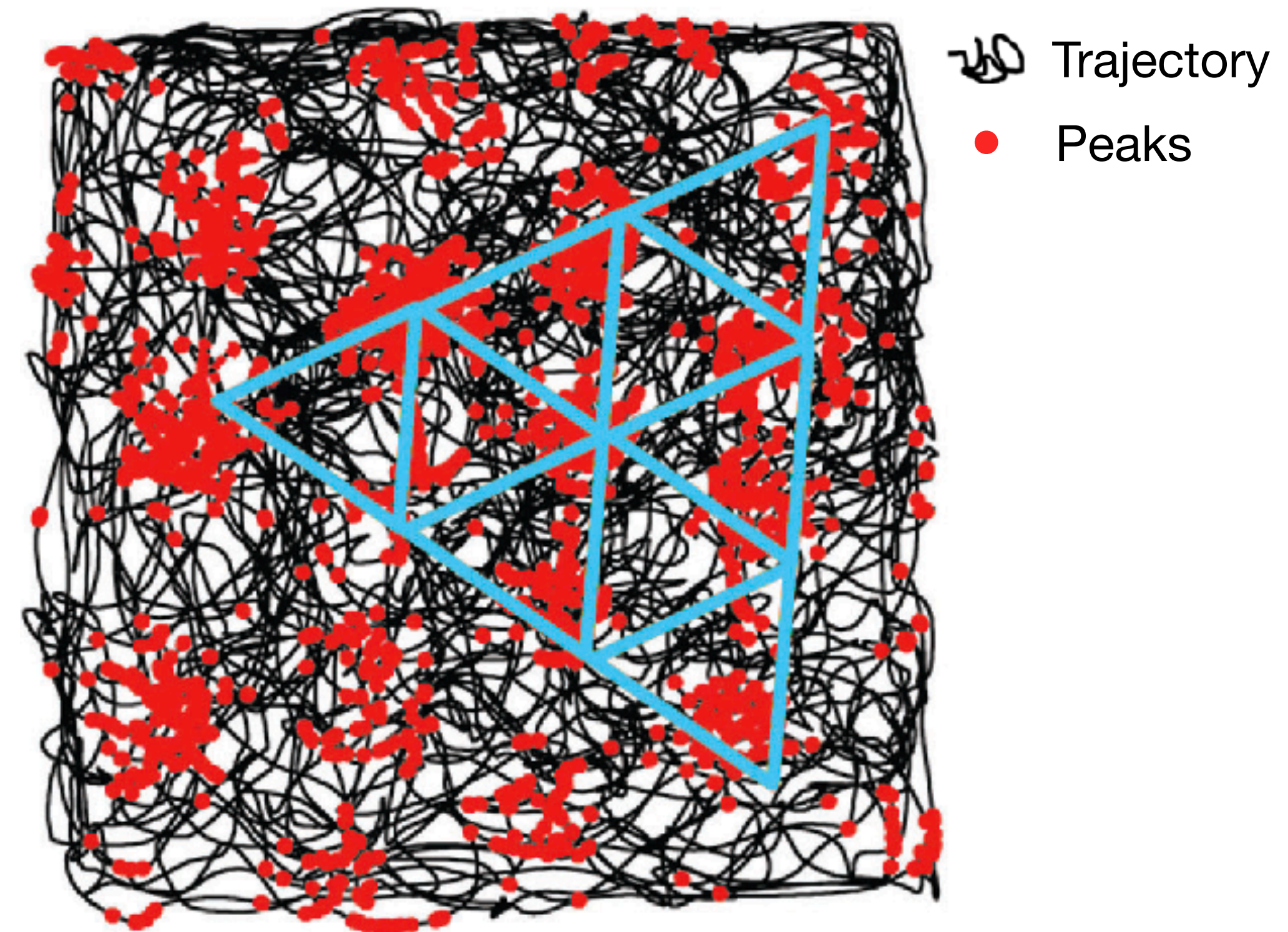
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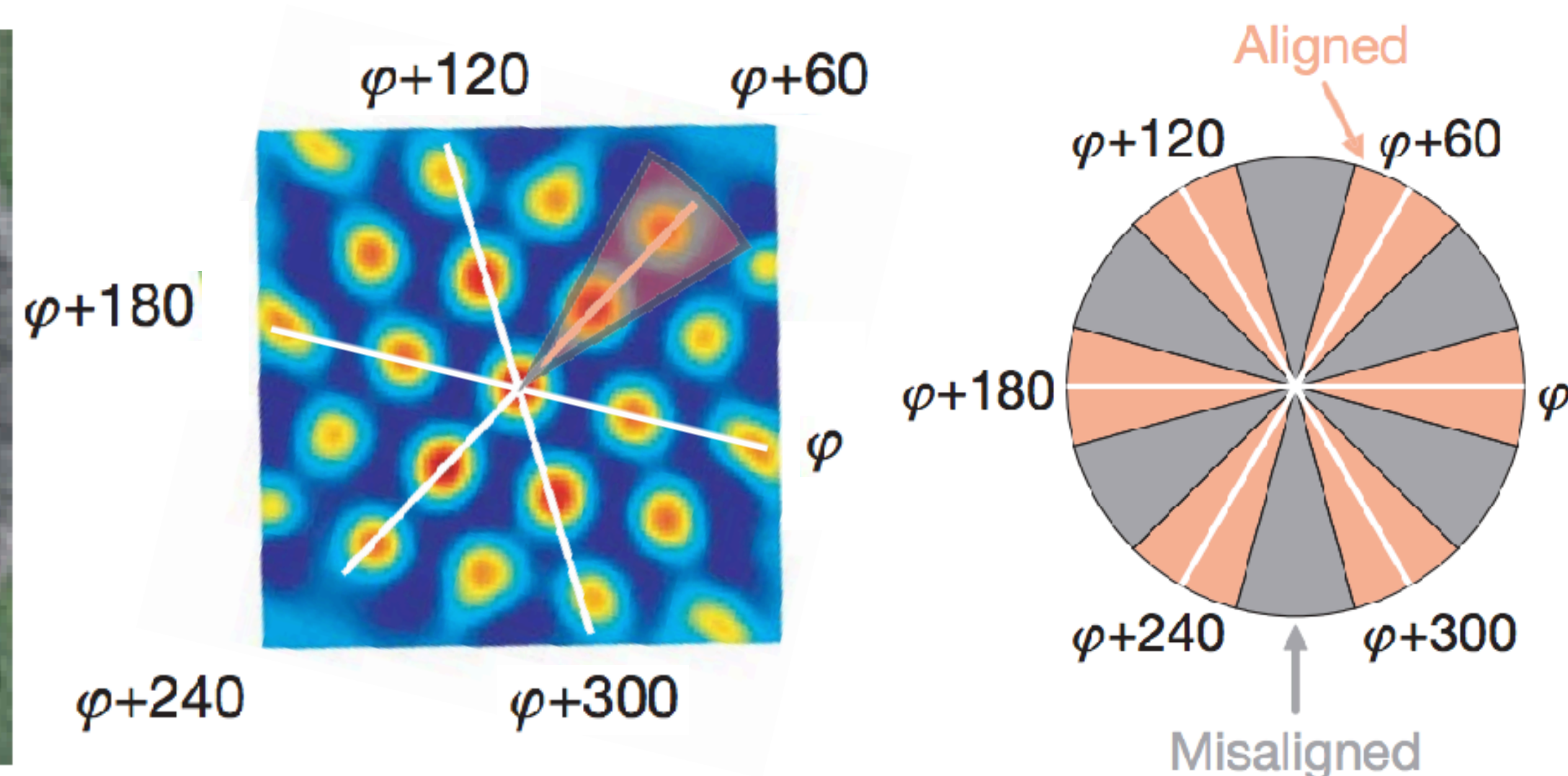
Grid Cells



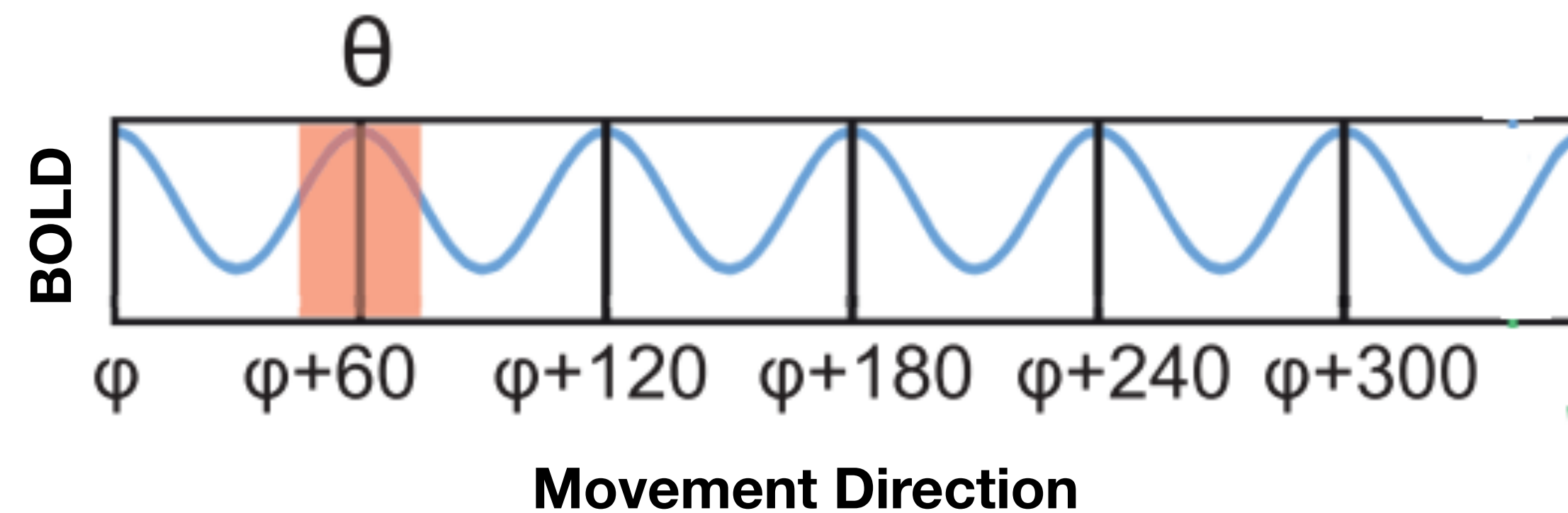
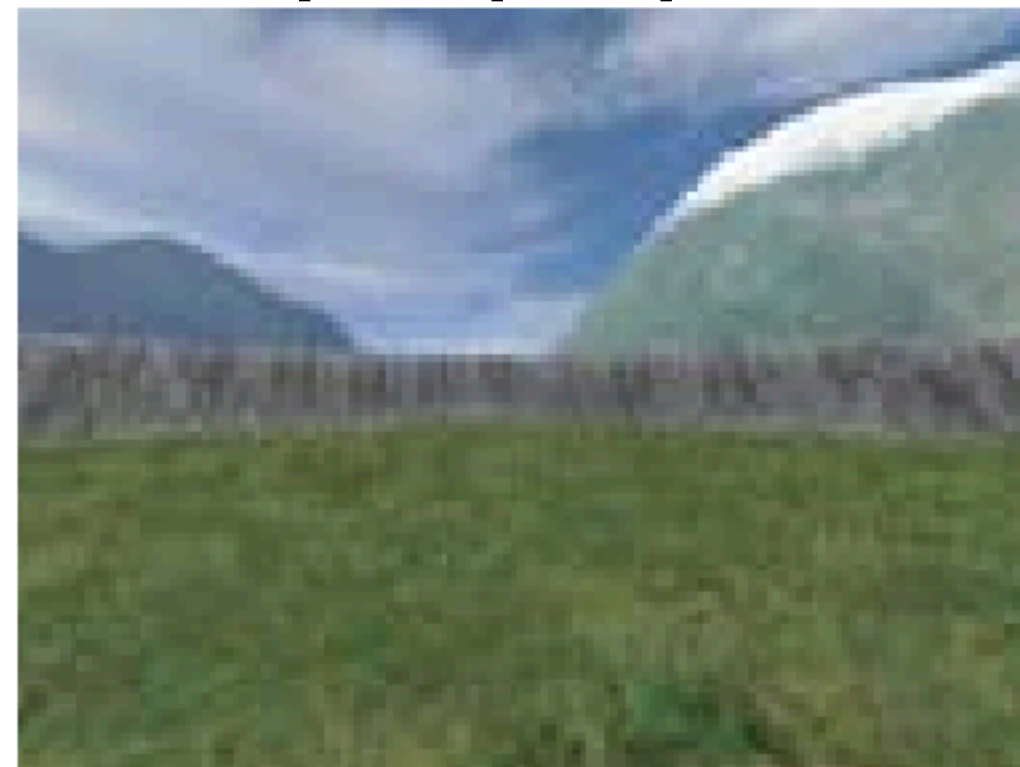
Hafting et al., (2005)
Moser, Rowland, & Moser (2015)

We can measure trajectories in human navigation

Spatial trajectory (Birds eye)

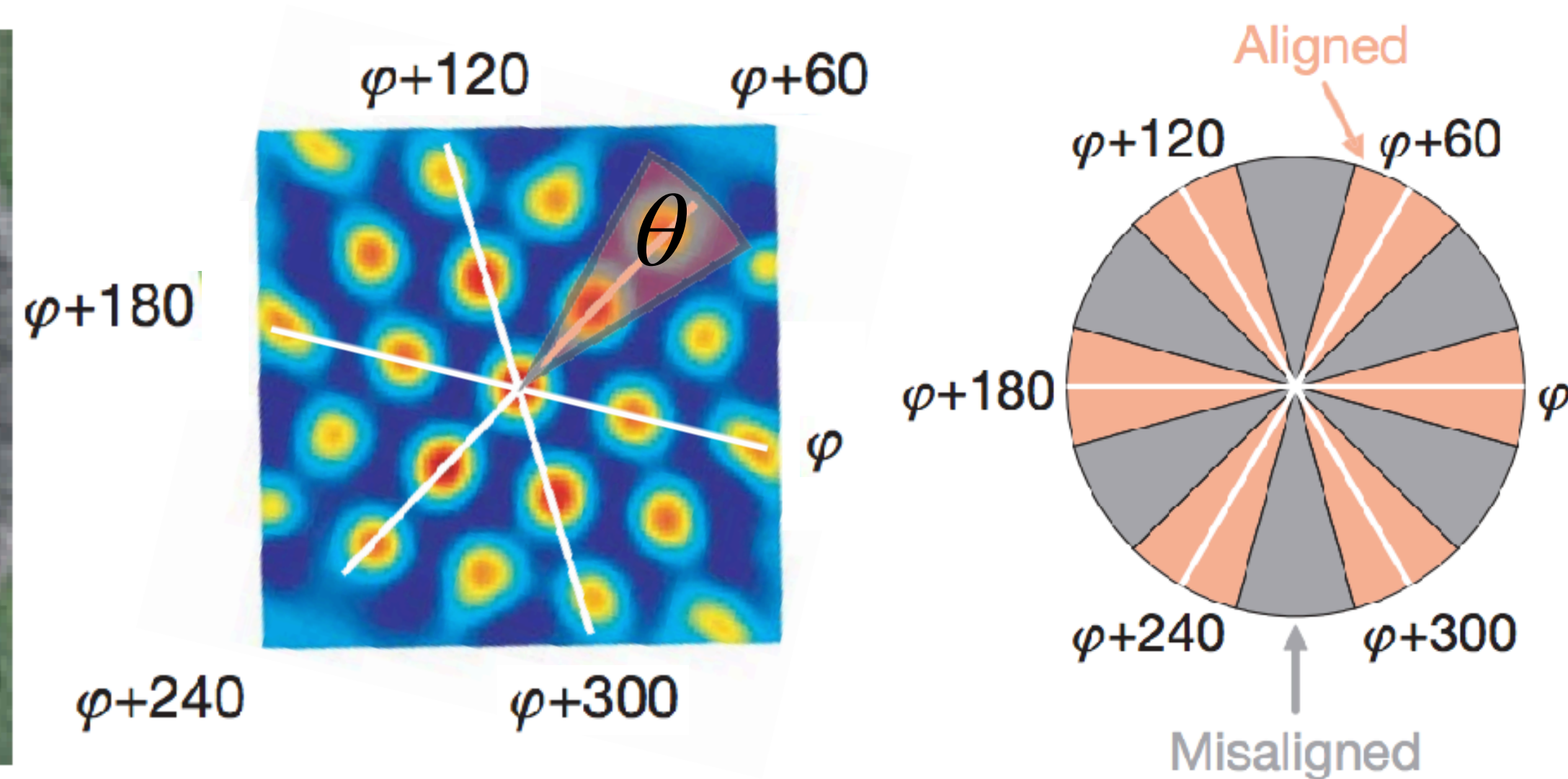


Participant perspective

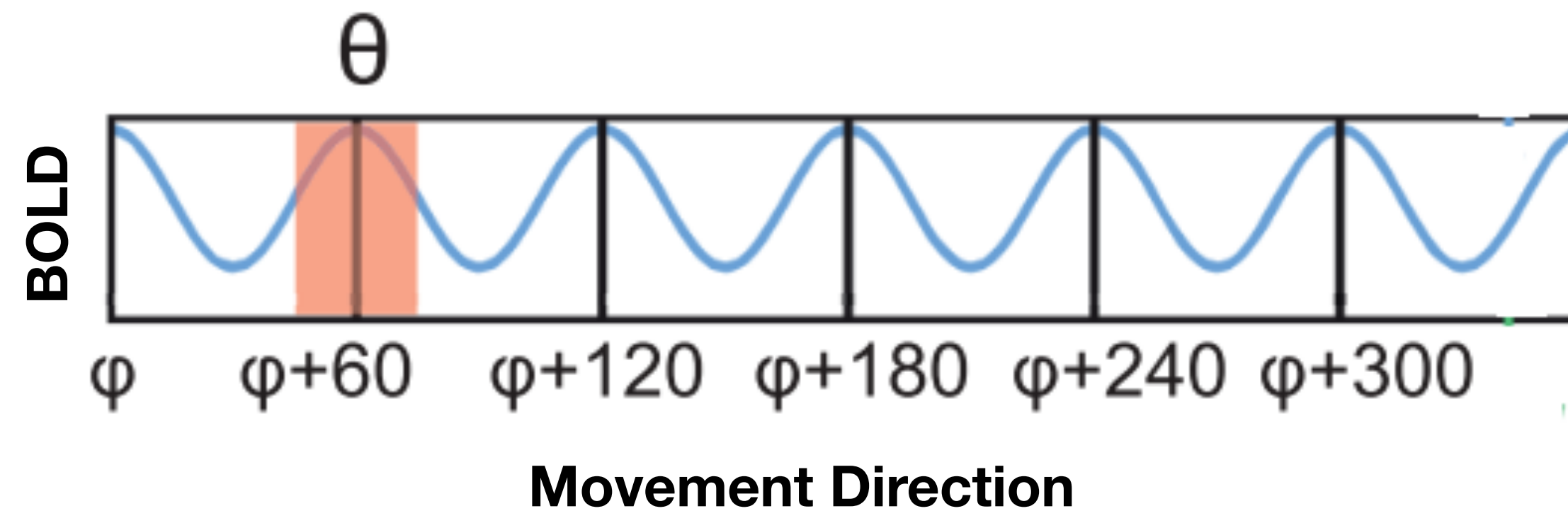


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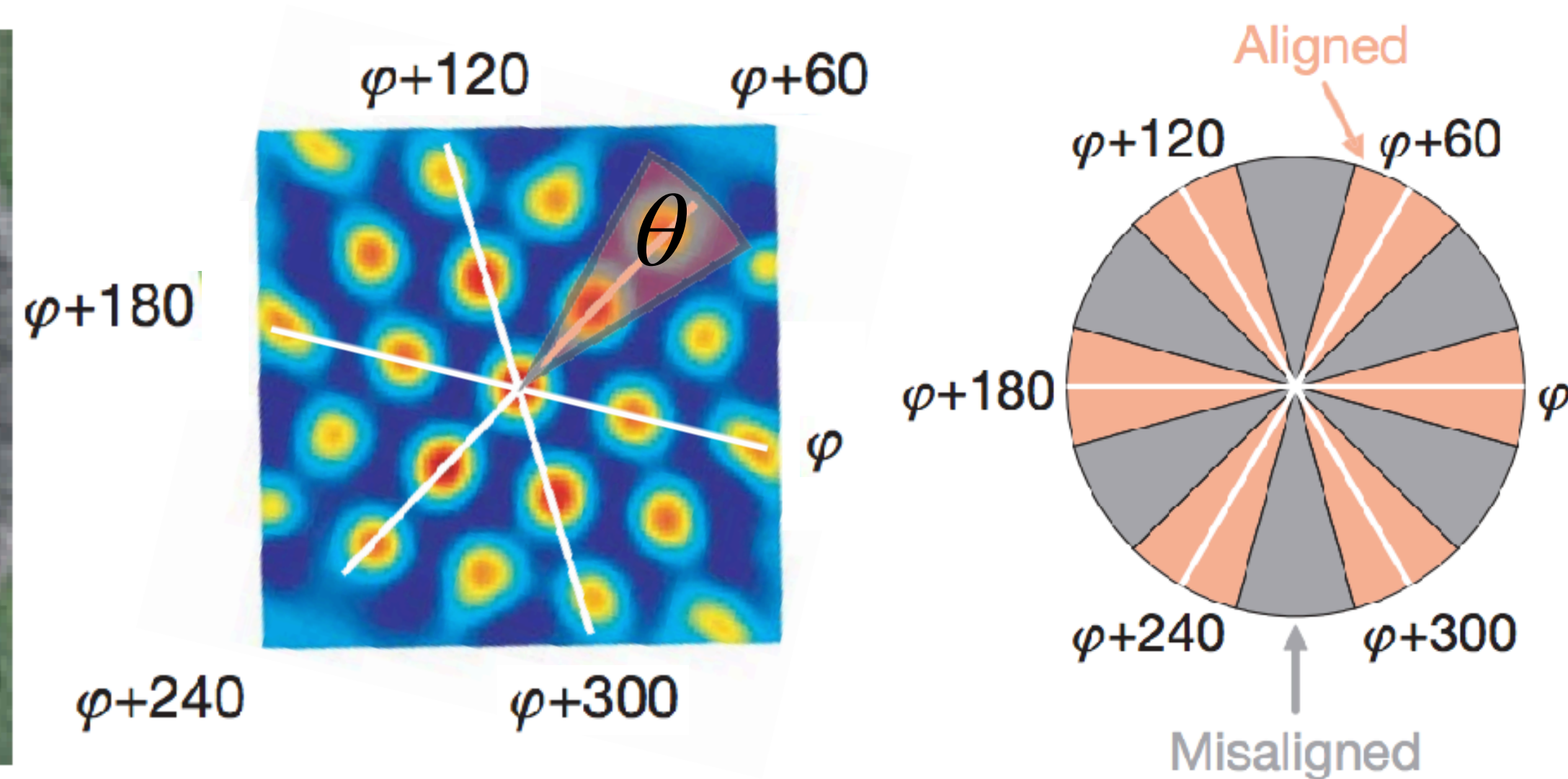
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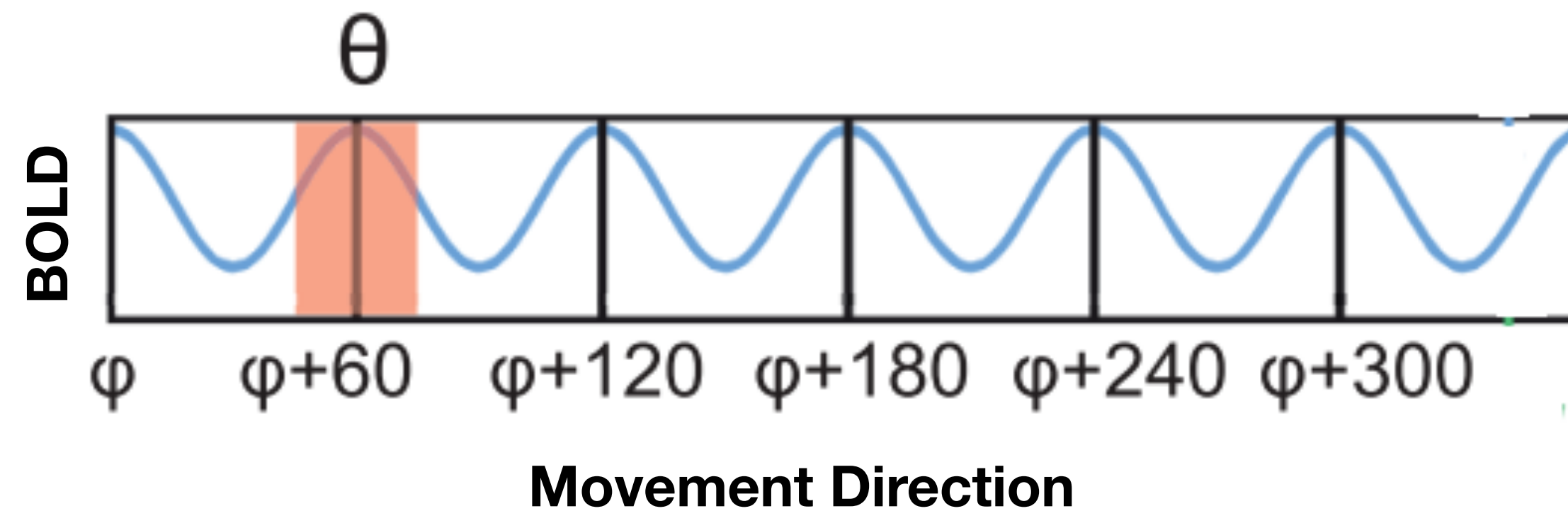
Doeller, Barry, & Burgess (*Nature*, 2010)

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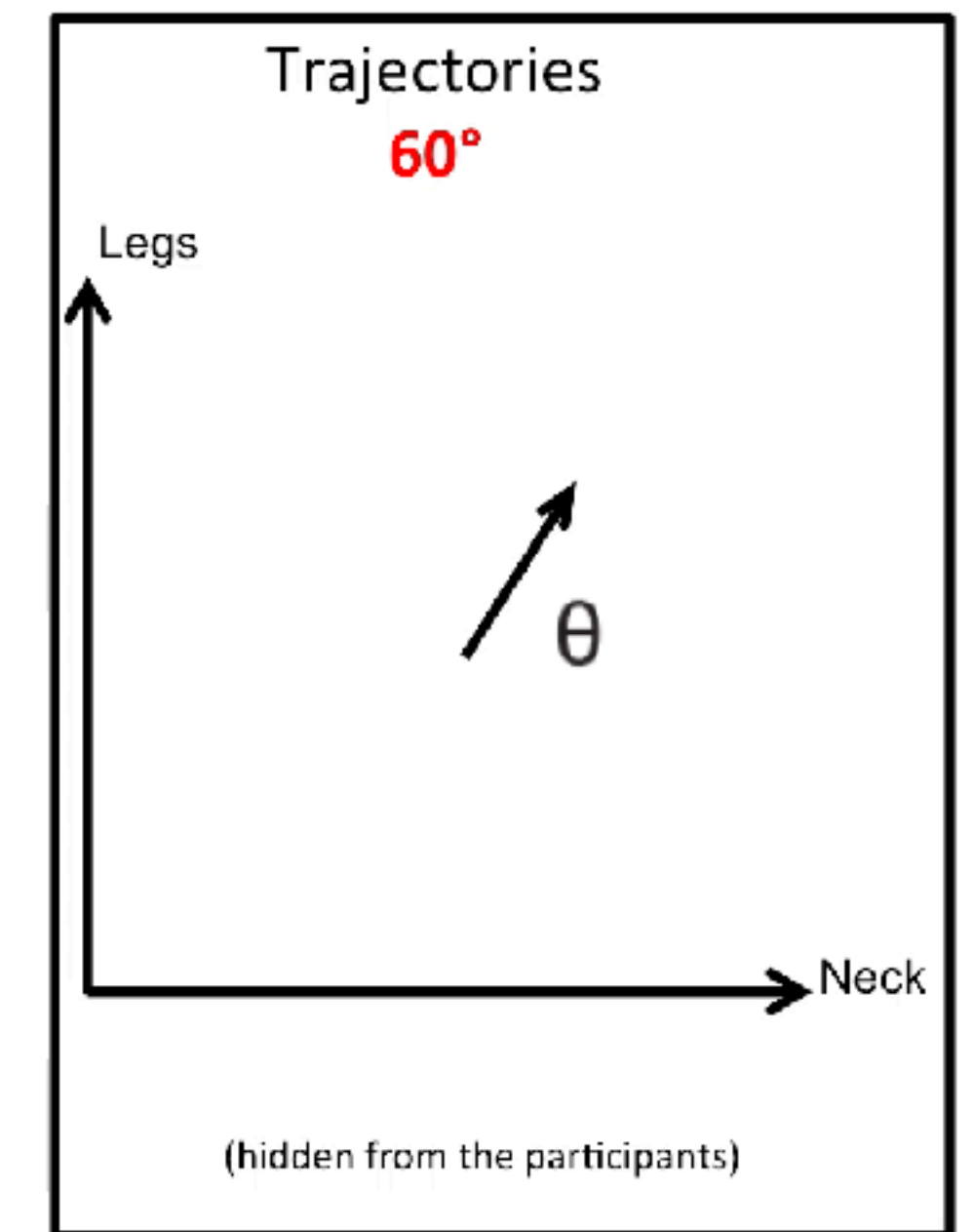
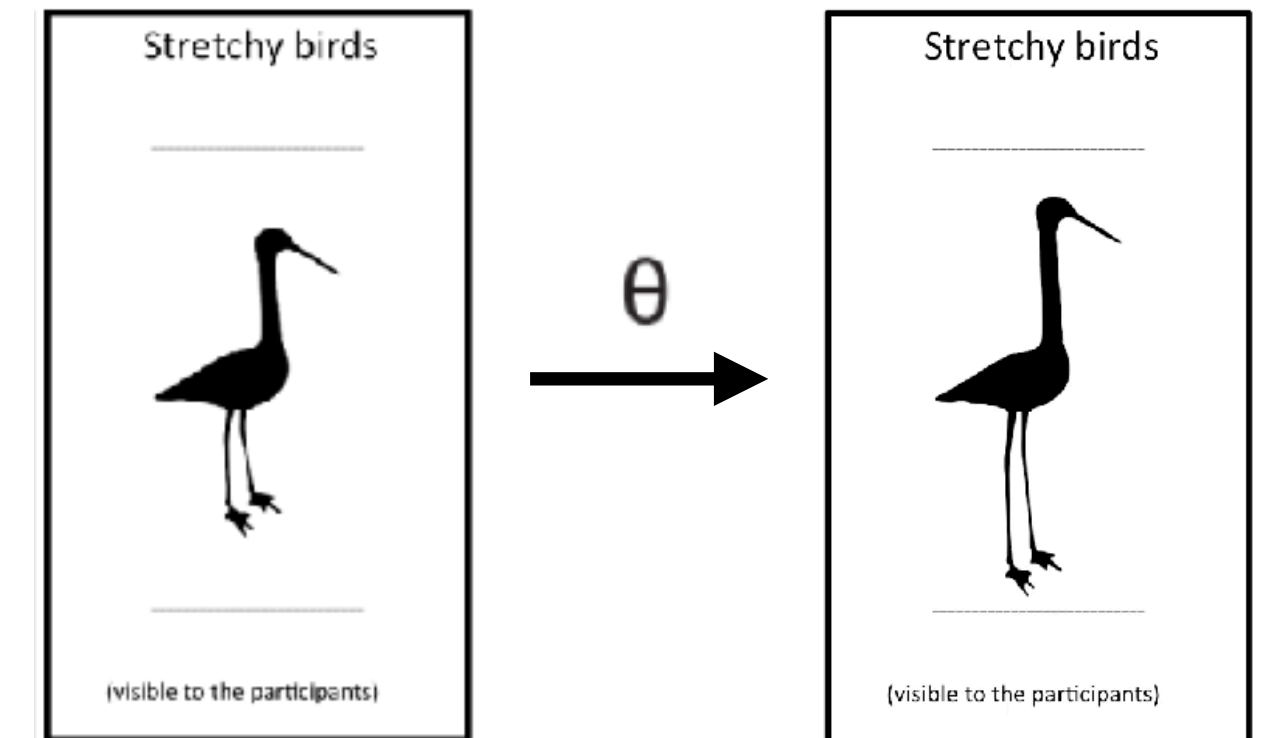
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Participant perspective



Also in non-spatial domains!



Spatial Rewards Influence Semantic Foraging

- Search in external and internal spaces follow similar principles of optimal foraging

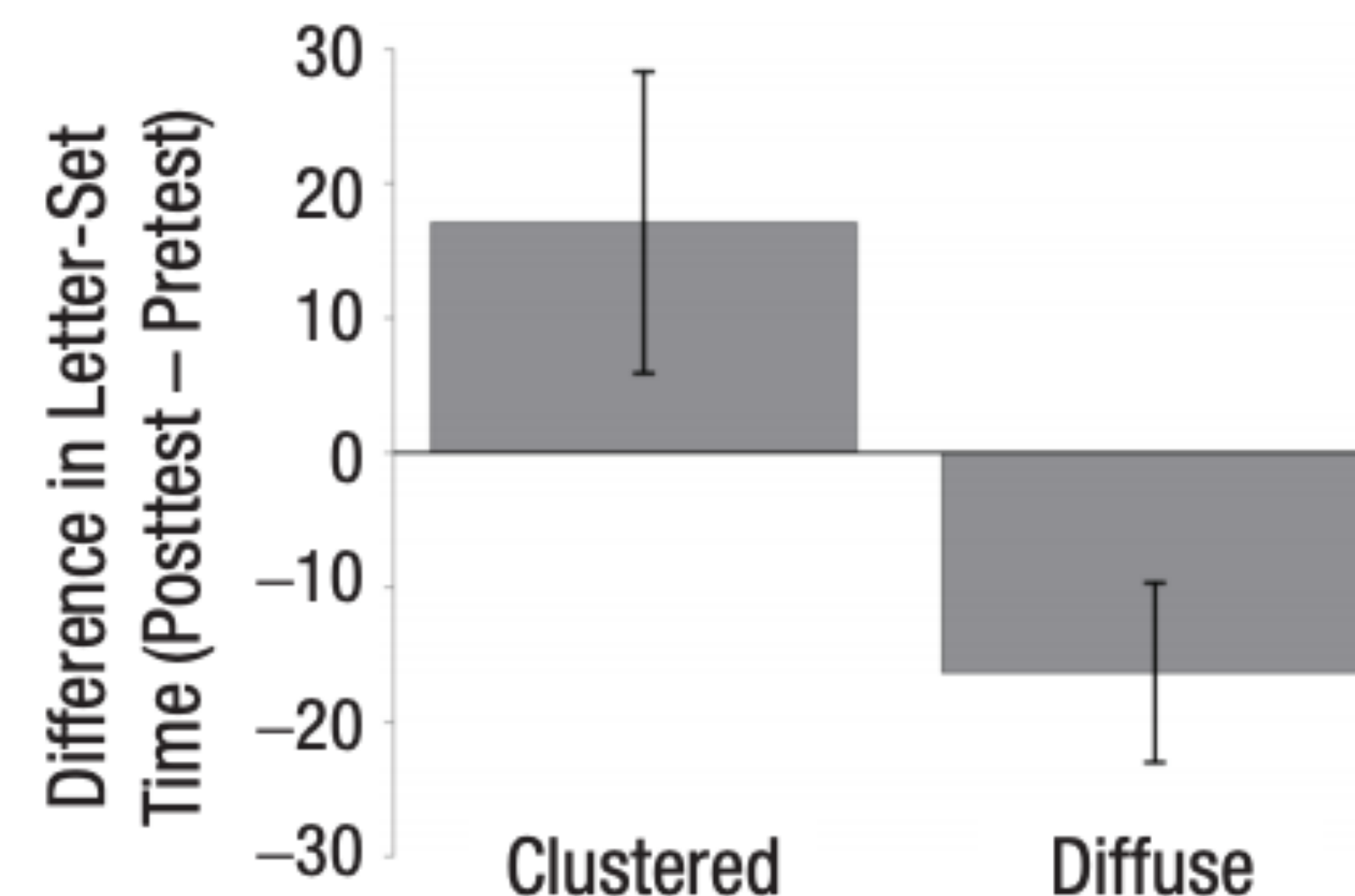
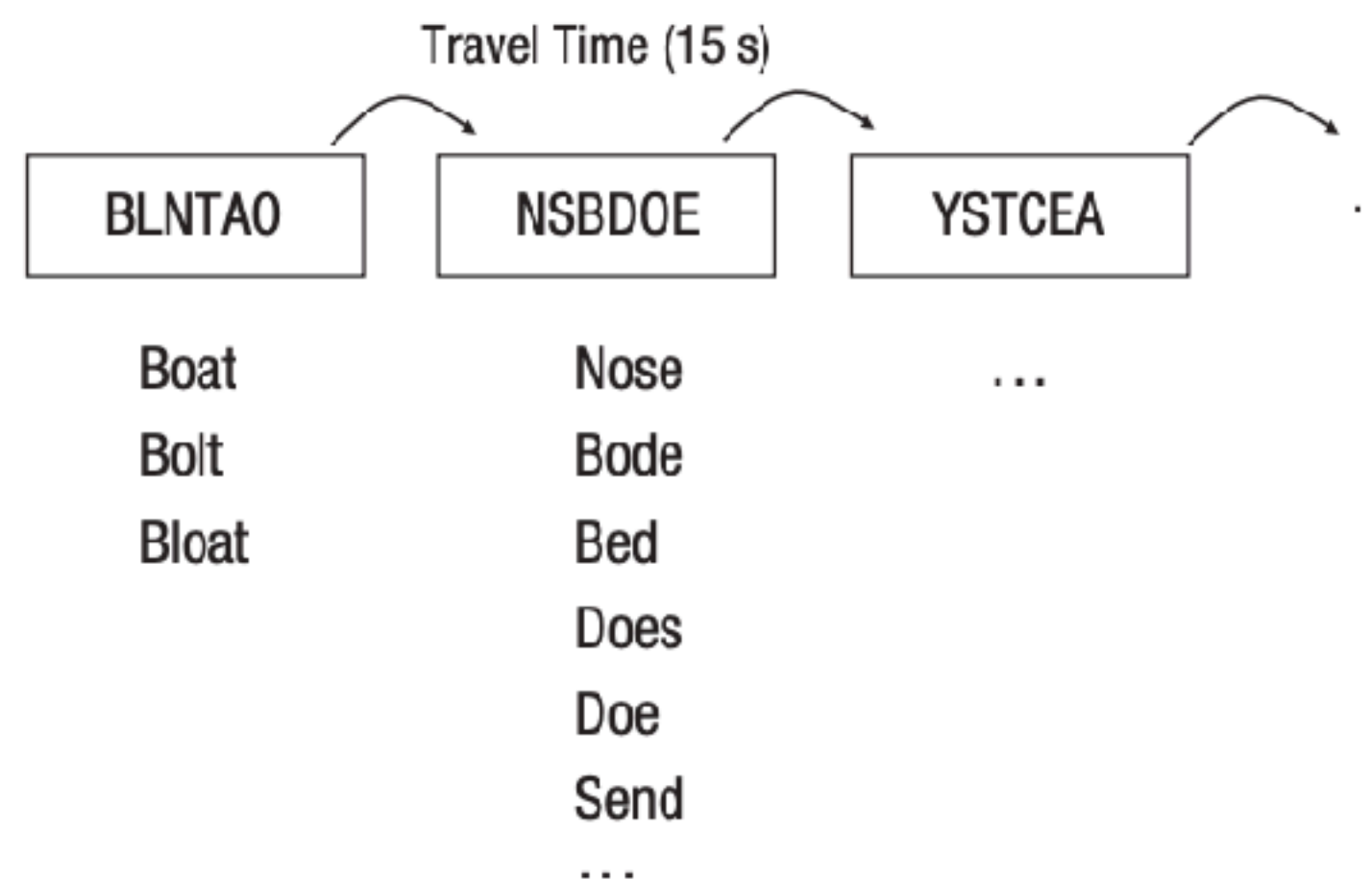
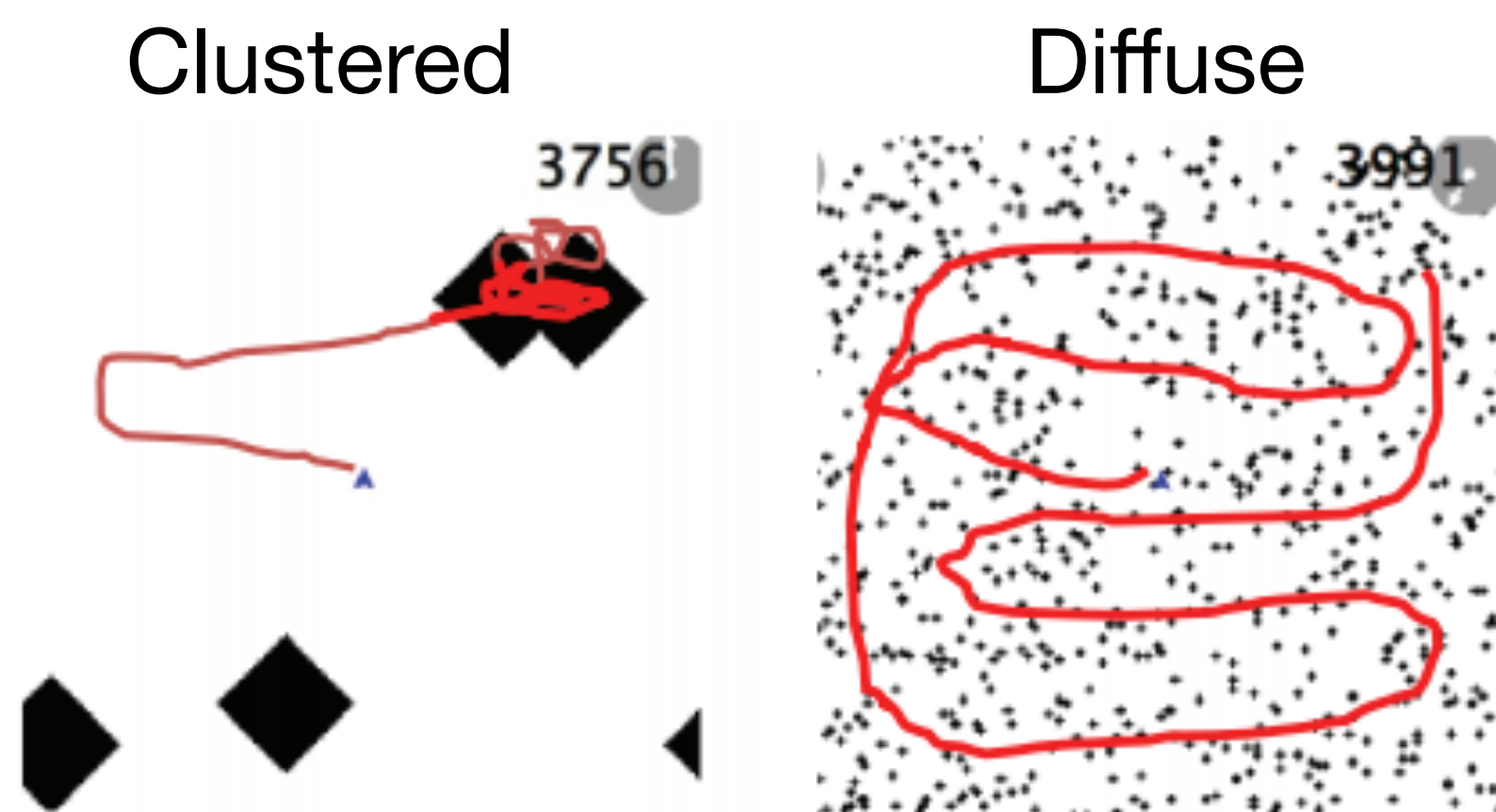
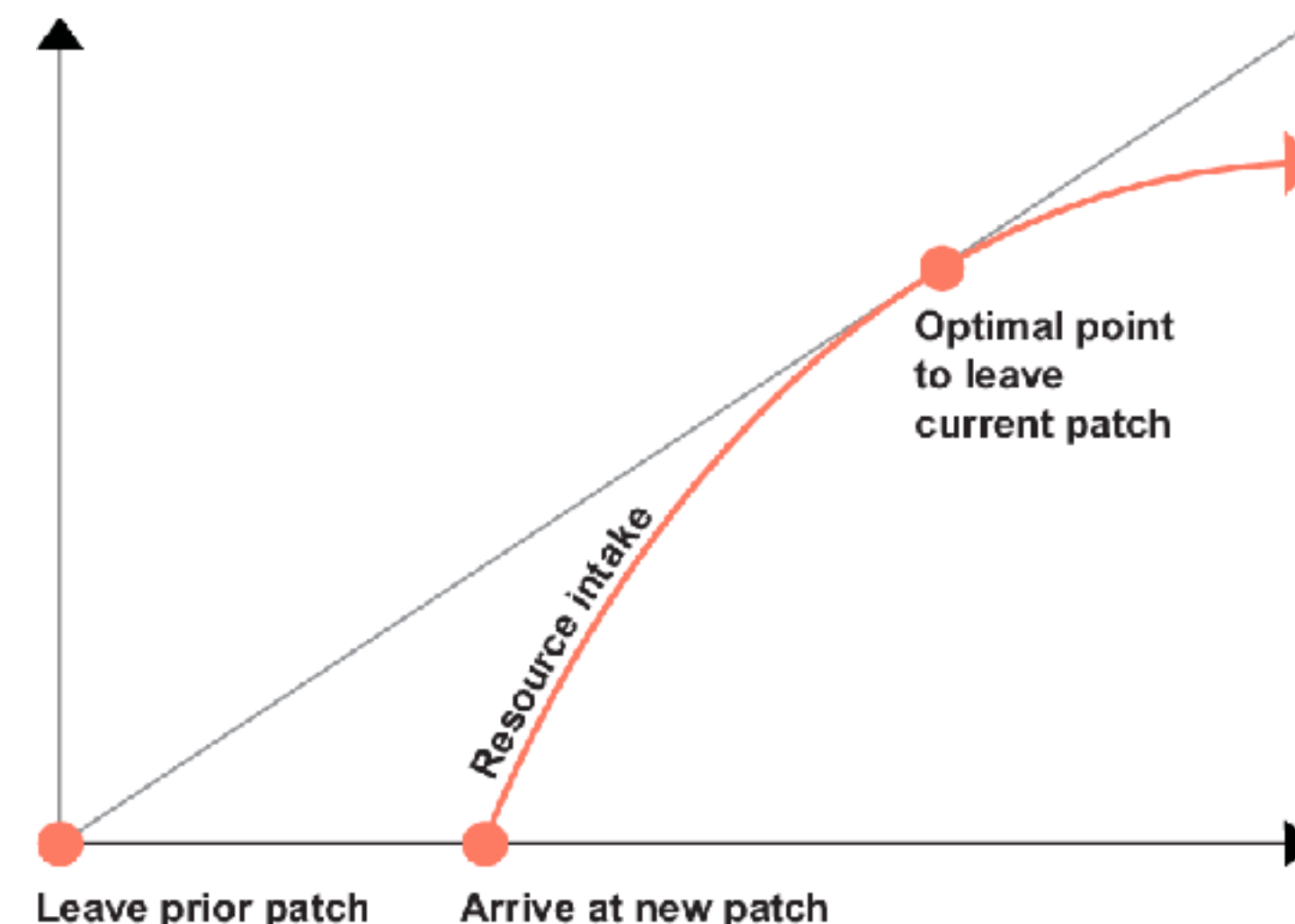
Charnov (1976); Pirolli & Card (1999)

- The distribution of resources in a spatial foraging task can influence semantic search patterns in a word generation task

Hills, Todd, & Goldstone (2008)

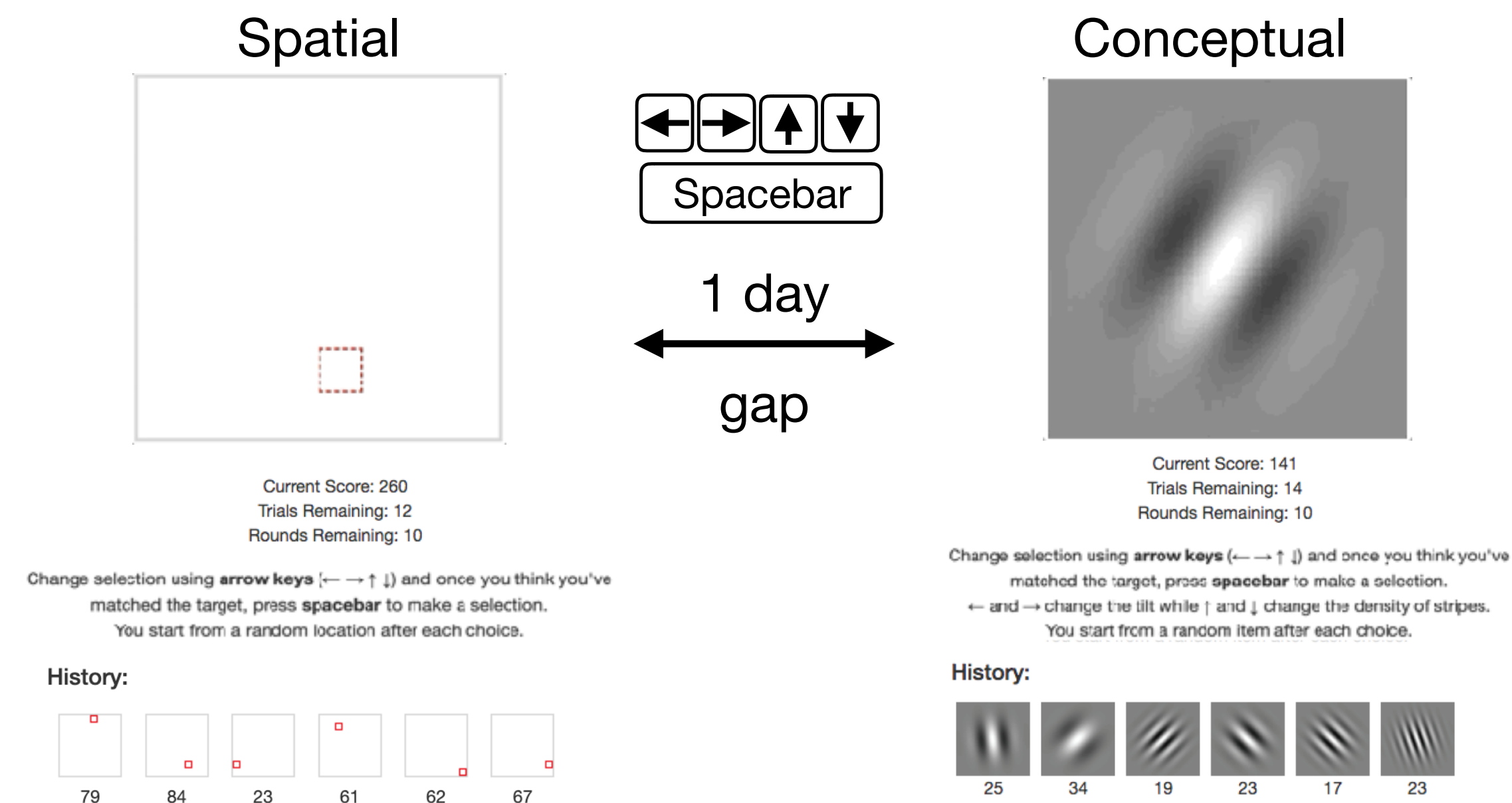
- “Exaptation” of spatial cognition to other domains

Hills (2006); Hills, Todd, & Goldstone (2008)



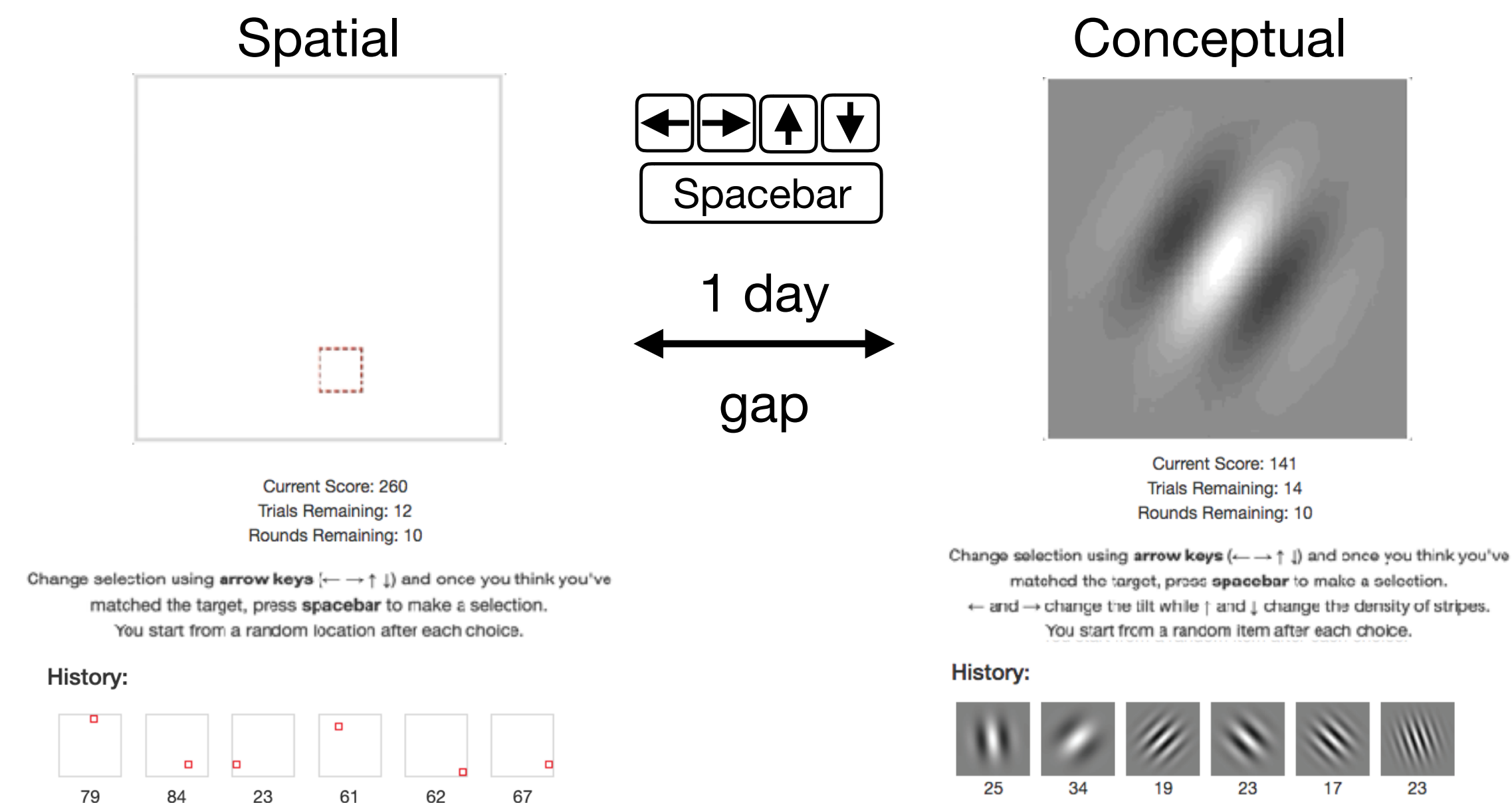
Connecting Spatial and Conceptual Search

- Since there is evidence for a common neural representation for both spatial and conceptual navigation, what are the downstream implications for behavior?
- Are there domain general principles for generalization (about novel stimuli) and exploration (in new environments)?
- Within-subject experiment, where participants used either spatial or conceptual features to guide the search for rewards



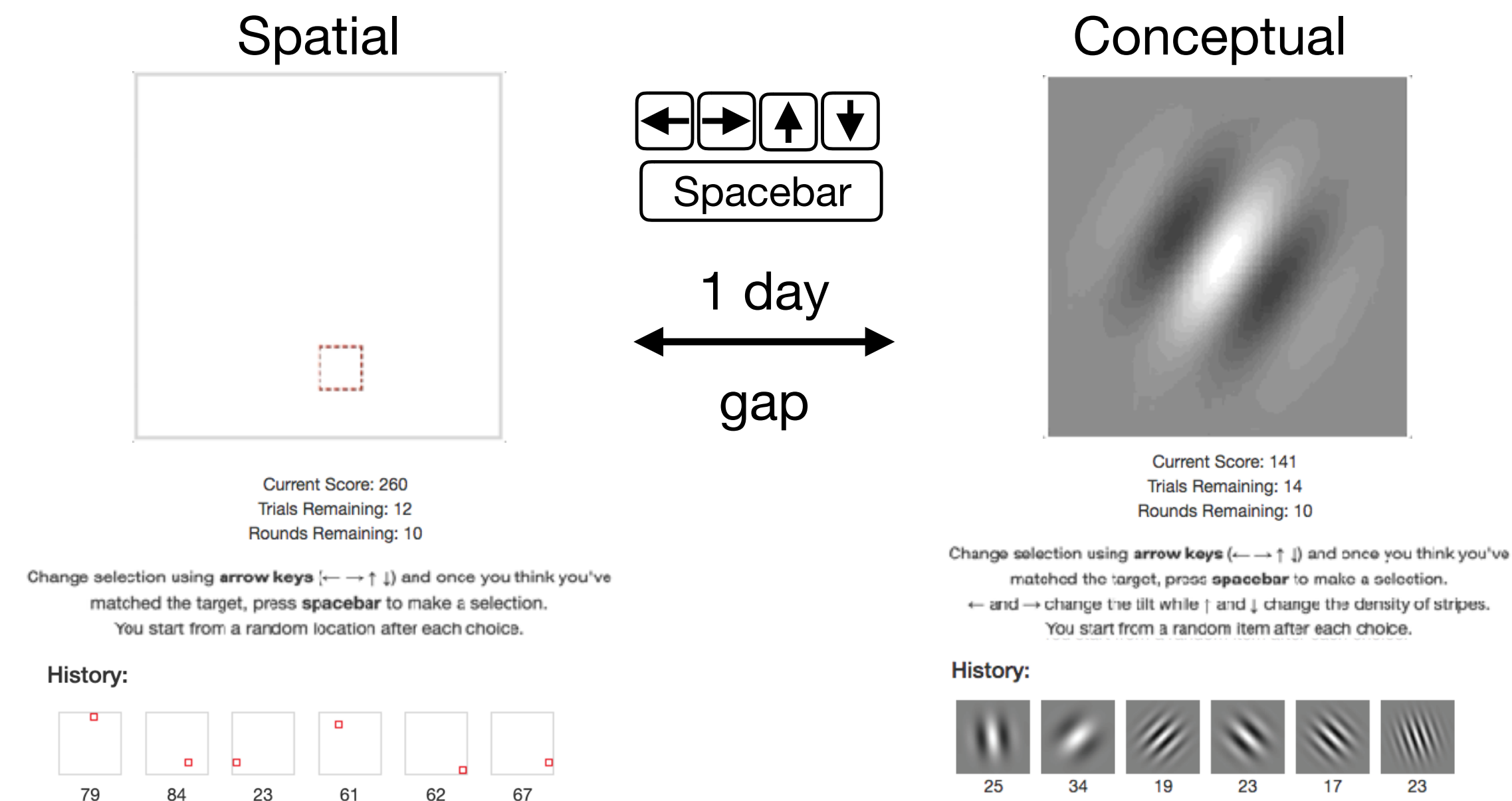
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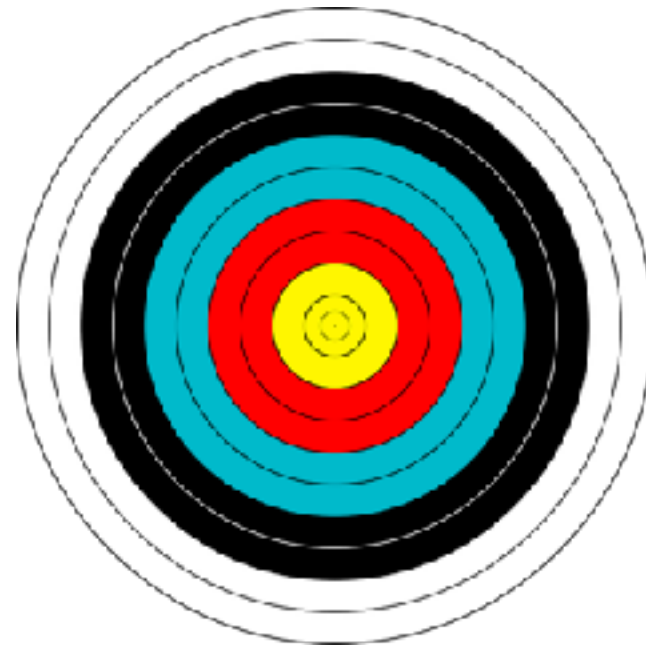
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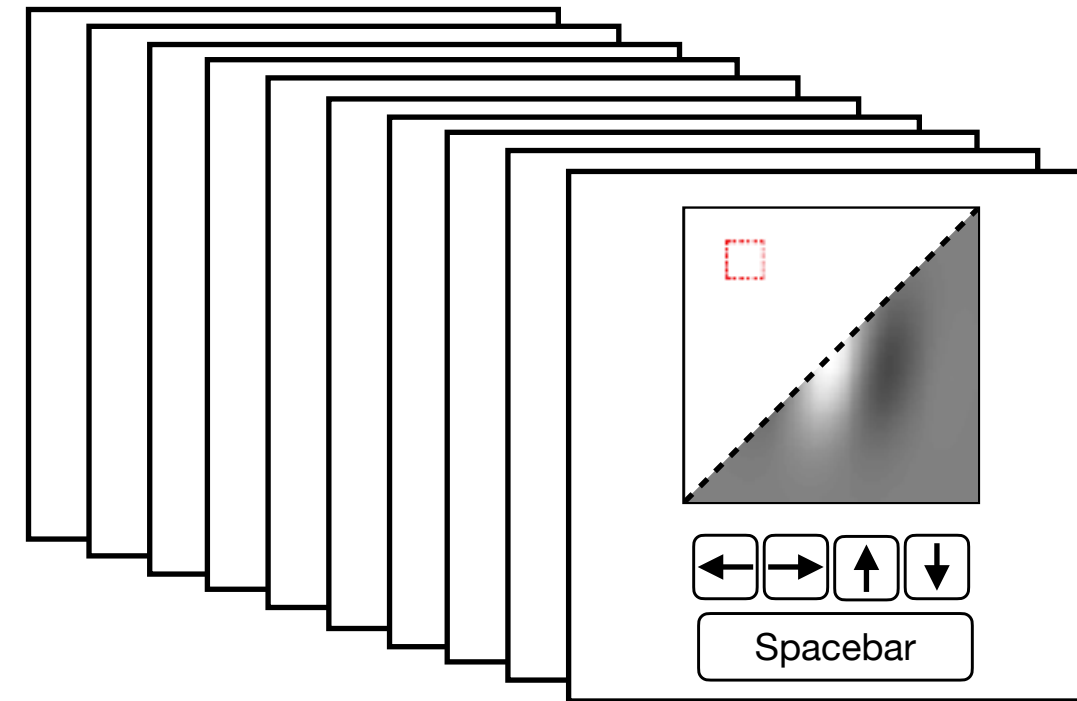
Task Design

Training Phase



Comprehension
Questions

Main Search Task



10 rounds
20 trials in each

Bonus
Round

Judgment and Confidence

Match target stimuli until learning criterion reached

Current Selection



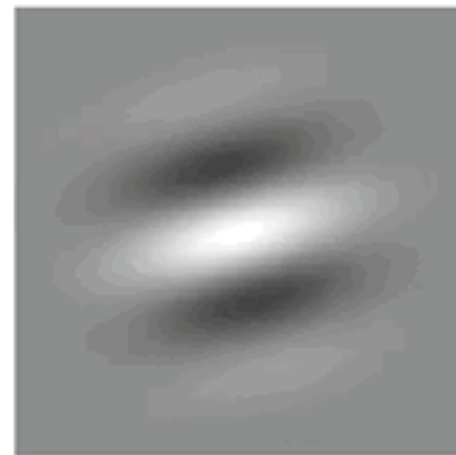
Correct Selections: 0 out of 0
Accuracy (last 10 choices): 0%

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You start from a random location after each choice.
The training session is complete when you have completed at least 32 trials and achieved a run of 9 out of 10 correct responses.

Target



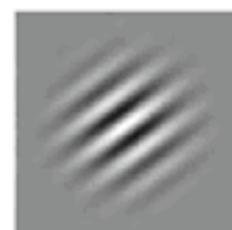
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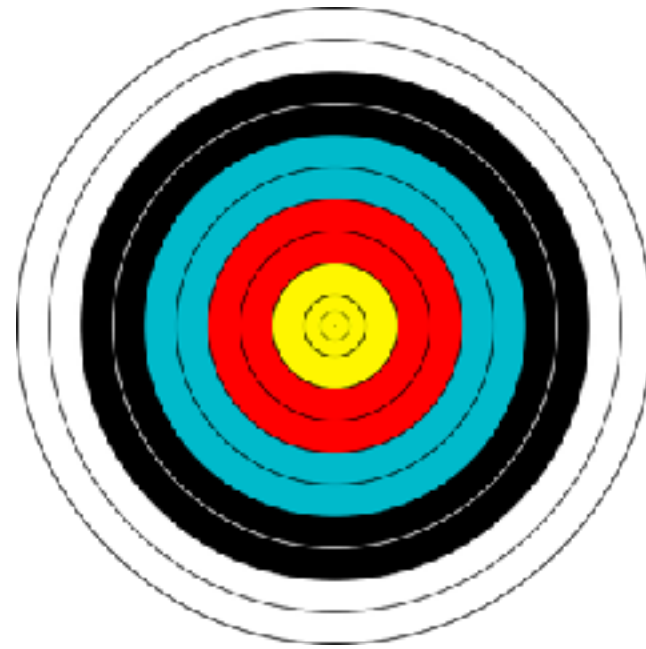
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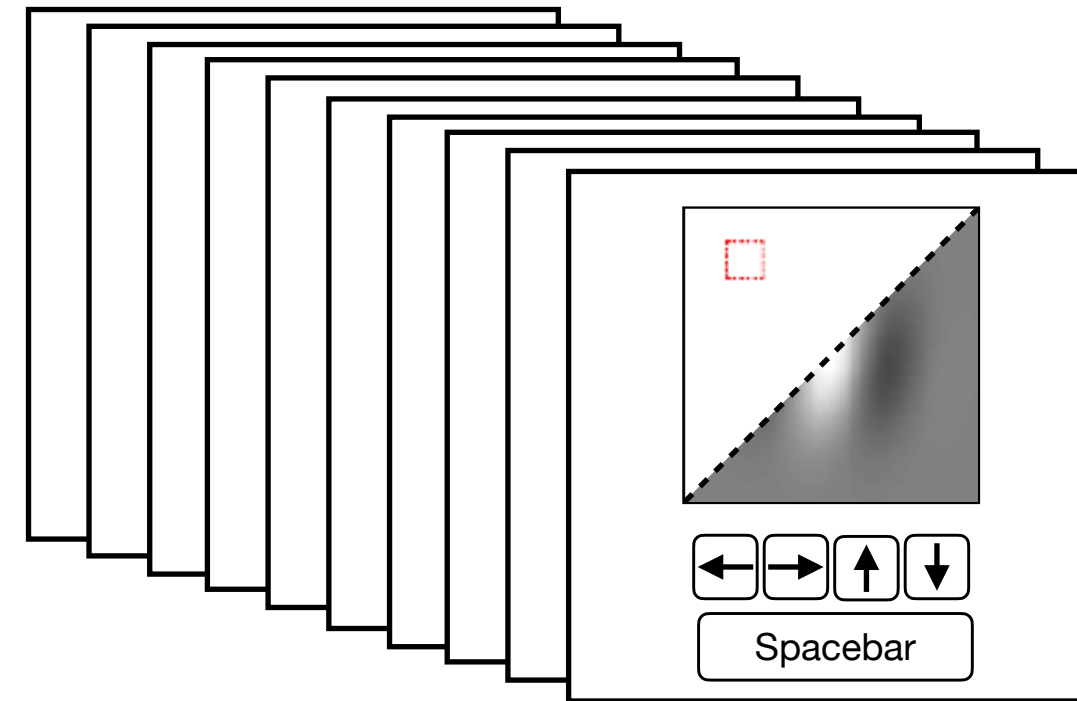
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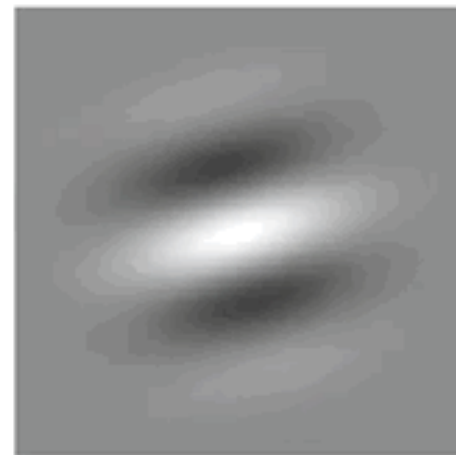
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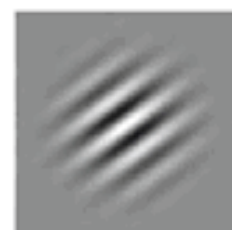
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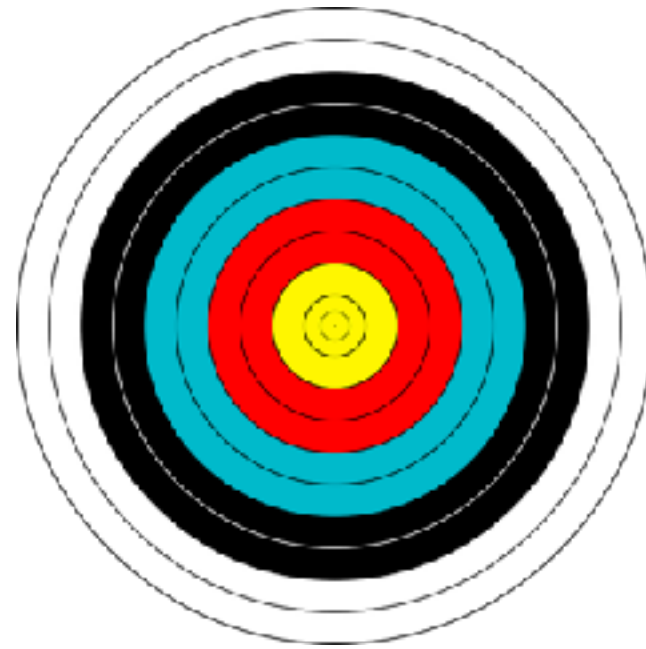
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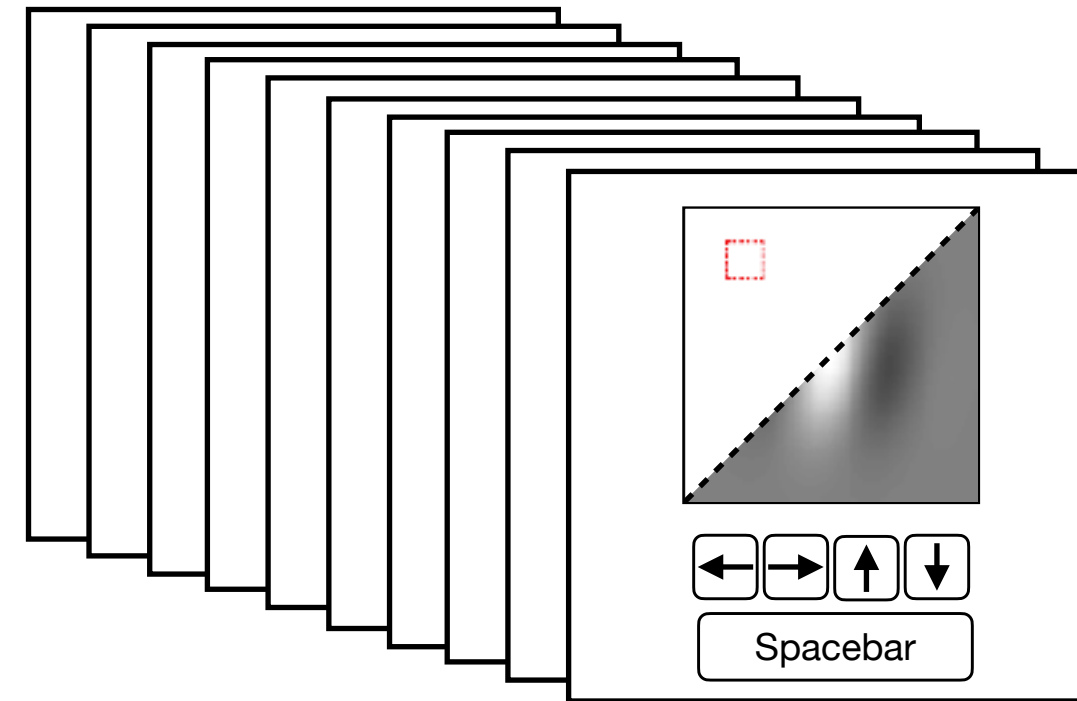
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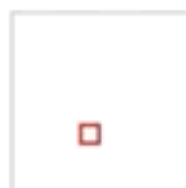
Current Selection



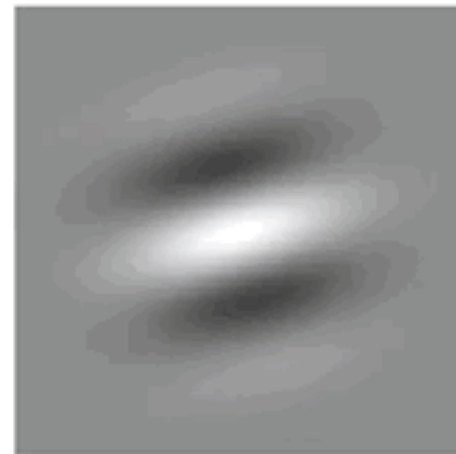
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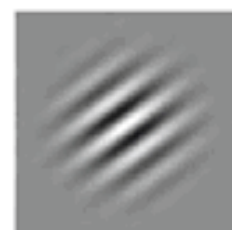
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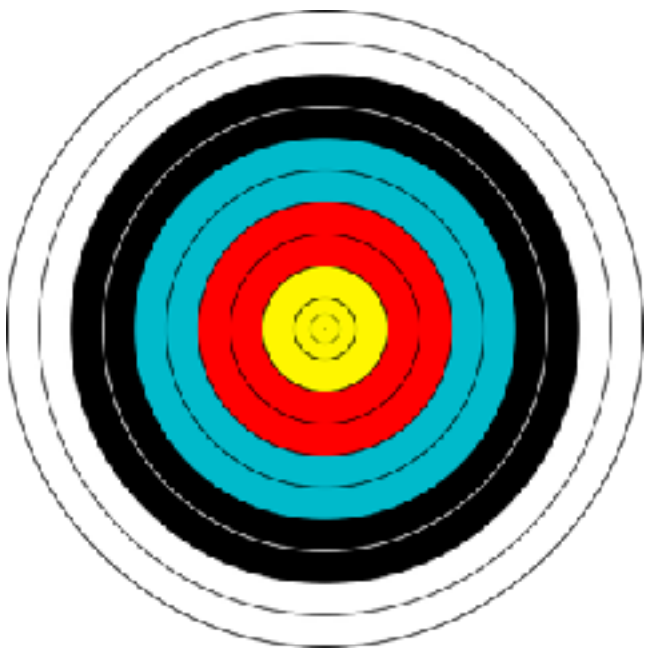
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Bandit Task:

1. Select stimuli using
2. Make selection using
3. Reward is displayed and then added to history
4. Start at a random stimuli

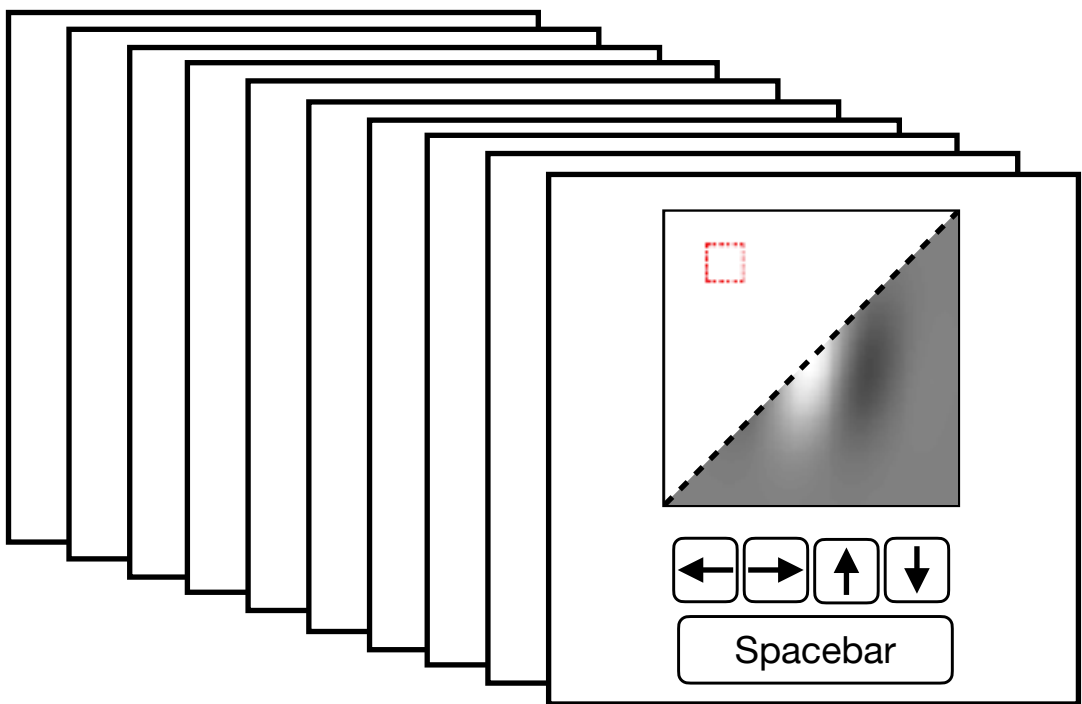
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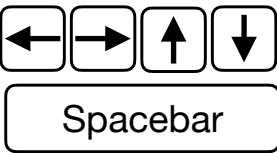
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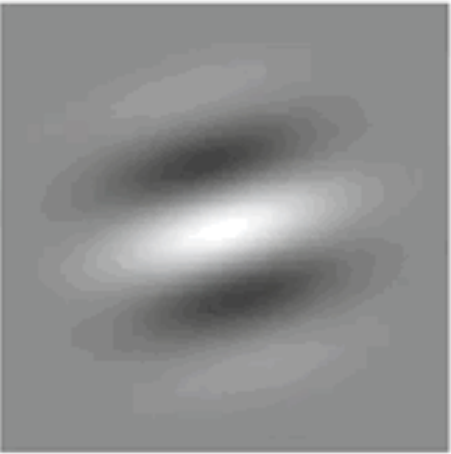
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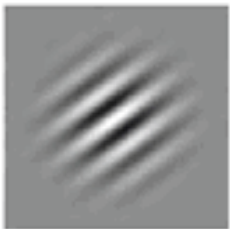
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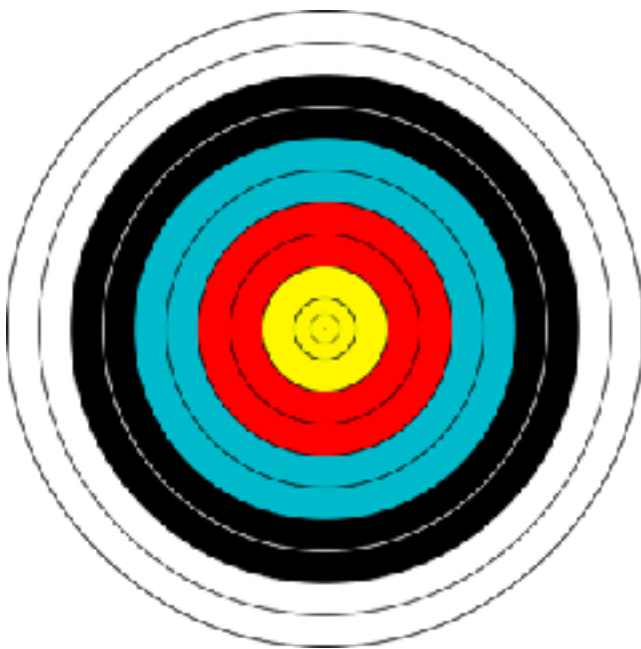
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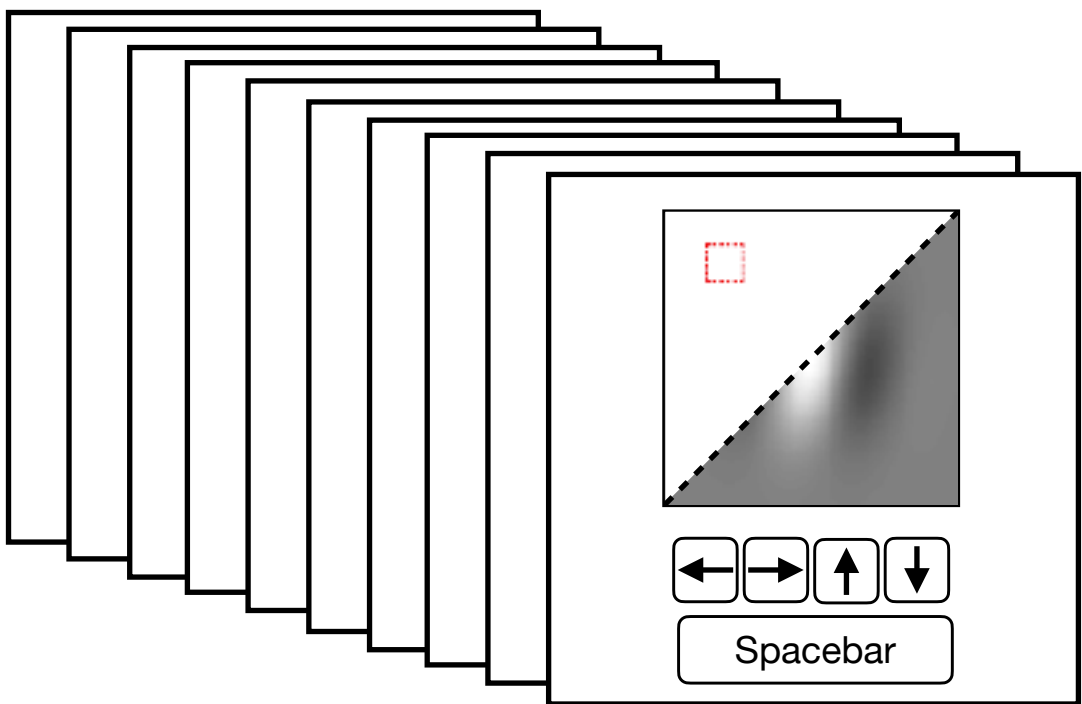
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Bonus
Round

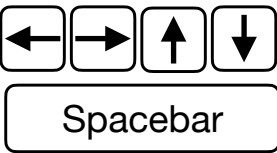
Judgment and Confidence

Match target stimuli until learning criterion reached

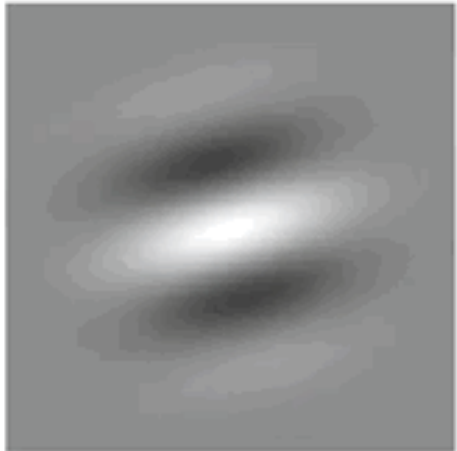
Current Selection



Correct Selections: 0 out of 0
Accuracy (last 10 choices): 0%



Current Selection



Correct Selections: 0 out of 0
Accuracy (last 10 choices): 0%

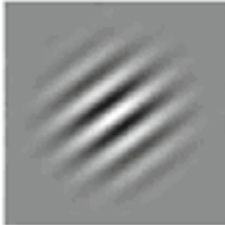
Change selection using **arrow keys** (← → ↑ ↓) and once you think you've matched the target, press **spacebar** to make a selection.
← and → change the tilt while ↑ and ↓ change the density of stripes.
You start from a random item after each choice.

The training session is complete when you have completed at least 32 trials and achieved a run of 9 out of 10 correct responses.

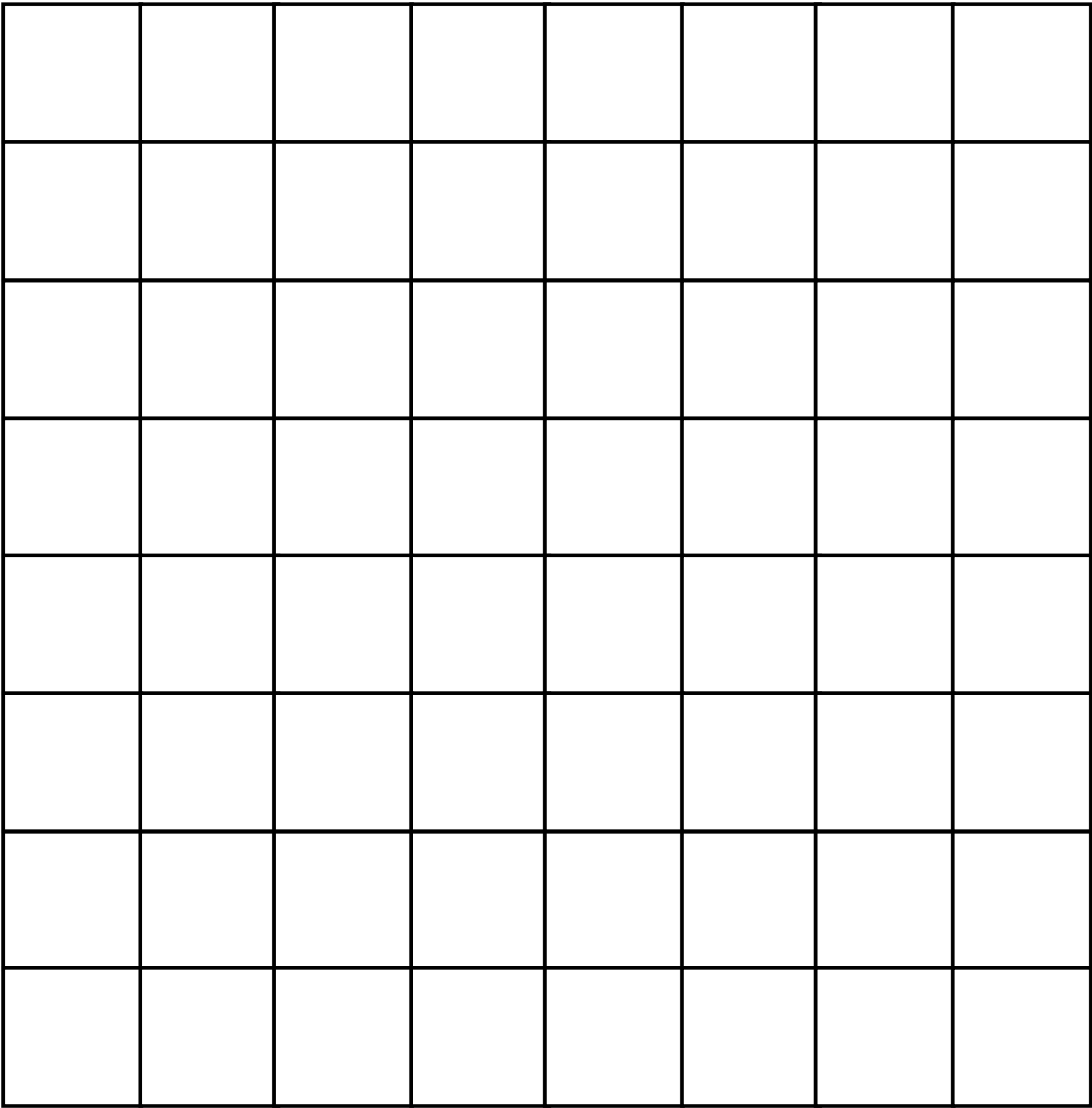
Target



Target

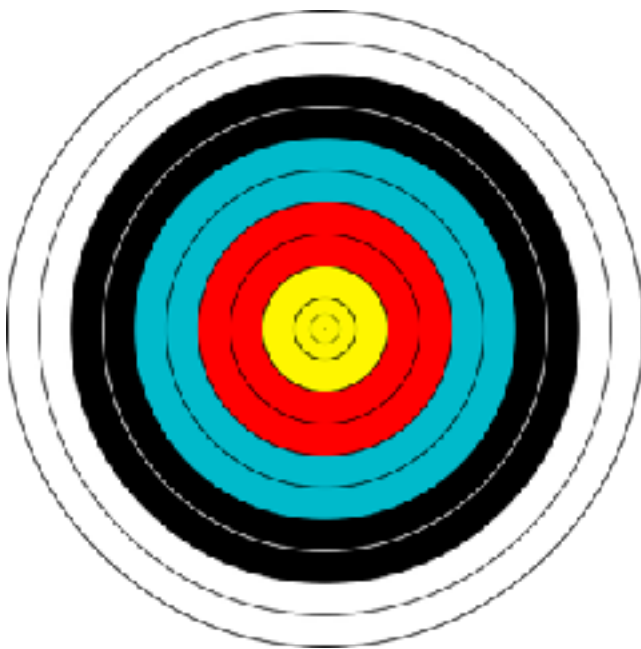


At least 32 trials AND a run of 9 out of 10 correct



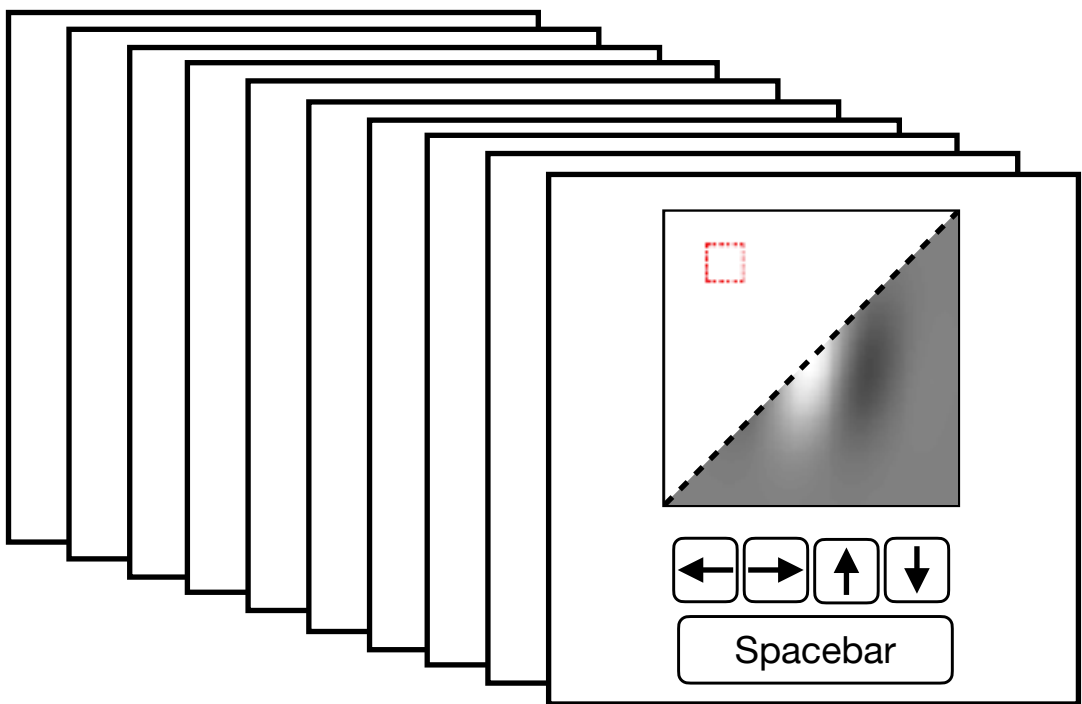
Task Design

Training Phase



Comprehension
Questions

Main Search Task



10 rounds
20 trials in each

Bonus
Round

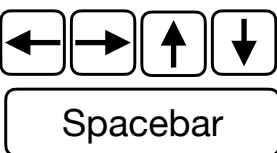
Judgment and Confidence

Match target stimuli until learning criterion reached

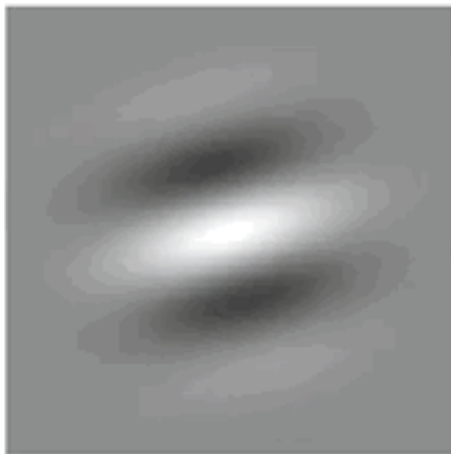
Current Selection



Correct Selections: 0 out of 0
Accuracy (last 10 choices): 0%



Current Selection



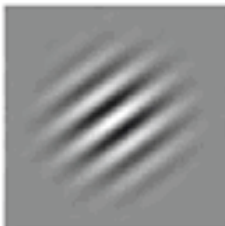
Correct Selections: 0 out of 0
Accuracy (last 10 choices): 0%

Change selection using **arrow keys** (← → ↑ ↓) and once you think you've matched the target, press **spacebar** to make a selection.
← and → change the tilt while ↑ and ↓ change the density of stripes.
You start from a random item after each choice.
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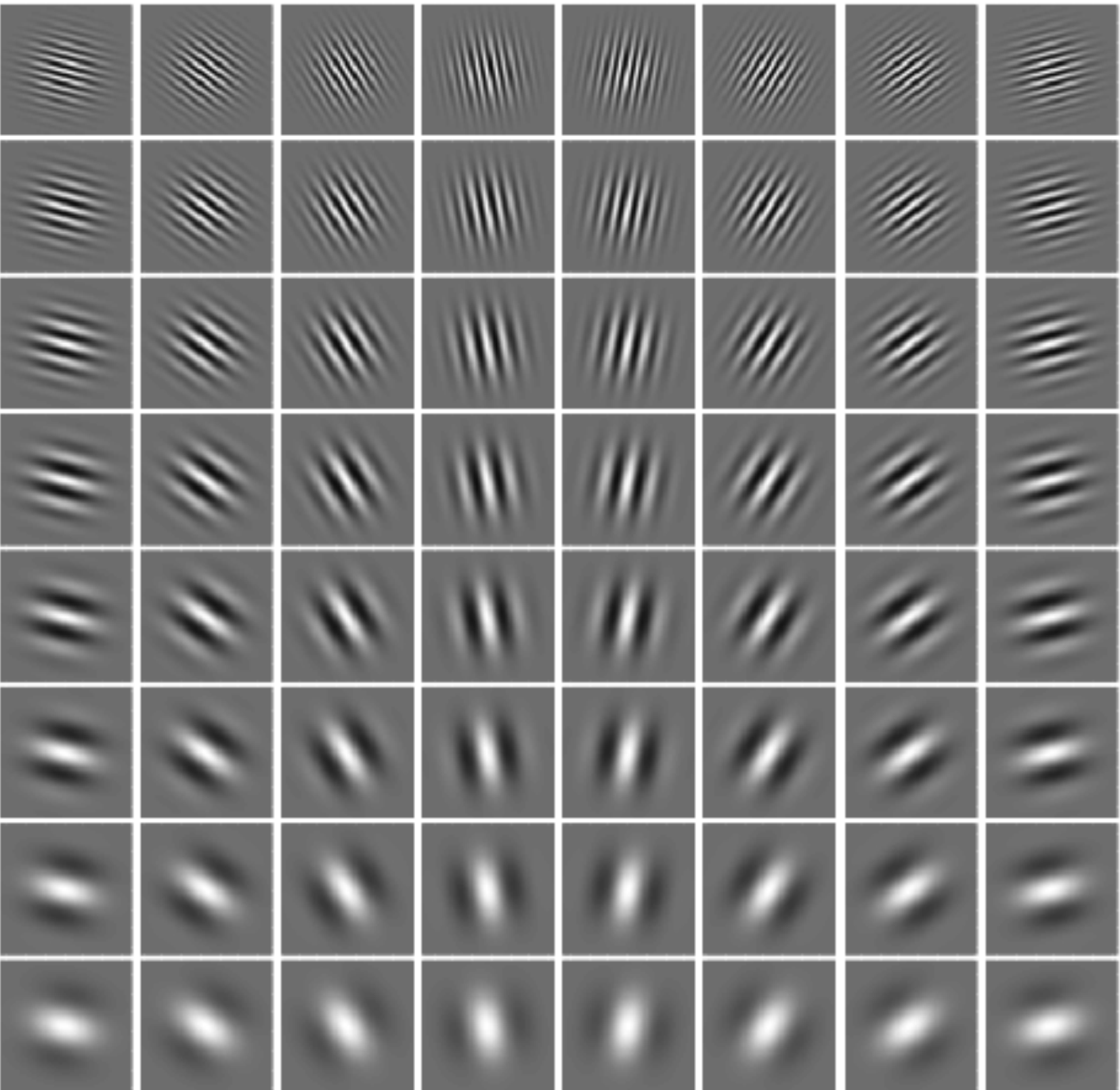
Target



Target



Stripe Density

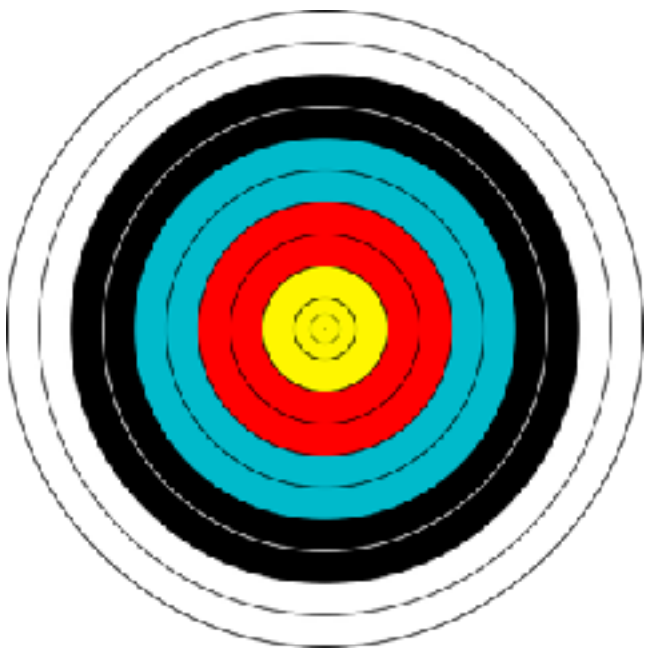


Tilt

At least 32 trials AND a run of 9 out of 10 correct

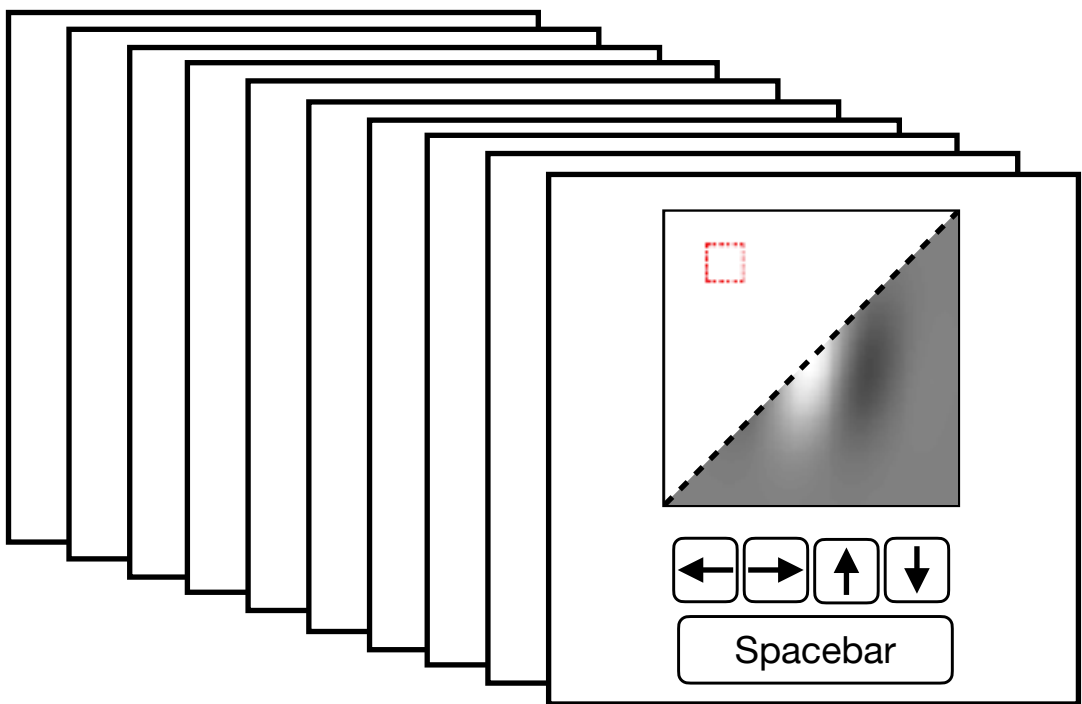
Task Design

Training Phase



Comprehension
Questions

Main Search Task



10 rounds
20 trials in each

Bonus
Round

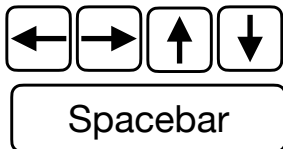
Judgment and Confidence

Match target stimuli until learning criterion reached

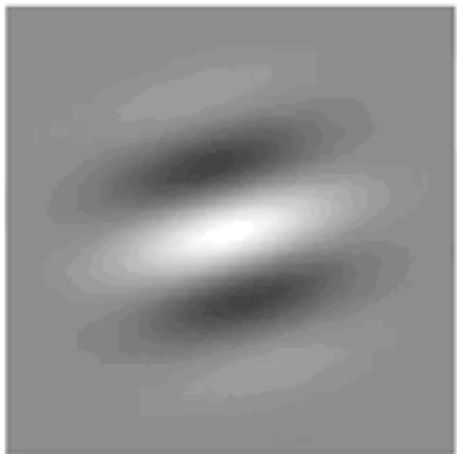
Current Selection



Correct Selections: 0 out of 0
Accuracy (last 10 choices): 0%



Current Selection



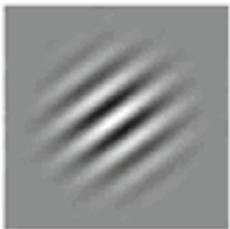
Correct Selections: 0 out of 0
Accuracy (last 10 choices): 0%

Change selection using **arrow keys** (← → ↑ ↓) and once you think you've matched the target, press **spacebar** to make a selection.
← and → change the tilt while ↑ and ↓ change the density of stripes.
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The training session is complete when you have completed at least 32 trials and achieved a run of 9 out of 10 correct responses.

Target

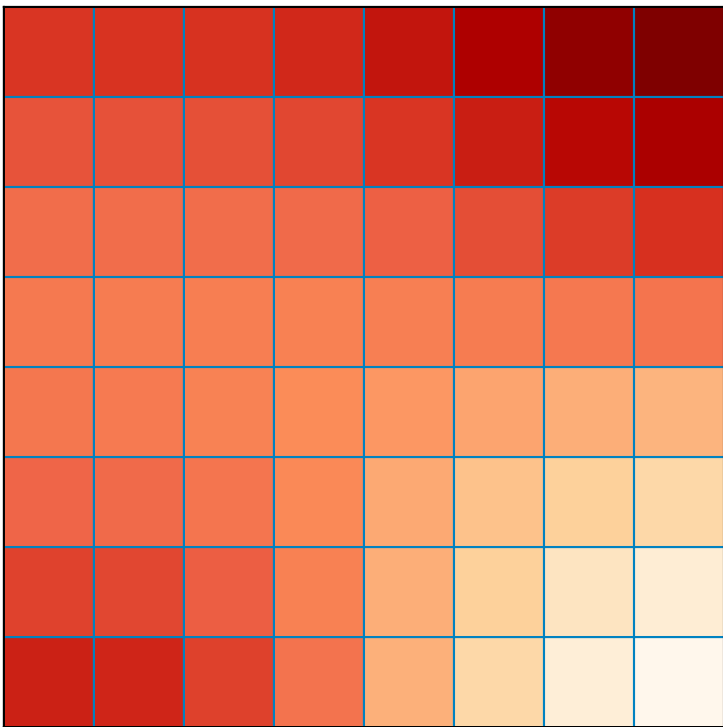
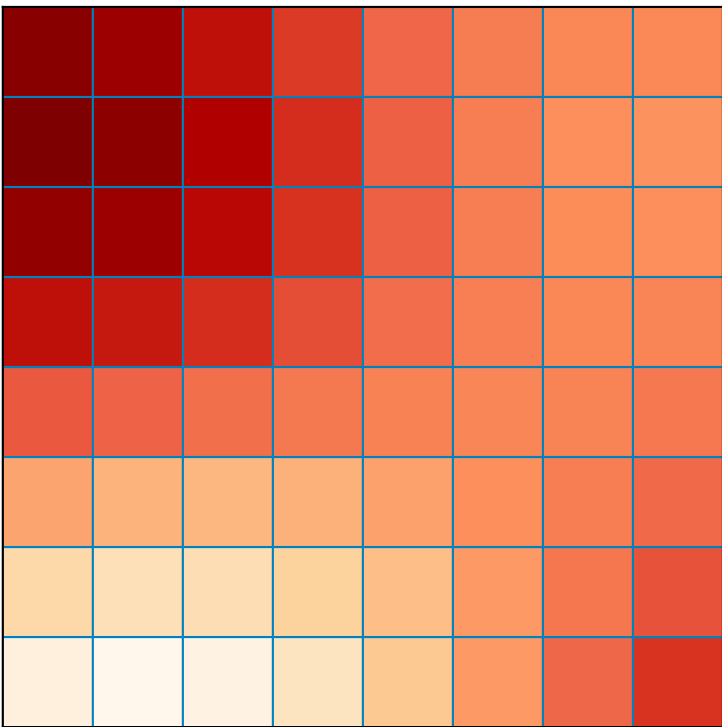


Target

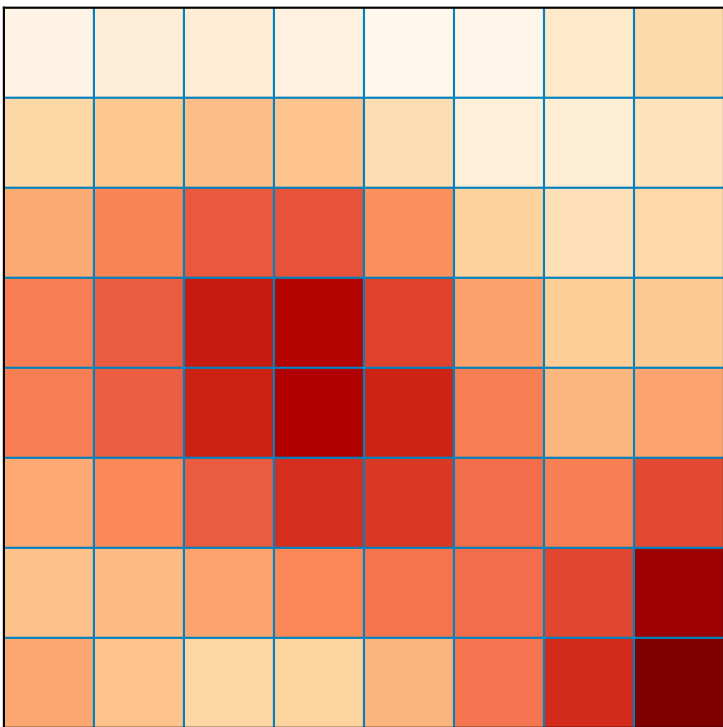
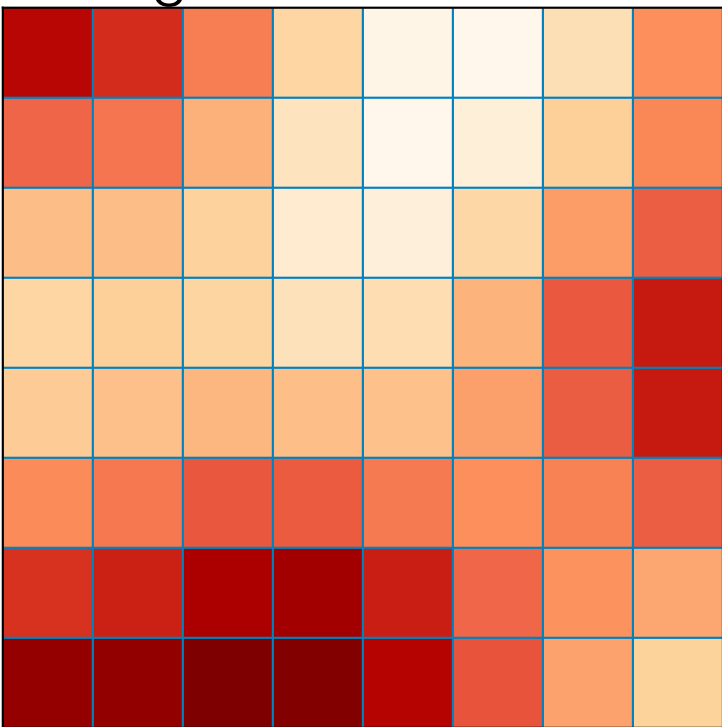


At least 32 trials AND a run of 9 out of 10 correct

Smooth Environments

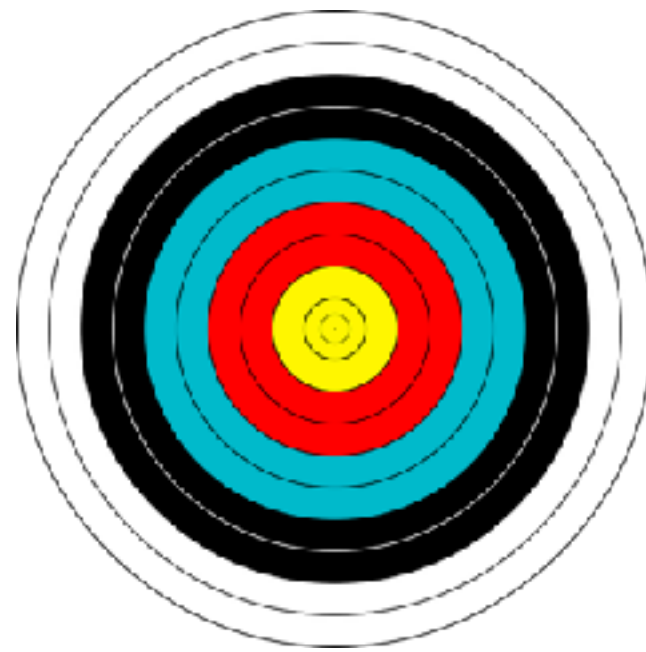


Rough Environments

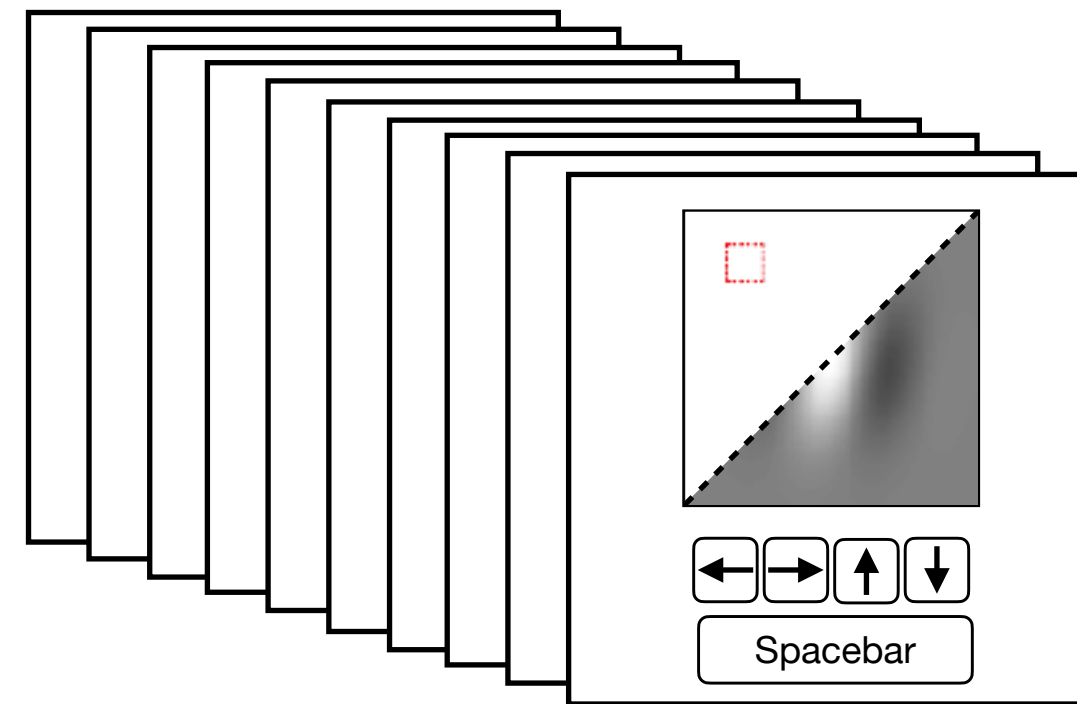


Task Design

Training Phase



Main Search Task



10 rounds
20 trials in each

Judgment and Confidence

Bonus
Round



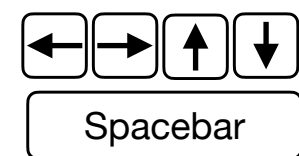
After the 15th trial of the 10th round

Match target stimuli until learning criterion reached

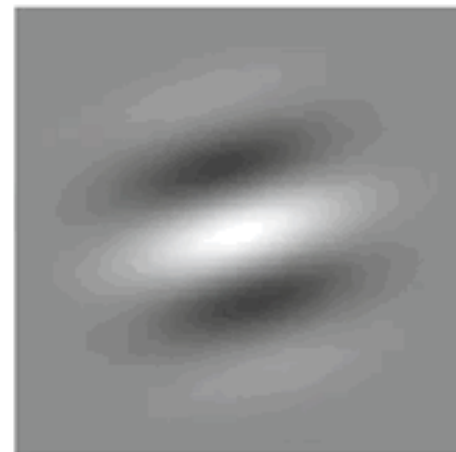
Current Selection



Correct Selections: 0 out of 0
Accuracy (last 10 choices): 0%



Current Selection



Correct Selections: 0 out of 0
Accuracy (last 10 choices): 0%

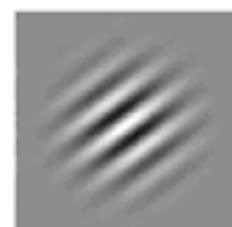
Change selection using **arrow keys** (← → ↑ ↓) and once you think you've matched the target, press **spacebar** to make a selection.
You start from a random location after each choice.
The training session is complete when you have completed at least 32 trials and achieved a run of 9 out of 10 correct responses.

Target



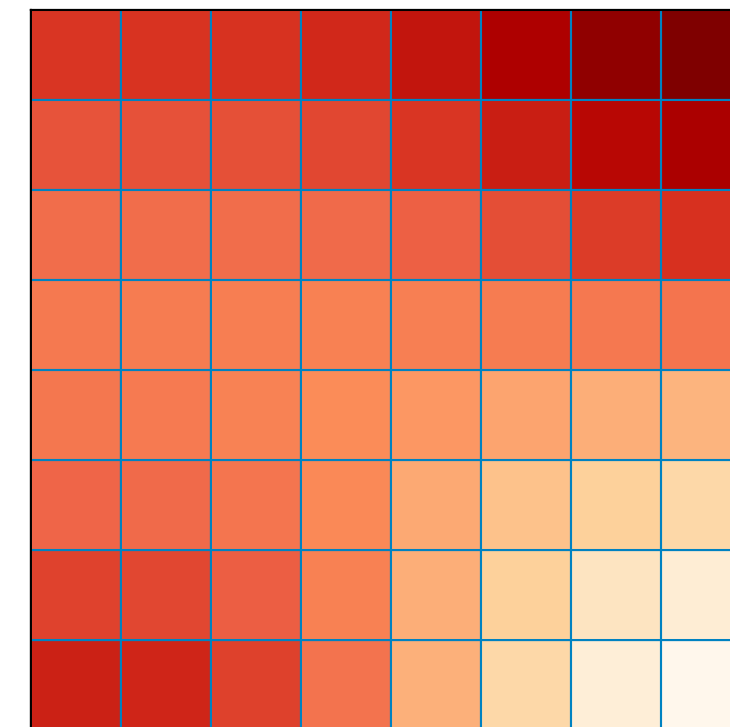
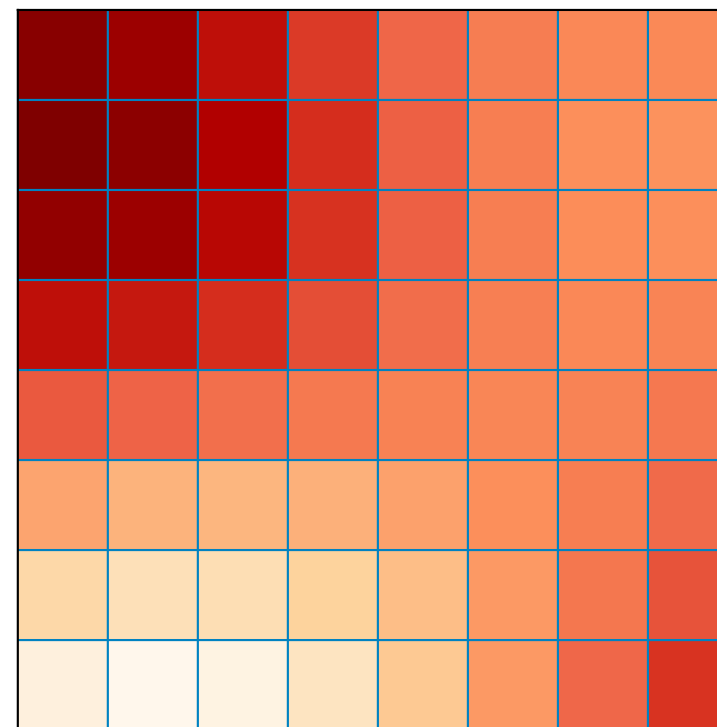
Change selection using **arrow keys** (← → ↑ ↓) and once you think you've matched the target, press **spacebar** to make a selection.
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The training session is complete when you have completed at least 32 trials and achieved a run of 9 out of 10 correct responses.

Target

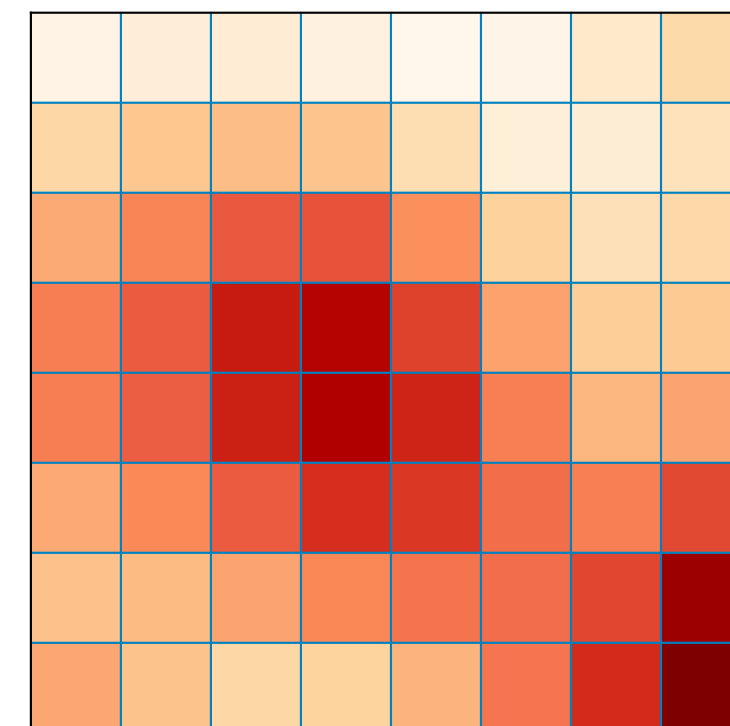
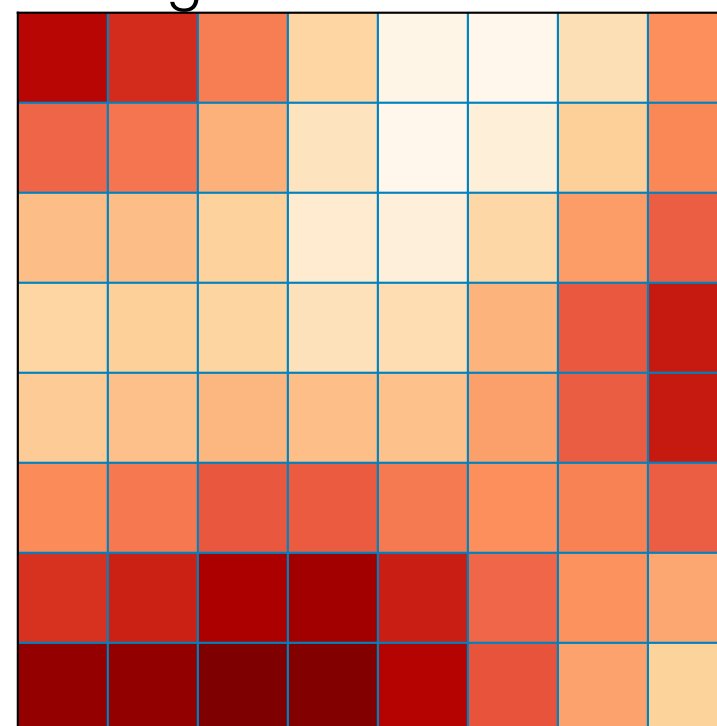


At least 32 trials AND a run of 9 out of 10 correct

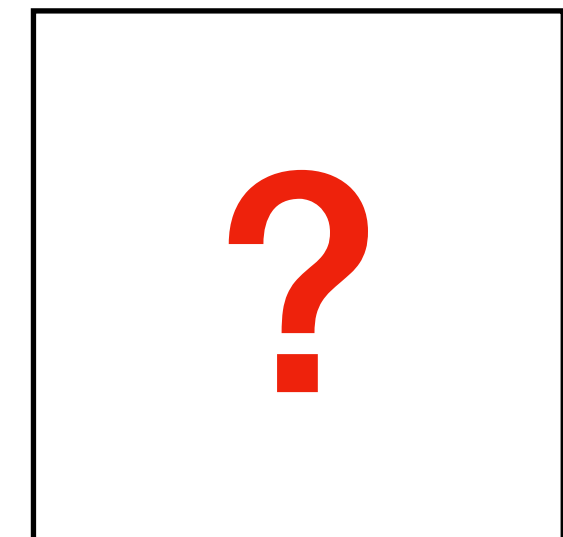
Smooth Environments



Rough Environments



Judgments on 10 unobserved stimuli



How many points do you think this item will earn?



45 points

How confident are you?



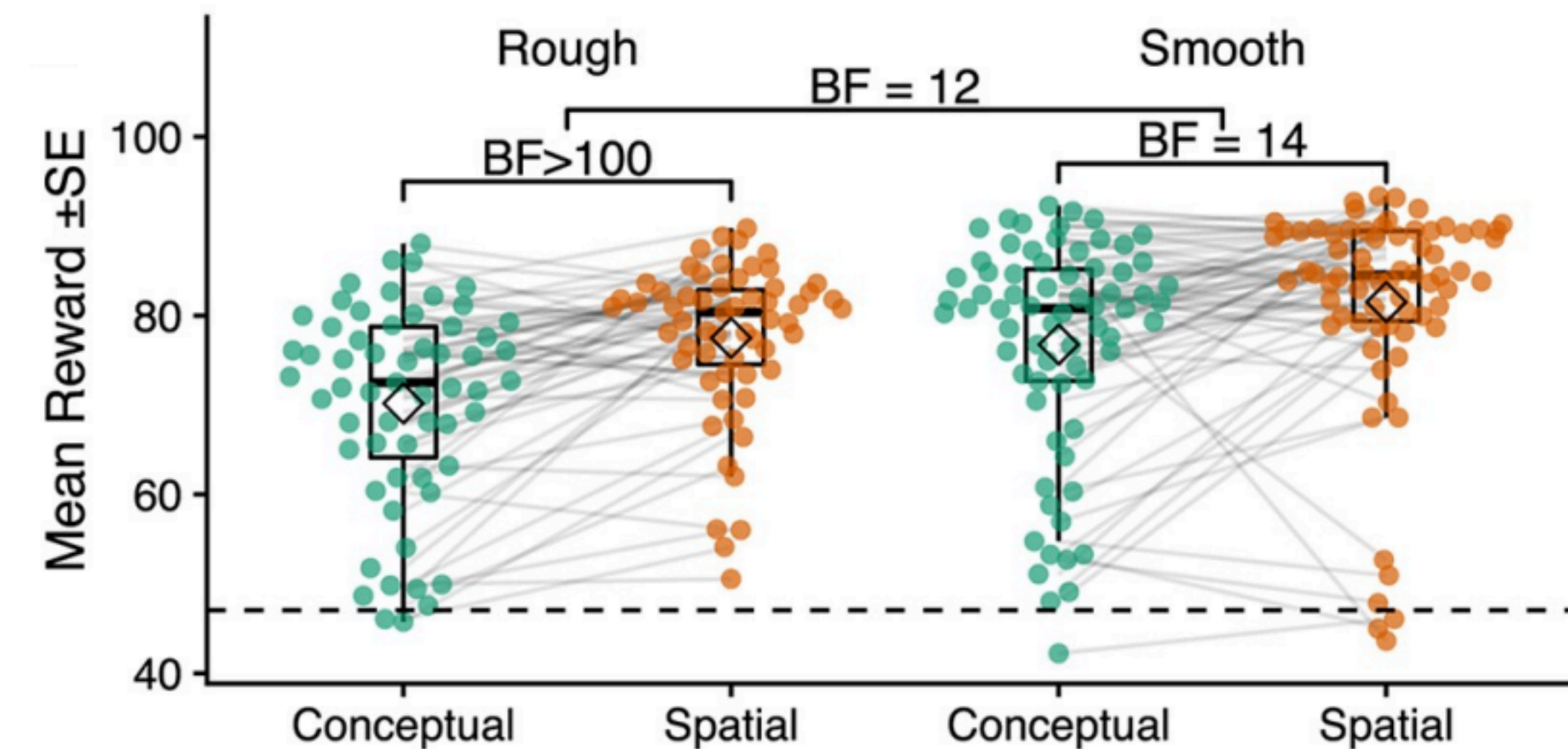
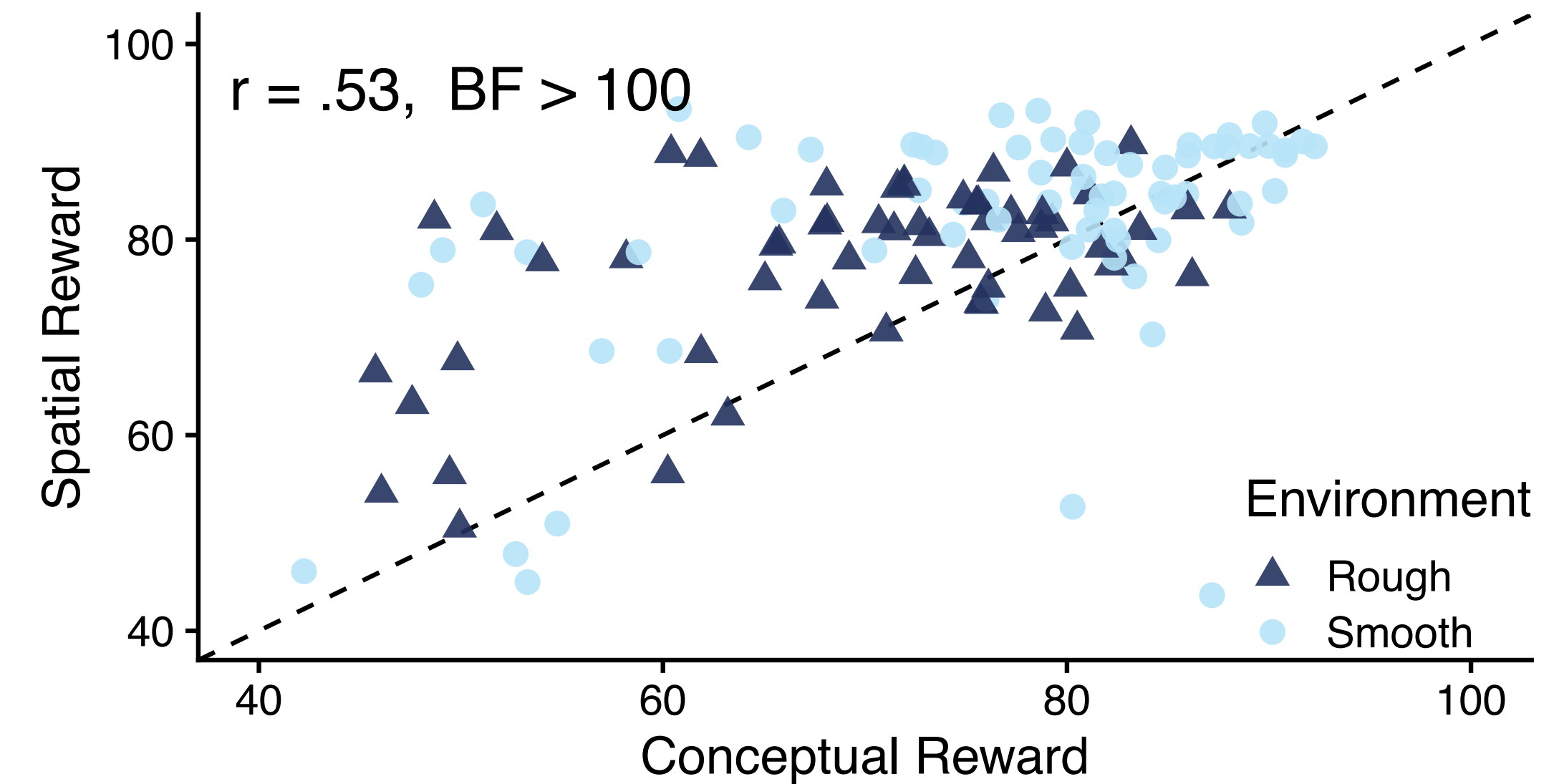
Least confident

Most confident

Submit

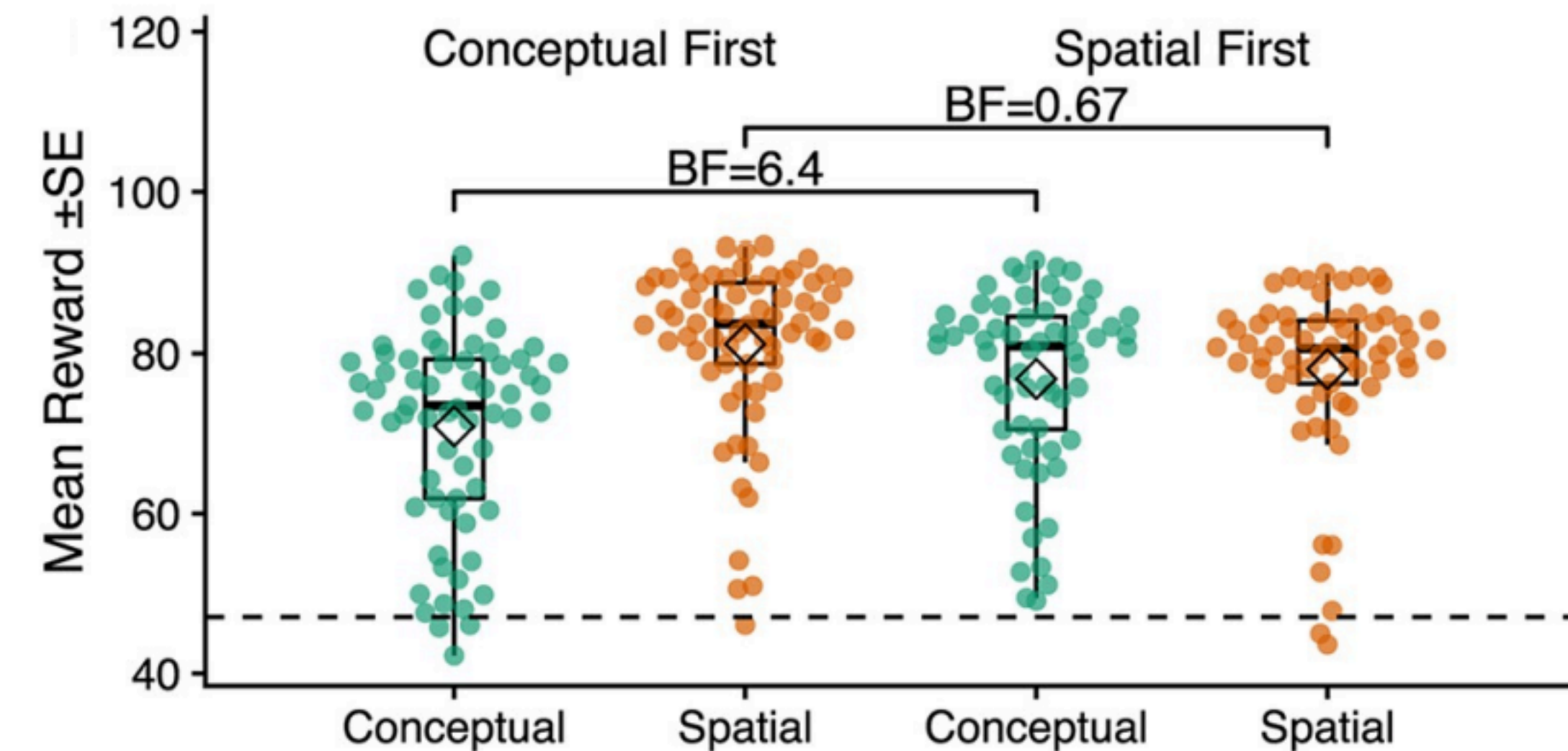
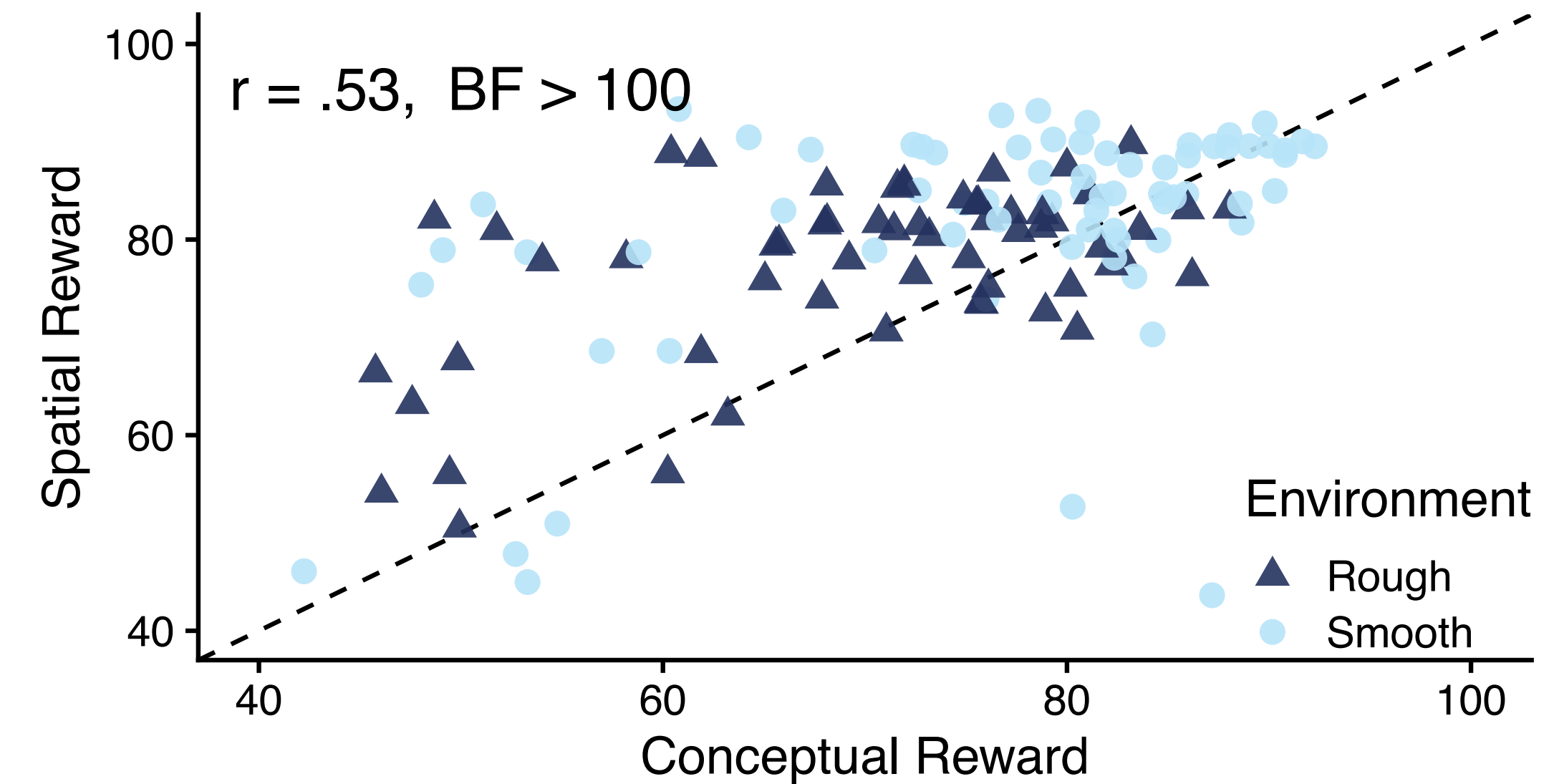
Behavioral Results

- Correlated performance, but generally better in the spatial task
- This difference can largely be explained by a one-directional transfer effect:
 - Experience with spatial search boosted performance on conceptual search, but not vice versa



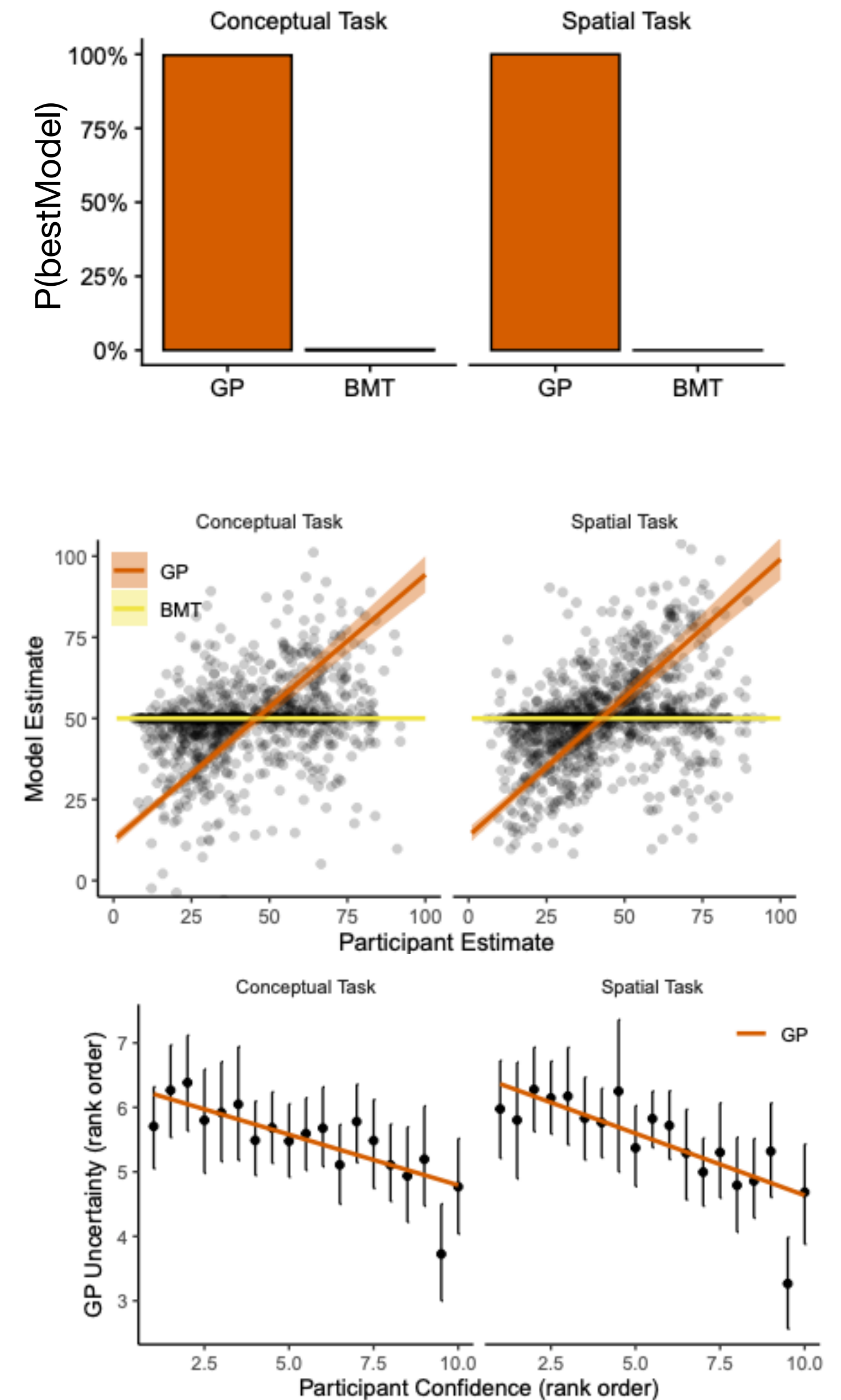
Behavioral Results

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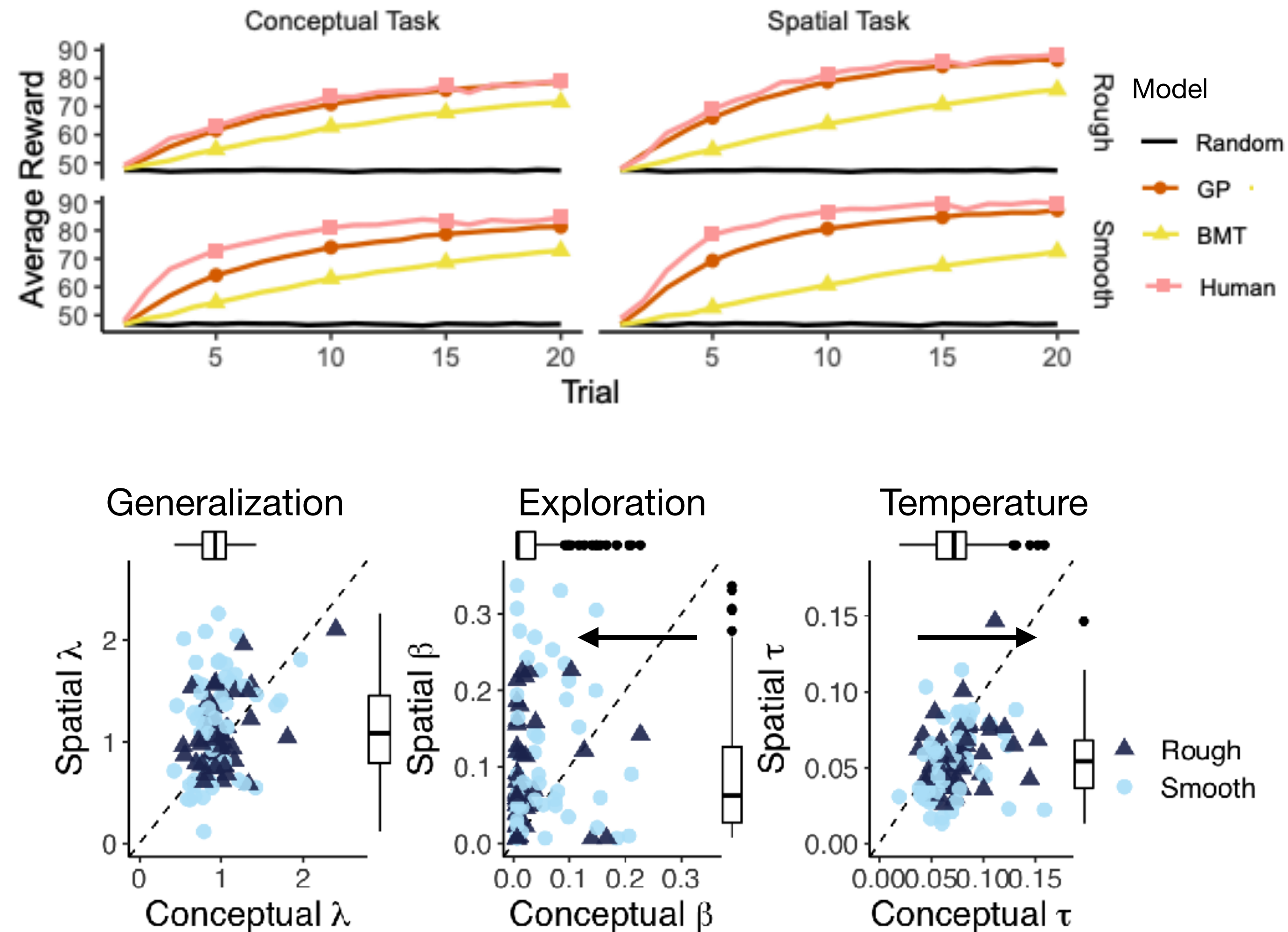
Modeling Results

- Using group-level Bayesian estimation, we find that **GP-UCB** is the best model of choice behavior
 - $P(\text{bestModel})$ estimates the most prevalent model (corrected for chance); also known as protected exceedance probability
- GP-UCB** also predicts bonus round judgments about expected reward and confidence
 - using parameters estimated from rounds 1-9, we can use model simulations to predict participant judgments for unobserved stimuli in round 10
 - BMT makes invariant predictions for novel options, but the GP predictions correspond to participant judgments, where uncertainty is the opposite of confidence



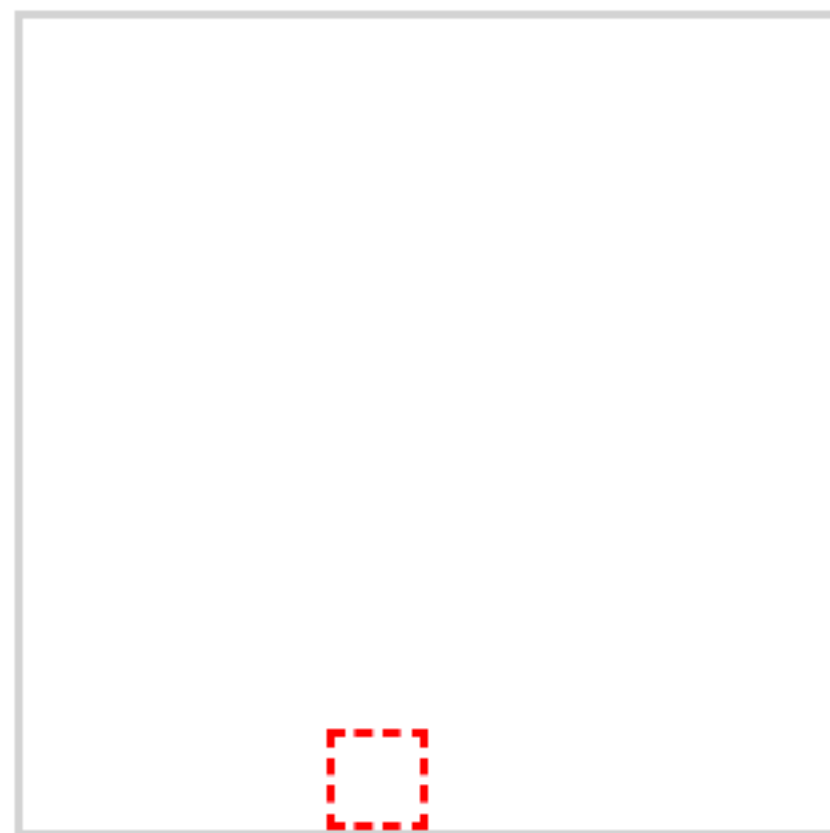
Modeling Results

- **GP-UCB** simulated learning curves resemble human performance
- Parameter estimates show similar levels of generalization but change in exploration
- Directed exploration vanishes in the conceptual task, replaced by higher temperature (i.e., random) sampling



Summary

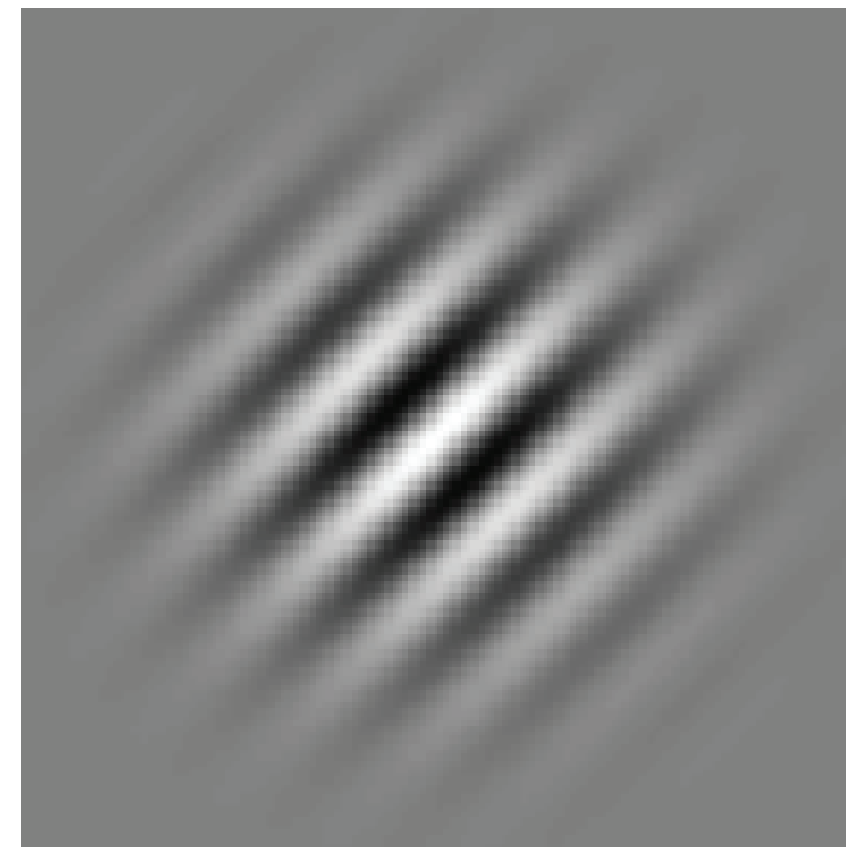
Spatial



Current Score: 260
Trials Remaining: 12
Rounds Remaining: 10

Change selection using **arrow keys** (← → ↑ ↓) and make a choice by pressing **spacebar**.
You start from a random tile after each choice and crossing over the edge of the grid brings you to the opposite side.

Conceptual

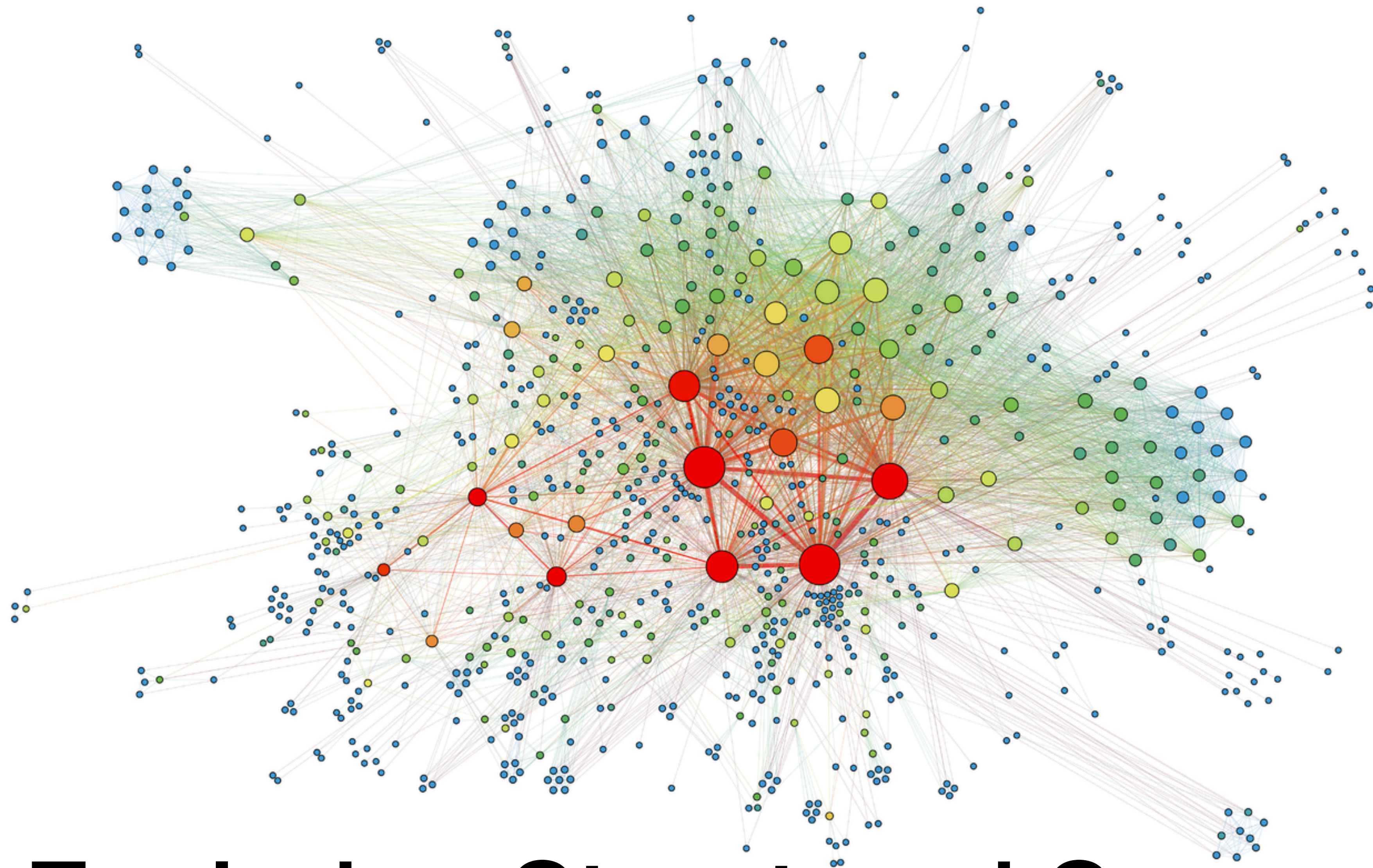


Current Score: 141
Trials Remaining: 14
Rounds Remaining: 10

Use your **arrow keys** to change the selection and make a choice by pressing **spacebar**.
← and → change the tilt while ↑ and ↓ change the number of stripes.
You start from a random item after each choice.

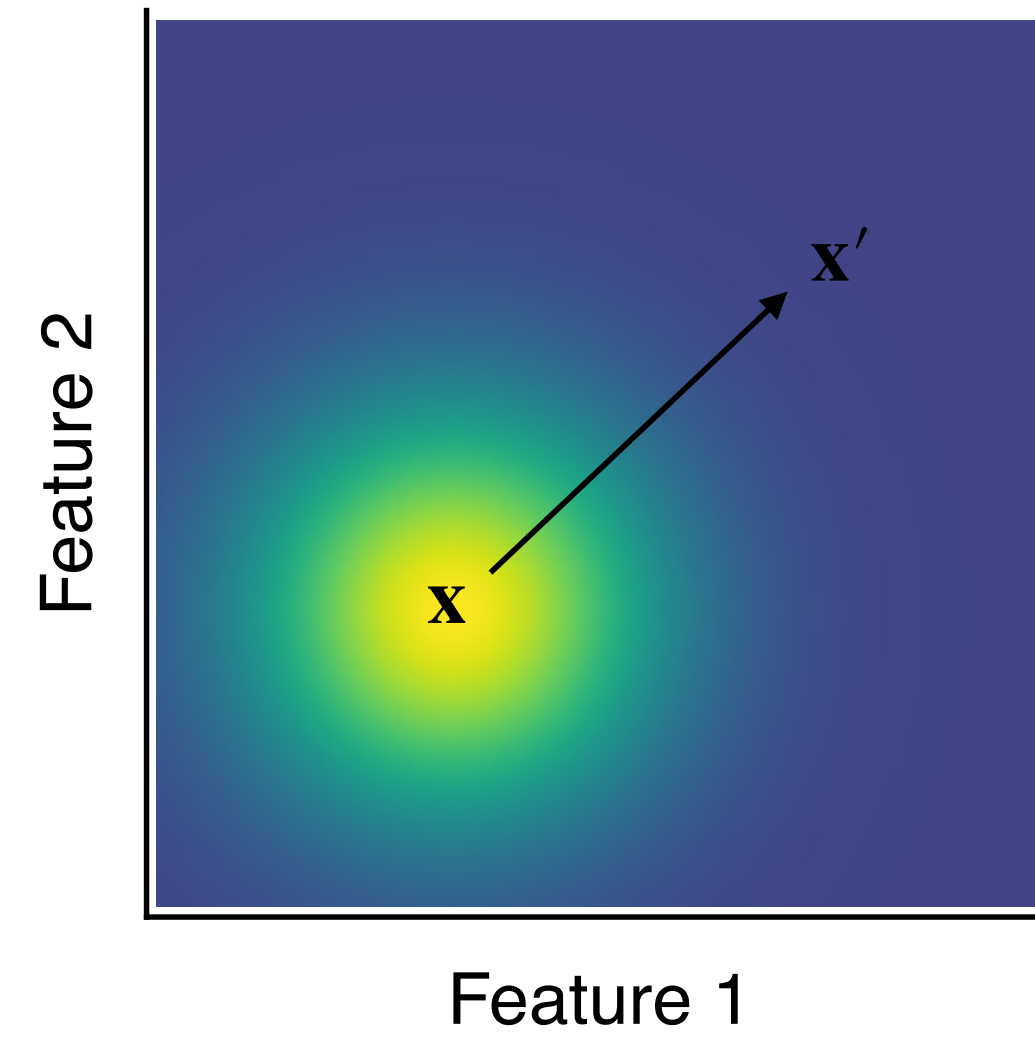
1 day
↔
gap

- Similar mechanisms of generalization-guided search in both domains
- But also diagnostic differences:
 - One-directional transfer effect suggest something fundamental about spatial reasoning
 - Switch from directed to random exploration
- Bonus round suggests participants have a good sense of uncertainty (confidence ratings) in both domains, but aren't able to leverage it to direct their exploration in the conceptual task

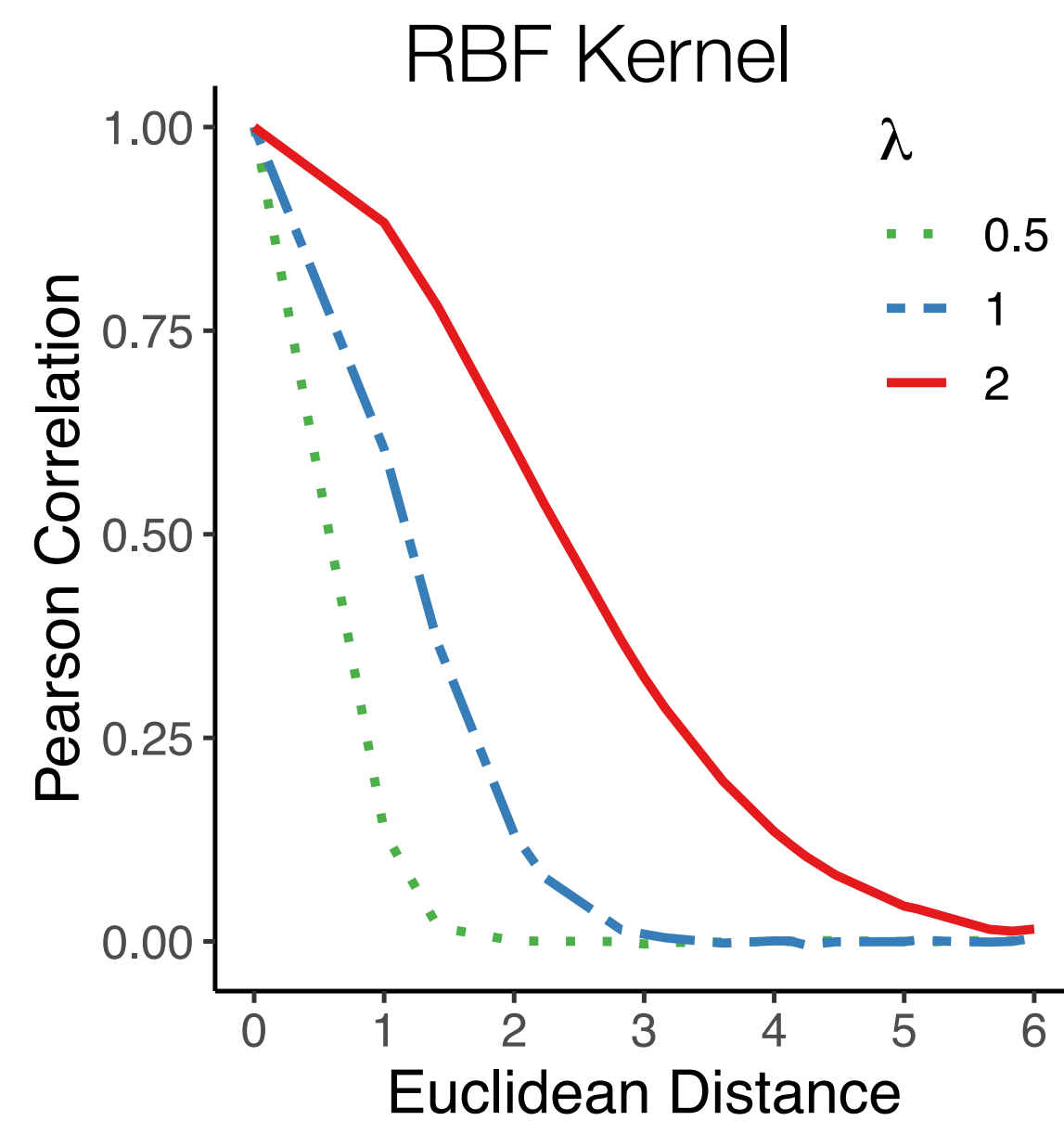
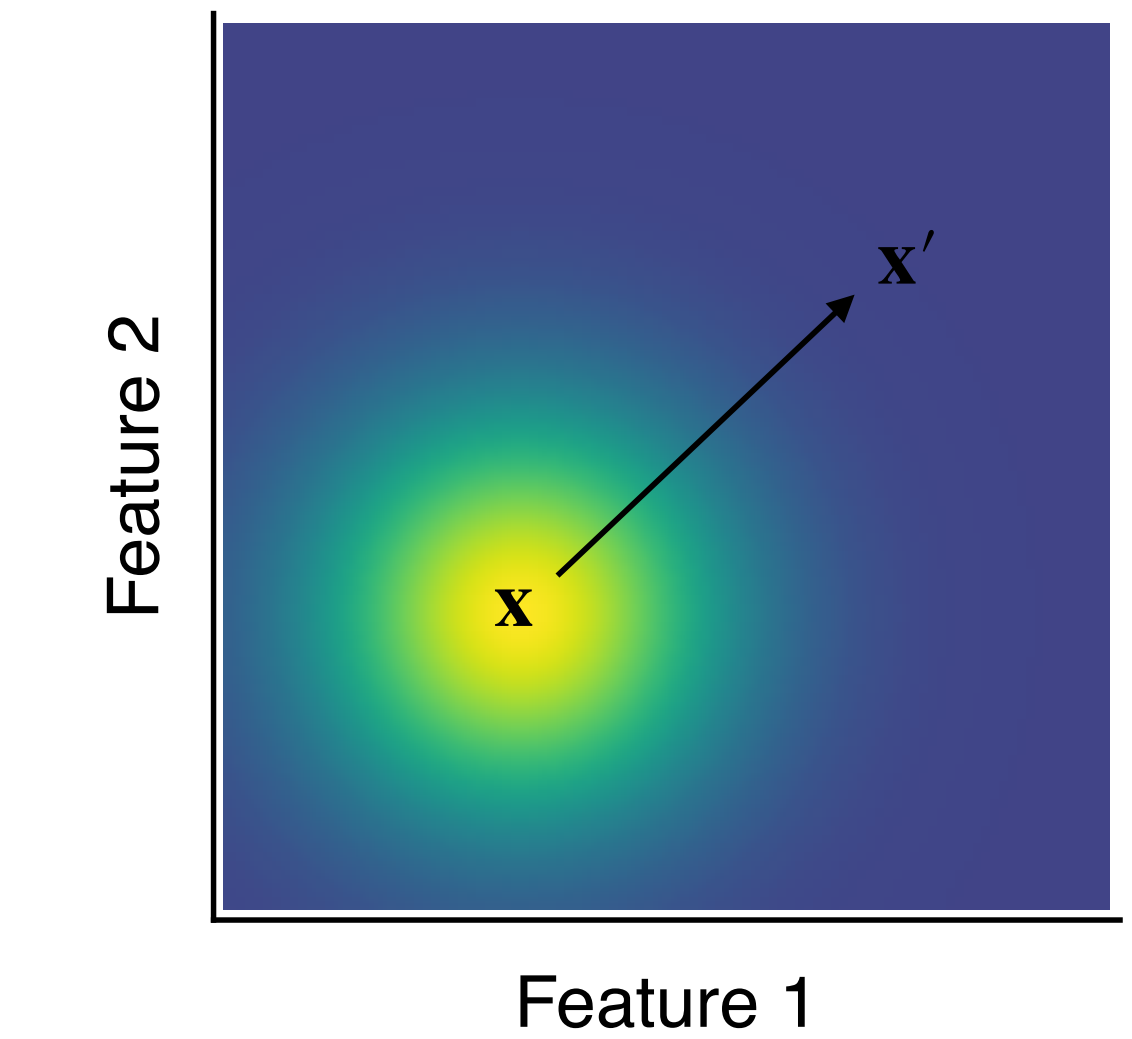


Exploring Structured Spaces

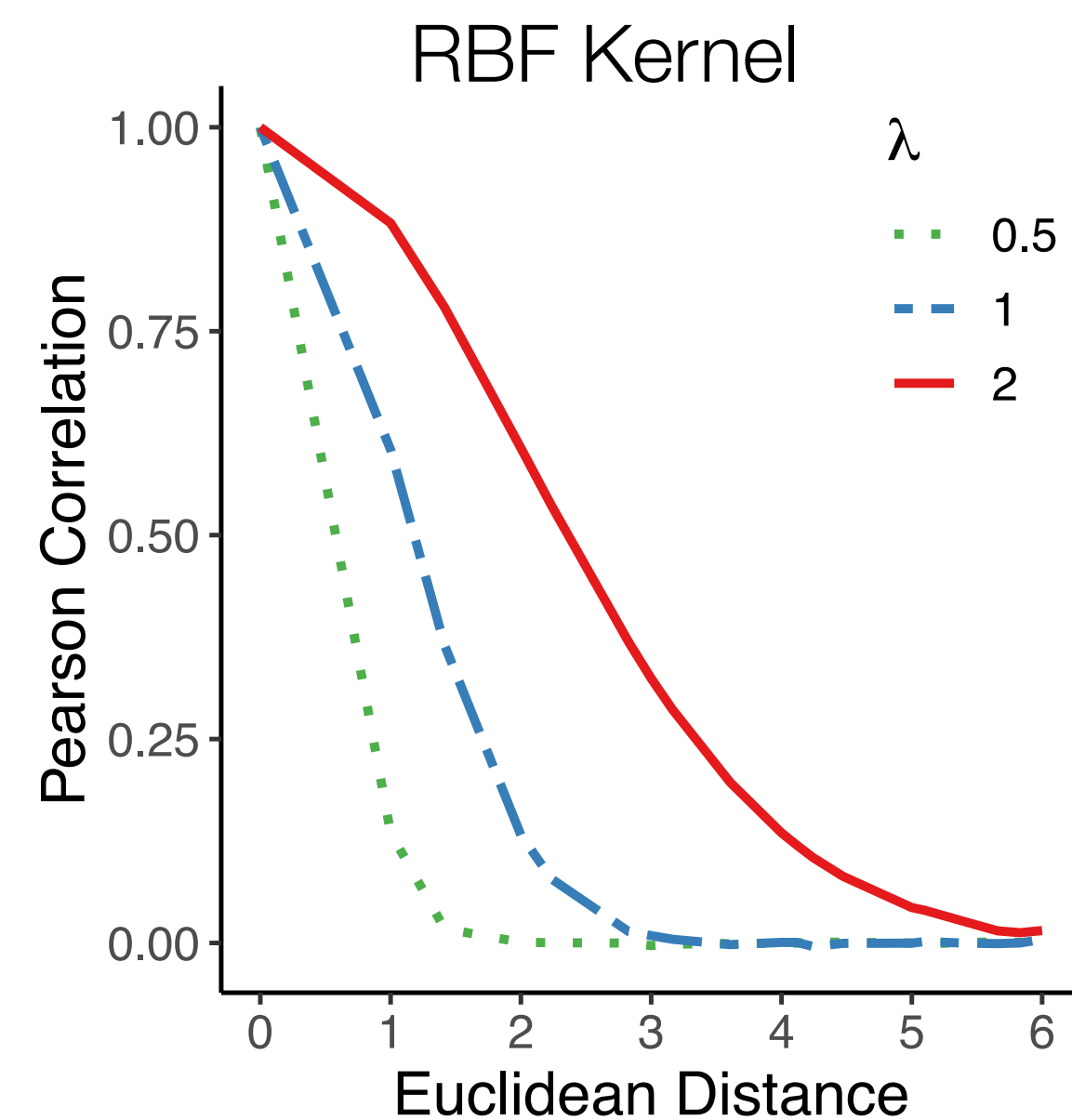
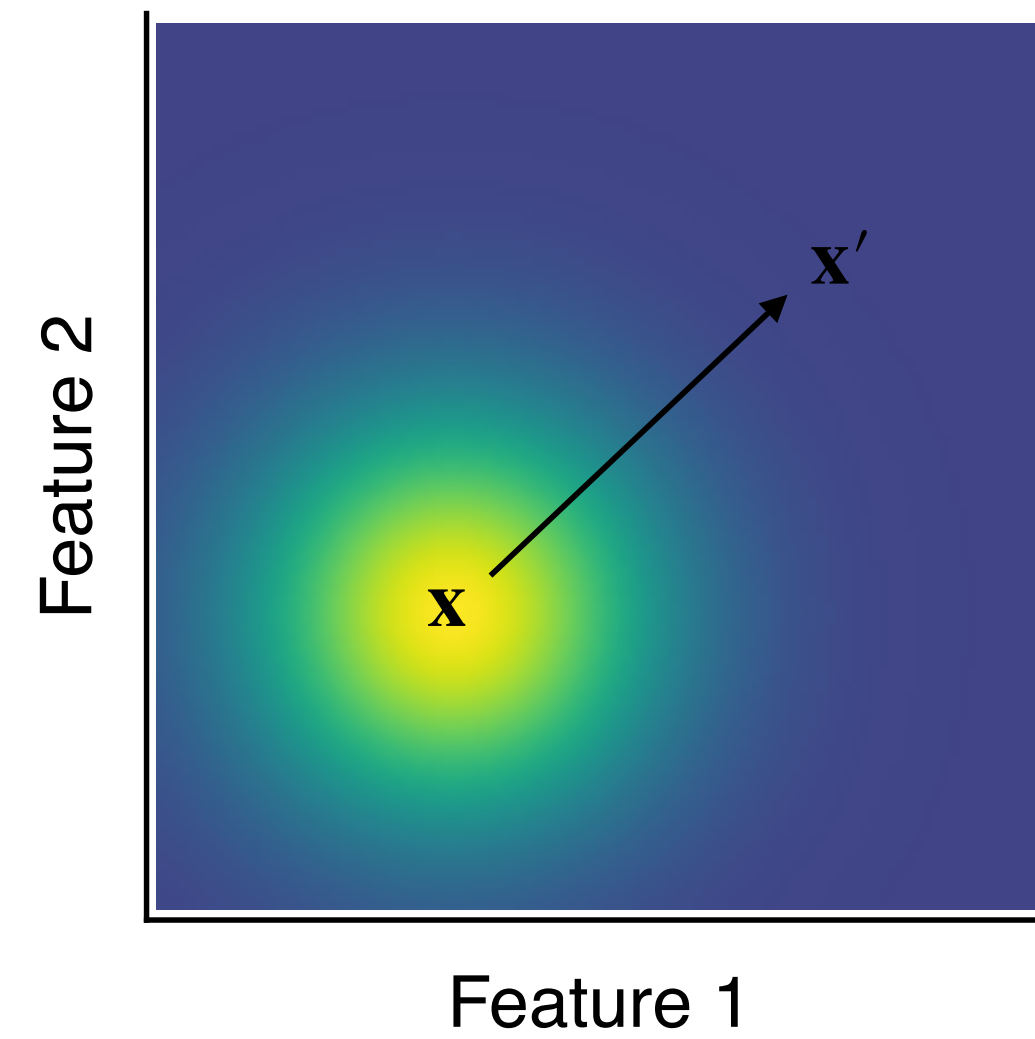
From continuous to structured spaces



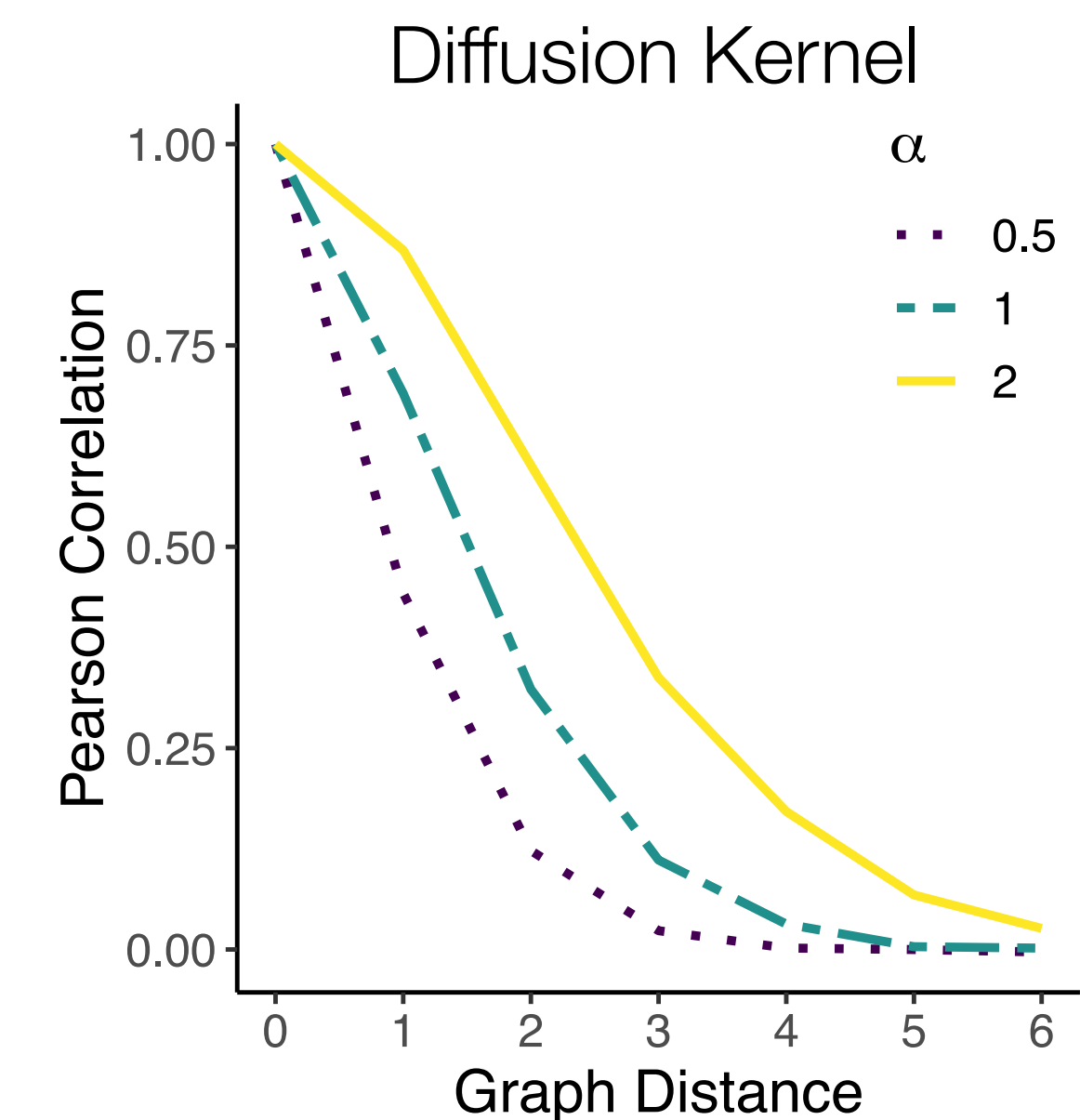
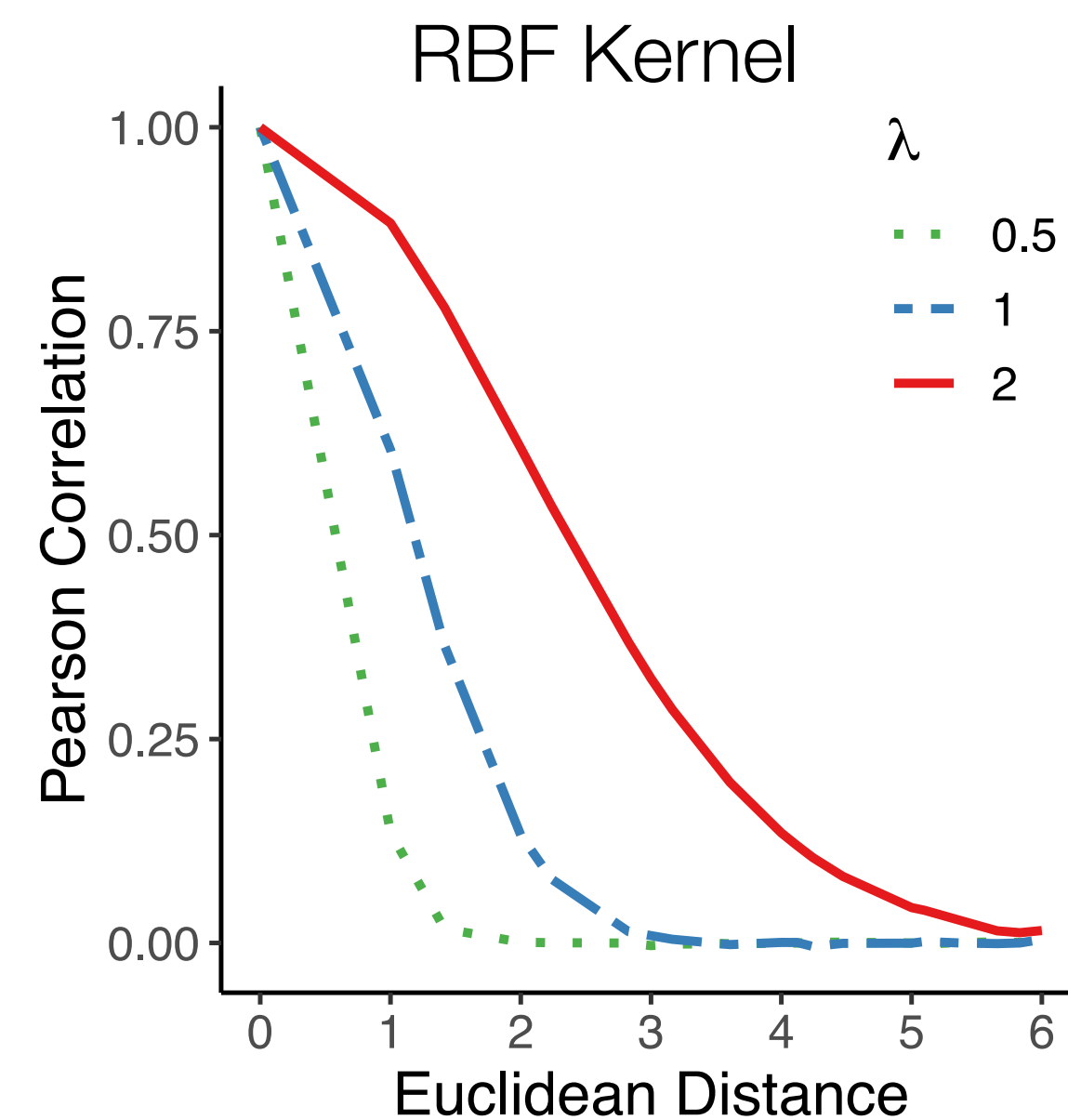
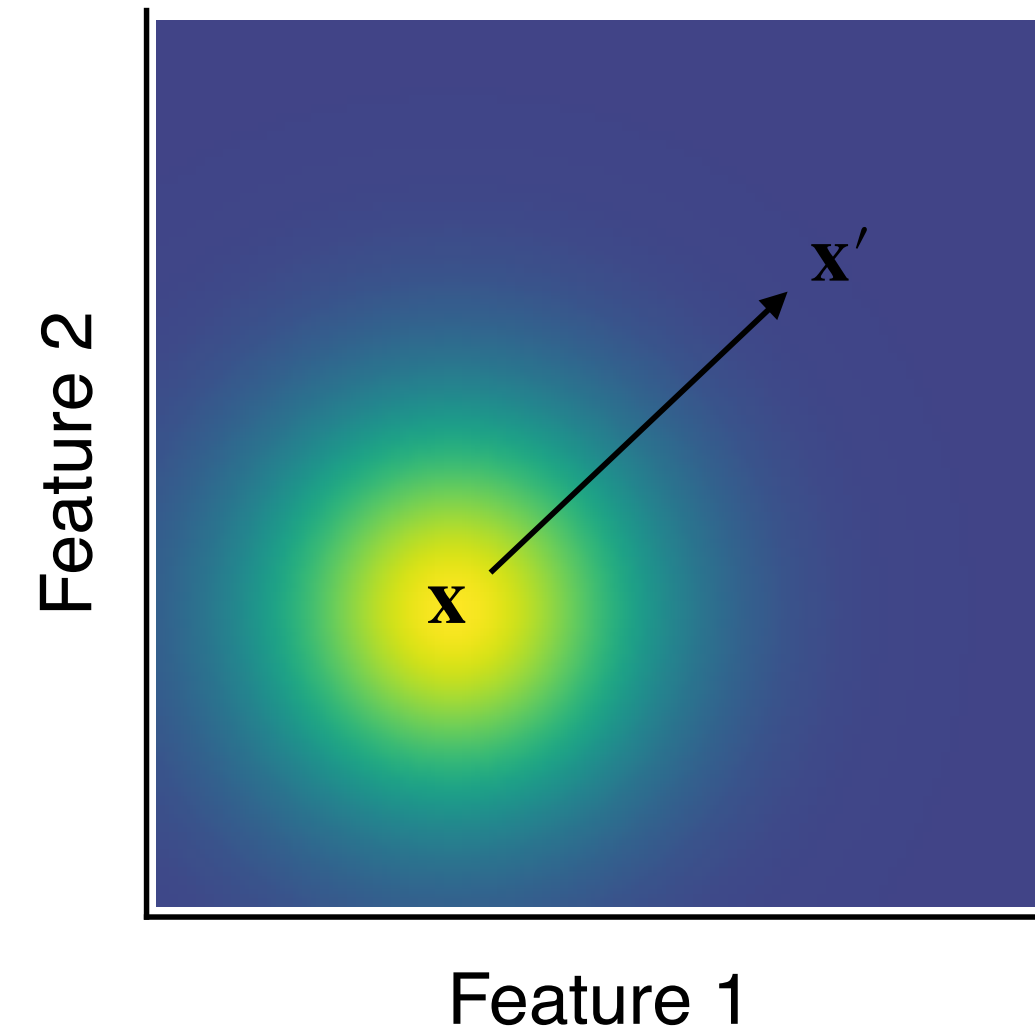
From continuous to structured spaces



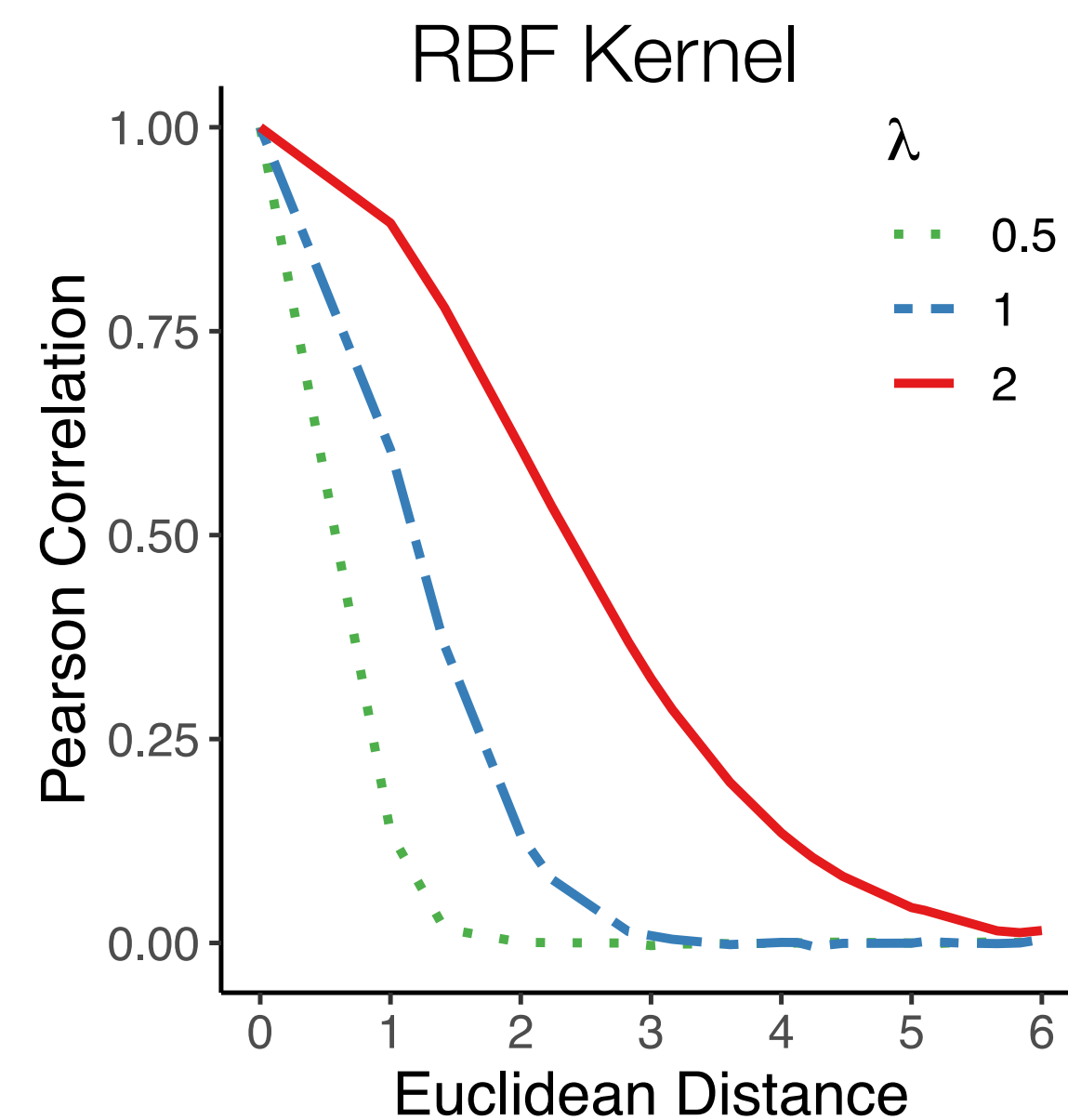
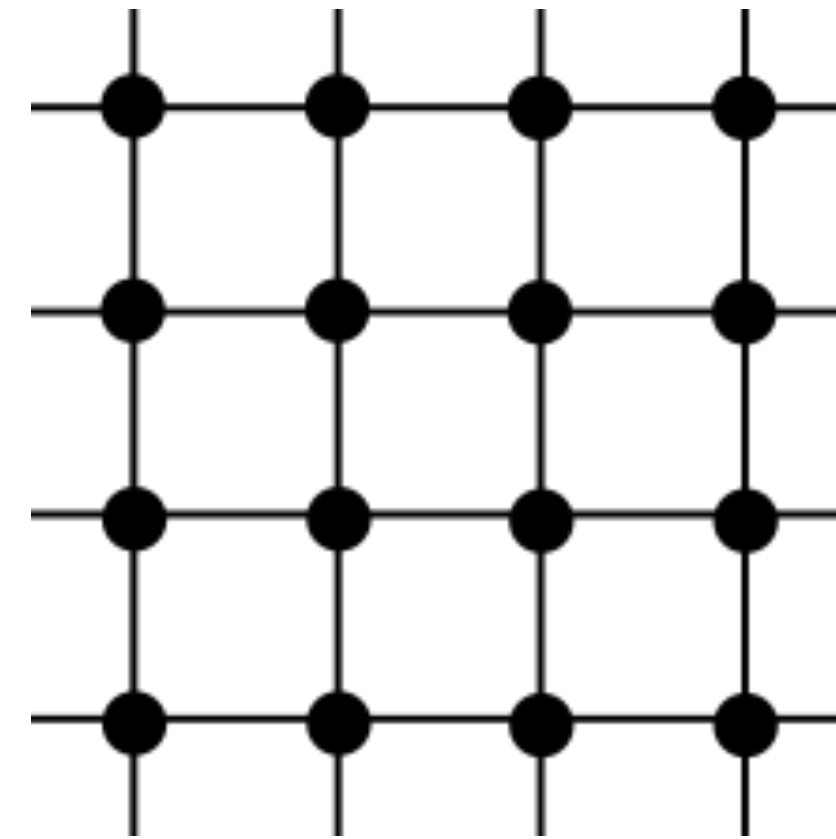
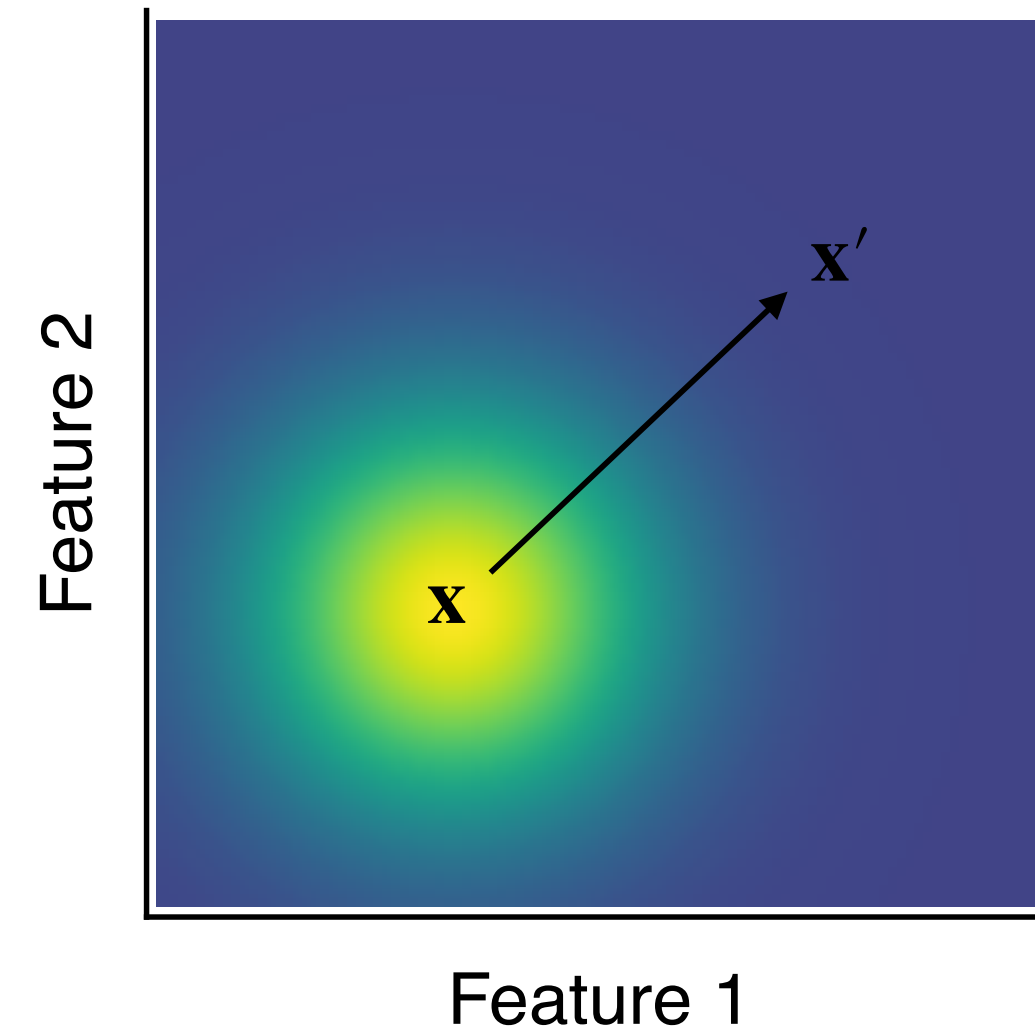
From continuous to structured spaces



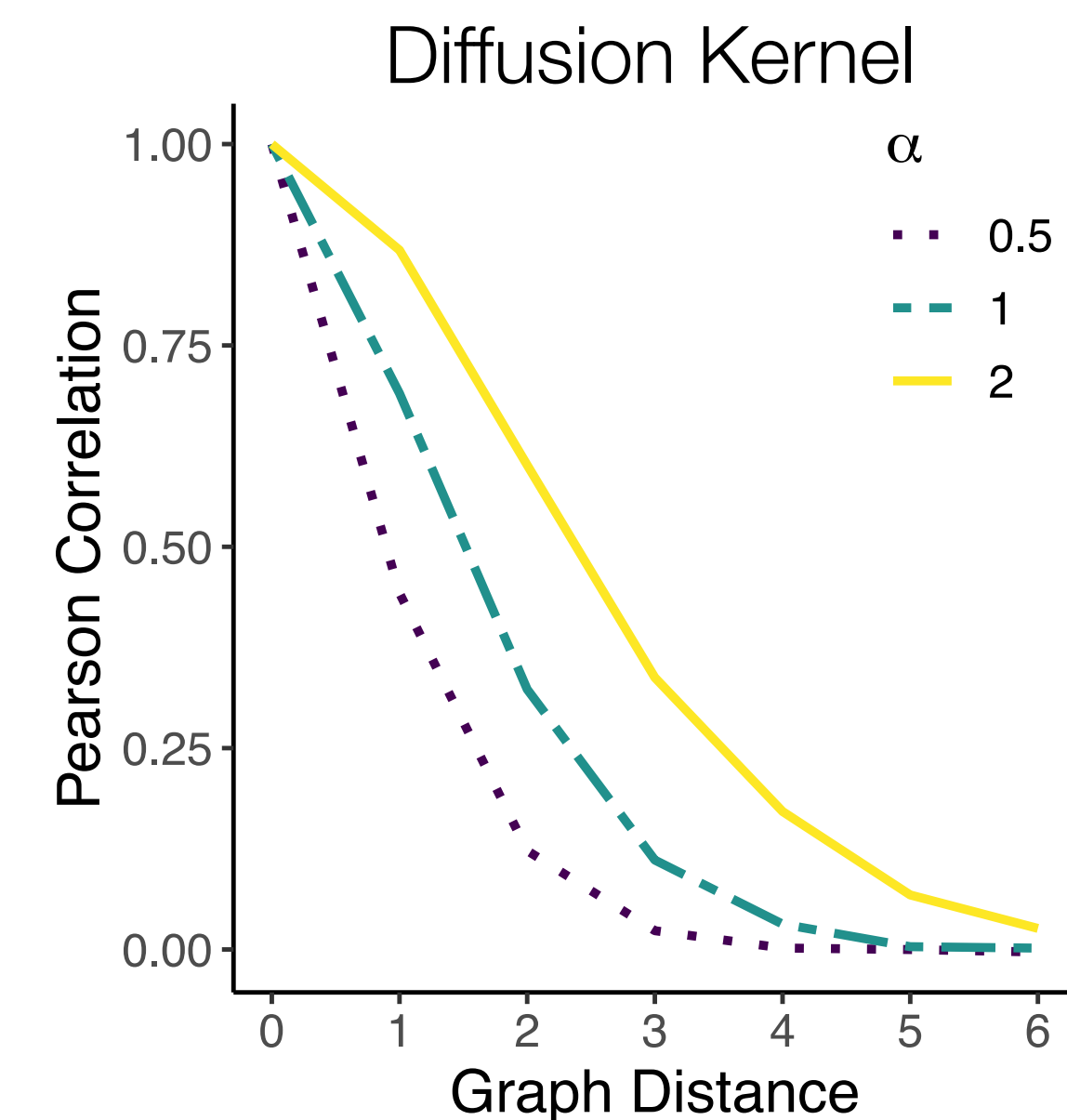
From continuous to structured spaces



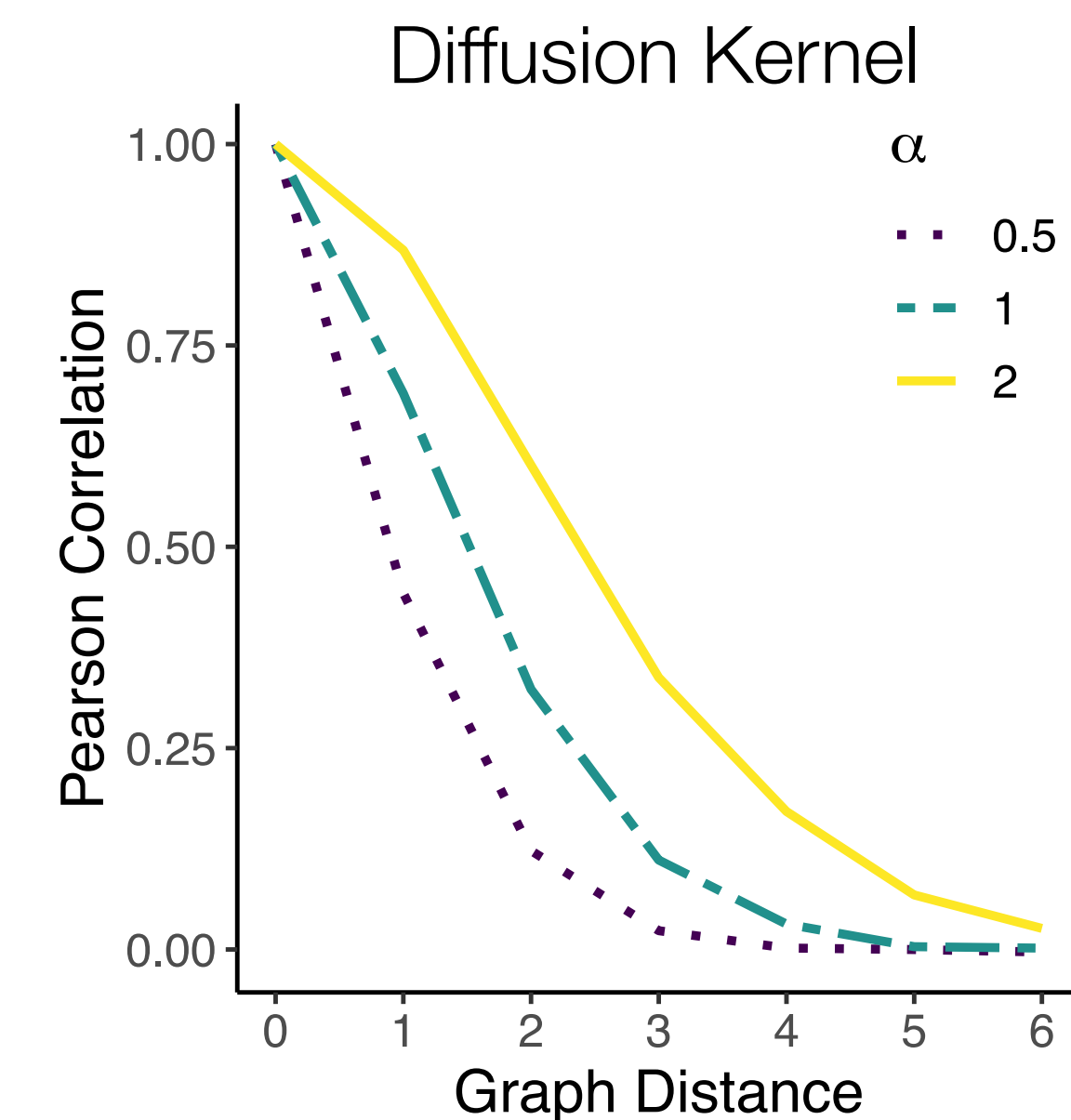
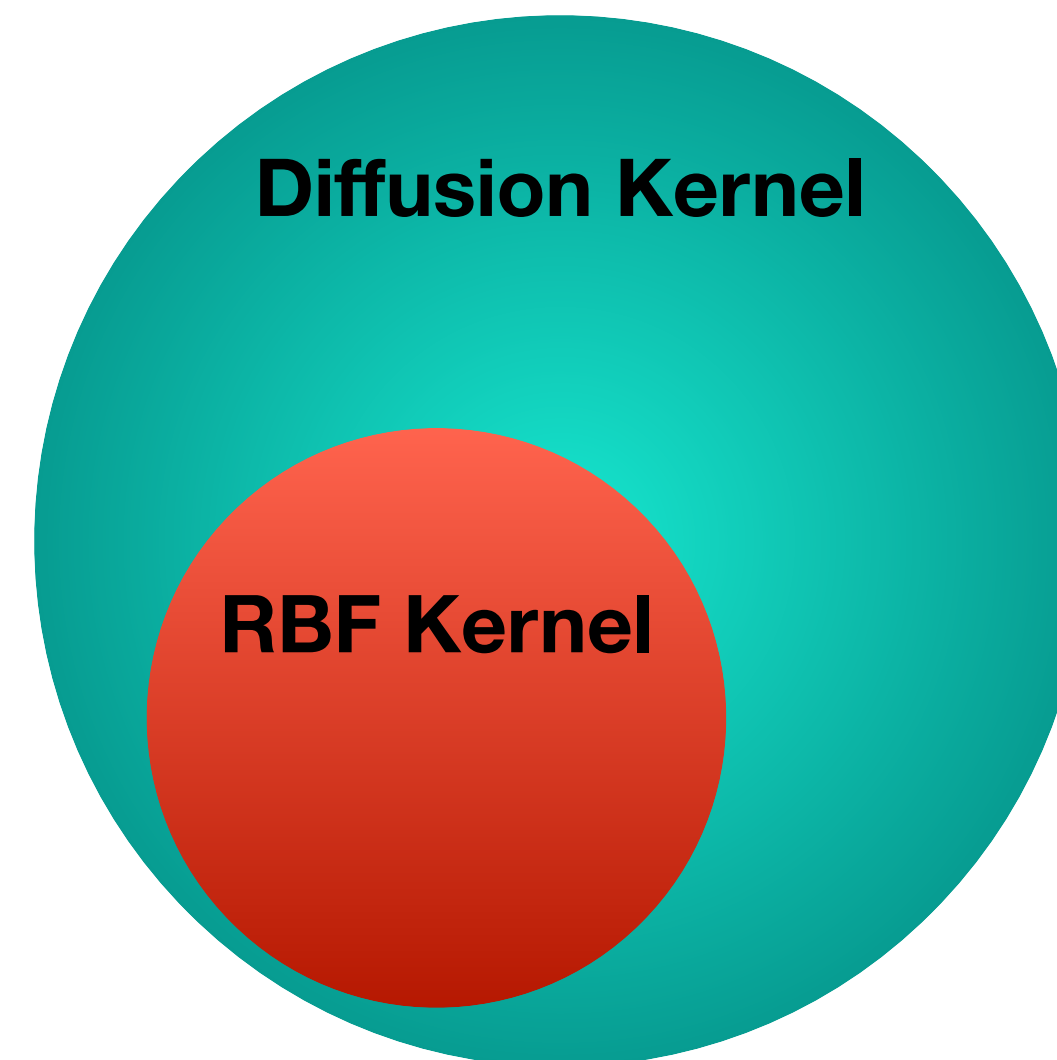
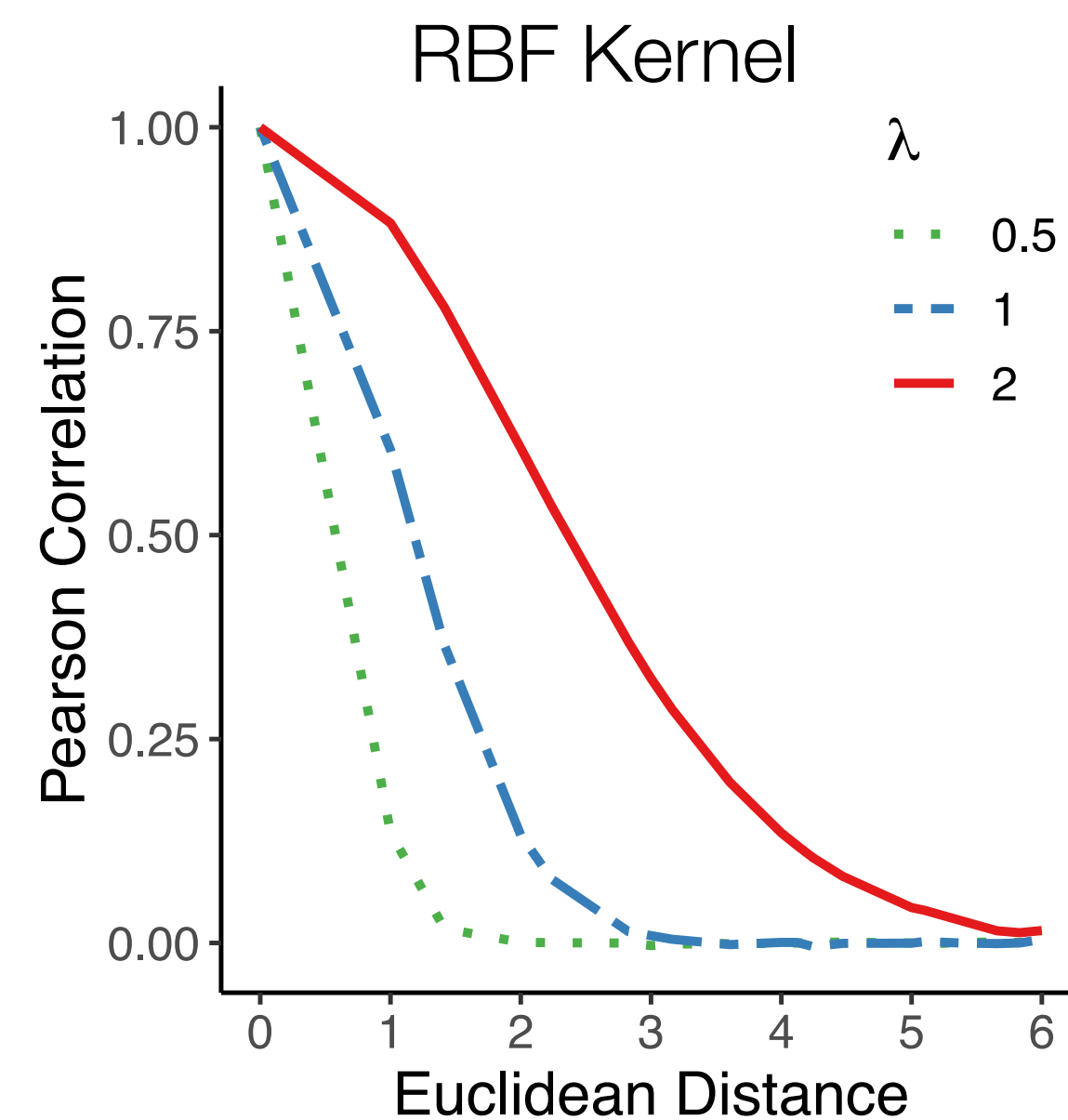
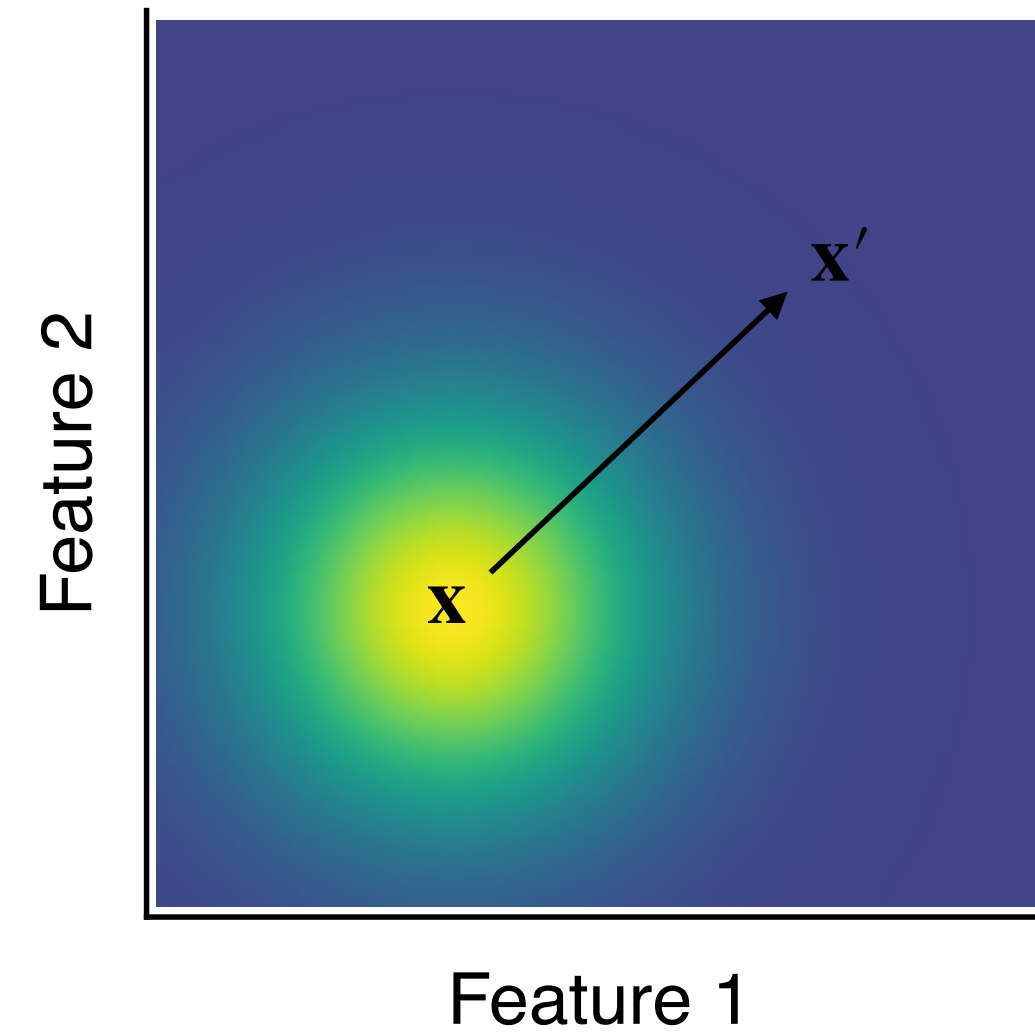
From continuous to structured spaces



==

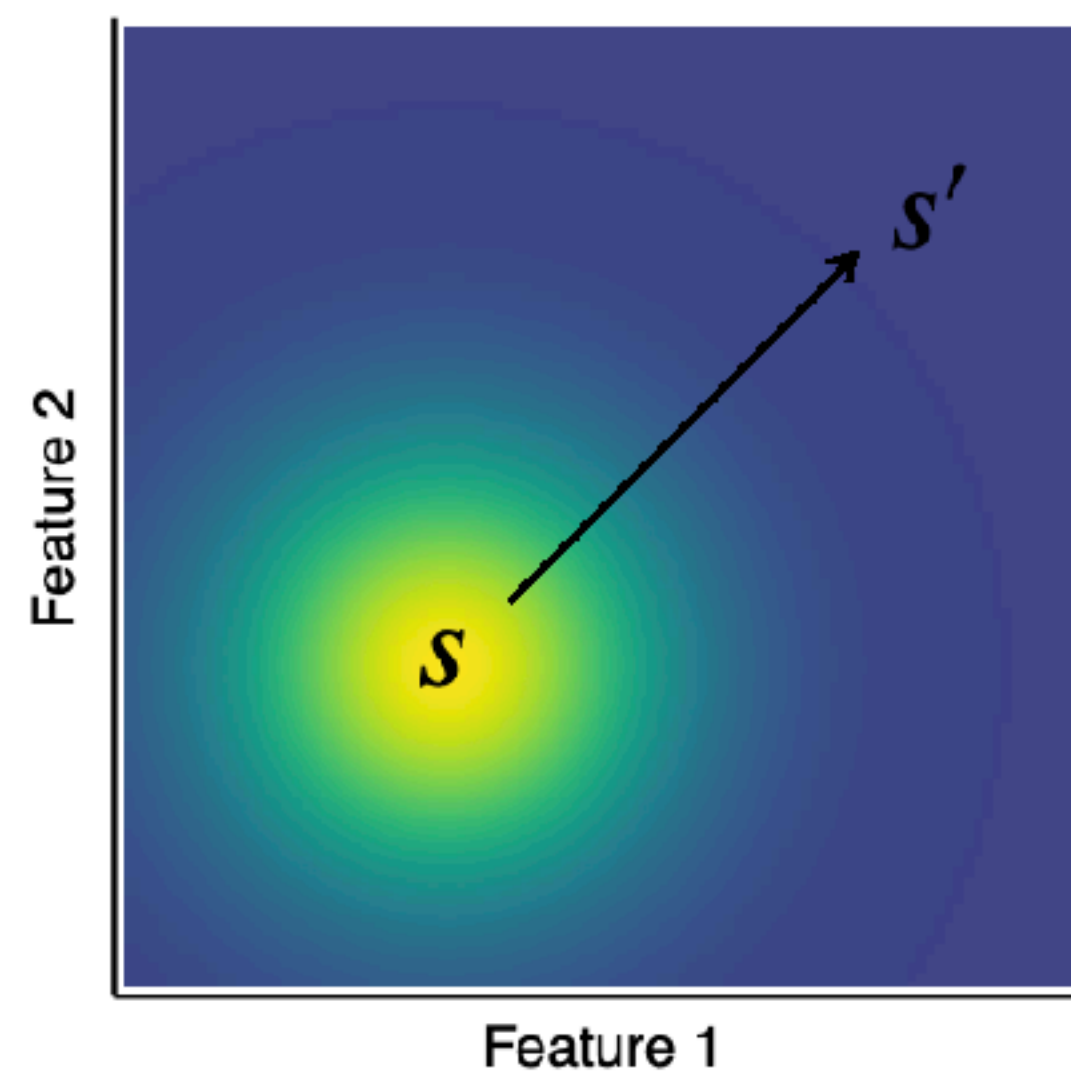


From continuous to structured spaces

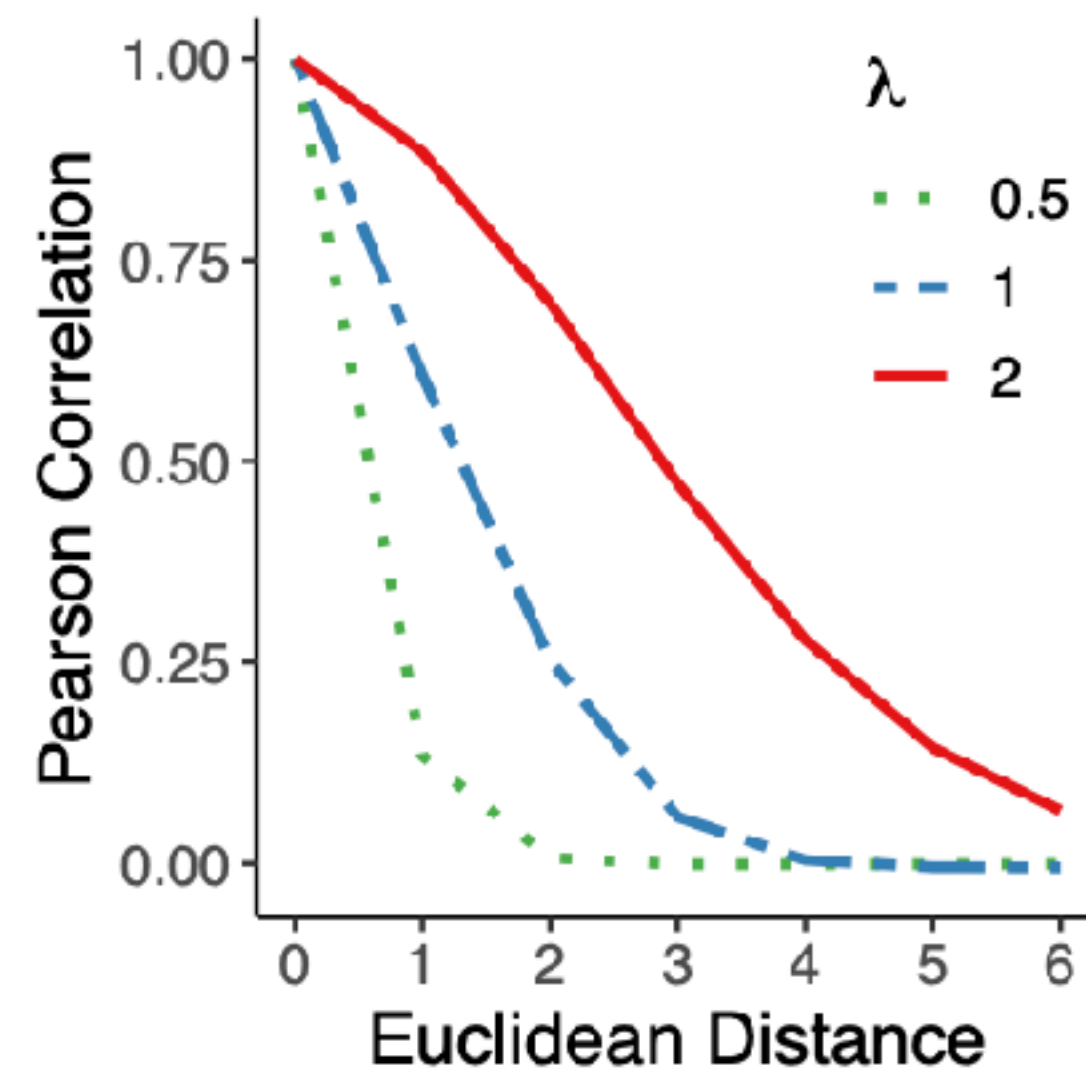


Continuous

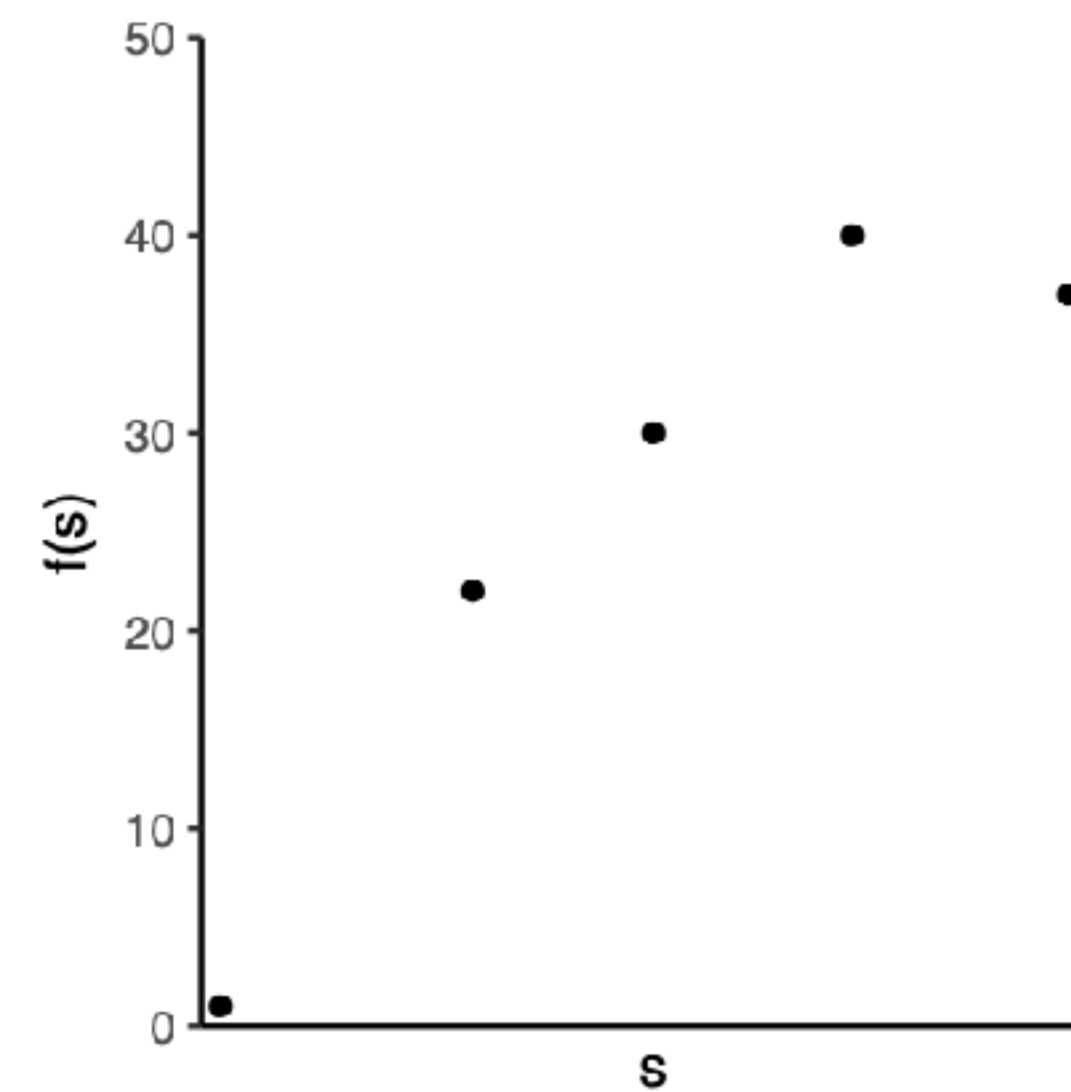
Similarity



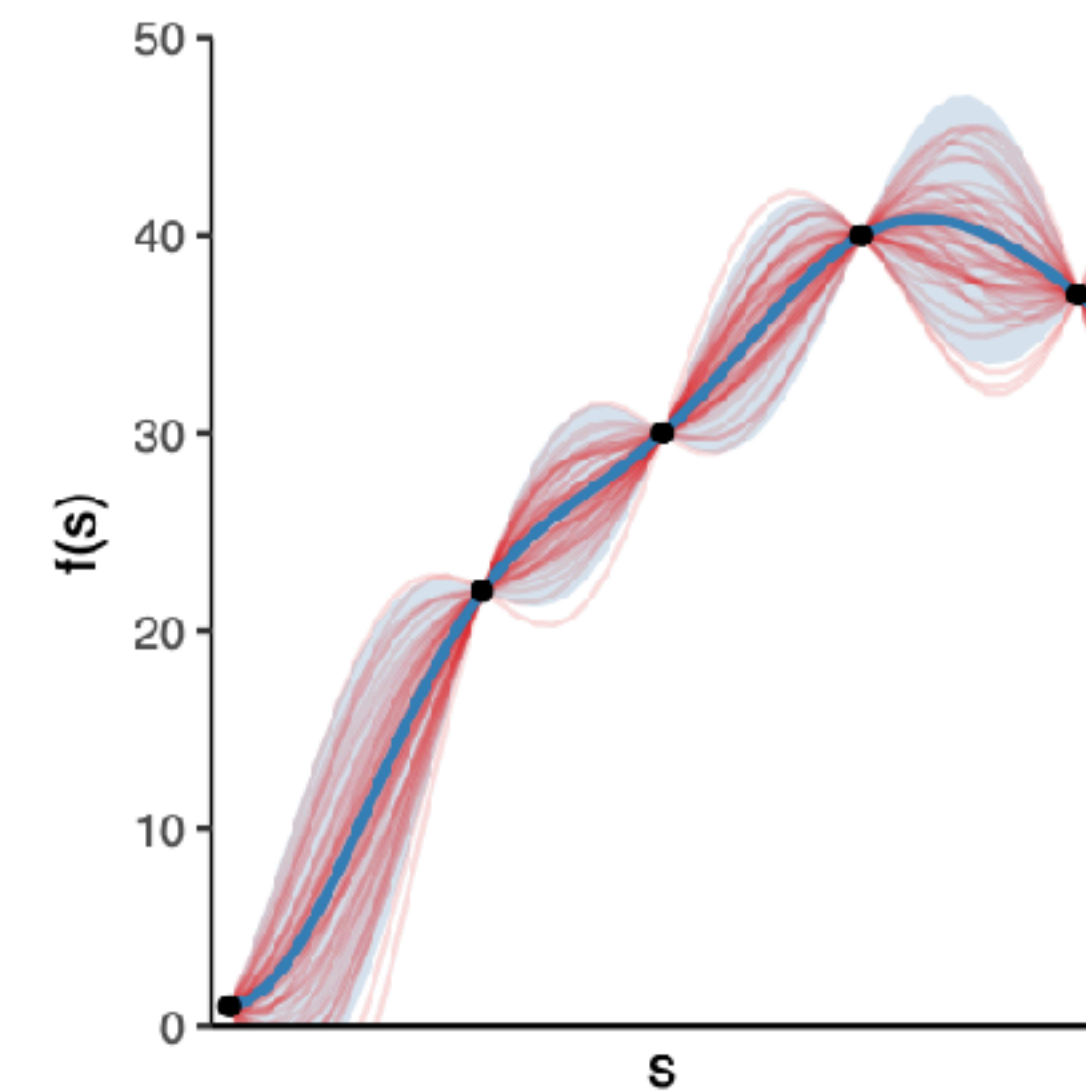
Kernel



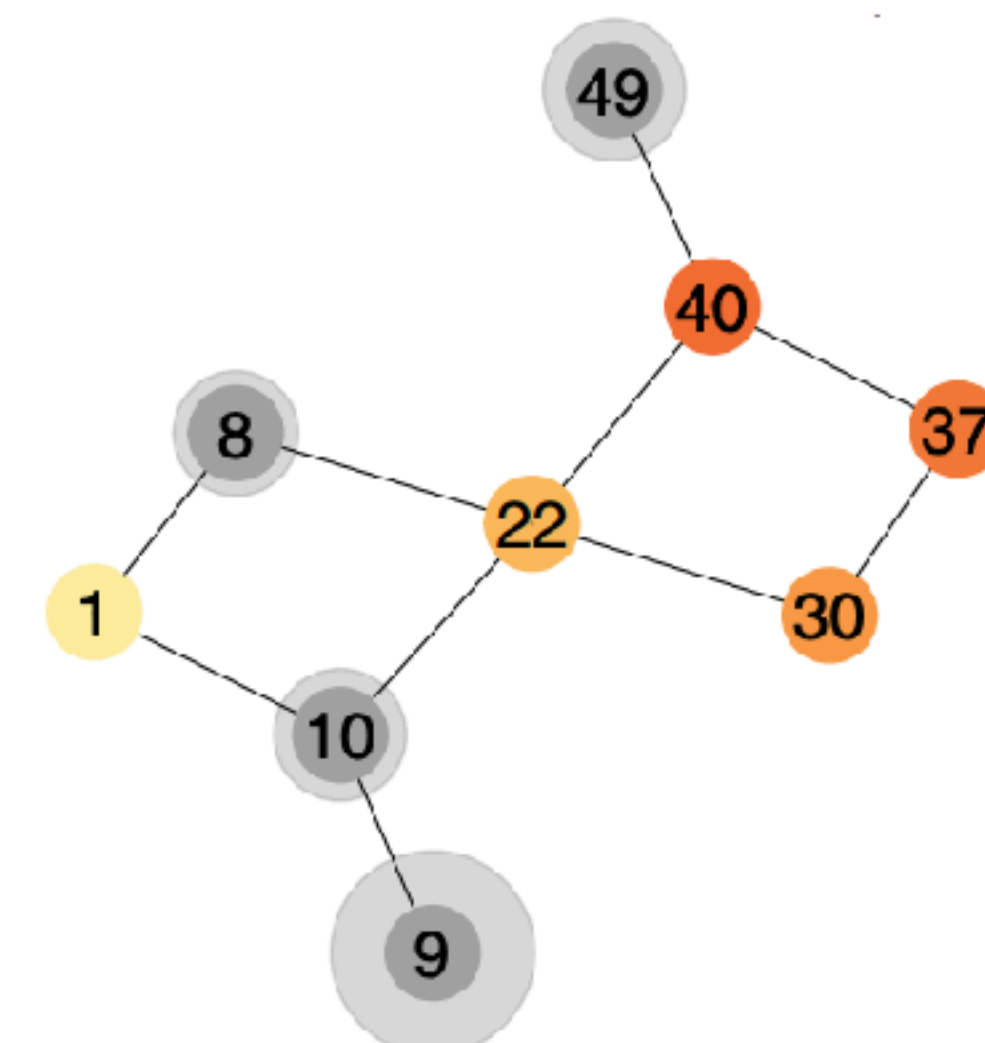
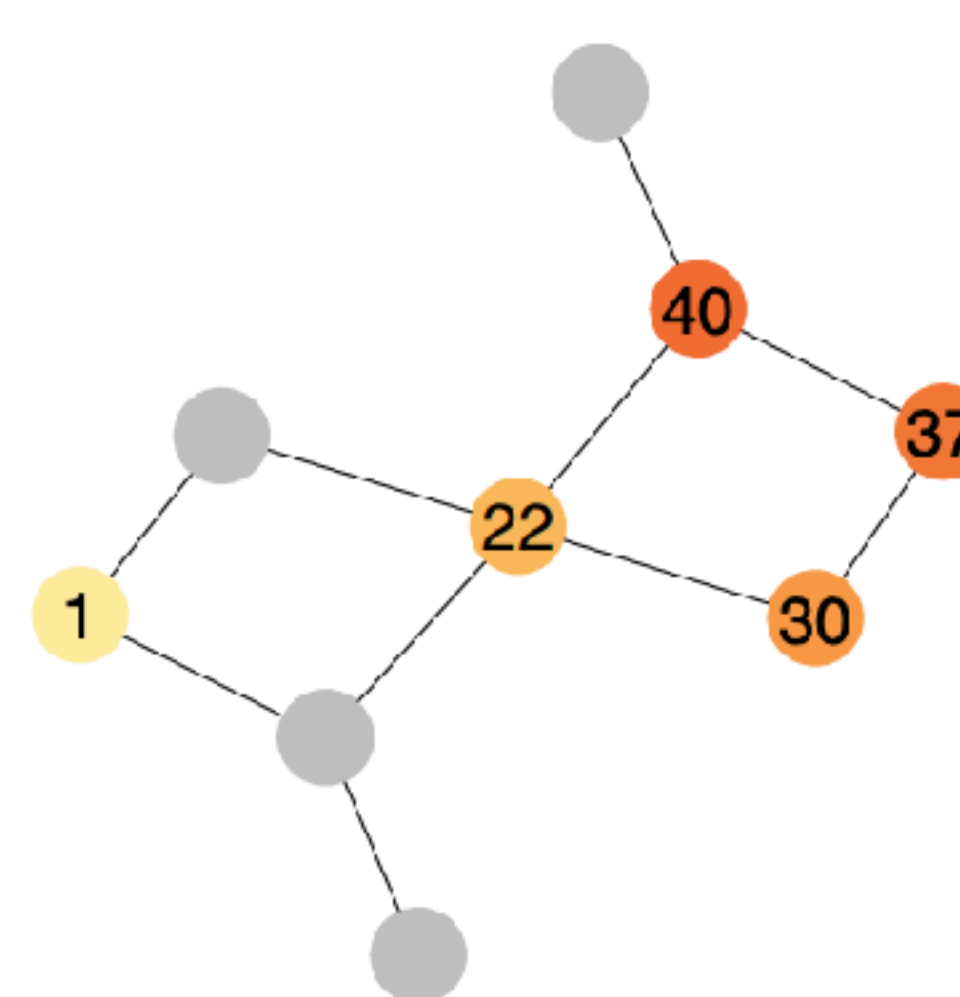
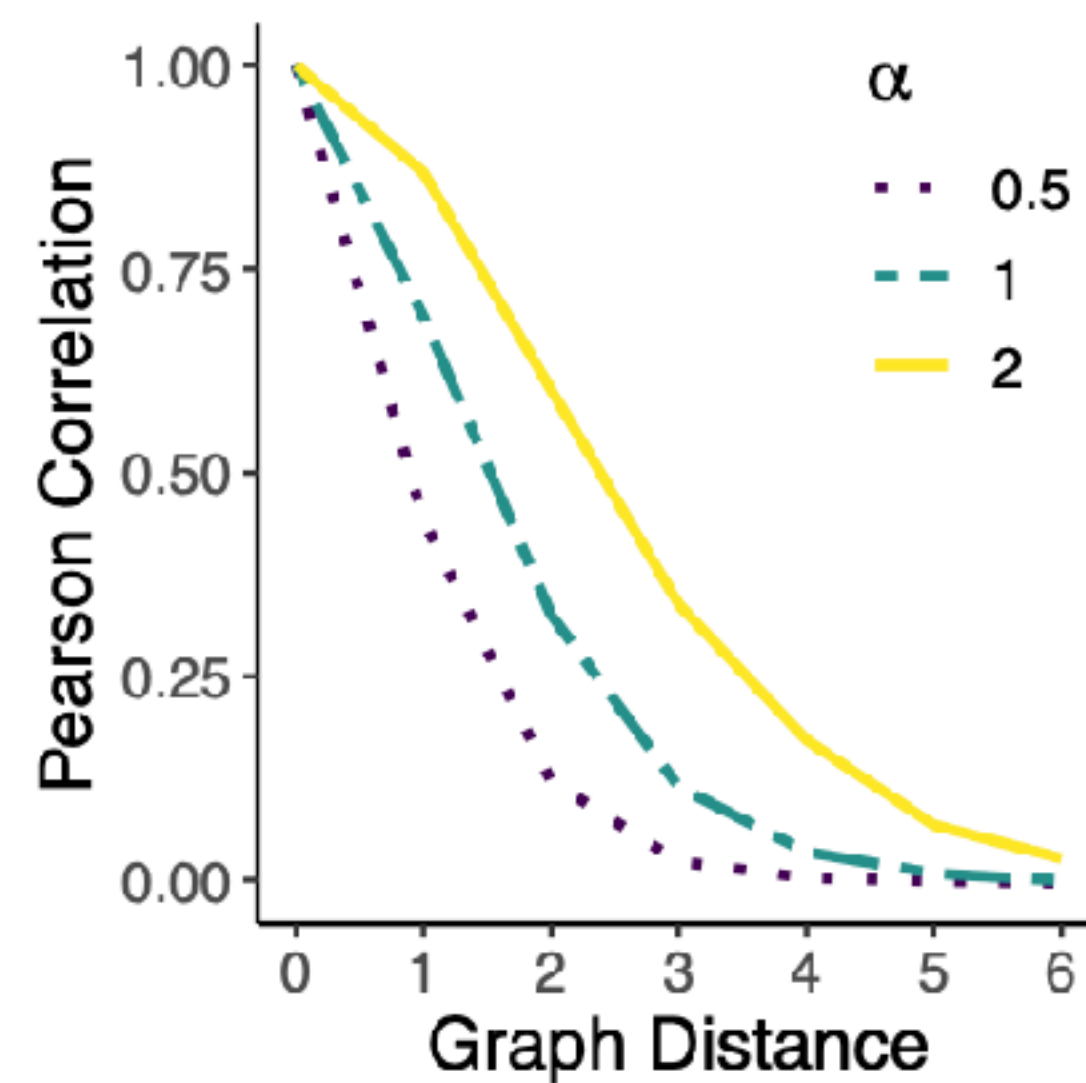
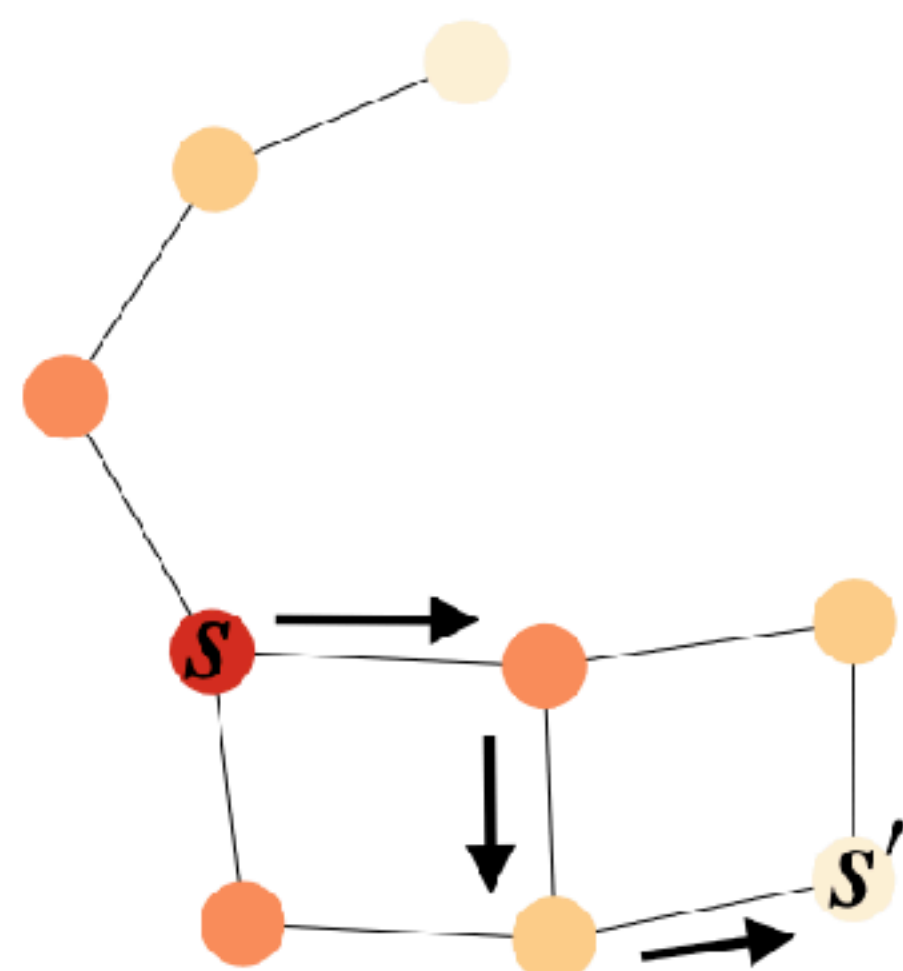
Observations



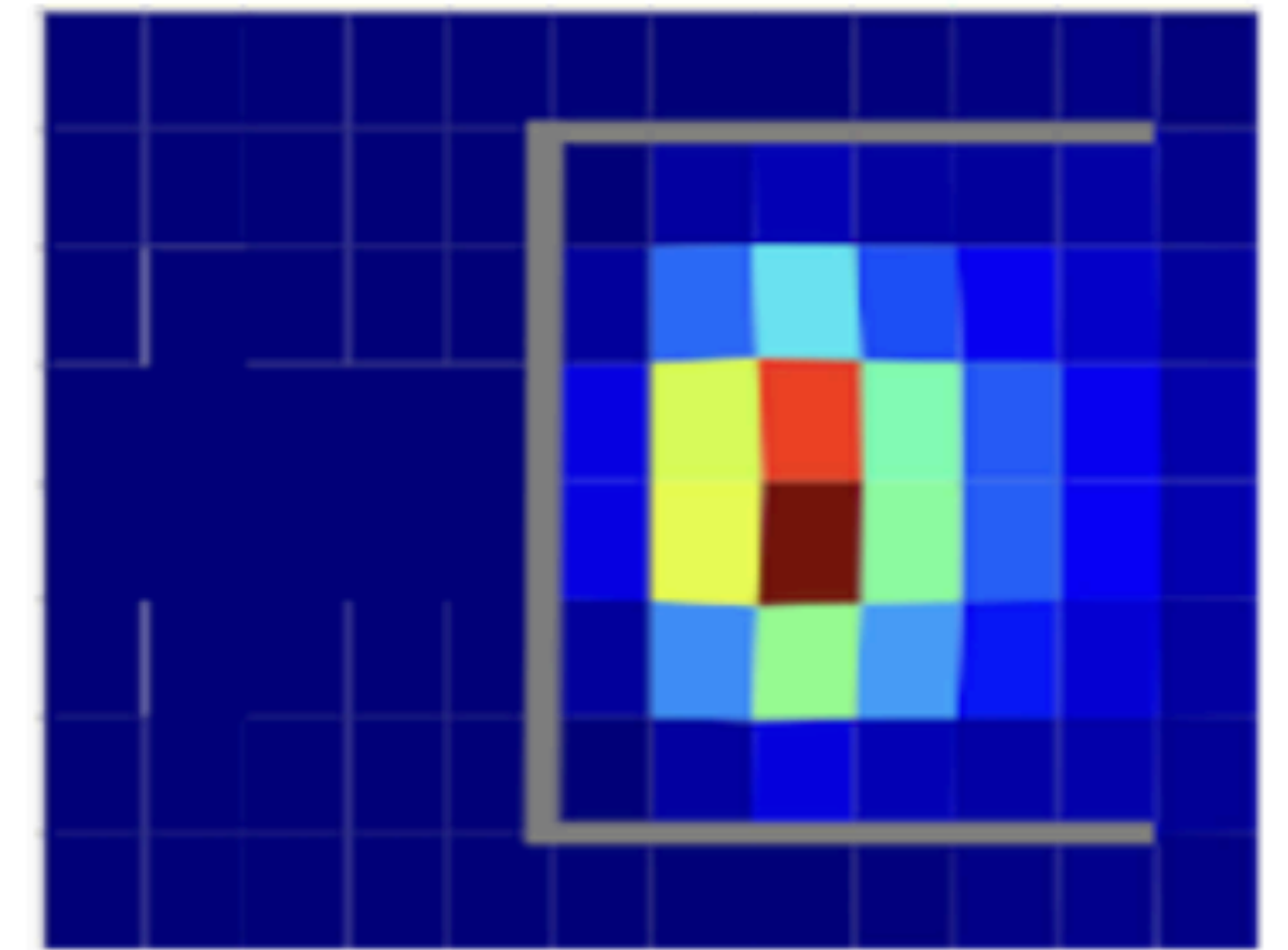
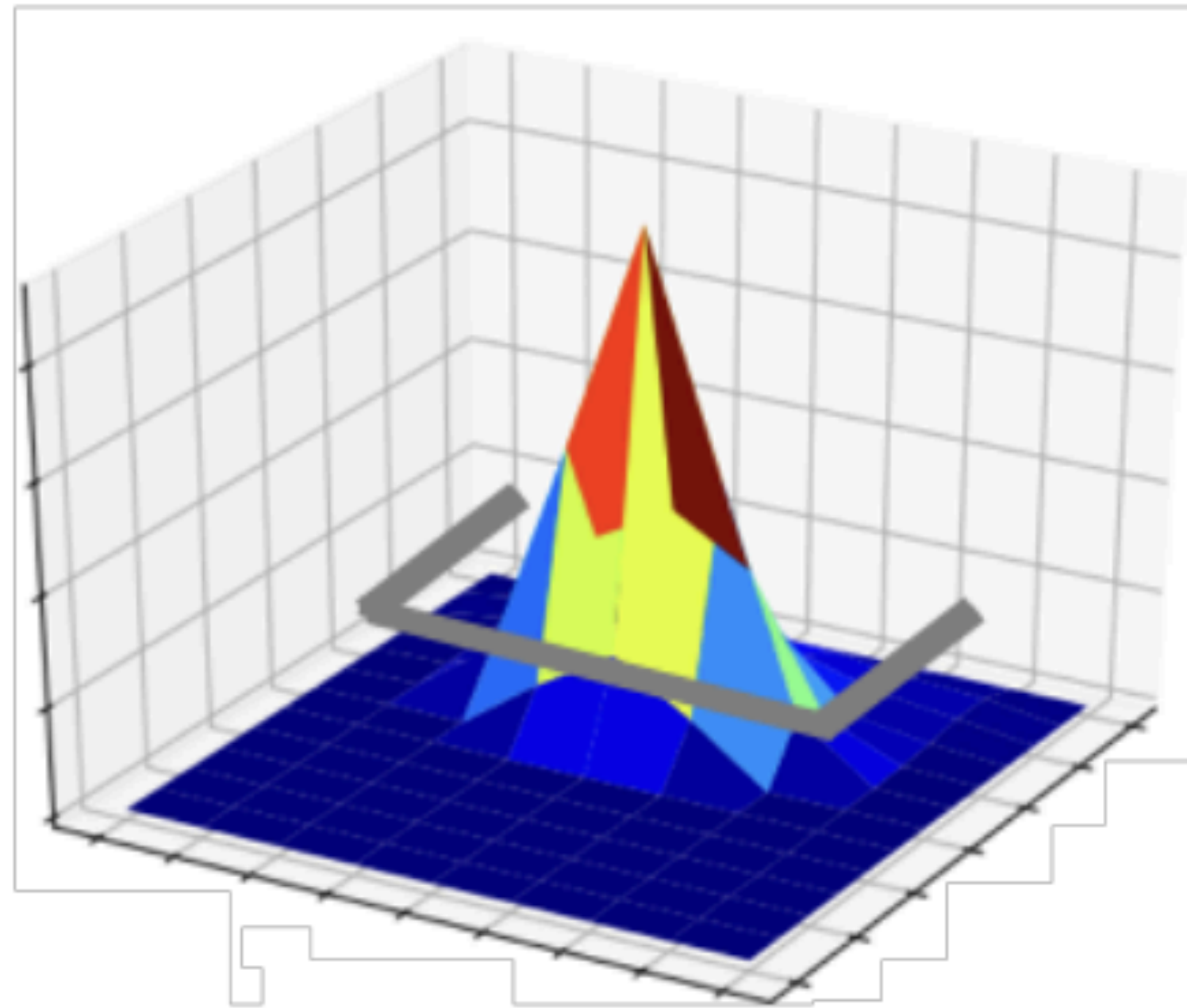
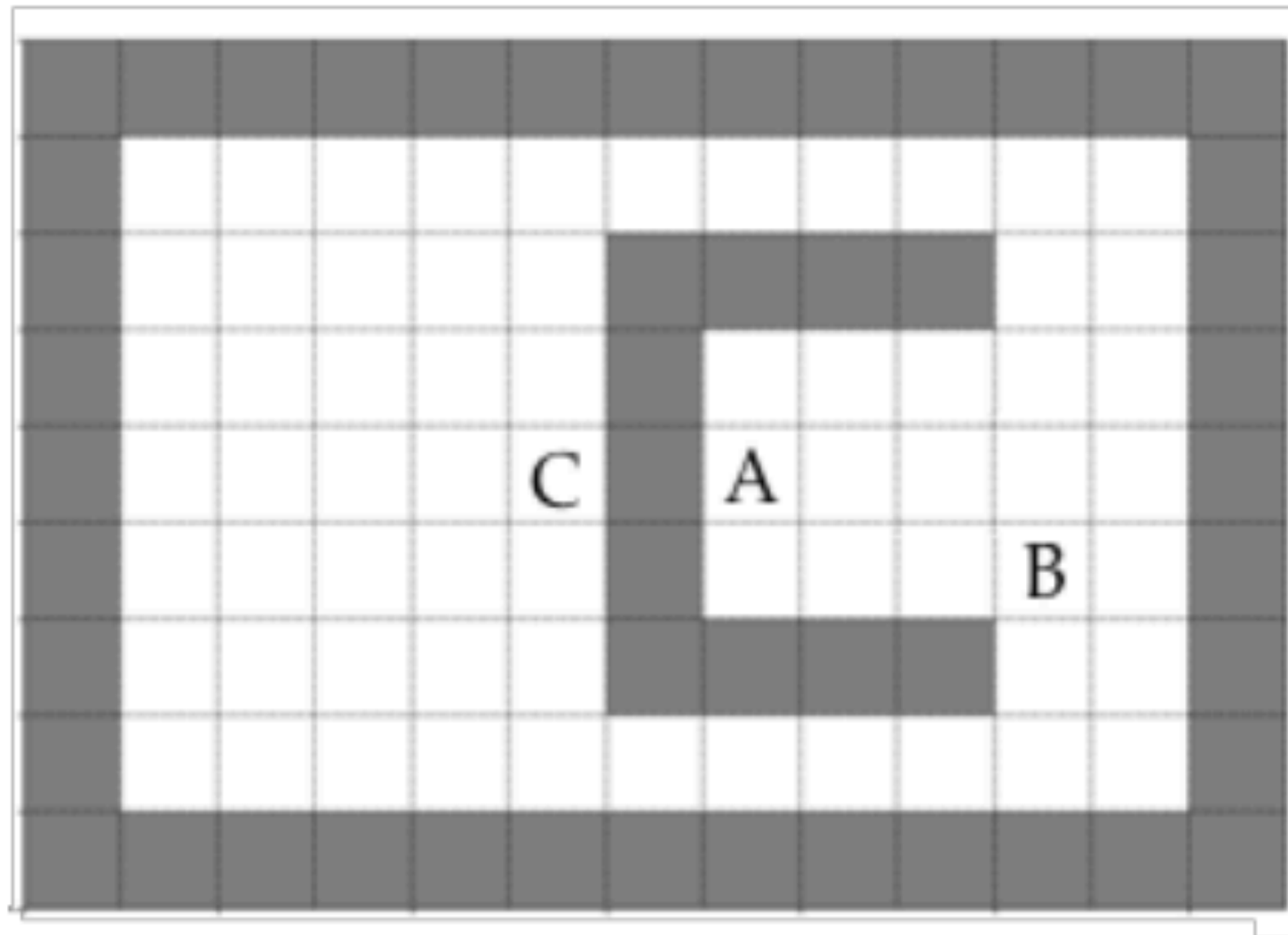
Predictions



Discrete



Generalization based on transition dynamics



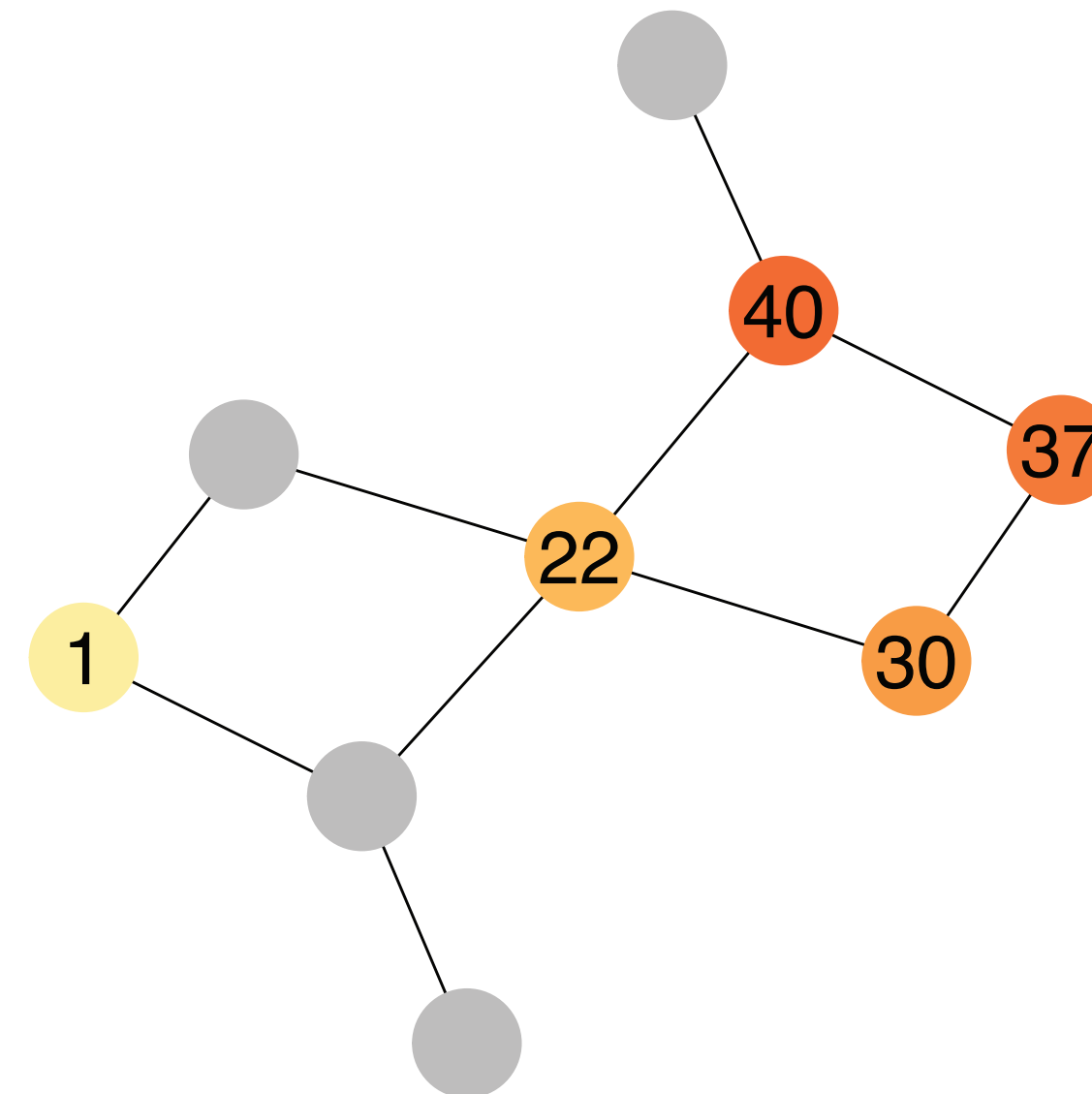
Machado et al. (*ICLR* 2018)

- A indicates a reward
- Even though C is closer than B, the transition dynamics of the environment make it easier for B to reach A

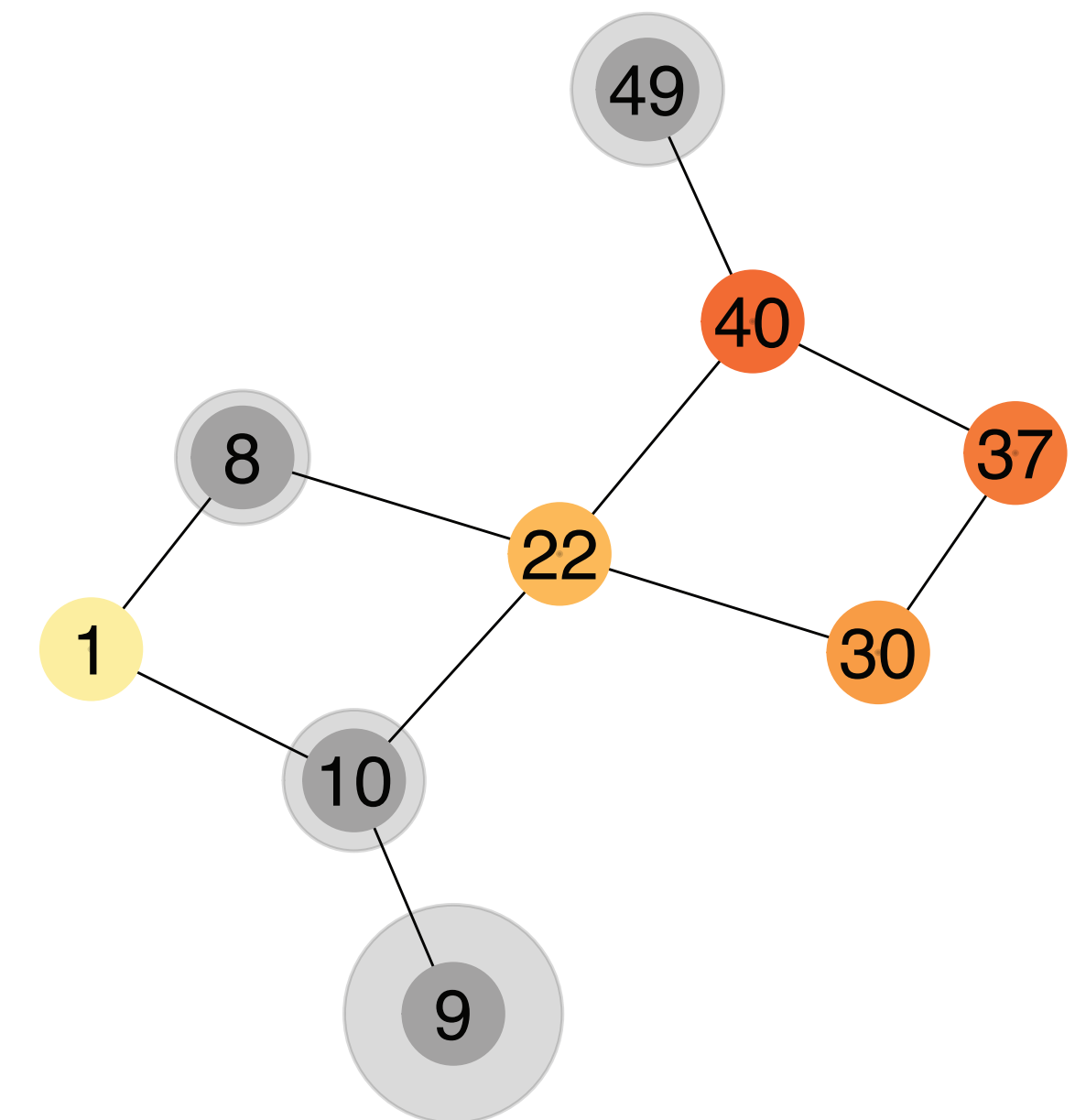
Diffusion Kernel

- Rather than similarity between features, we use the connectivity structure of the graph to define similarity
- $$k_{DF}(s, s') = \exp(-\alpha L)$$
- Where L is the graph Laplacian
 - α is a free parameter (diffusion level)
 - The diffusion kernel assumes function values diffuse across the graph according to a random walk

Observations



Predictions (with uncertainty)

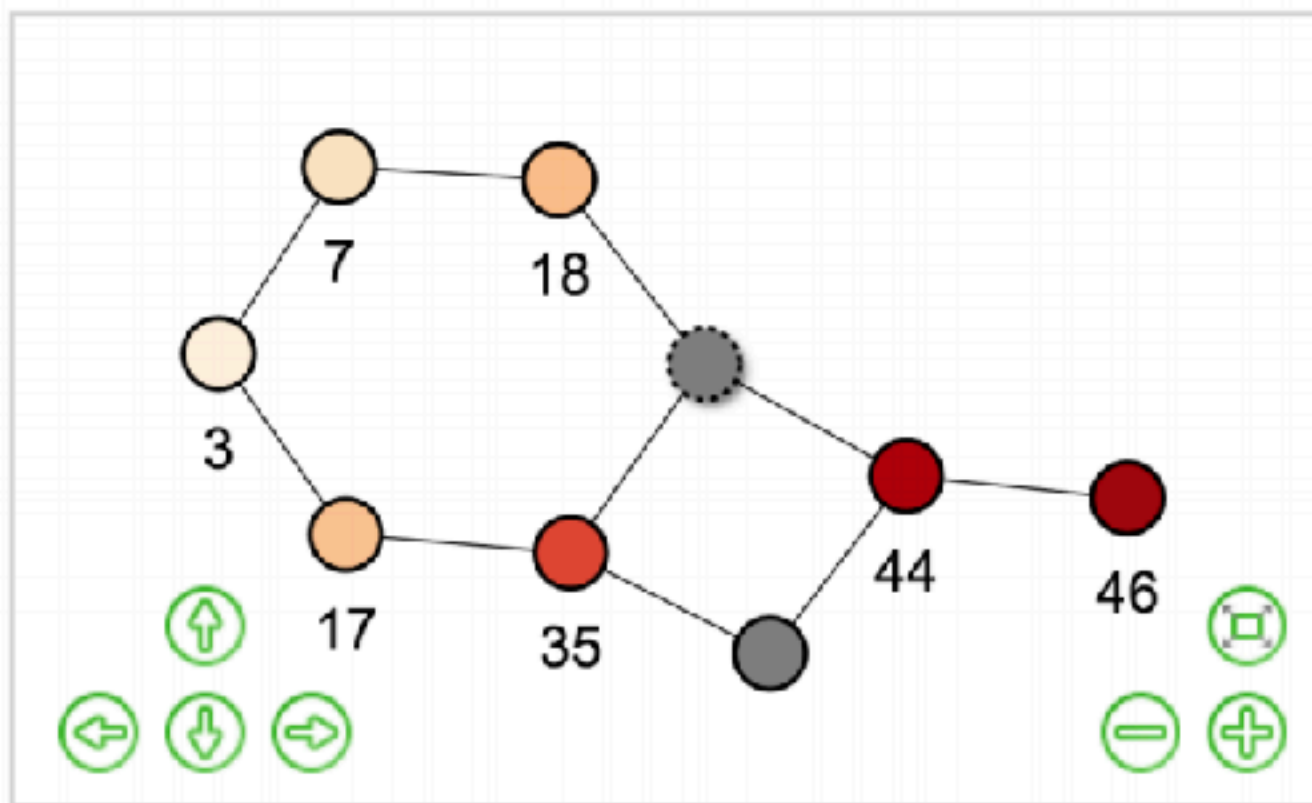


Experiment 1

Prediction Task

Current Network: 4/30

Current Weighted Error: 10.19



How many passengers do you think will be observed at the selected station?

Few Many

How confident are you?

Not very confident Highly confident

Submit

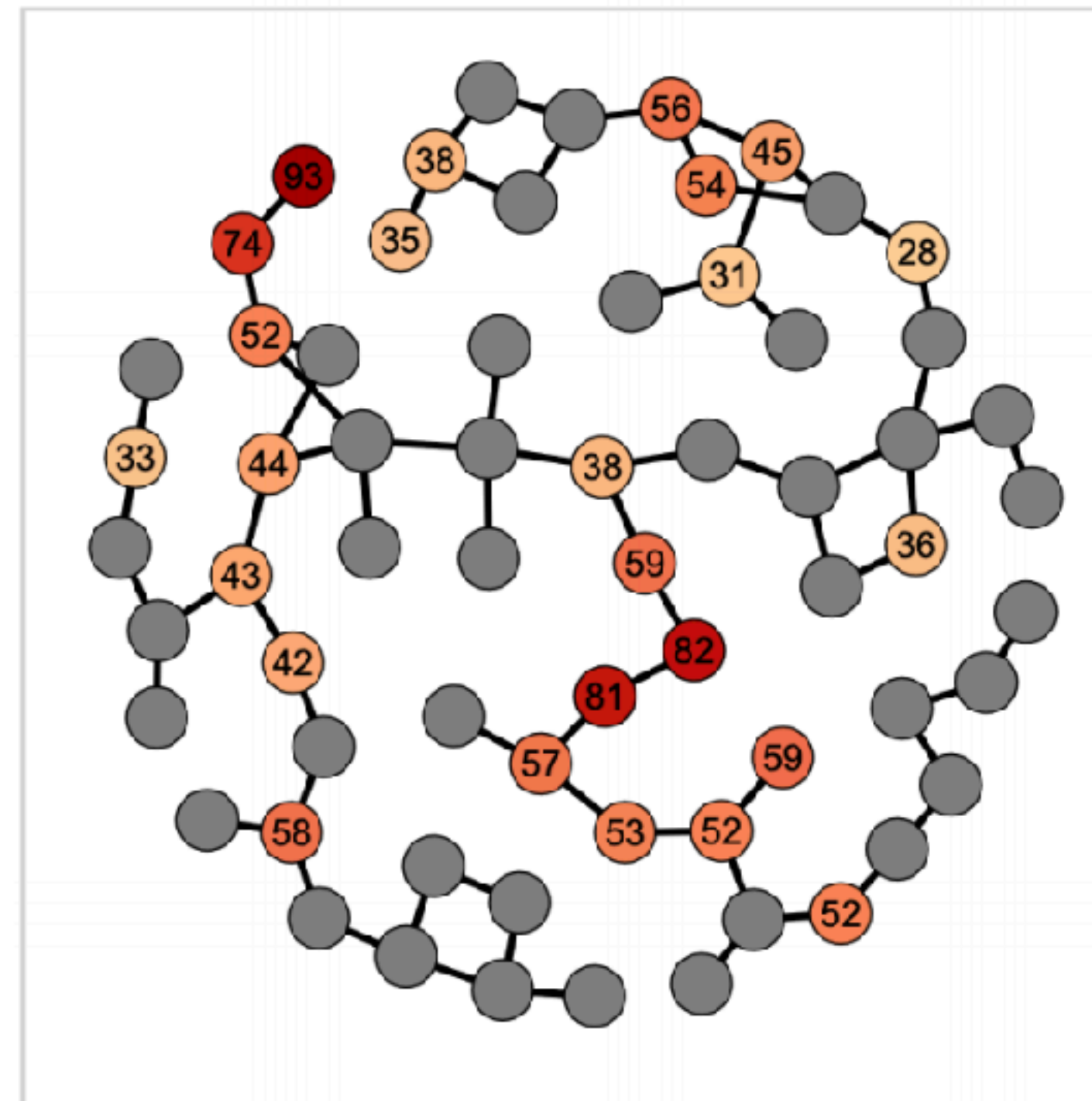
Experiment 2

Bandit Task

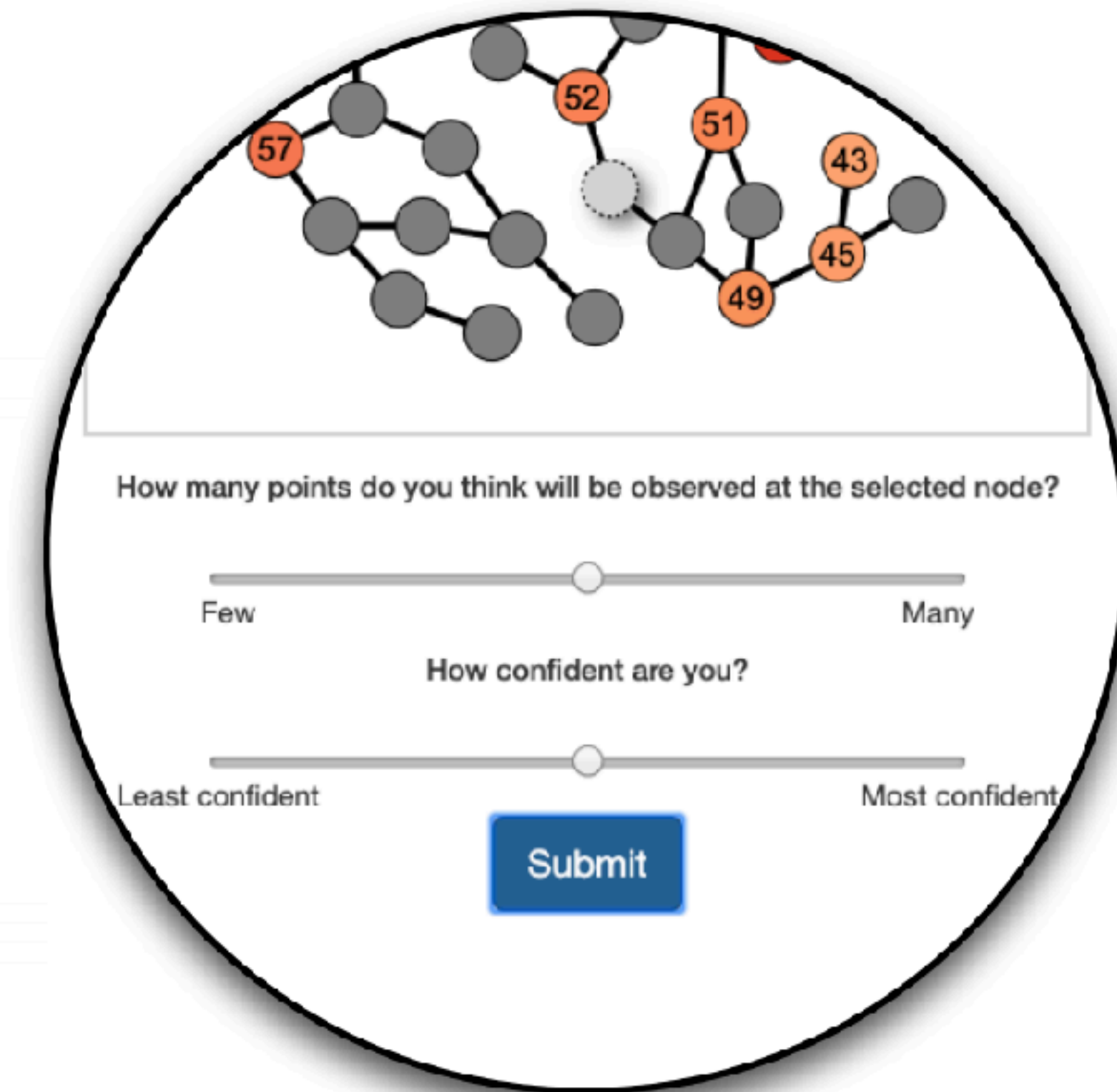
Current Score: 1296

Clicks remaining: 1

Current round: 1/10



Bonus Round

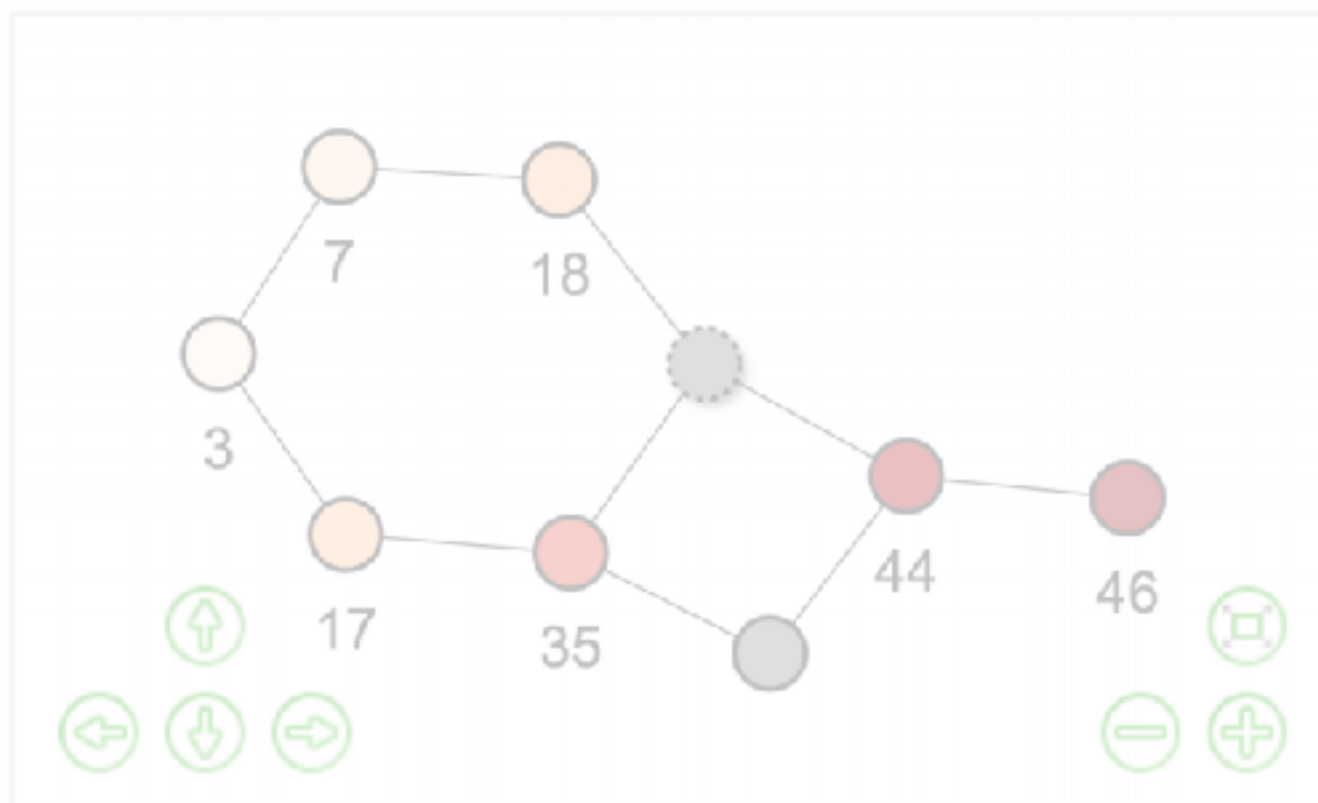


Experiment 1

Prediction Task

Current Network: 4/30

Current Weighted Error: 10.19



How many passengers do you think will be observed at the selected station?

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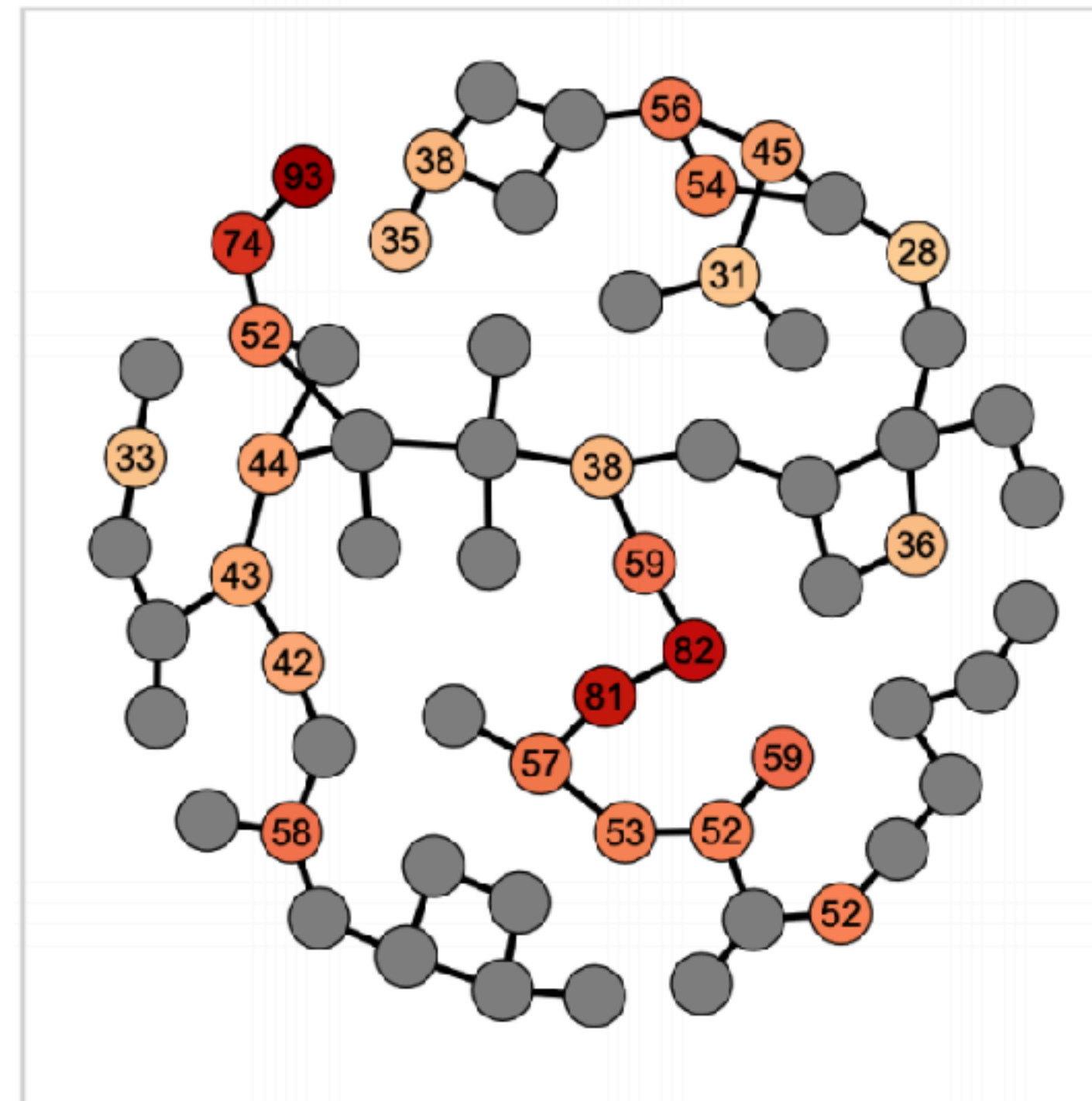
Experiment 2

Bandit Task

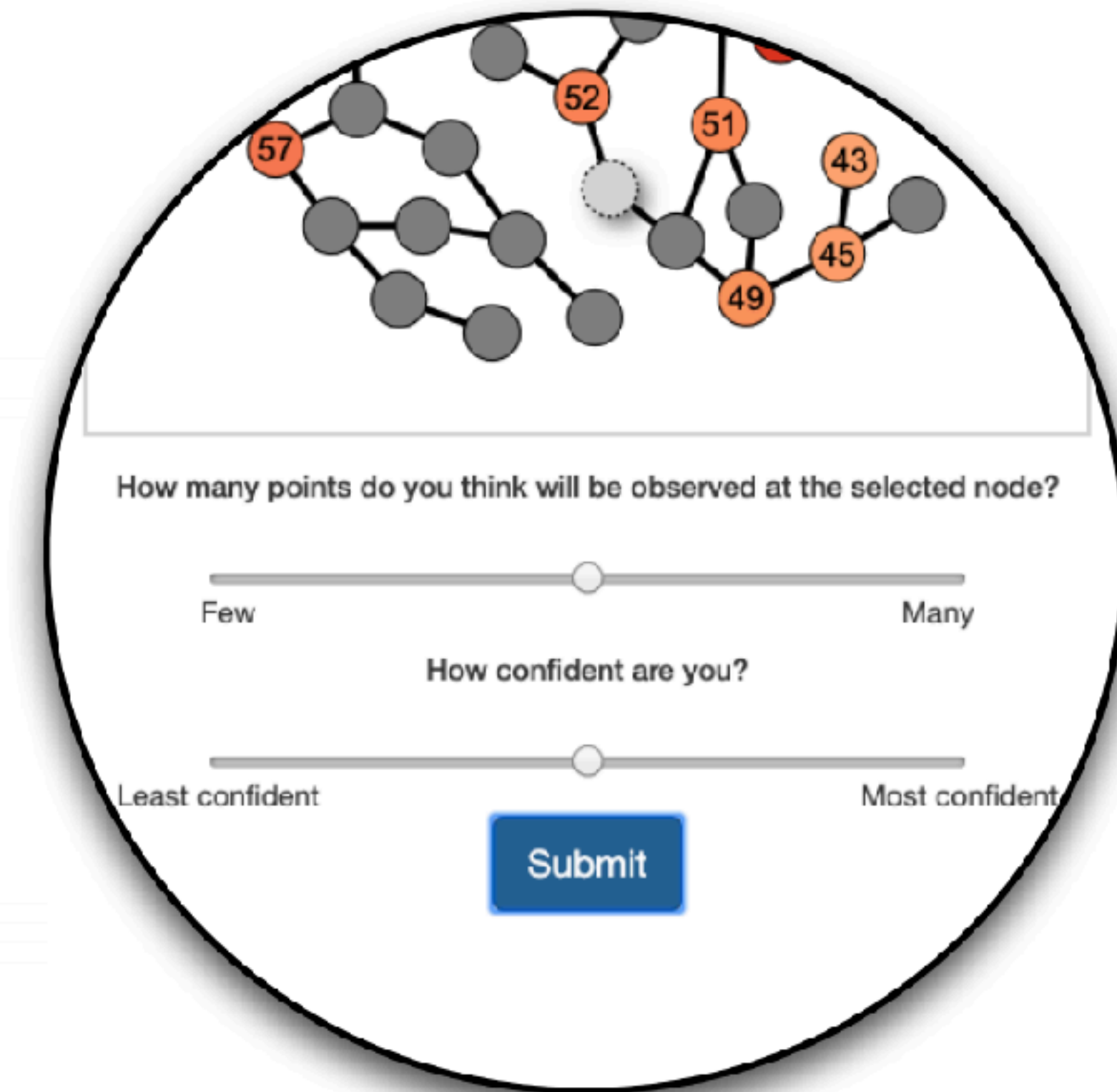
Current Score: 1296

Clicks remaining: 1

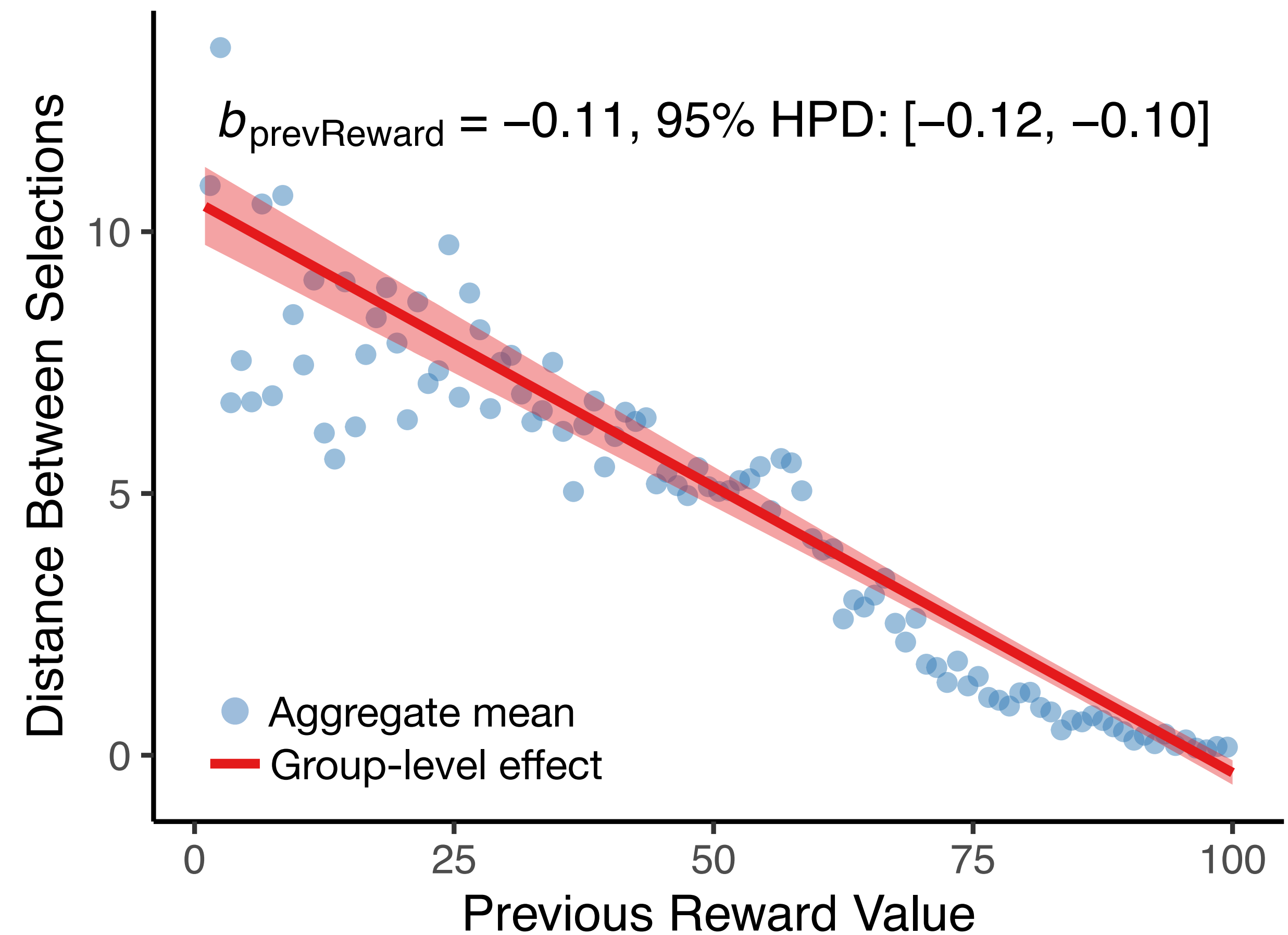
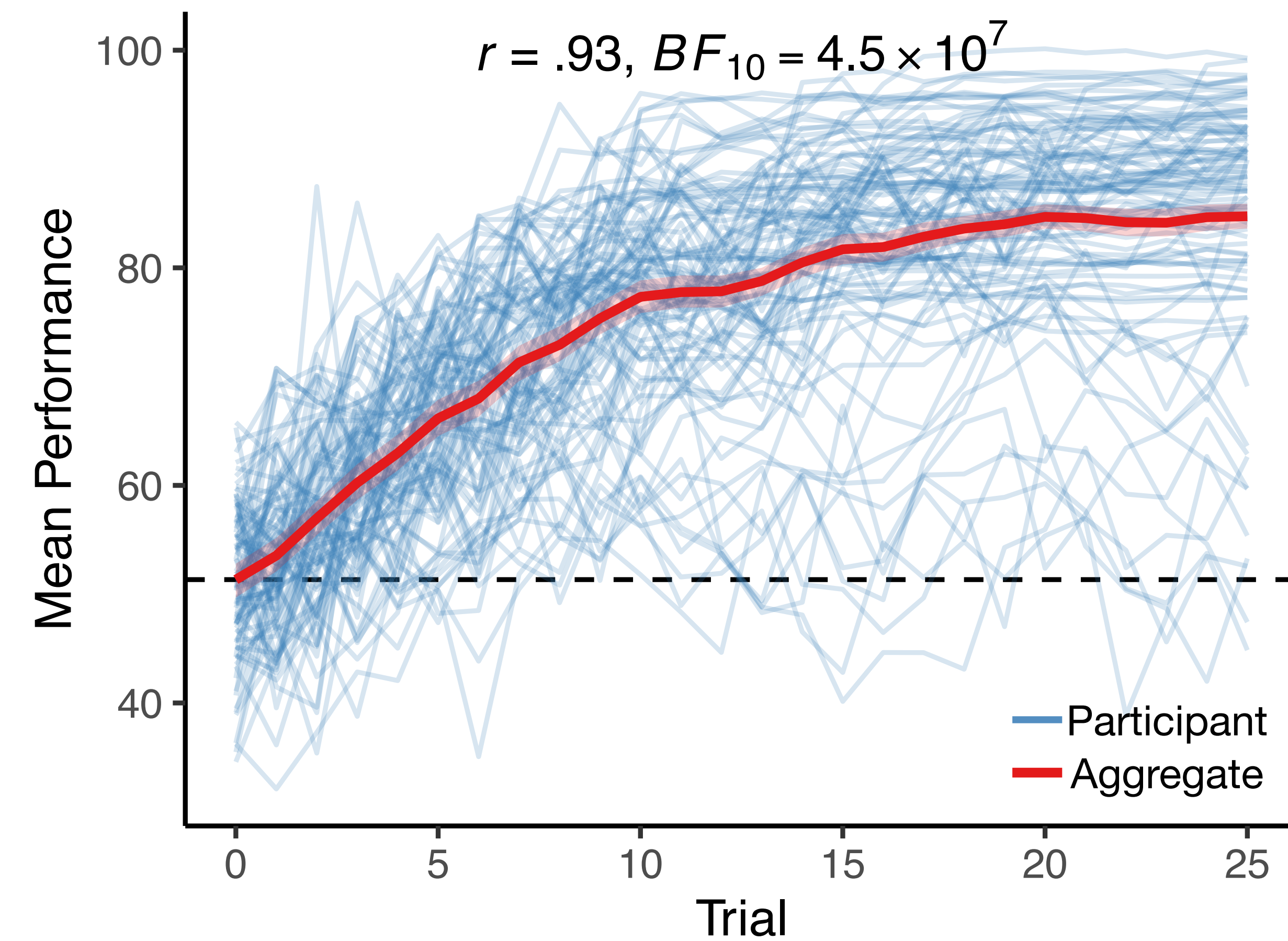
Current round: 1/10



Bonus Round

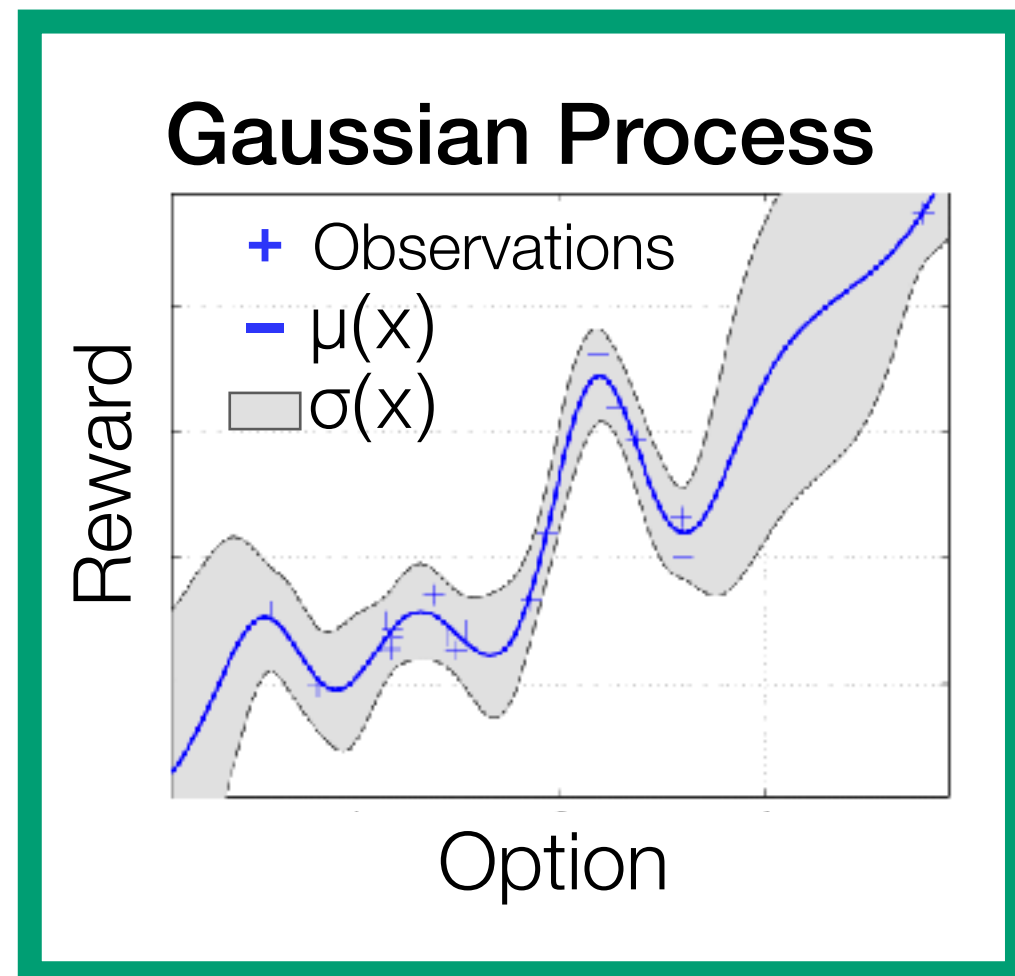


Behavioral Results

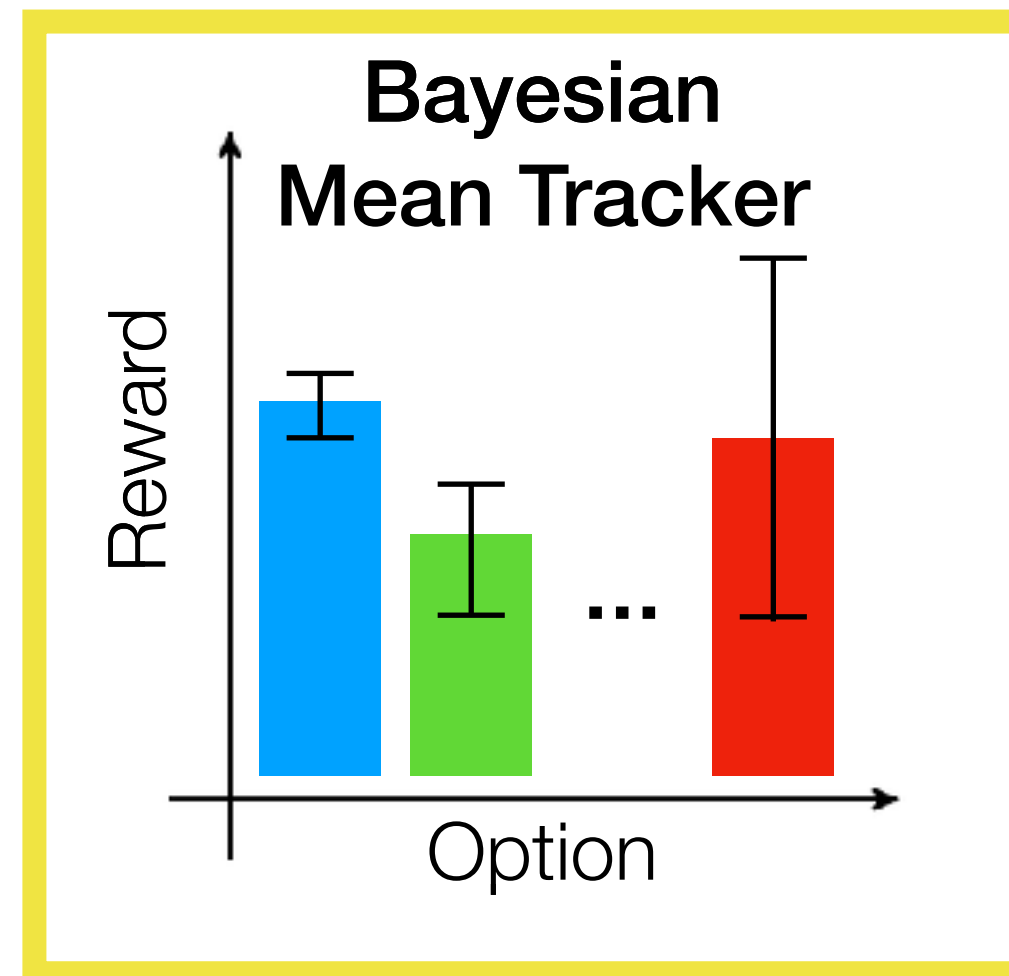


Model Results

Generalization

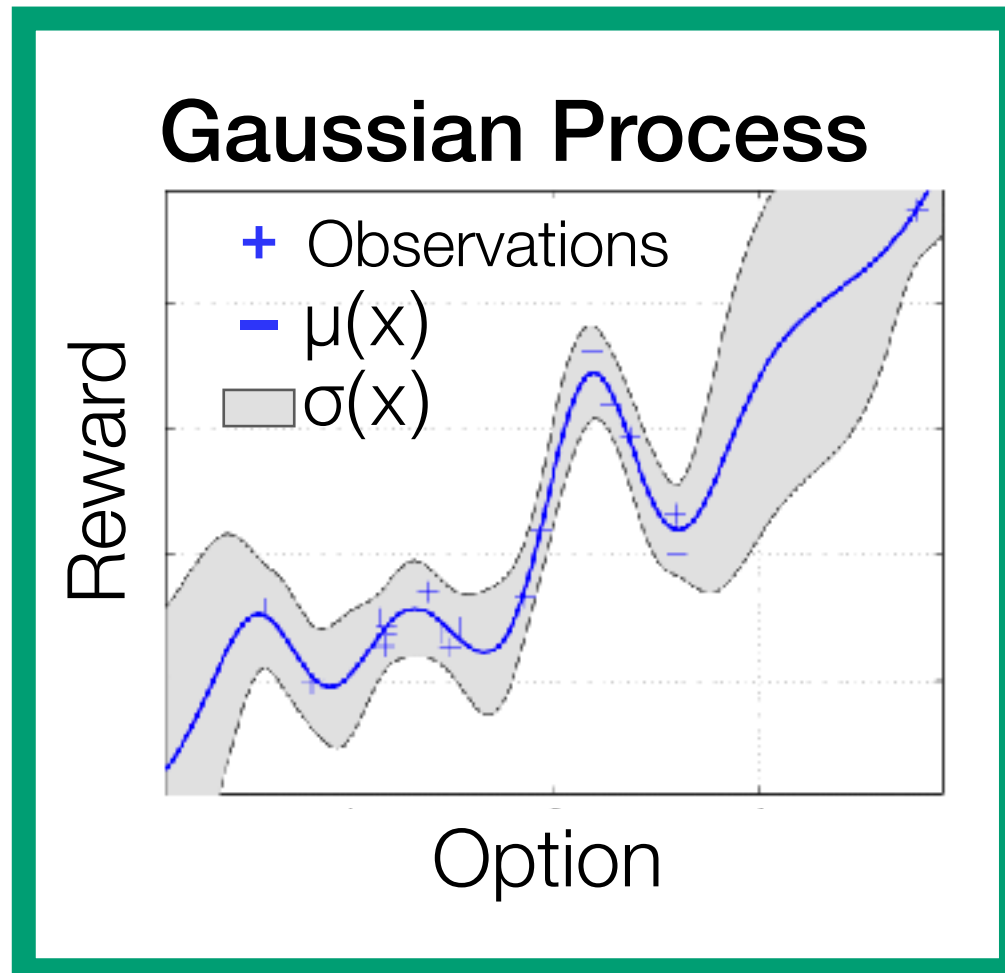


No generalization

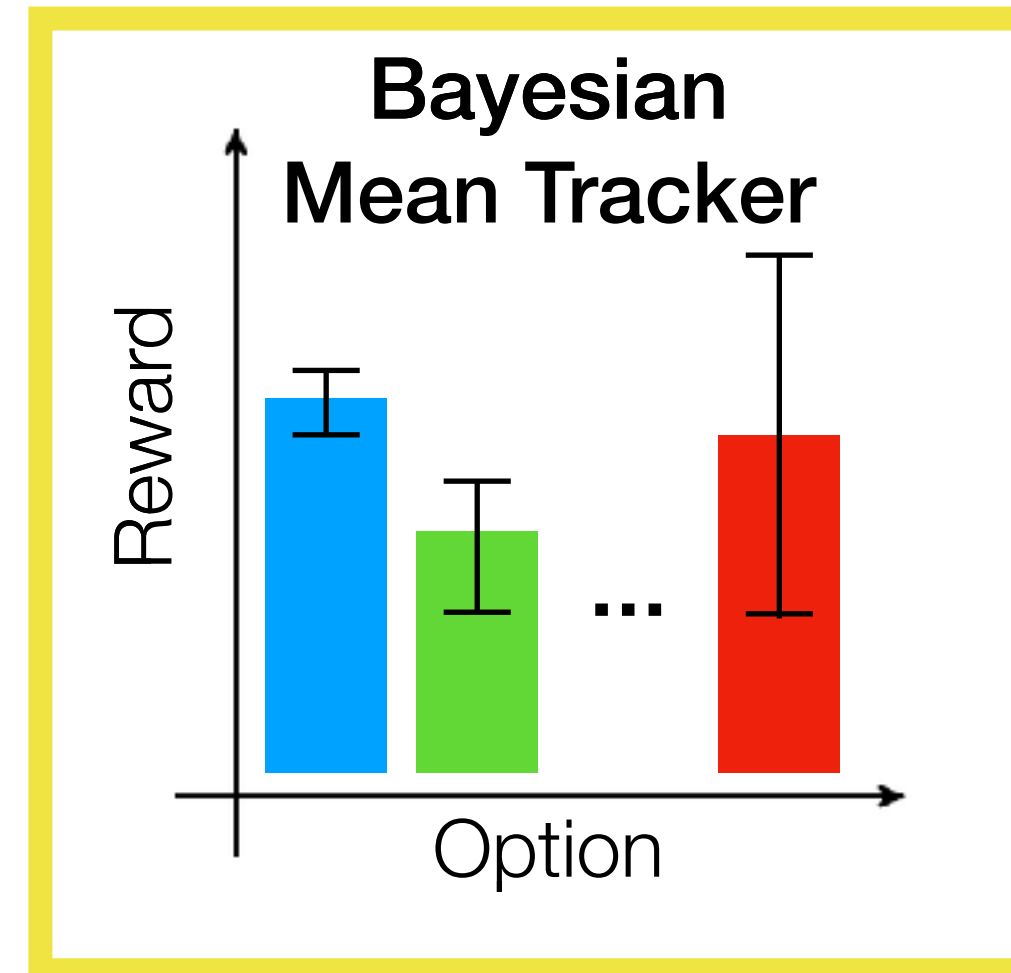


Model Results

Generalization

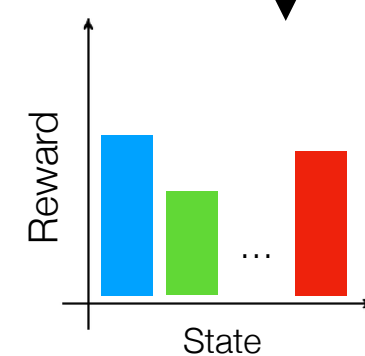


No generalization



Successor Representation

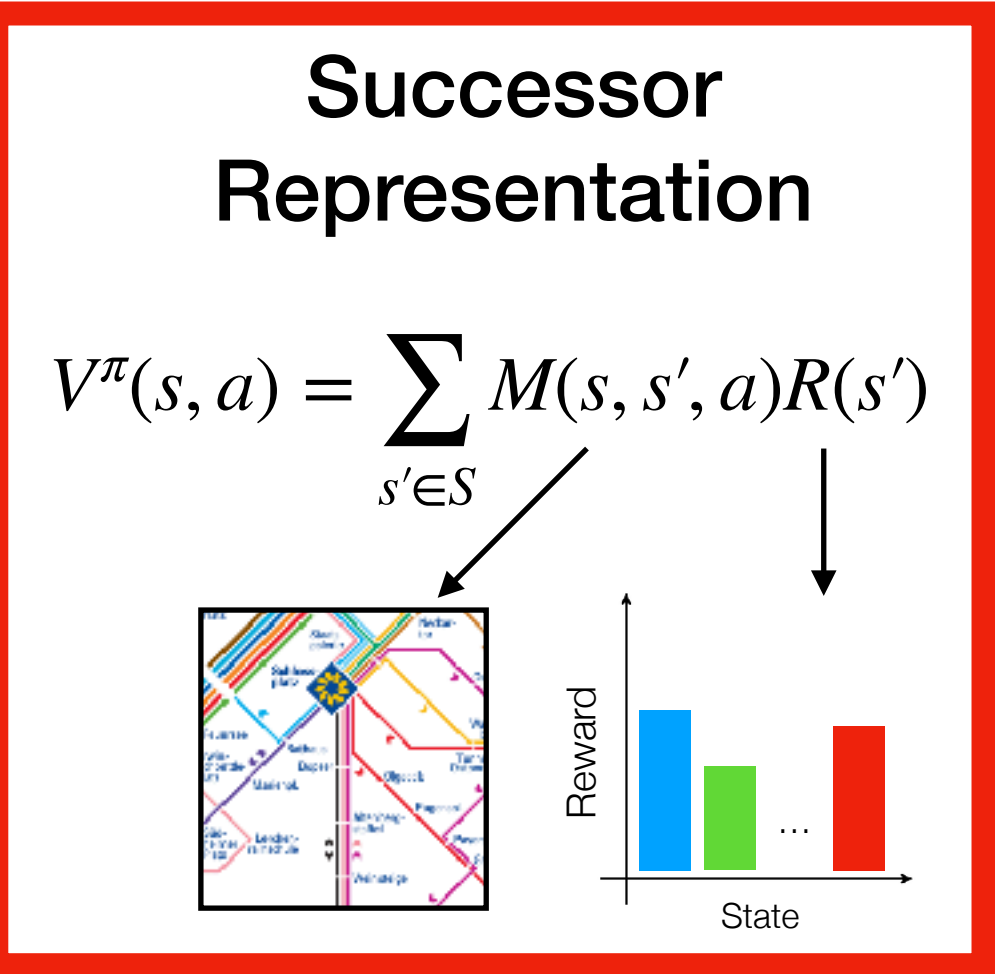
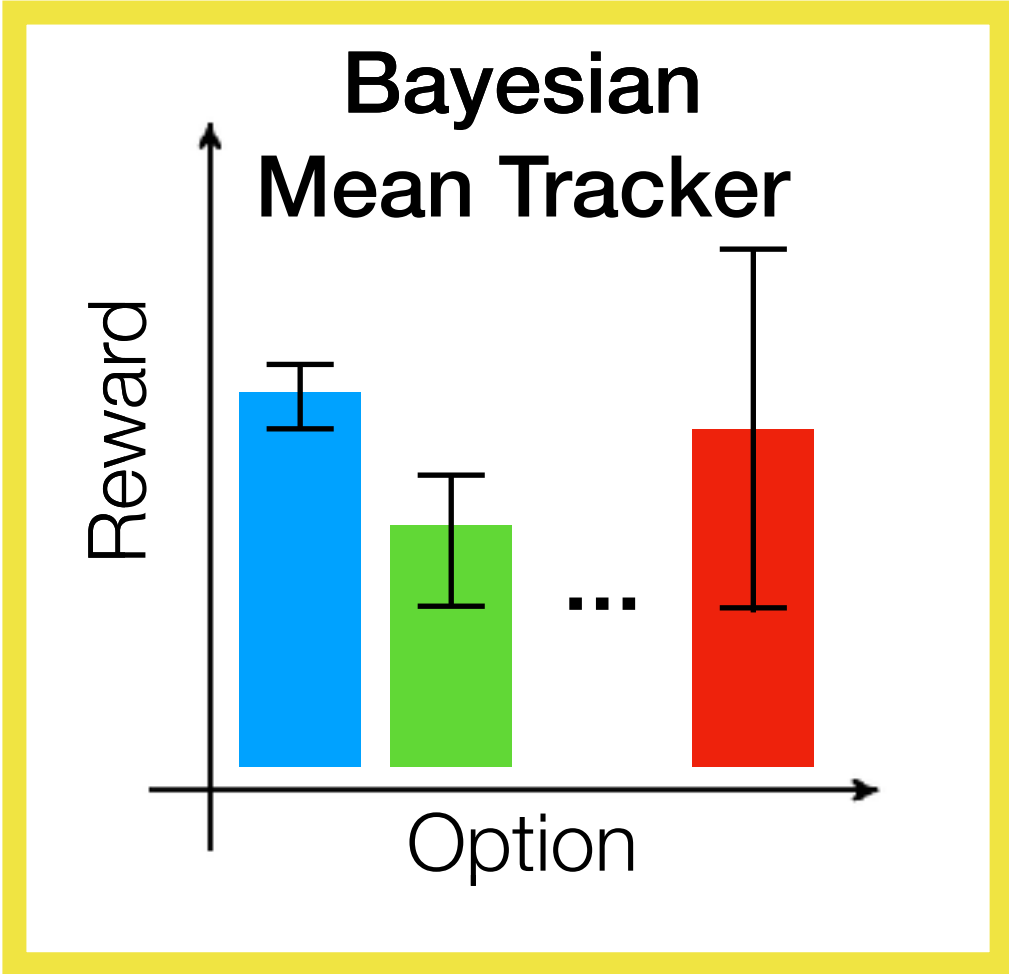
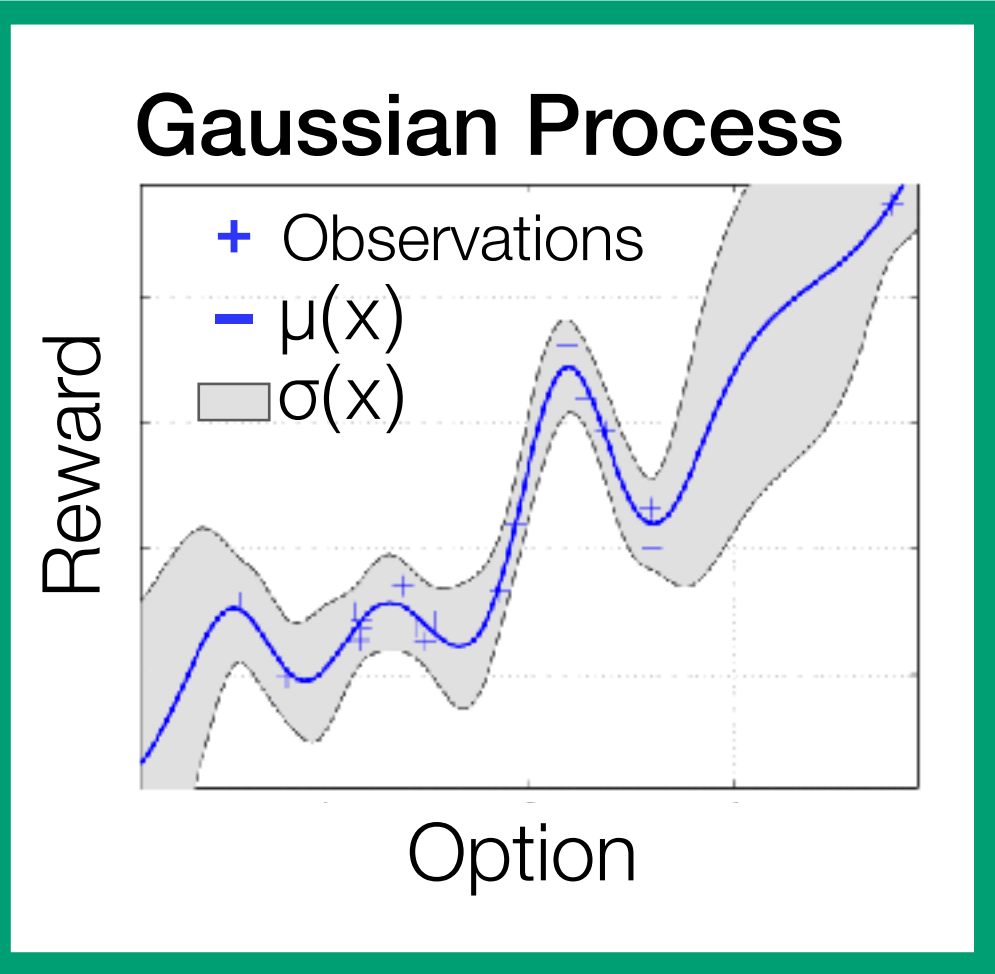
$$V^\pi(s, a) = \sum_{s' \in \mathcal{S}} M(s, s', a) R(s')$$



Model Results

Generalization

No generalization



directed + random exploration

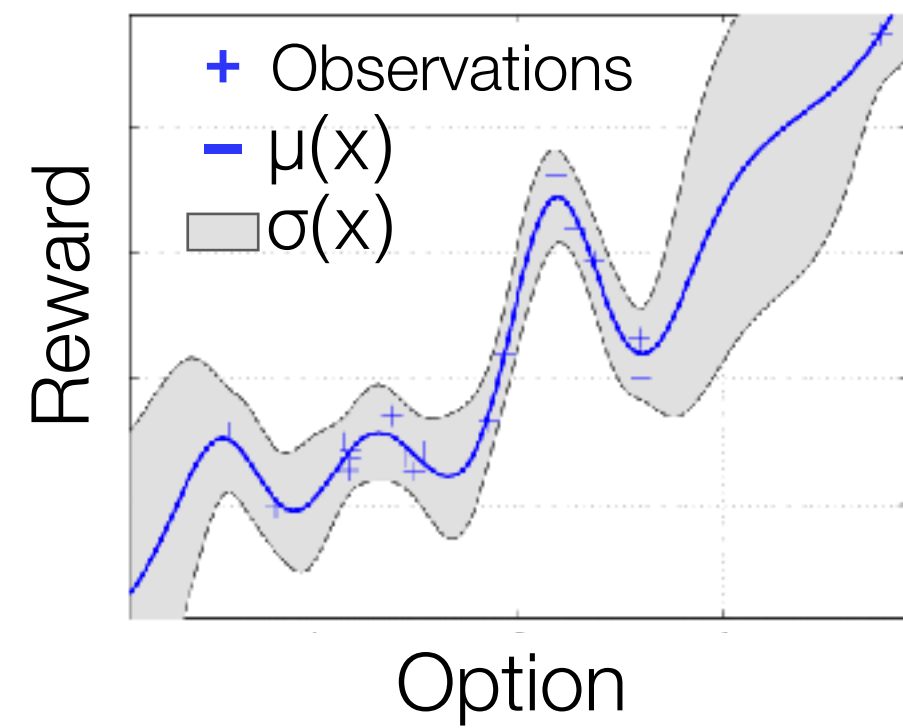
random exploration

Model Results

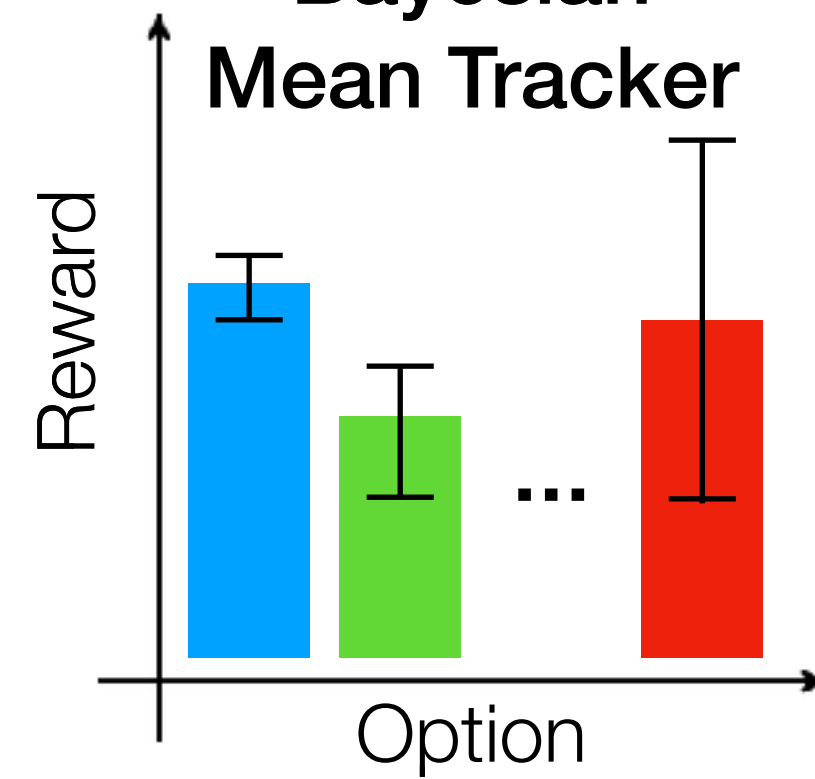
Generalization

No generalization

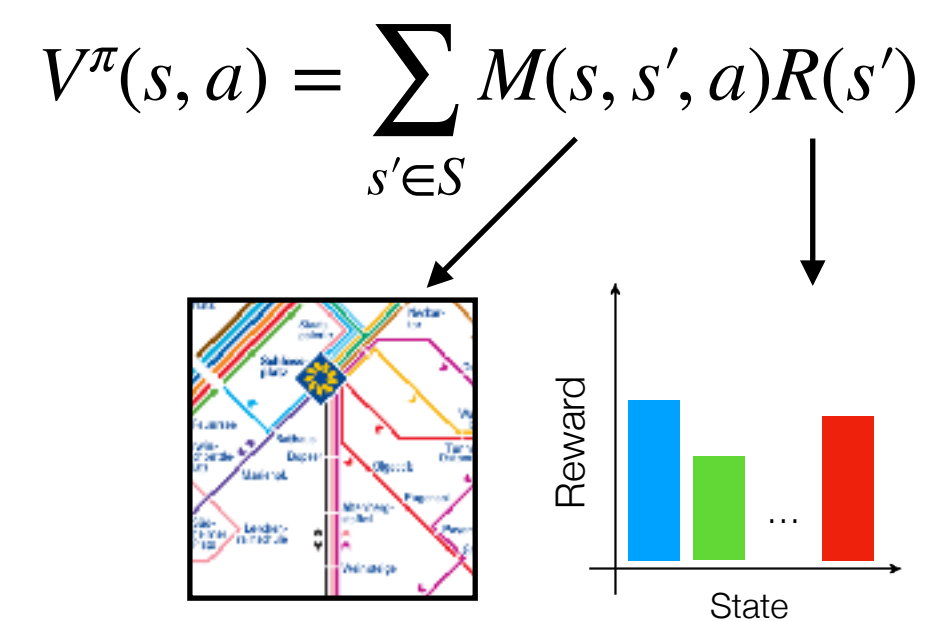
Gaussian Process



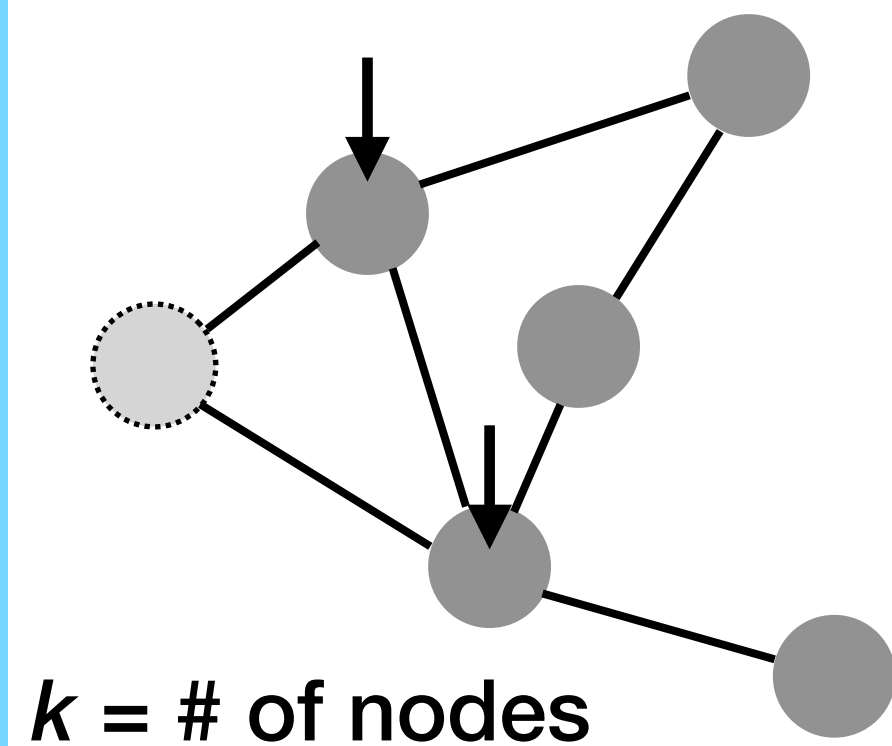
Bayesian Mean Tracker



Successor Representation



k-Nearest Neighbors



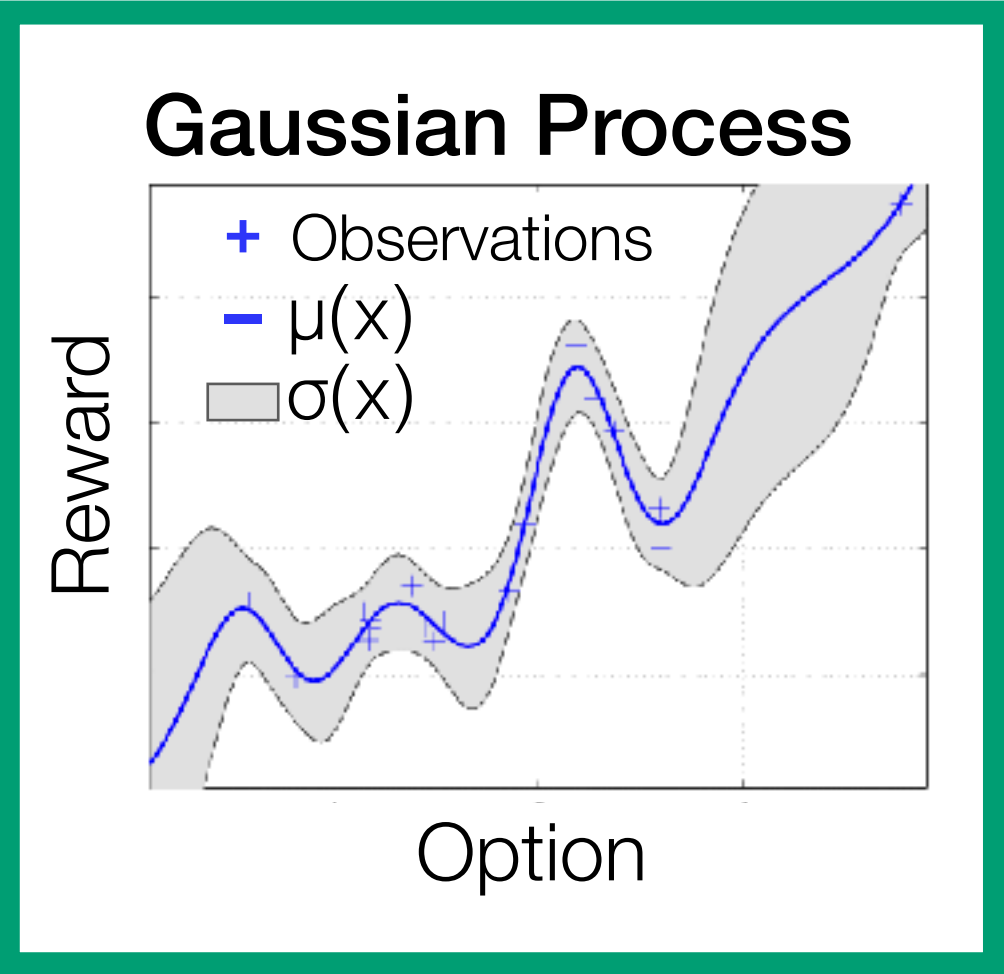
directed + random exploration

random exploration

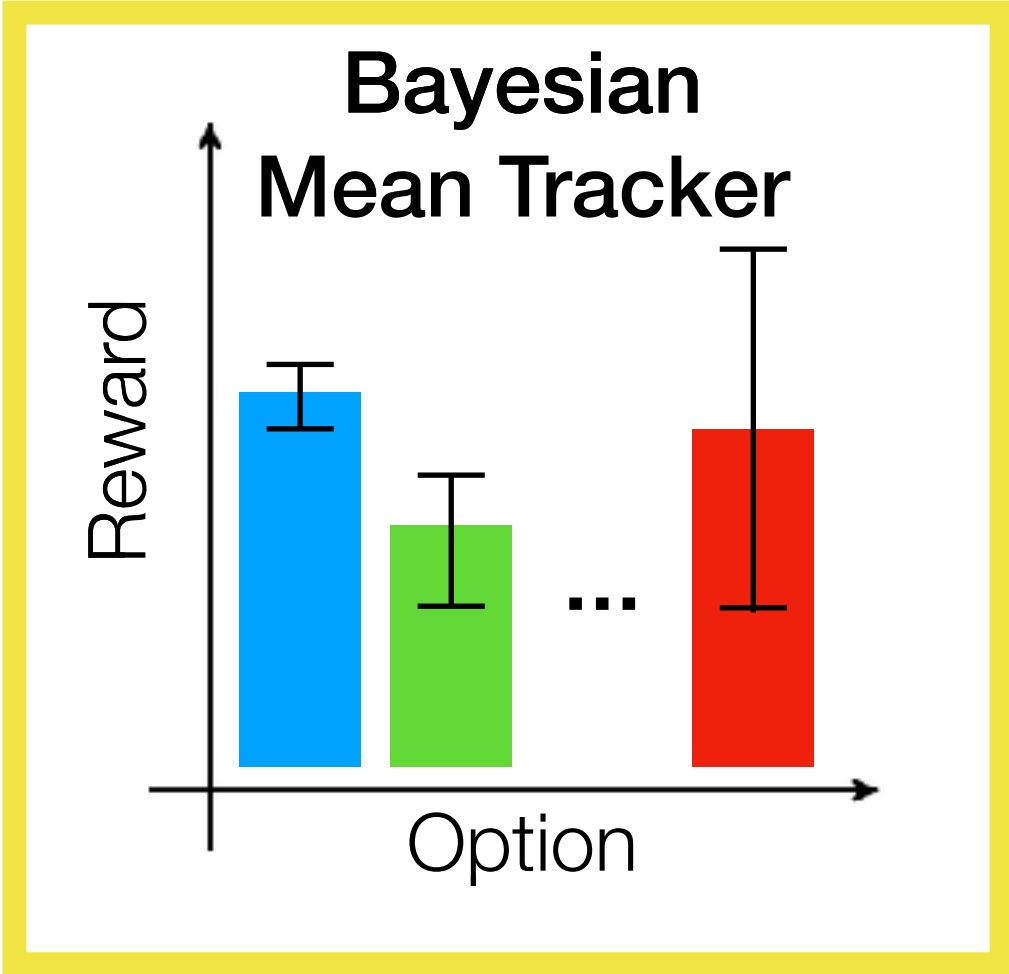
Model Results

directed + random exploration

Generalization

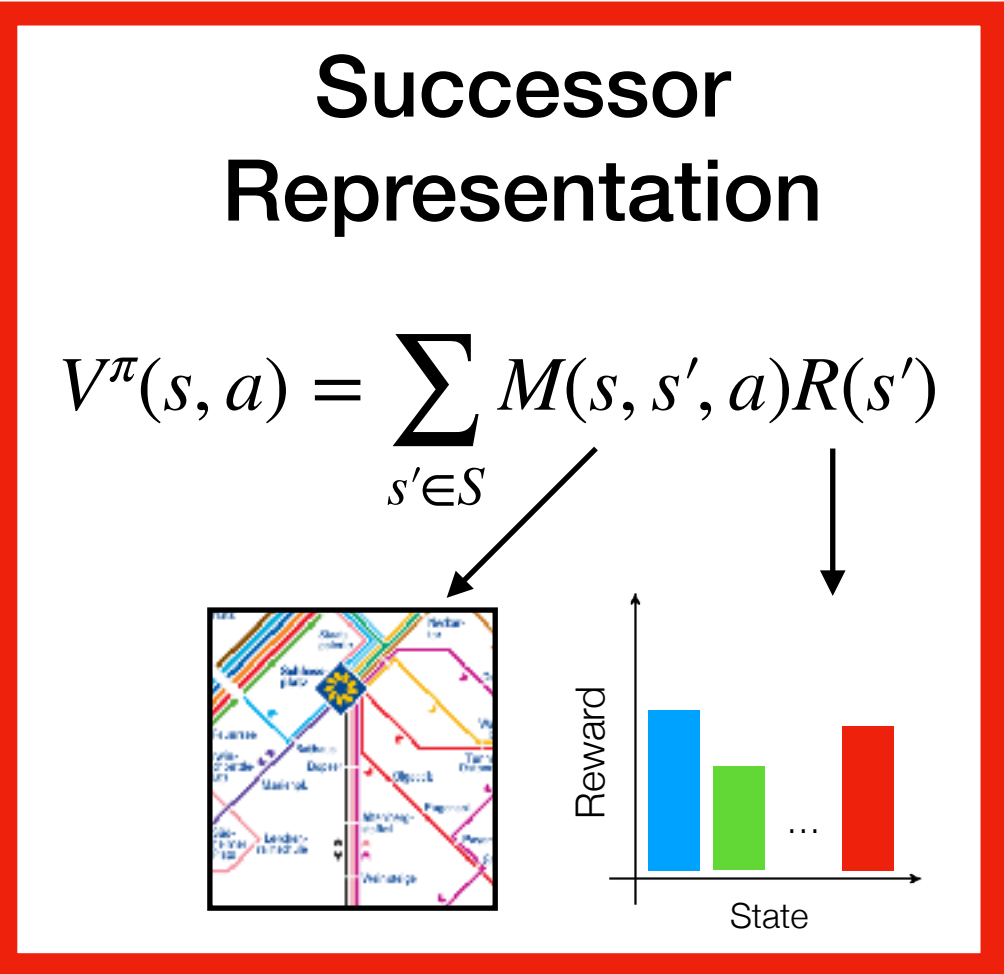


No generalization

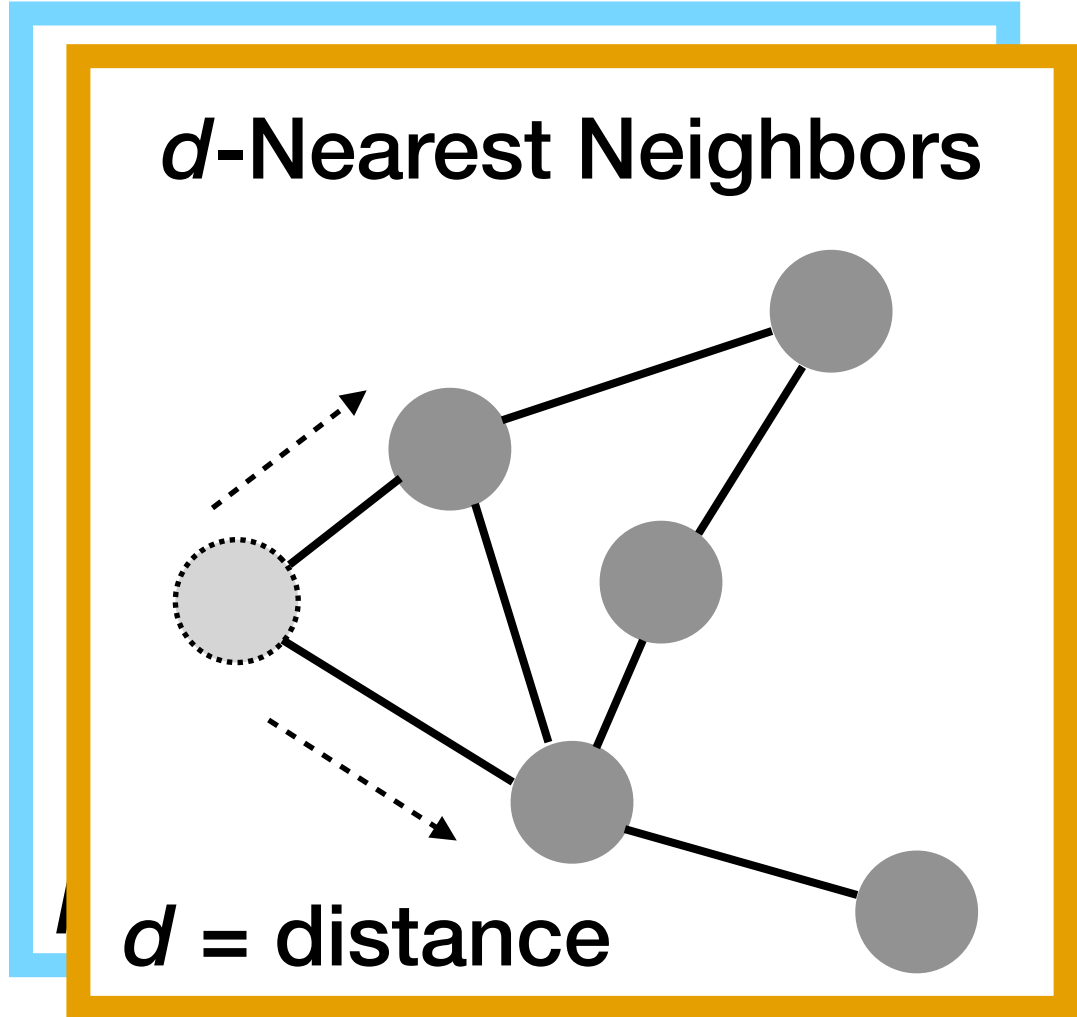


random exploration

Successor Representation



d -Nearest Neighbors



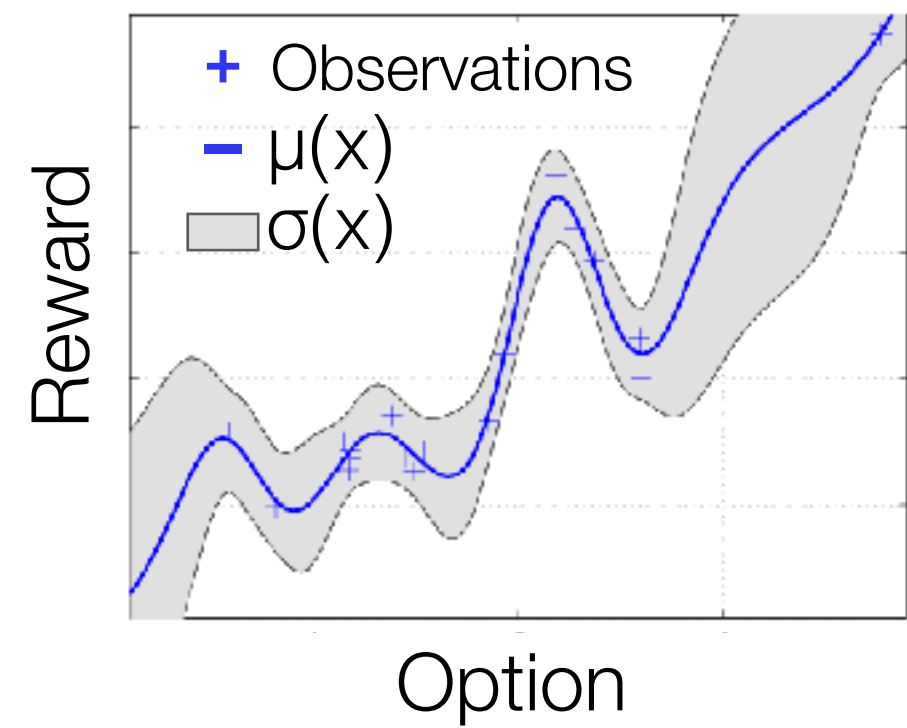
Model Results

directed + random exploration

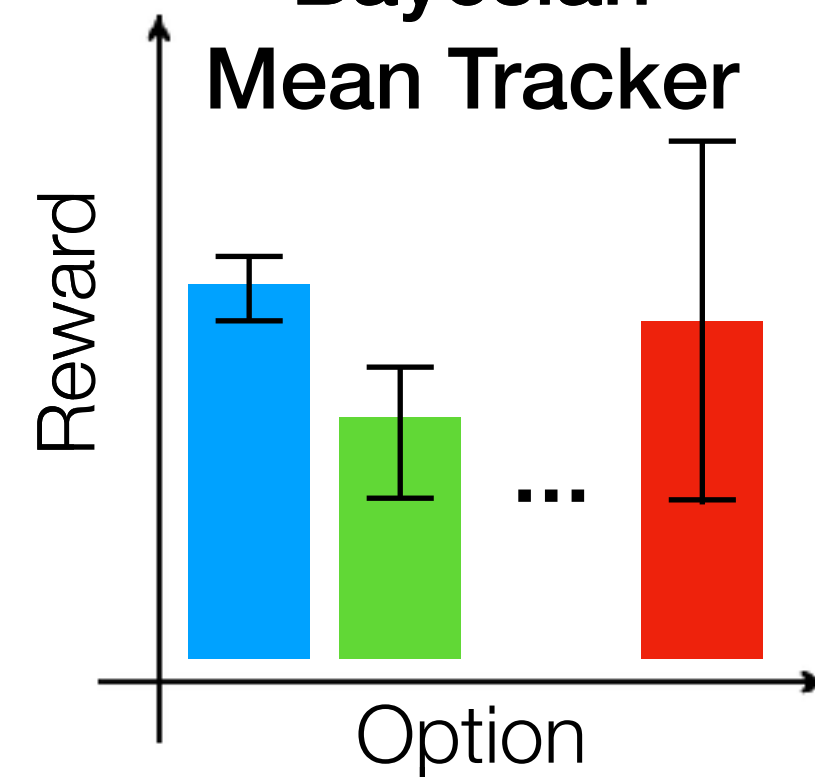
Generalization

No generalization

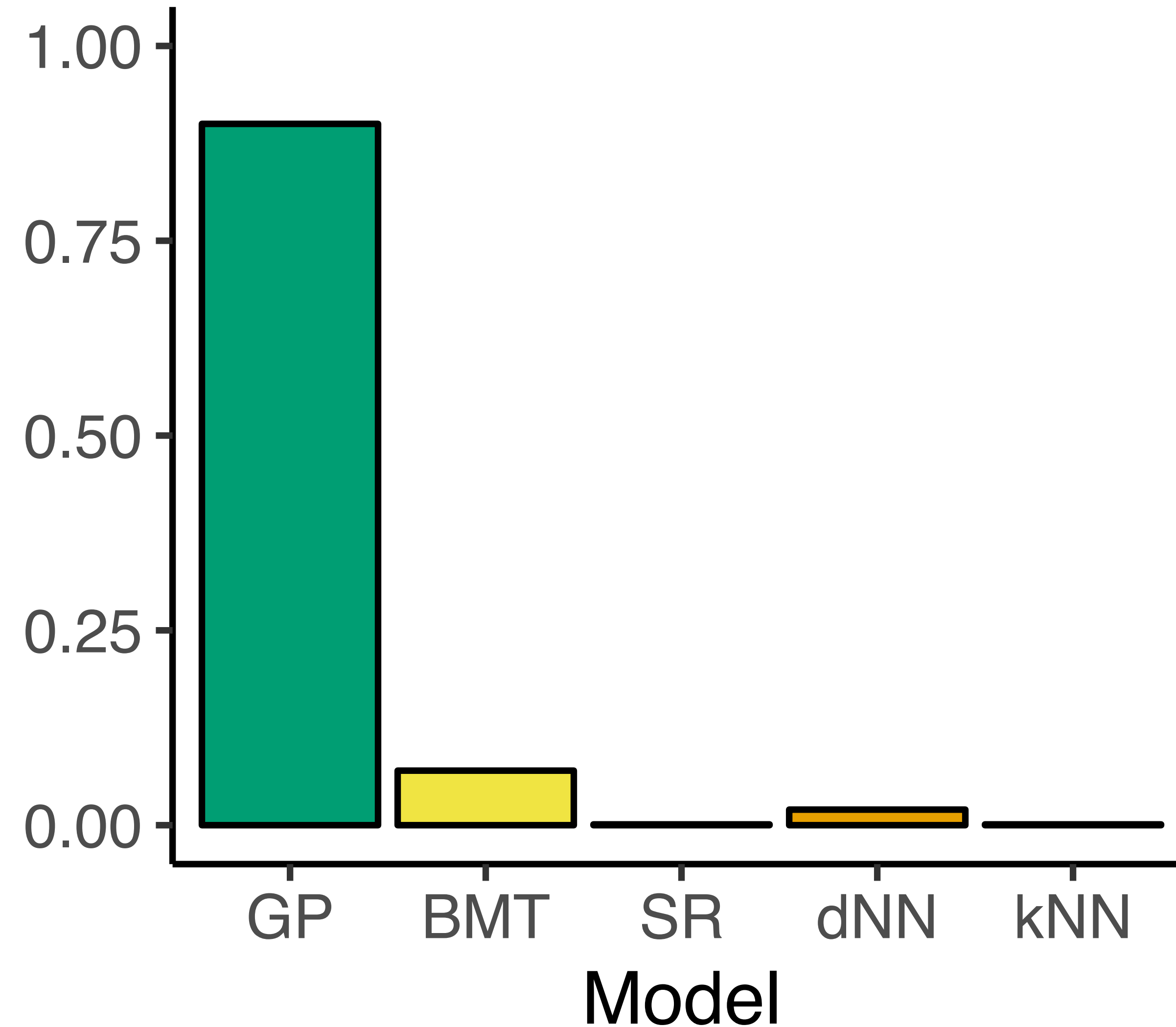
Gaussian Process



Bayesian Mean Tracker

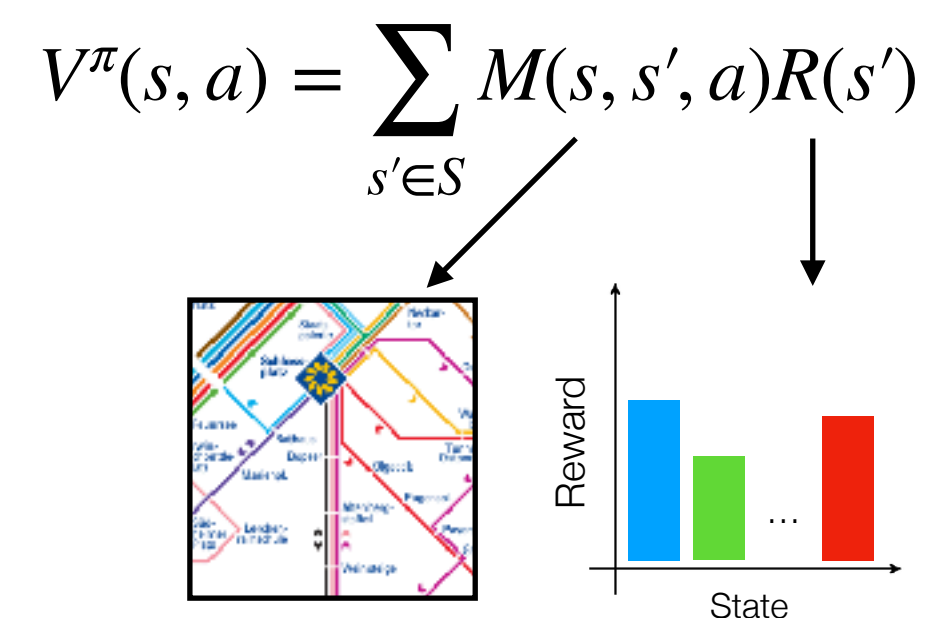


P(Best Model)

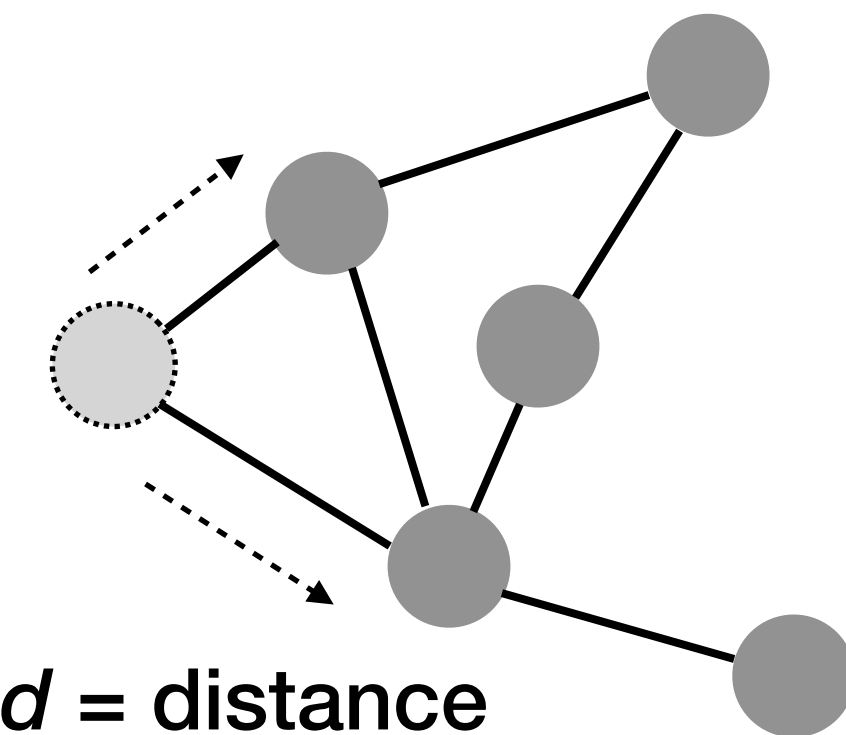


random exploration

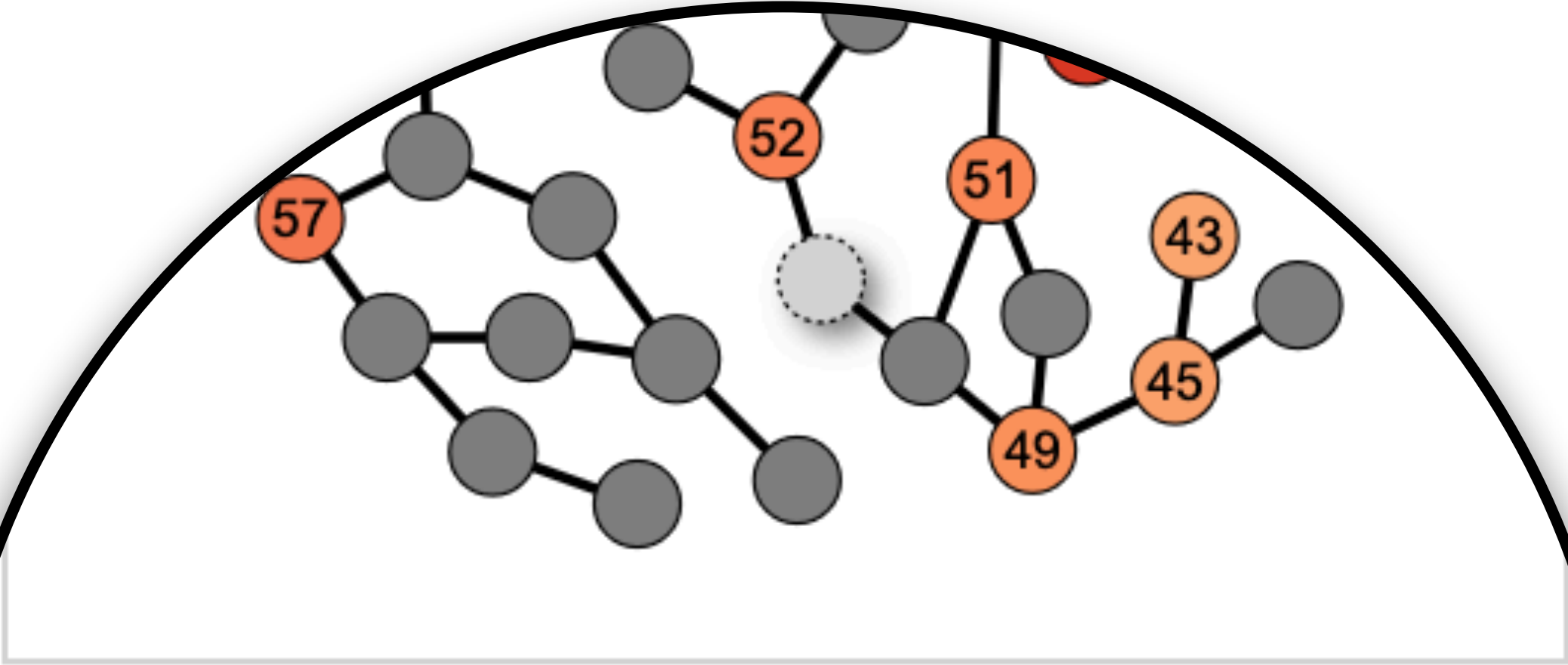
Successor Representation



d-Nearest Neighbors



Validation on judgments



How many points do you think will be observed at the selected node?

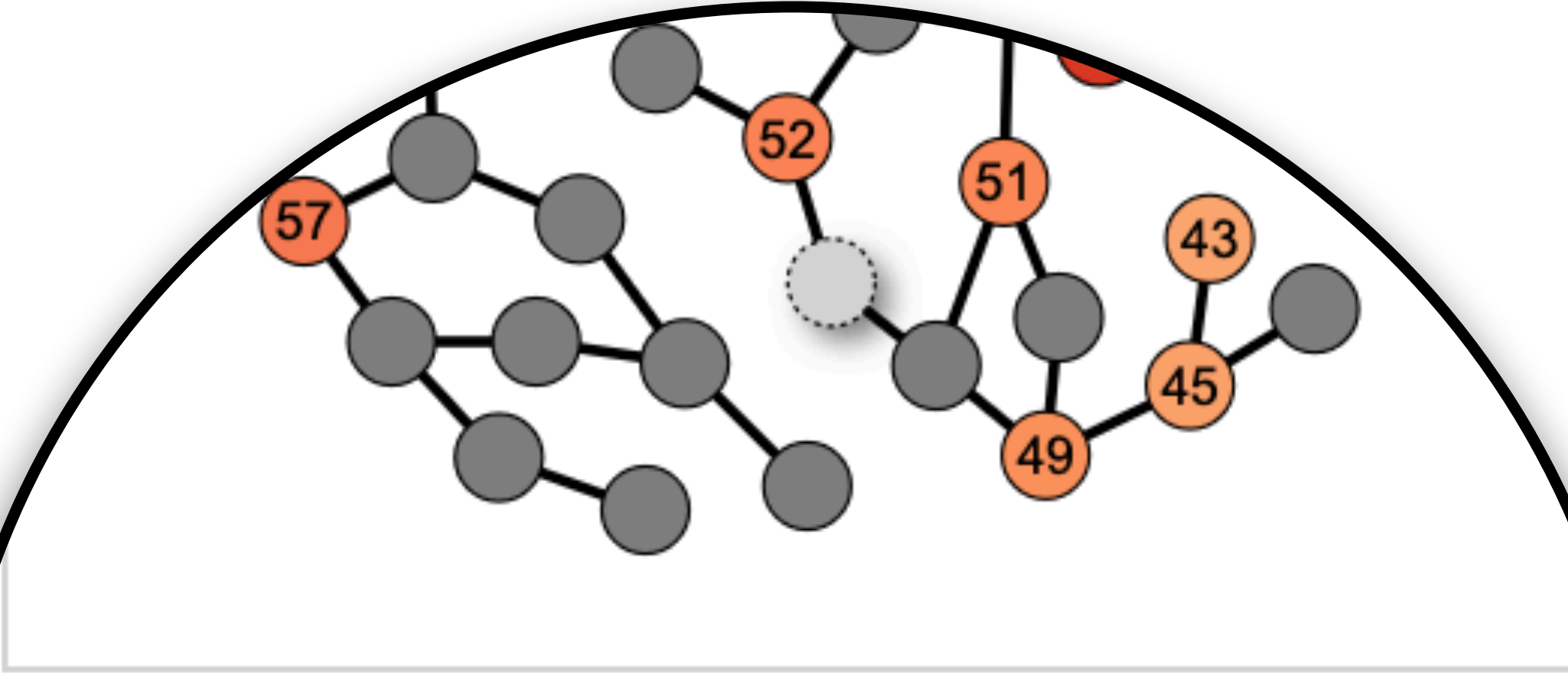
Few Many

How confident are you?

Least confident Most confident

Submit

Validation on judgments



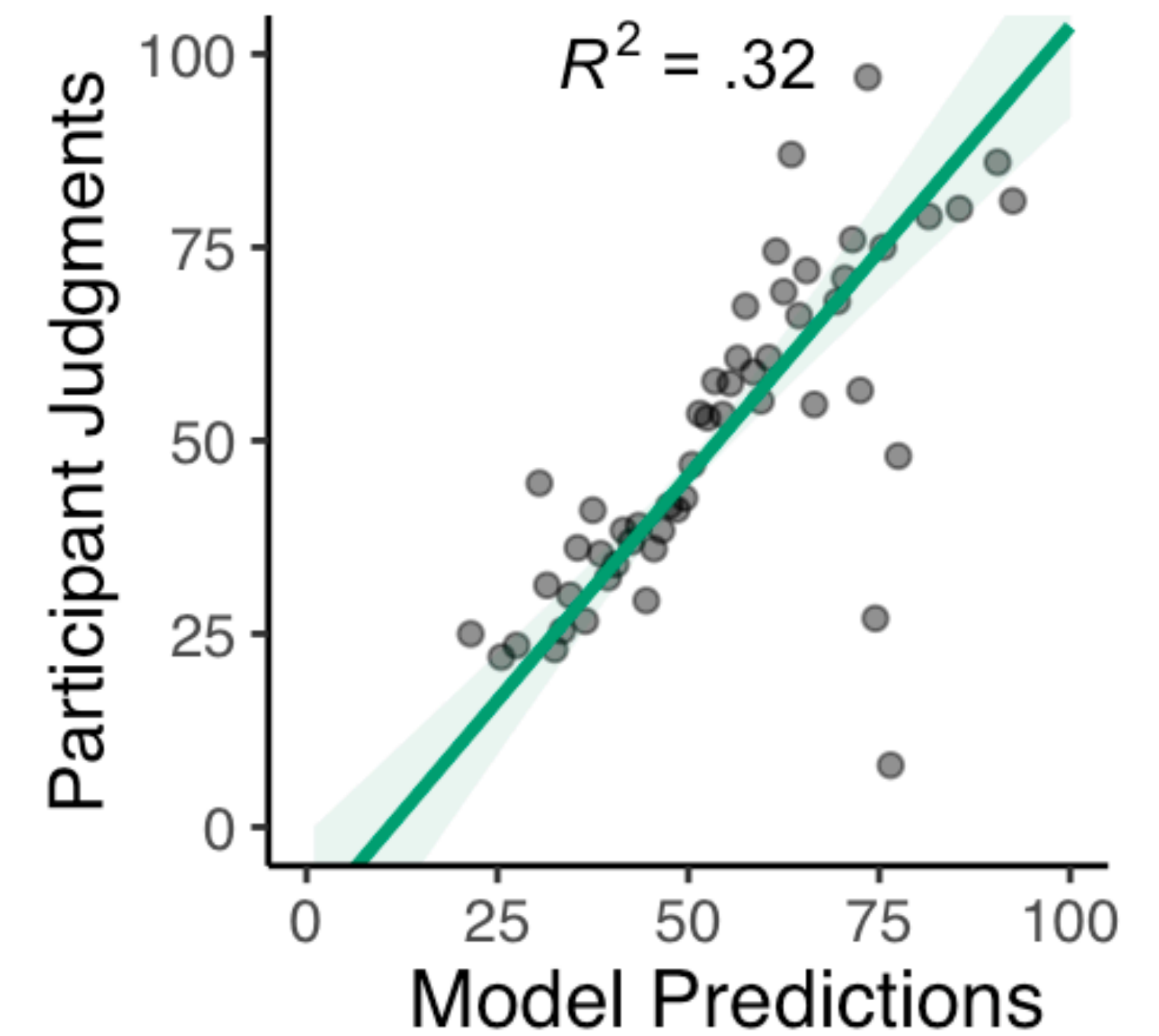
How many points do you think will be observed at the selected node?

Few Many

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Validation on judgments

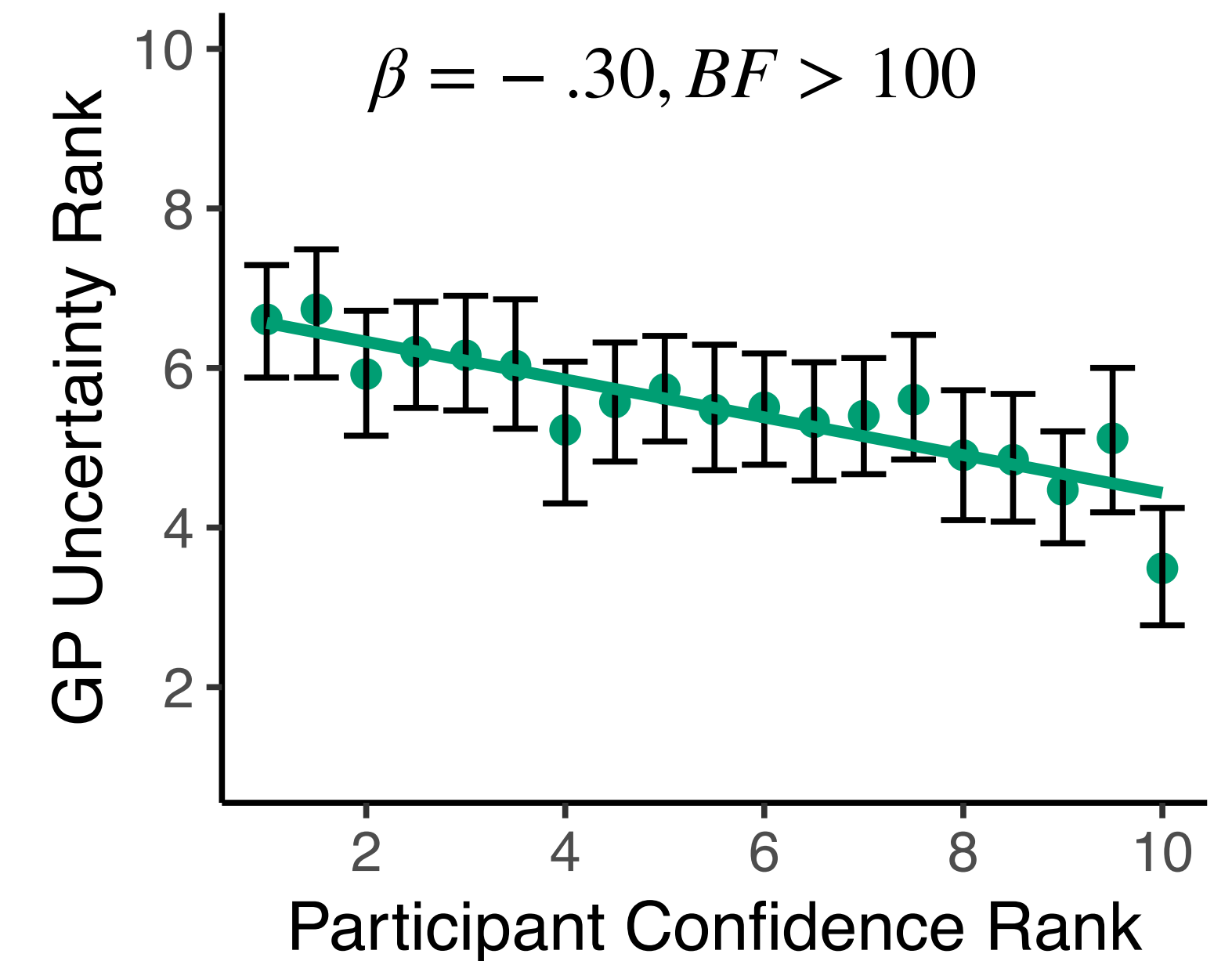
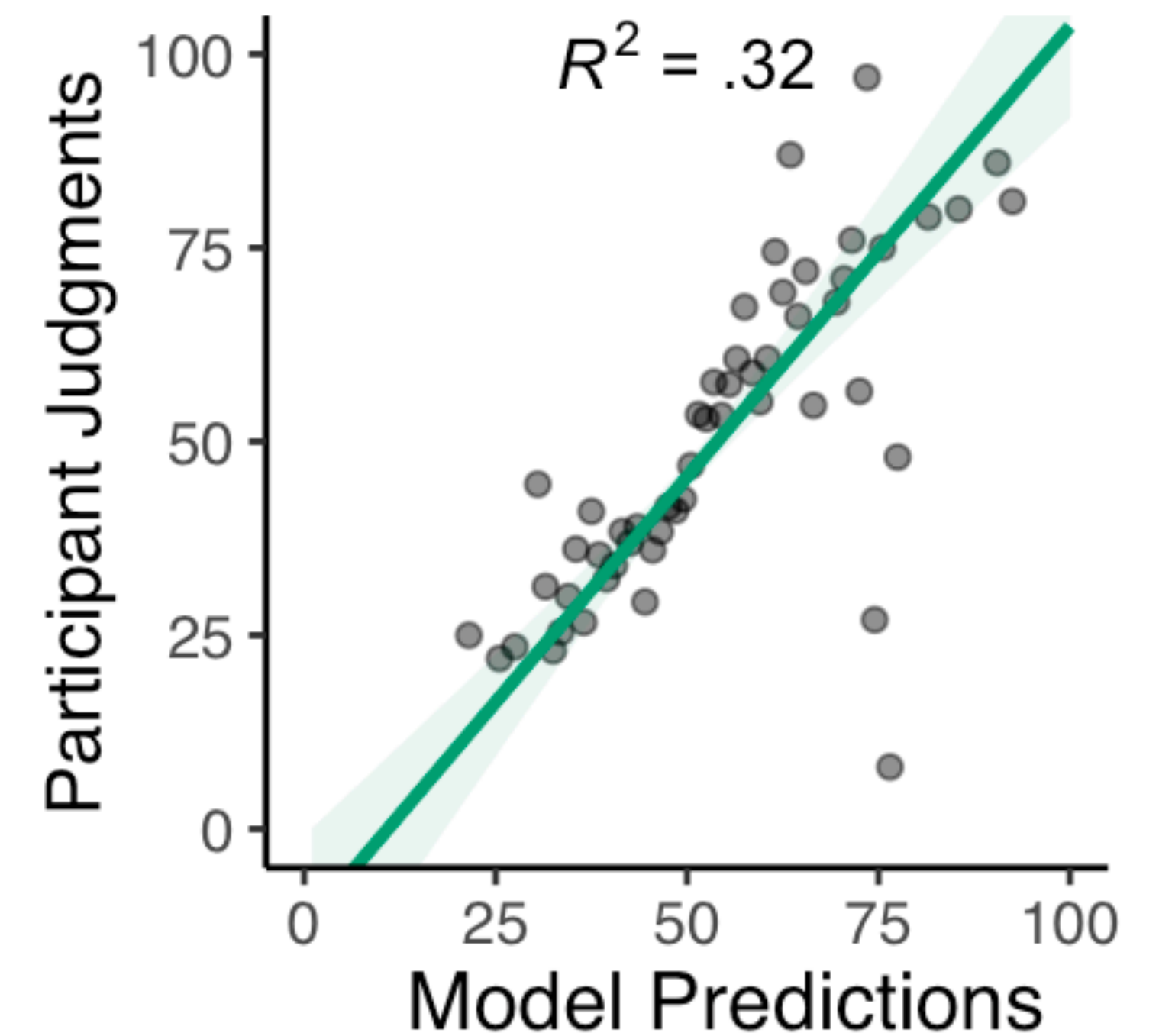
How many points do you think will be observed at the selected node?

Few Many

How confident are you?

Least confident Most confident

Submit



Conclusions

- How do we navigate vast problem spaces?
 - Generalization and directed exploration provide a powerful model for efficient learning across many domains
- By modeling generalization as functional inference, we can:
 - Predict search decisions
 - Simulate human-like performance
 - Predict judgments of expected reward and confidence
- Underlying mechanisms of Bayesian inference, kernel similarity, and episodic RL have deep theoretical connections to other models in Neuroscience and Computer Science

Future directions

- How is the structure of similarity learned?
 - **Successor Representation:** online prediction error about future states? (Dayan, *NeurComp*1993; Stachenfeld et al., *Nat Neuro* 2017)
 - **Tolman Eichenbaum Machine:** associative learning mechanisms (Whittington et al., *Cell* 2020)
 - **Structure induction:** Bayesian inference about hypothesized structure? (Kemp & Tenenbaum, *PNAS* 2008)
- How do humans keep functional inference tractable as we gain more experience?
 - GPs scale cubically with the size of the data $\mathcal{O}(n^3)$
 - A large part of this complexity is in computing the underlying uncertainty
 - Perhaps population codes can support flexible generalization with uncertainty (Tano, Dayan, & Pouget, *NeurIPS* 2020)

Thanks to my collaborators and funders



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Azzurra Ruggeri
MPI Berlin



Nico Schuck
MPI Berlin



Sam Gershman
Harvard



Simon Ciranka
MPI Berlin



Anna Giron
Uni Tübingen



Mona Garvert
MPI Leipzig



Maarten Speekenbrink
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Jonathan Nelson
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Wouter van den Bos
Uni Amsterdam



EBERHARD KARLS
UNIVERSITÄT
TÜBINGEN



TÜBINGEN AI CENTER
BMBF Competence Center for Machine Learning



UNIVERSITÄT
TÜBINGEN



CyberValley



Intelligente Systeme

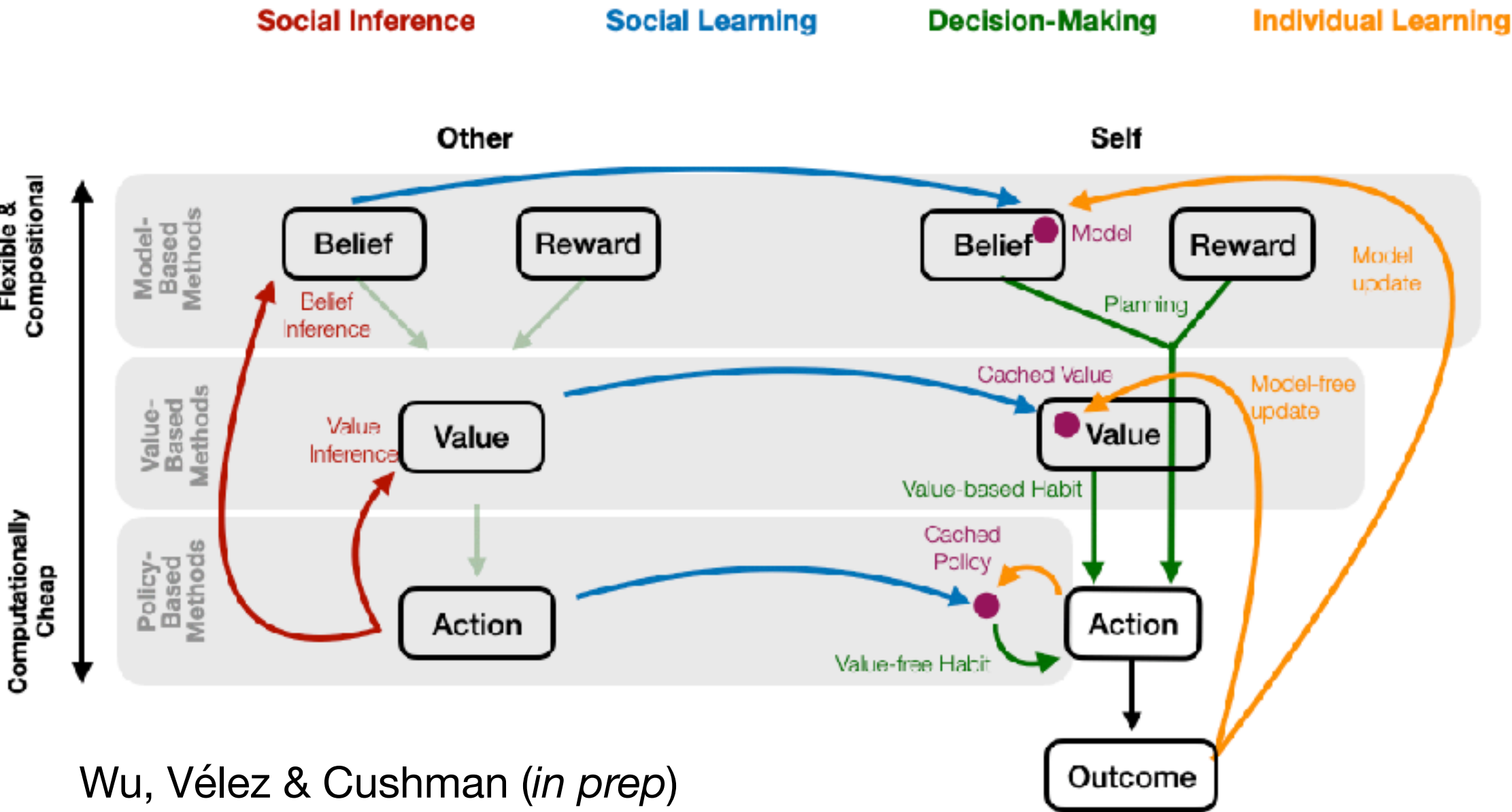
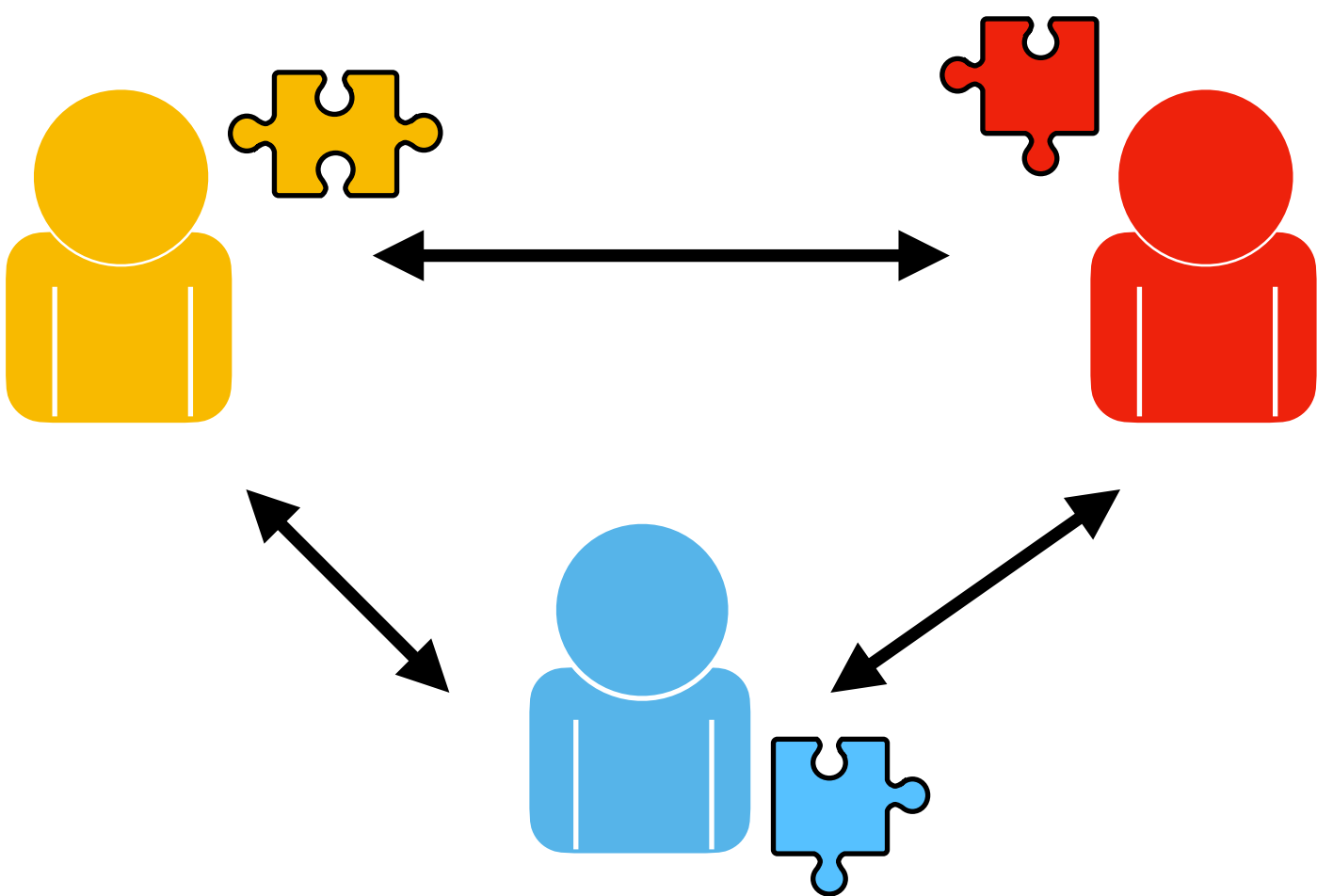
ADVANCING MACHINE INTELLIGENCE WITH ROBUST MACHINE LEARNING

Fuly Funded PhD position: Computational mechanisms of Social Learning

Potential topics include:

- Theory of Mind inference using inverse RL
- Selectivity and specialization in social learning using VR experiments programmed in minecraft
- Cumulative cultural evolution
- Integration of individual and social information

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Recreated Visual Field



POV Recording

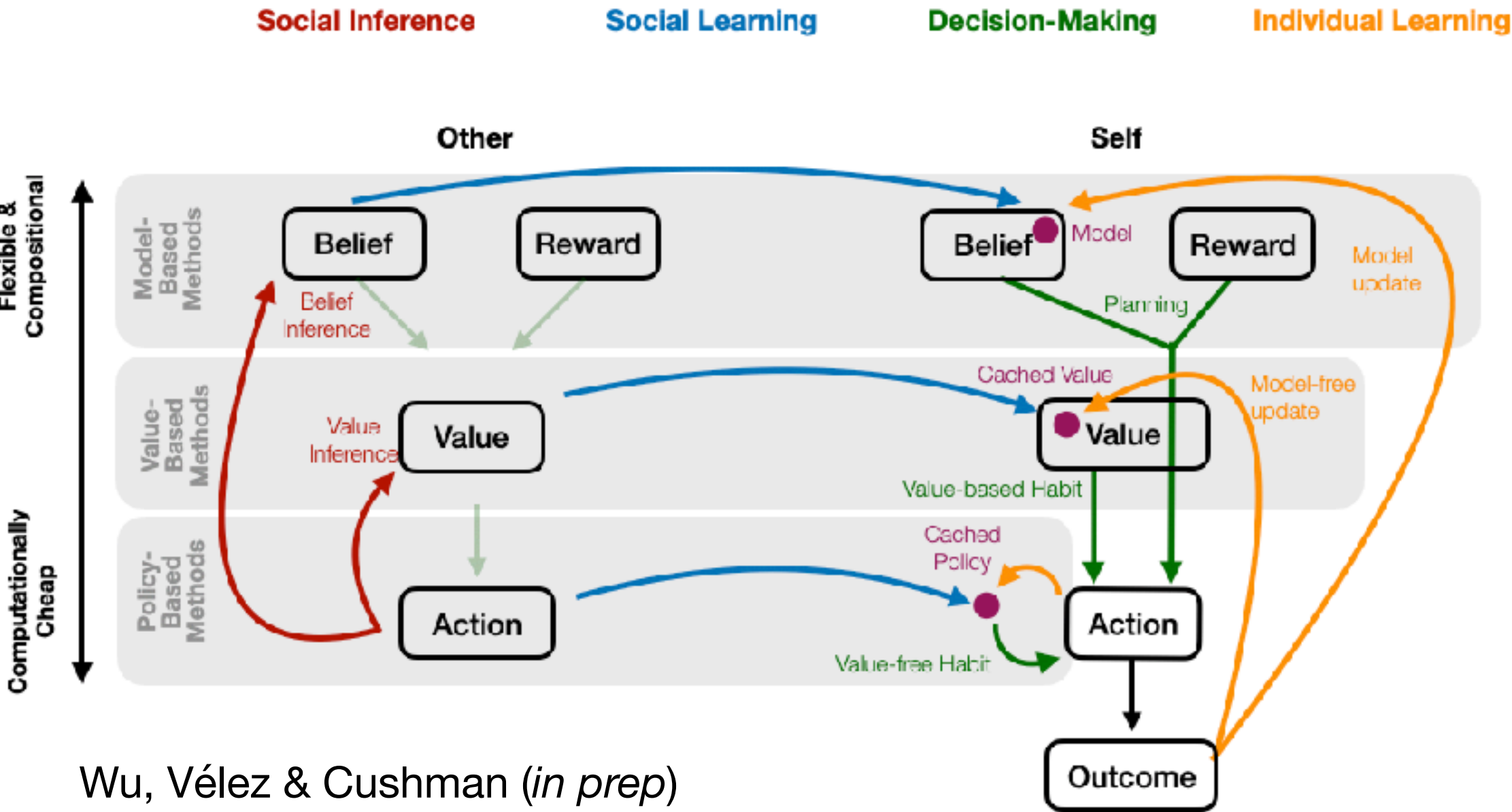
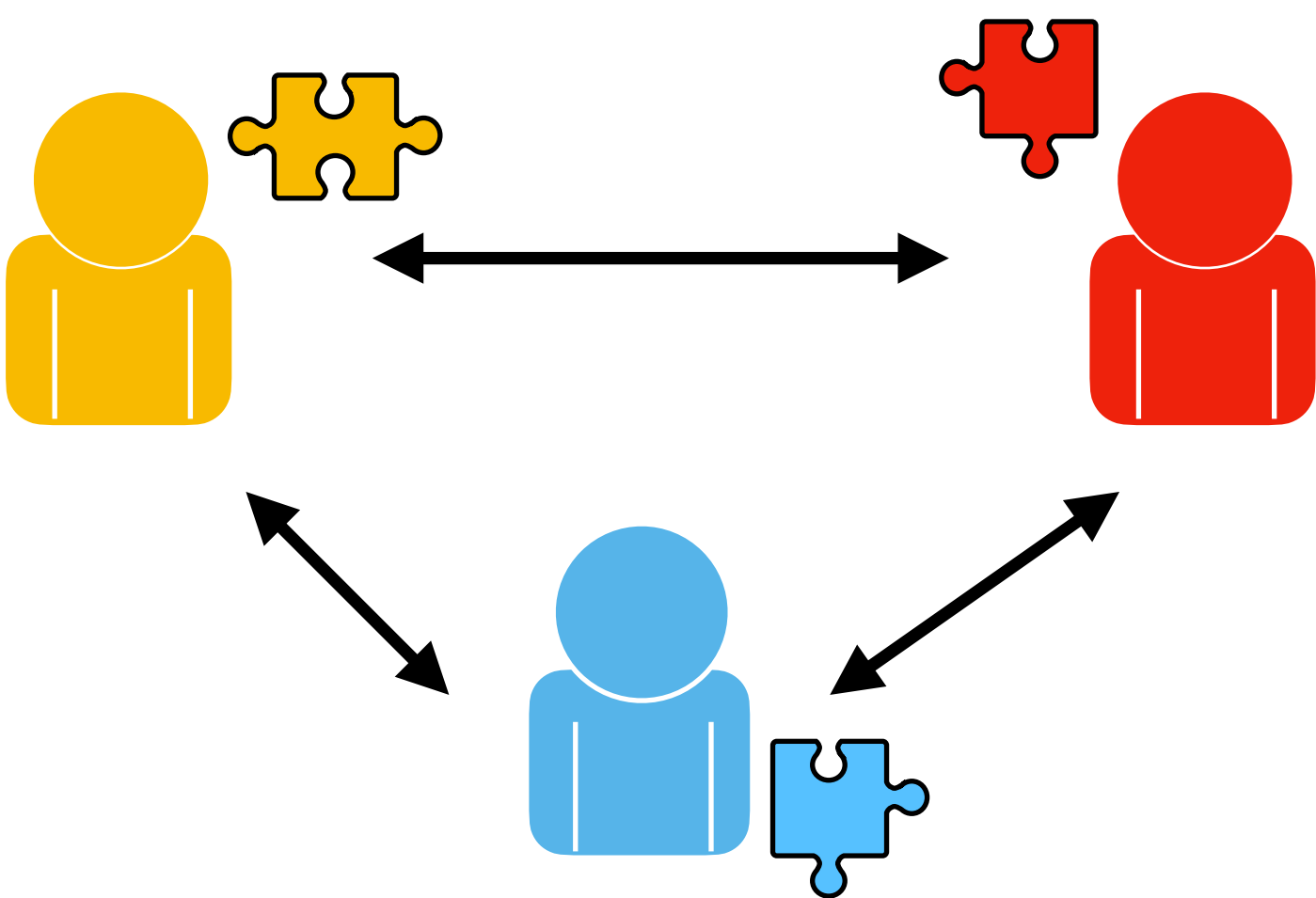


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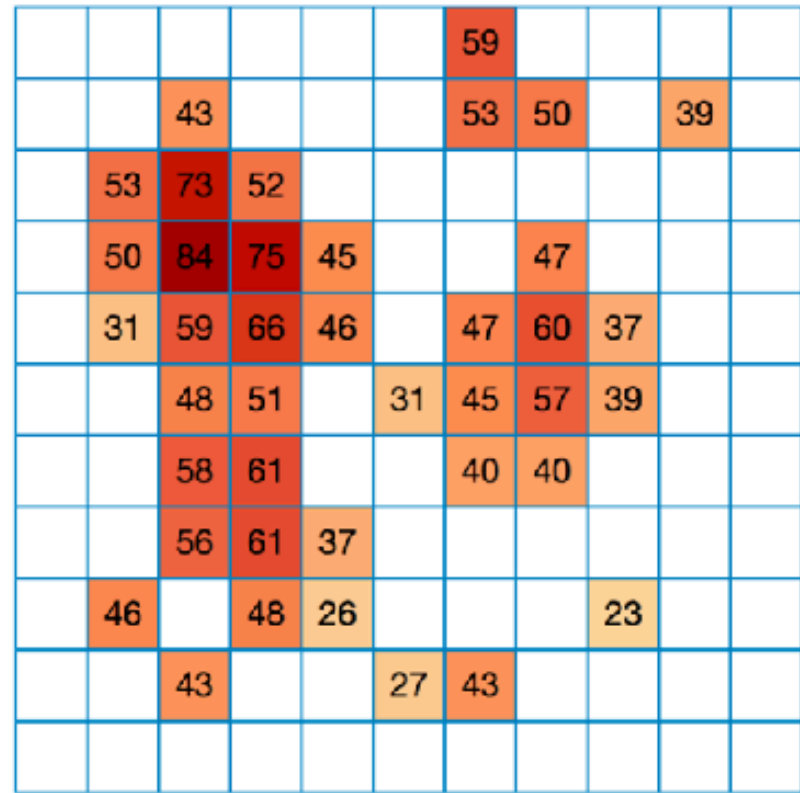
Recreated Visual Field



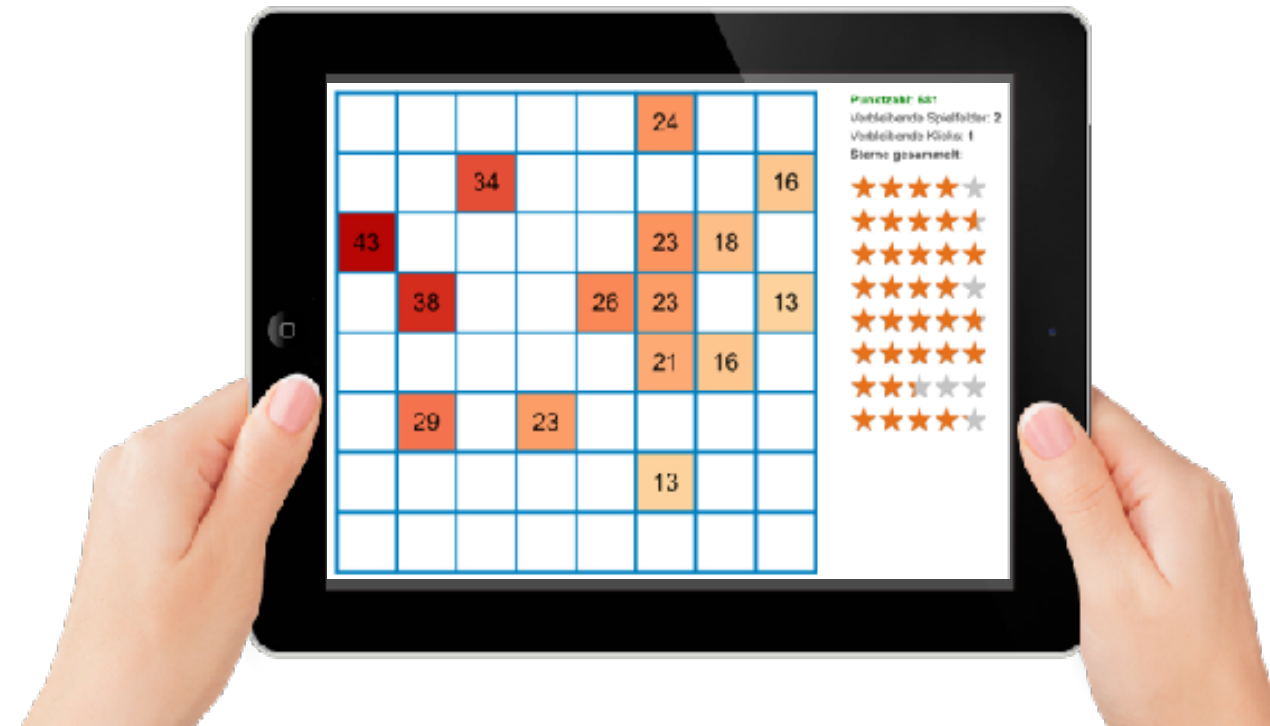
POV Recording

Questions?

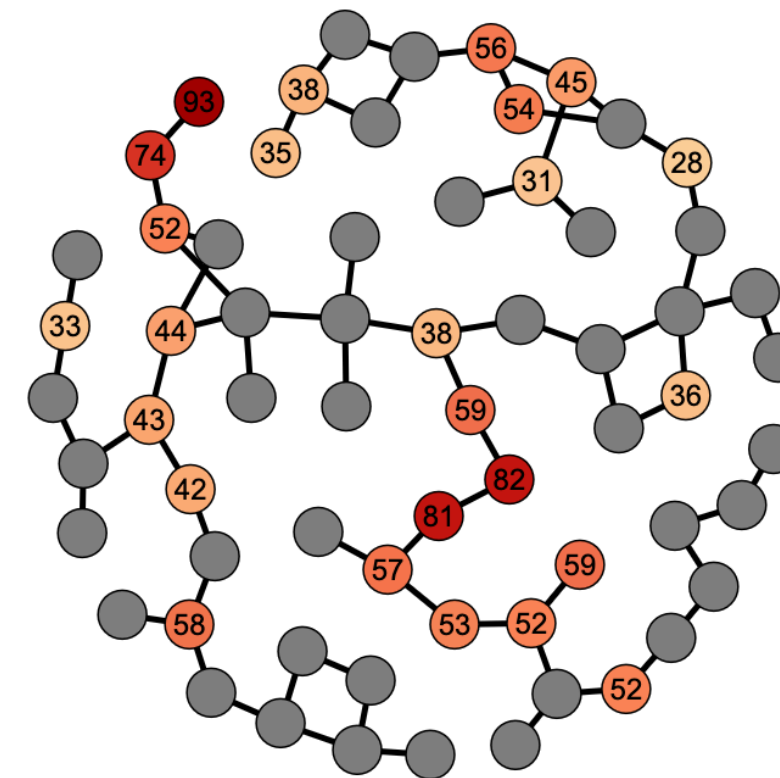
Grid Search



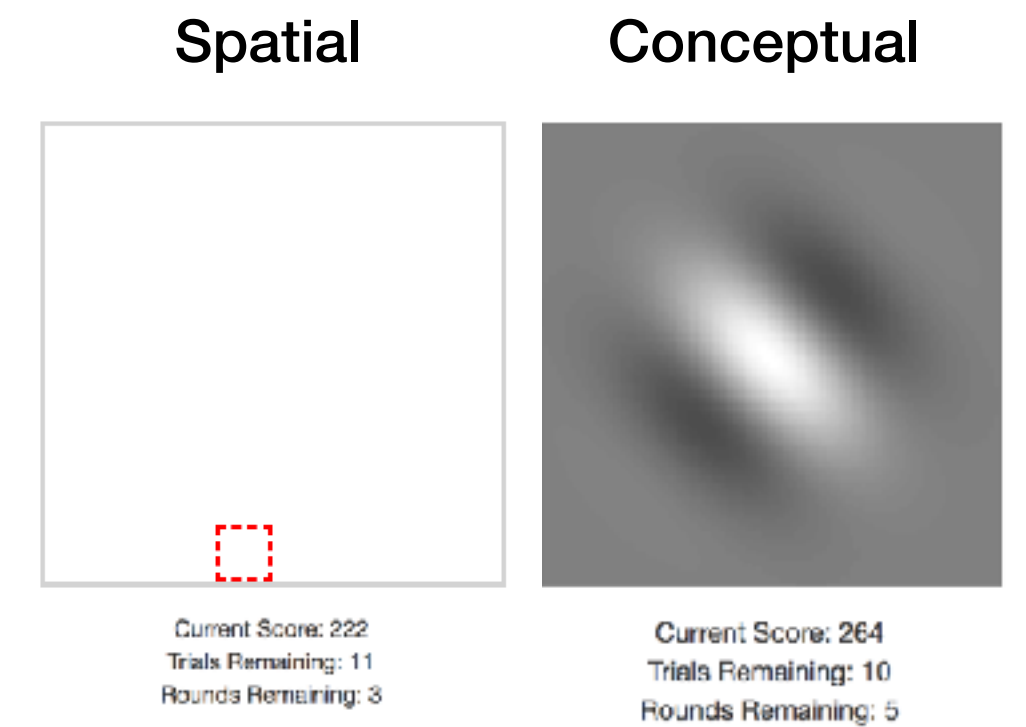
Learning Like a Child



Graph Search



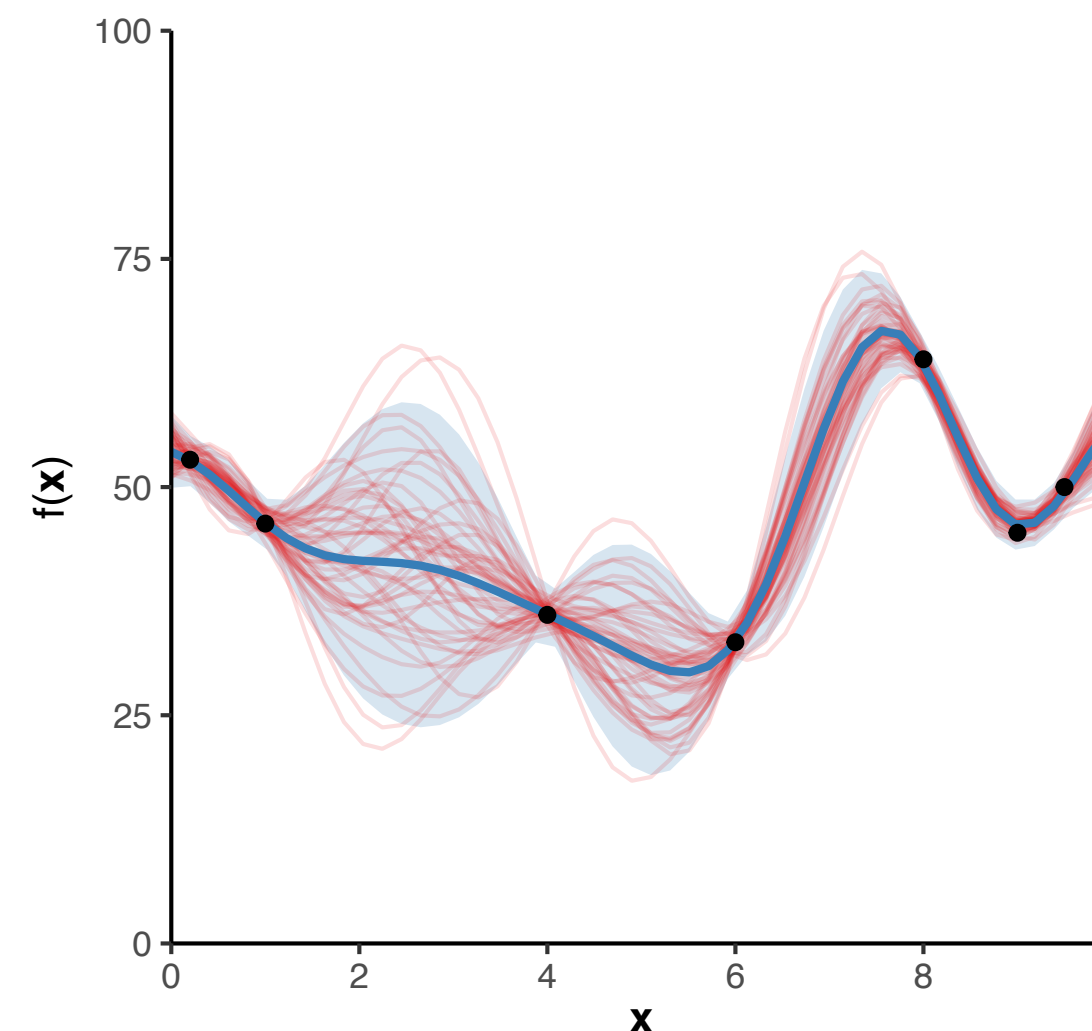
Conceptual Search



Safe Search



Gaussian Processes



Generalization

