An introduction to reinforcement learning

@ Harvard RL Workshop 2022

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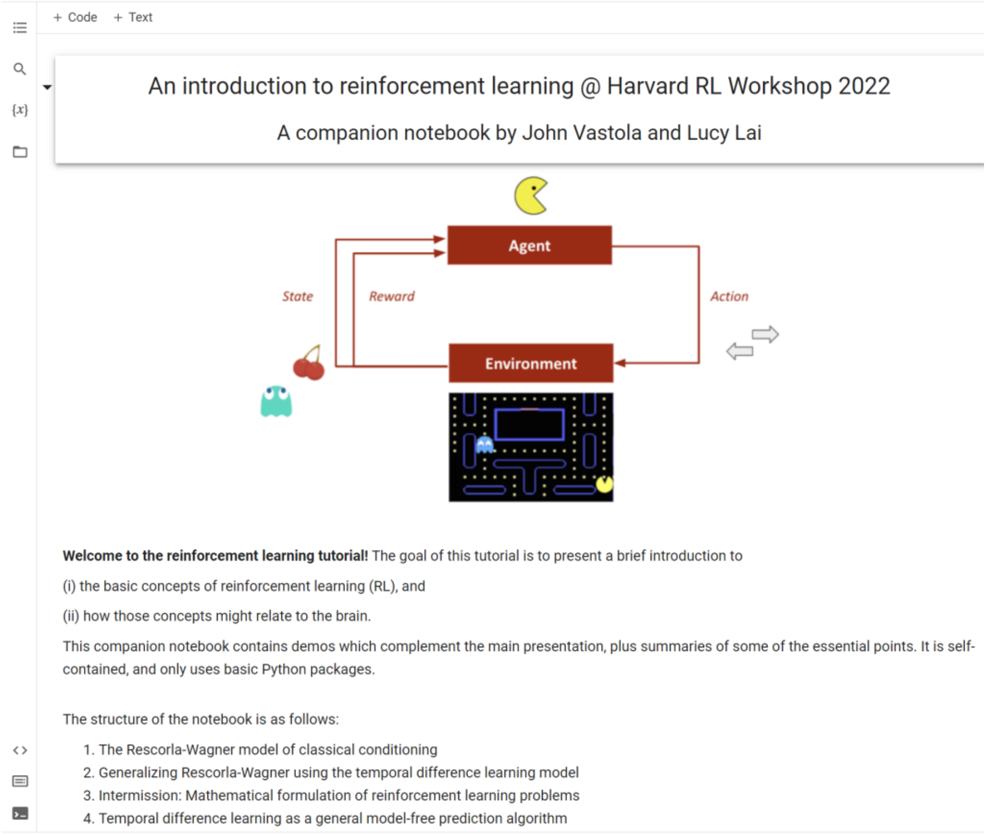
- Slides: https://bit.ly/RLtutorialslides
- Companion notebook (courtesy of John!): bit.ly/RLnotebook



Welcome to the reinforcement learning tutorial! The goal of this tutorial is to present a brief introduction to

(i) the basic concepts of reinforcement learning (RL), and

(ii) how those concepts might relate to the brain.

This companion notebook contains demos which complement the main presentation, plus summaries of some of the essential points. It is self-contained, and only uses basic Python packages.

The structure of the notebook is as follows:

1. The Rescorla-Wagner model of classical conditioning
2. Generalizing Rescorla-Wagner using the temporal difference learning model
3. Intermission: Mathematical formulation of reinforcement learning problems
4. Temporal difference learning as a general model-free prediction algorithm

Can run online using Google Colab; don’t need your own Python installation.

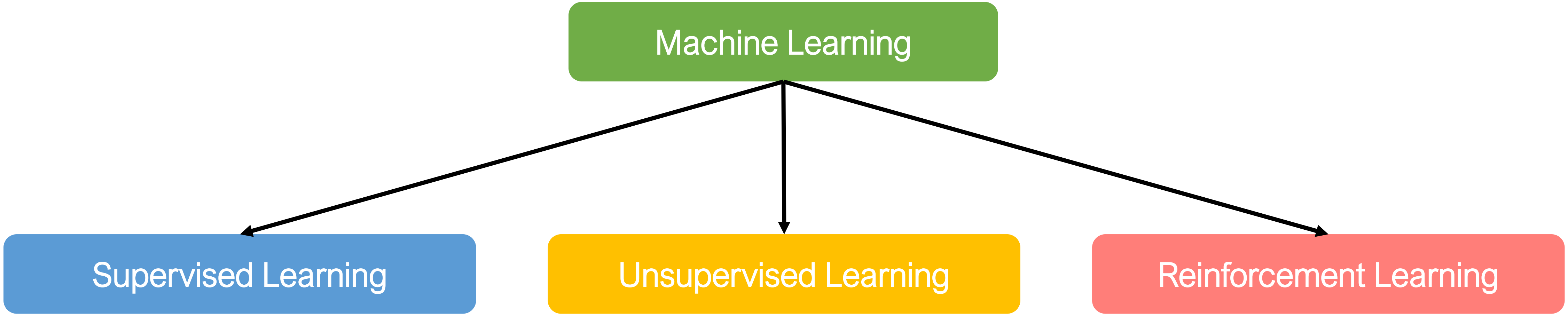
- Career level?
- Discipline?
- Knowledge of RL?

Let’s get started!

Learning objectives & Key takeaways

- After today's session, you will be able to:
  - **Define** the key ingredients of RL: agent, state, action, reward, policy, value and **how they work together** in an algorithm
    - Gives you a primer for common terms used in talks
  - **Implement** the Rescola-Wagner rule and the TD-learning algorithm
  - **Explain** why dopamine encodes a temporal difference (TD) or reward prediction error (RPE)
  - **Identify** some open questions in RL

Three types of learning

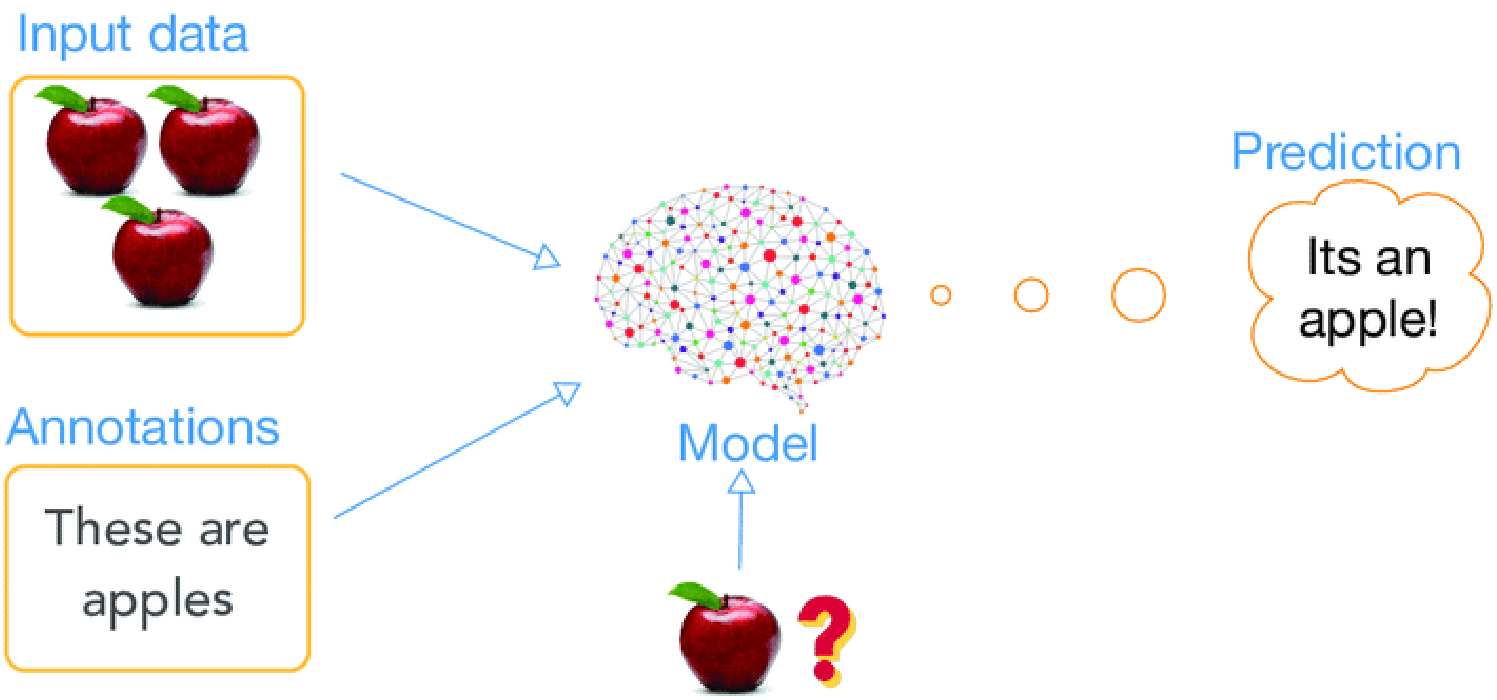


Three types of learning

Machine Learning

Supervised Learning | Unsupervised Learning | Reinforcement Learning

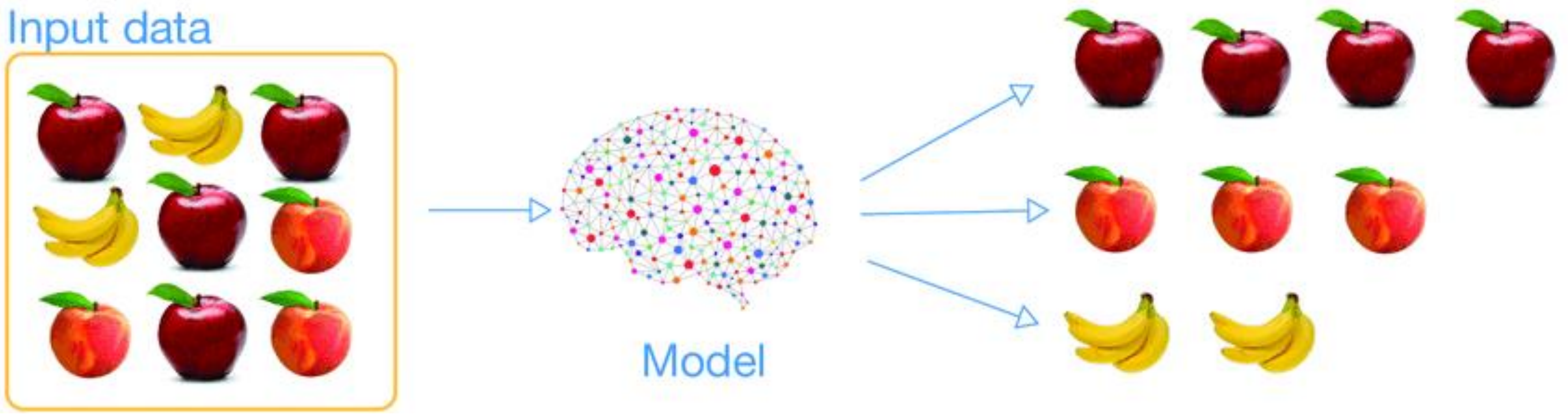
learning with a teaching signal; e.g. assigning pictures to labels



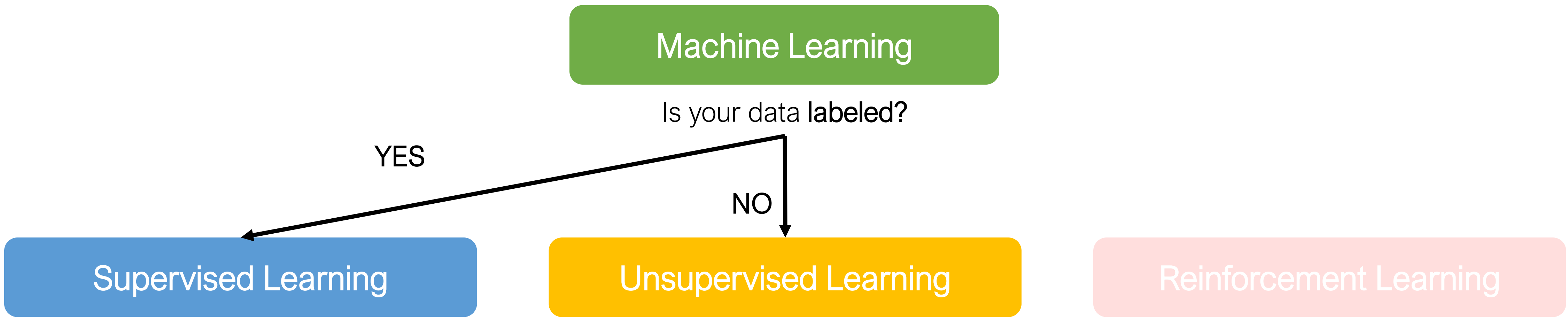
Three types of learning

Machine Learning

- Supervised Learning
  learning with a teaching signal; e.g. assigning pictures to labels
- Unsupervised Learning
  learning the statistics of the world; e.g. perceptual category learning
- Reinforcement Learning



Three types of learning



learning with a teaching signal; e.g. assigning pictures to labels

learning the statistics of the world; e.g. perceptual category learning

Three types of learning

Machine Learning

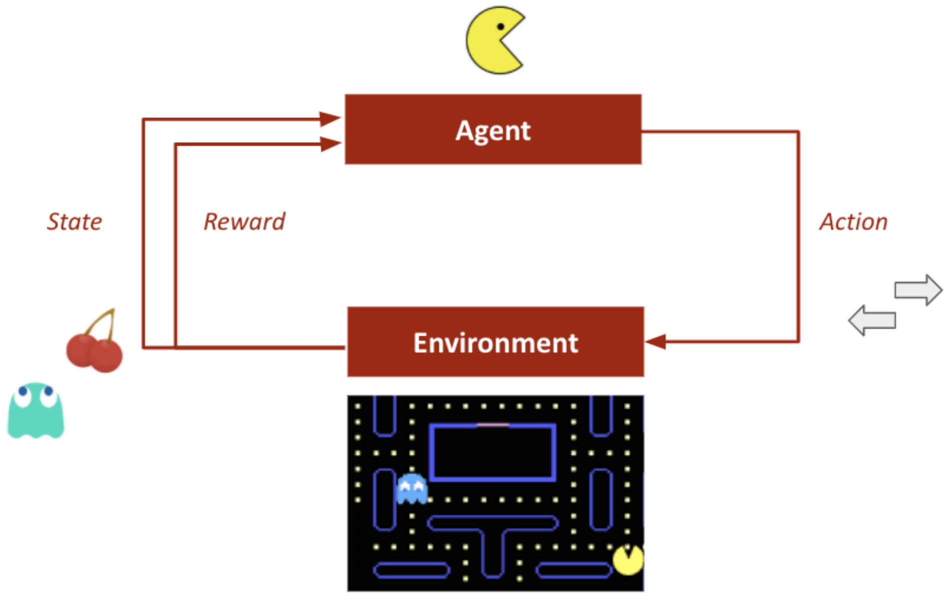
Is your data **labeled?**

YES

NO

N/A – data not given, agent generates data via interactions with the environment

Supervised Learning	Unsupervised Learning	Reinforcement Learning
learning with a teaching signal; e.g. assigning pictures to labels	learning the statistics of the world; e.g. perceptual category learning	learning what to do from interactions with the world; a reinforcement signal rather than teaching signal



Three types of learning

Machine Learning

Is your data **labeled?**

YES

NO

N/A – data not given, agent generates data via interactions with the environment

Supervised Learning

learning with a teaching signal; e.g. assigning pictures to labels

- Classification
    - Logistic regression
    - Support vector machines (SVMs)
    - Convolutional neural networks (CNNs)
- Regression
    - Linear regression

Unsupervised Learning

learning the statistics of the world; e.g. perceptual category learning

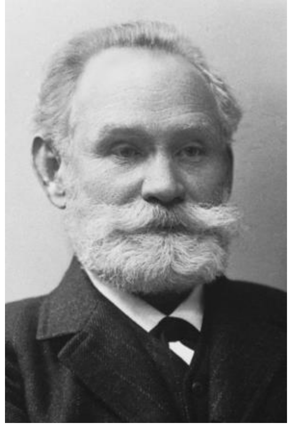
- Dimensionality reduction
    - PCA
    - LDA
- Clustering
    - K-nearest neighbors (KNN) clustering
    - Hierarchical clustering

Reinforcement Learning

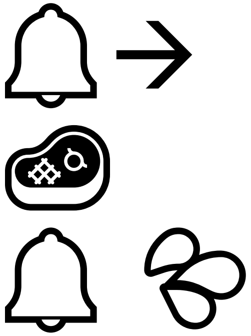
learning what to do from interactions with the world; a reinforcement signal rather than teaching signal

- Model-based RL
    - AlphaZero
- Model-free RL
    - Actor-critic (policy & value)
    - Policy learning
        - Policy gradient
    - Value learning
        - Tabular Q-learning
        - Deep Q-learning
        - Function approximation

Pavlovian conditioning



Ivan Pavlov



pair stimulus with some significant event

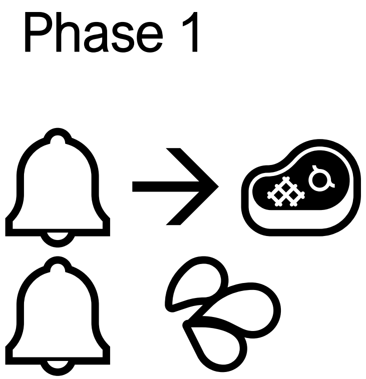
measure anticipatory behavior

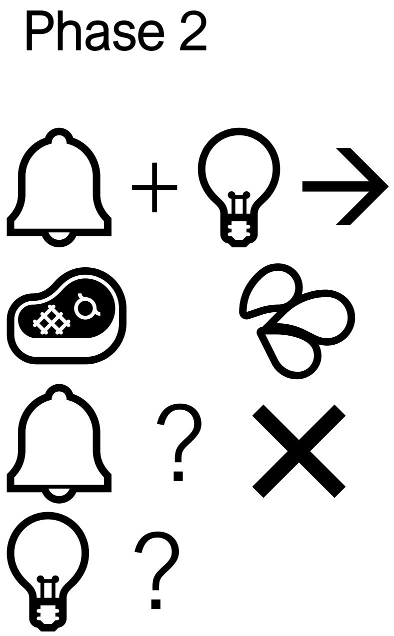
Terminology:

- Unconditional stimulus (US)
- Conditional stimulus (CS)
- Conditional response (CR)

Kamin’s blocking

- What happens when you pair another predictor with the US after animal has already been conditioned to one CS?





- First CS blocks acquisition of the second CS!
- CS-US pairing is not enough, also need surprise!

Rescorla-wagner rule

- **Core idea:** an animal only learns when surprised, i.e., when events violate its expectations

- The change in the value of a CS () is proportional to the difference between the value of the US () and value predicted by the CS (, can be multiple!), a.k.a. the *prediction error*:

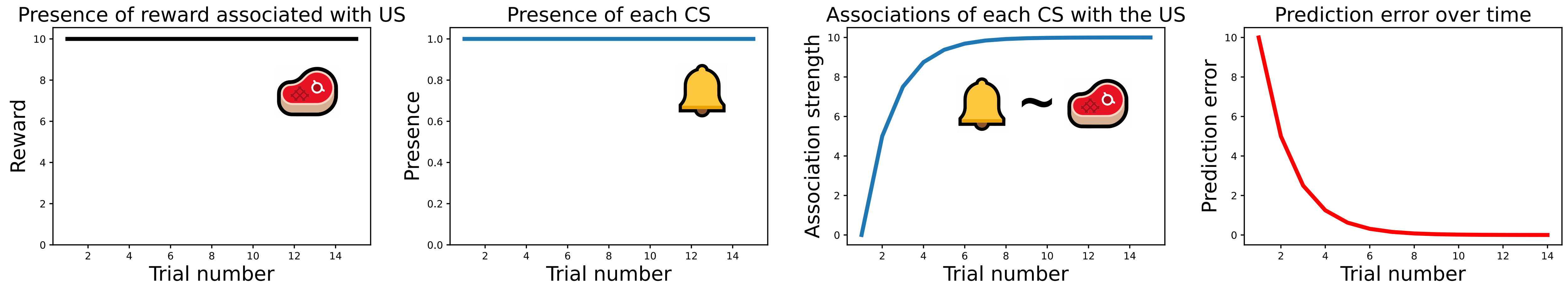
$$\Delta V(CS_j) = \alpha(R_{US} - \sum_{i\in\text{trial}} V(CS_i))$$

- Two assumptions/hypotheses:
  - (1) learning is driven by *error* (formalizes the notion of surprise)
  - (2) prediction error driven by *summation* of predictors

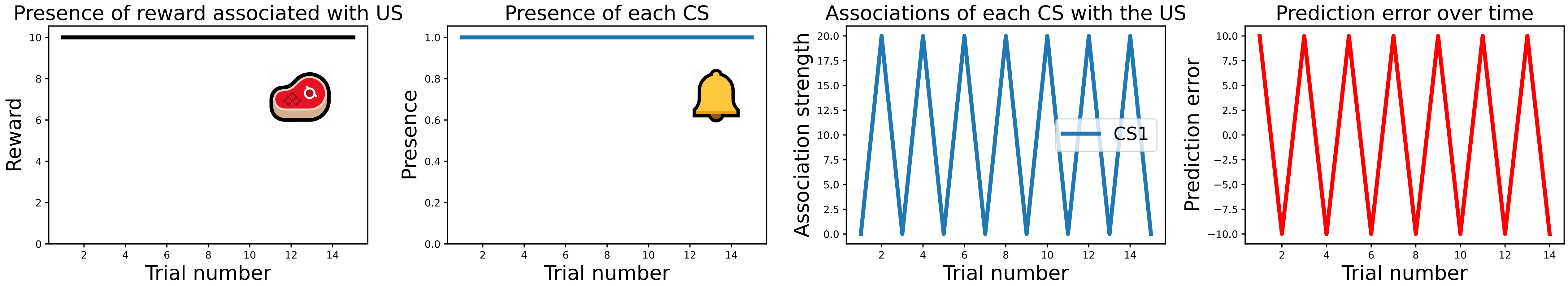
- What happens to the *prediction error* after a couple iterations of this?

- What happens to the value if the learning rate α is high? If α is low?

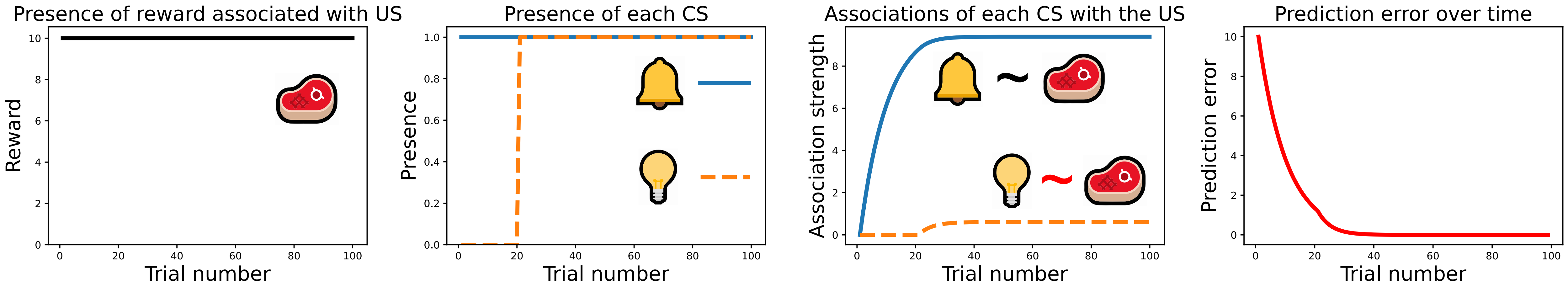
Low learning rate



High learning rate



Rescorla-Wagner can model blocking experiments:

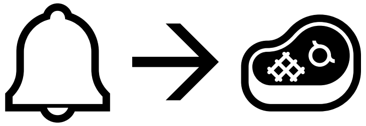


Summary so far

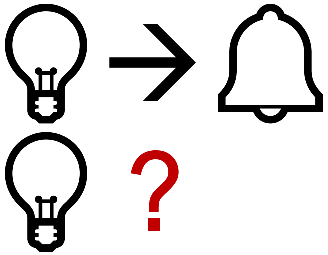
- Rescorla-Wagner learning suggests that we learn from prediction errors
- In this framework, learning = erasing previous beliefs
- Slow learning is not necessarily bad!!!
- We can think of the “learning rate” as an important factor determining how we balance old and new information

But…second-order conditioning

Phase 1



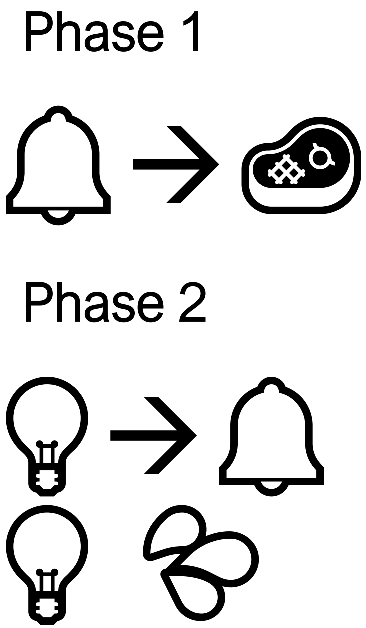
Phase 2



$$\Delta V(CS_j) = \alpha(R_{US} - \sum_{i \in \text{trial}} V(CS_i))$$

- What does the Rescorla-Wagner model predict?
  A. animals will salivate to the light
  B. animals will not salivate to the light

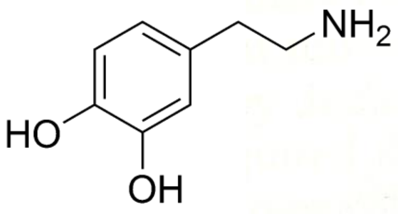
But…second-order conditioning

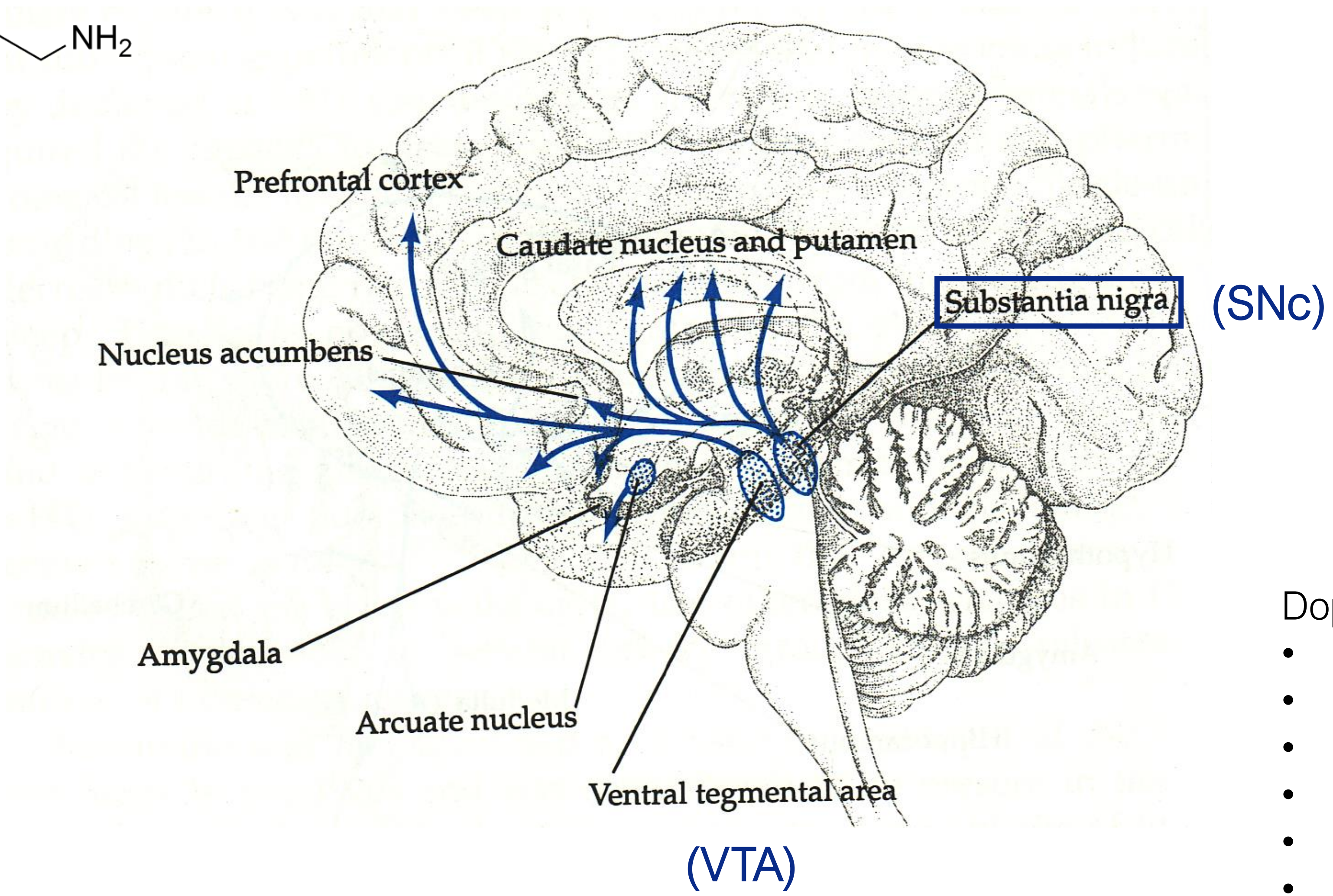


Second-order conditioning: a neutral conditional stimulus (CS) acquires the ability to elicit a conditioned response (CR) without ever being directly paired with an unconditioned stimulus (US)

- What do YOU think actually happens?
  A. animals will salivate to the light
  B. animals will not salivate to the light

Another puzzle…dopamine

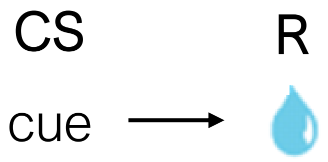


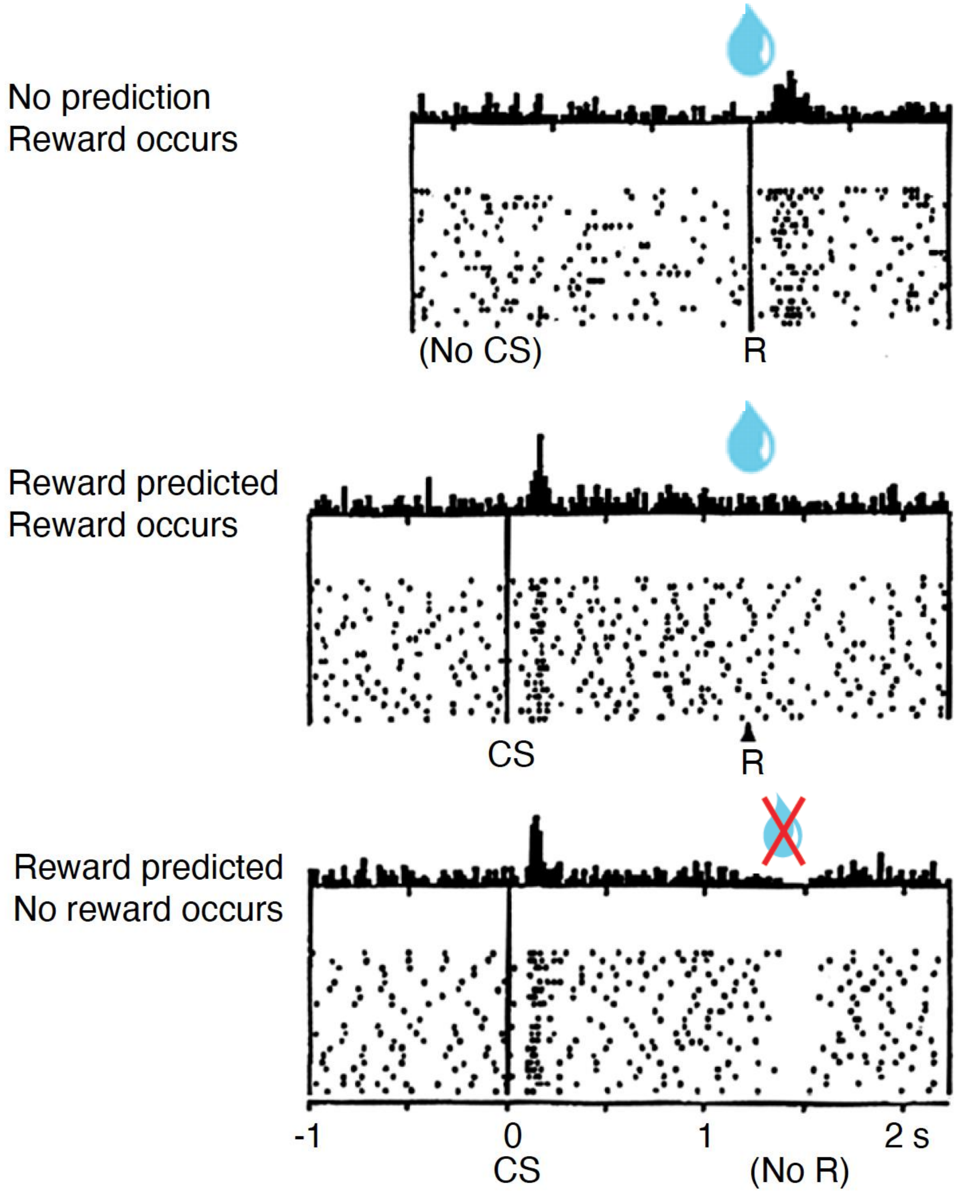


Dopamine plays a role in:

- motivation
- learning
- action-selection
- addiction
- schizophrenia
- Parkinson's disease
- etc…

Another puzzle…dopamine





Dopamine responds to reward-predicting stimuli instead of to rewards themselves

Schultz, Dayan, & Montague, 1997

So…two puzzles

Behavioral puzzle: second order conditioning

Neural puzzle: dopamine responds to reward-predicting stimuli instead of to rewards

How to solve these puzzles?

TD learning

- **Core idea:** Temporal difference learning extends the ideas from Rescorla-Wagner learning from immediate rewards to **all rewards in the future**.

Rescorla- Wagner: $\Delta V(CS_j) = \alpha[R_{US} - \sum_{i \in \mathrm{trial}} V(CS_i)]$

TD learning: $\Delta V(t) = \delta = \alpha[R(t) + \gamma \cdot \hat{V}(t+1) - \hat{V}(t)]$

Value (at the current point in time): the *discounted* sum of all future rewards

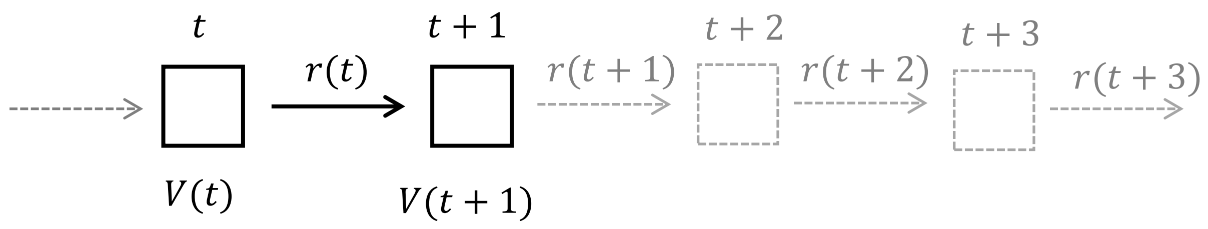
Predicted reward

- New idea: a discount factor γ that tells you how much to care about rewards in the future

Sutton & Barto 1983, 1990

TD learning

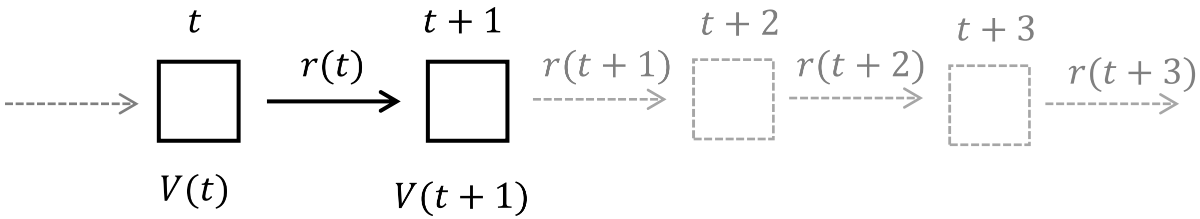
States



t : time
r : reward
V : value

TD learning

States



t : time
r : reward
V : value

Value: the discounted sum of all future rewards

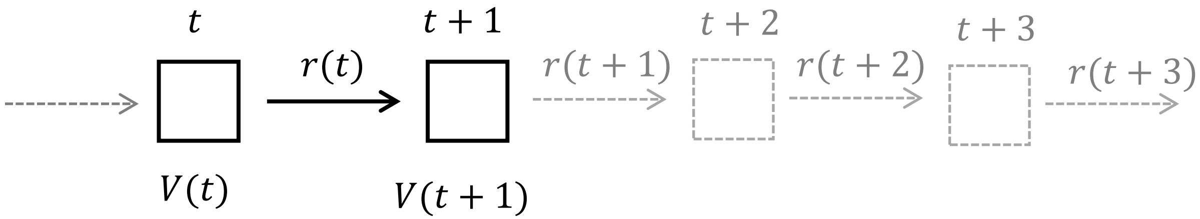
Discount factor

$$0 < \gamma < 1$$

$$V(t) = \sum_{k=0}^{\infty} \gamma^k \, r_{t+k}$$

TD learning

States



t : time
r : reward
V : value

Value: the discounted sum of all future rewards

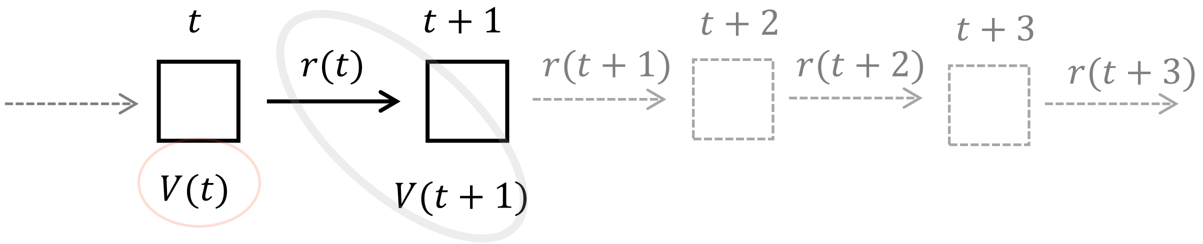
Discount factor
$0 < \gamma < 1$

$$V(t) = \sum_{k=0}^{\infty} \gamma^k \, r_{t+k} = r(t) + \underbrace{\boxed{\gamma \cdot r(t+1) + \gamma^2 \cdot r(t+2) + \cdots}}_{\gamma \cdot V(t+1)}$$

$$V(t) = r(t) + \gamma \cdot V(t+1)$$

TD learning

States



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$$V(t) = \sum_{k=0}^{\infty} \gamma^k r_{t+k} = r(t) + \underbrace{\boxed{\gamma \cdot r(t+1) + \gamma^2 \cdot r(t+2) + \cdots}}_{\gamma \cdot V(t+1)}$$

$$V(t) = r(t) + \gamma \cdot V(t+1)$$

Temporal difference (TD) prediction error

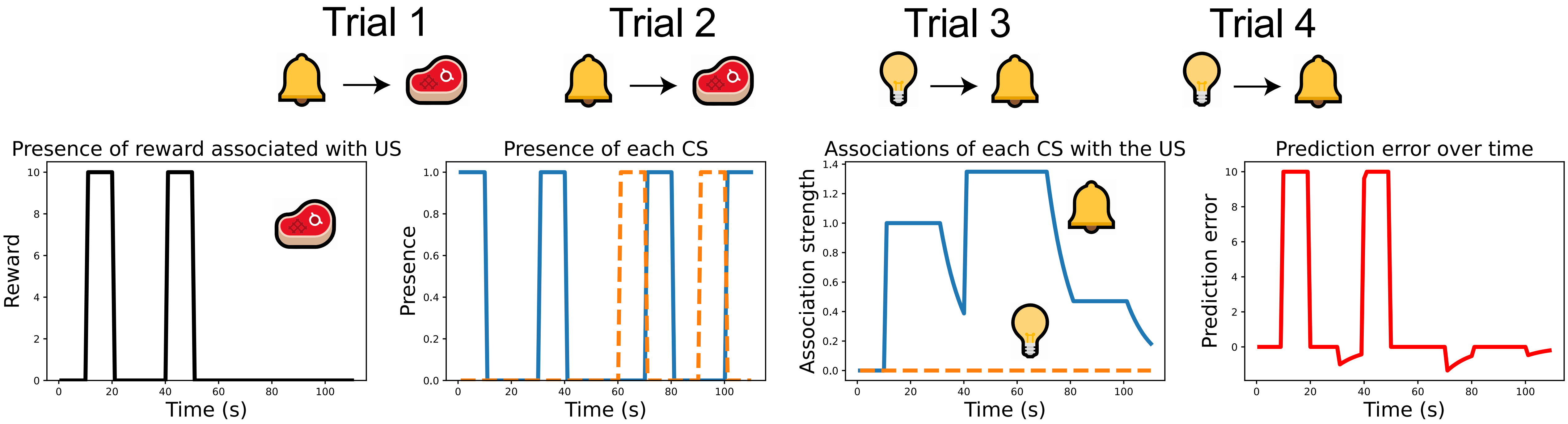
$$\delta = r(t) + \gamma \cdot \hat{V}(t+1) - \hat{V}(t) \quad \Rightarrow \quad \text{Update } V(t)$$

$$\hat{V}(t) \leftarrow \hat{V}(t) + \alpha \cdot \delta \qquad (\alpha\text{: learning rate})$$

Sutton, 1988; Sutton & Barto, 1998; Montague et al., 1996; Schultz et al., 1997

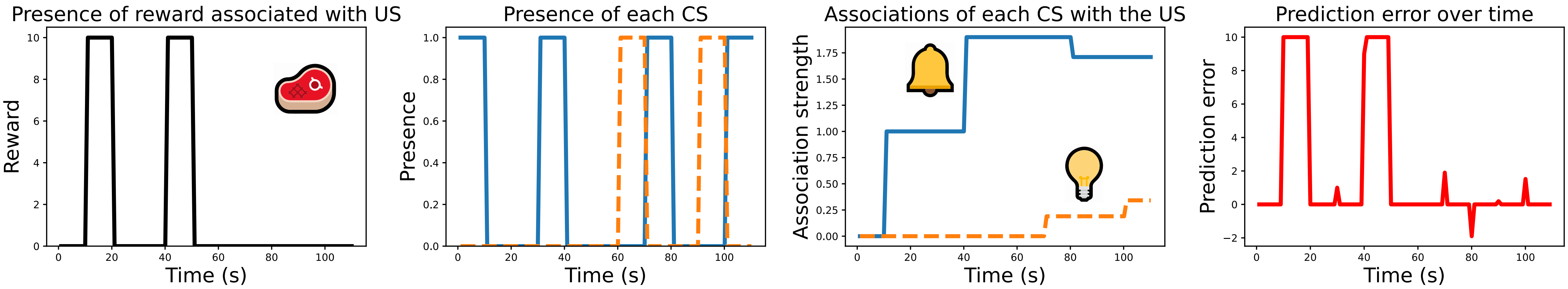
Discount factor γ determines how much you care about future reward

When there is no anticipating the future (γ = 0), second order conditioning doesn't happen:



Discount factor γ determines how much you care about future reward

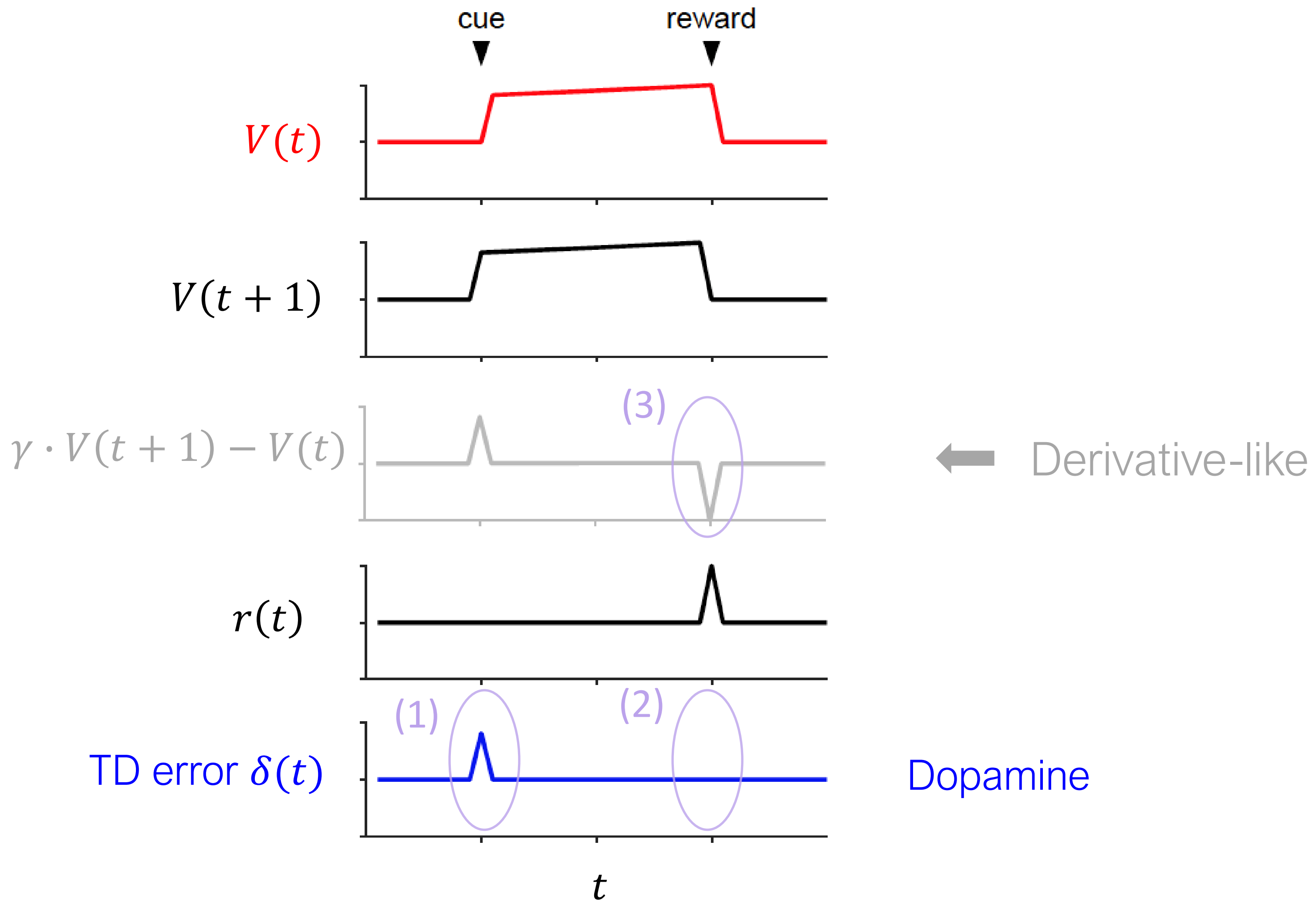
When anticipating *eventual* reward (γ = 1), second order conditioning *does* happen:



Dopamine responses as TD errors

$$\delta(t) = r(t) + \gamma \cdot V(t+1) - V(t)$$

$r(t)$: reward
γ: discount factor
$V(t)$: Value

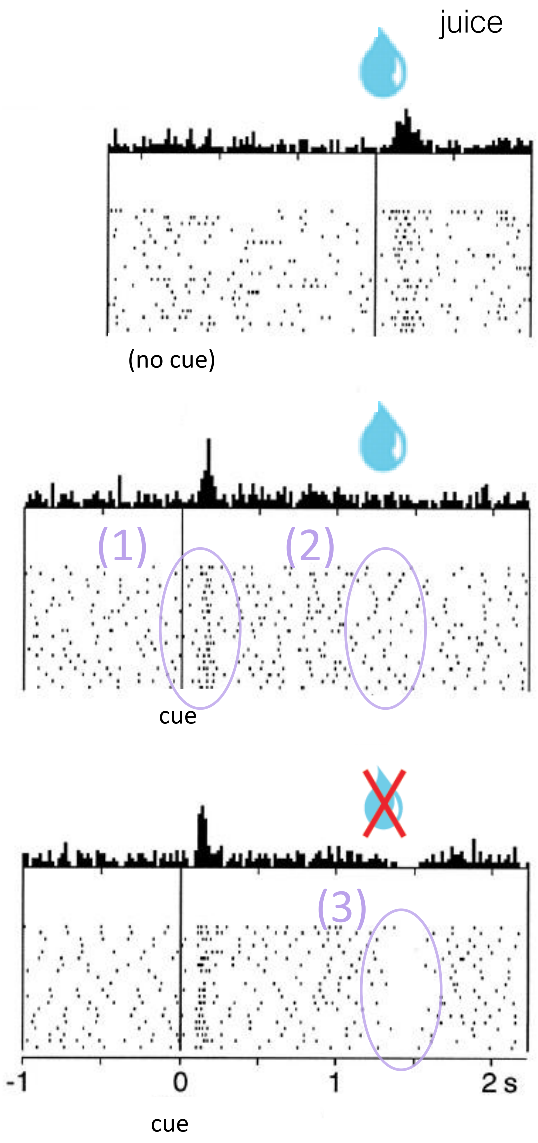


Dopamine responses as TD errors

No prediction
Reward occurs

Cue predicts reward
Reward occurs

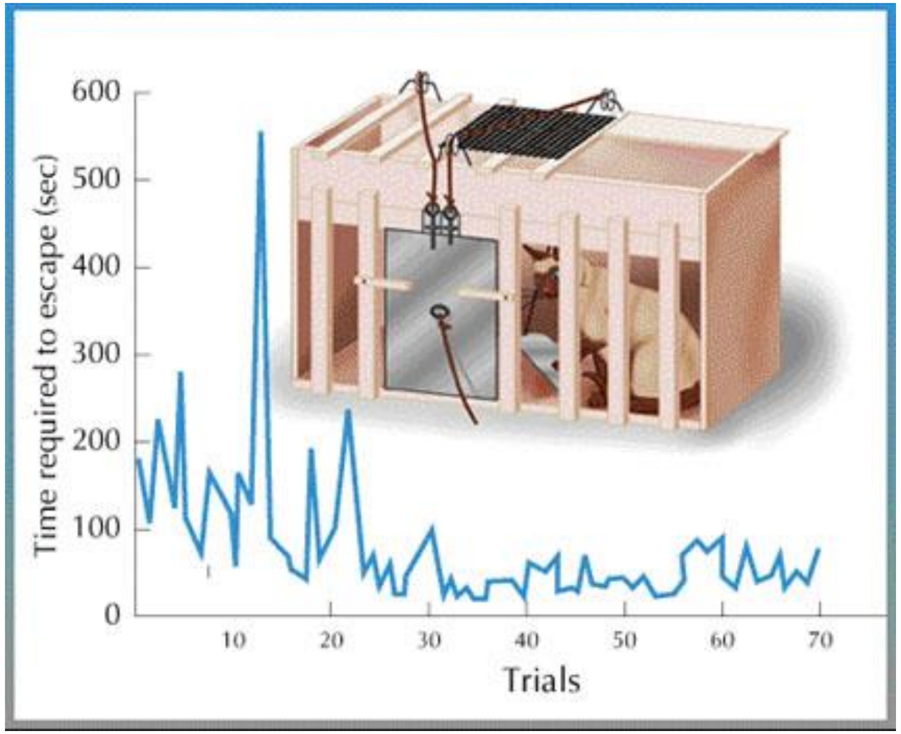
Cue predicts reward
No reward occurs

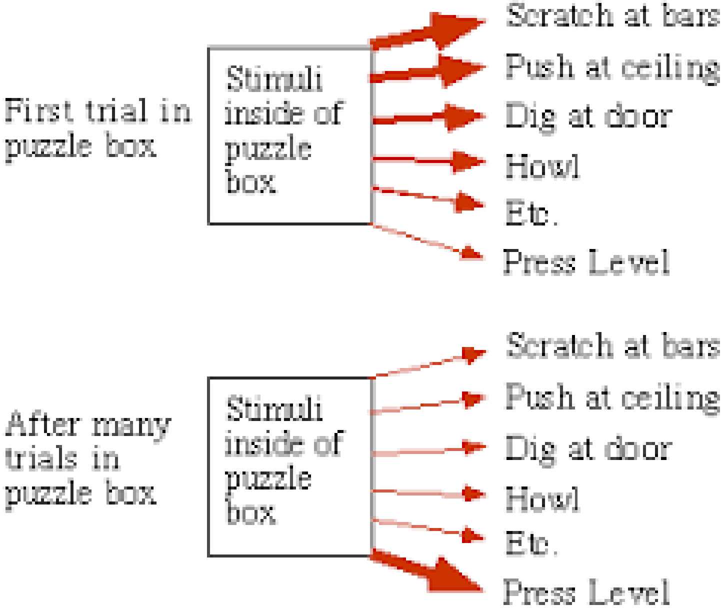


Schultz, Dayan & Montague (1997)

Action selection

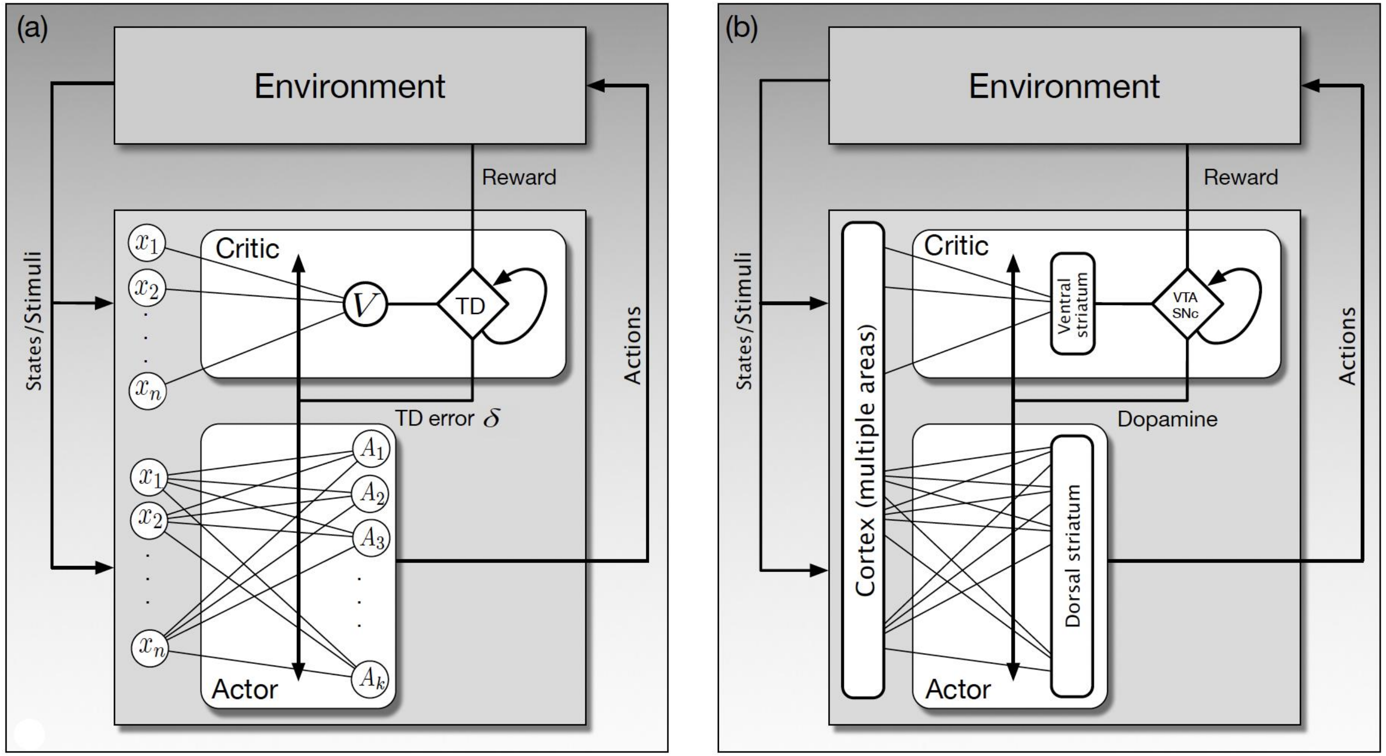
- Prediction learning is not enough by itself, need something that helps you change behavior!
- Instrumental learning: Thorndike's Law of Effect





- Successful actions will be reinforced!

Actor-critic models



"Actor" learns policies (mappings from state to actions)

"Critic" evaluates whether the actions that the actor chose were high or low in value

TD error updates both state and action values

Dorsal striatum: implicated in influencing action selection

Ventral striatum: reward processing and assigning affective value to sensory input

Dopamine modulates synaptic plasticity in both the dorsal and ventral striatum

Correspondences between psychology and RL

Behavioral psychology ⇄ RL in computer science

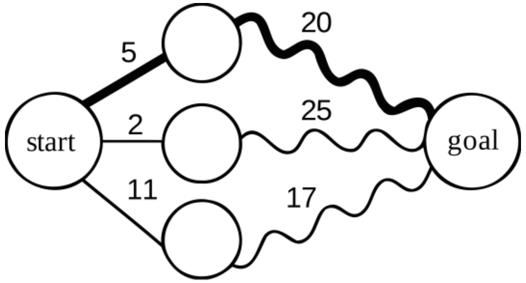
Behavioral psychology		RL in computer science
Pavlovian (classical)	predicting upcoming events (stimuli/reward)	**Algorithms for prediction** can I predict the future values of states?
vs		vs
instrumental conditioning	behavior contingent on environment	**algorithms for control** what should my policy be?

RL in neuroscience

RL in machine learning

Historical threads

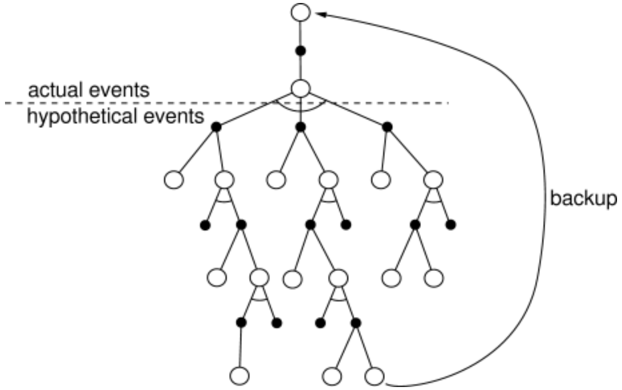
Optimal control theory



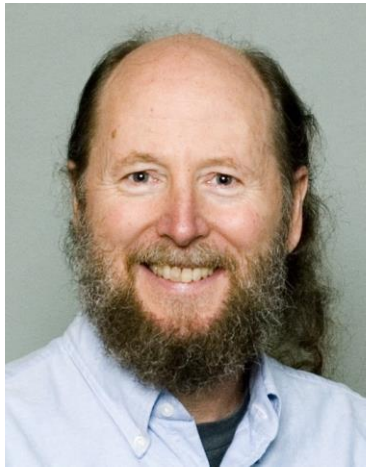
Dynamic programming:
Bellman (~1950s)

Trial-and-error learning

e.g. Samuel's checker-playing program (~1959)



Temporal difference learning, Q-learning…

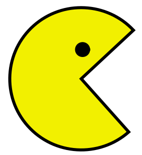


Sutton ~ 1988:
First systematic treatment of TD methods

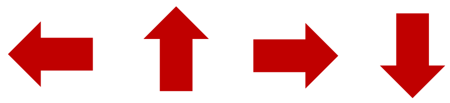
Watkins 1989: Q-learning

Tesauro 1992: TD-Gammon

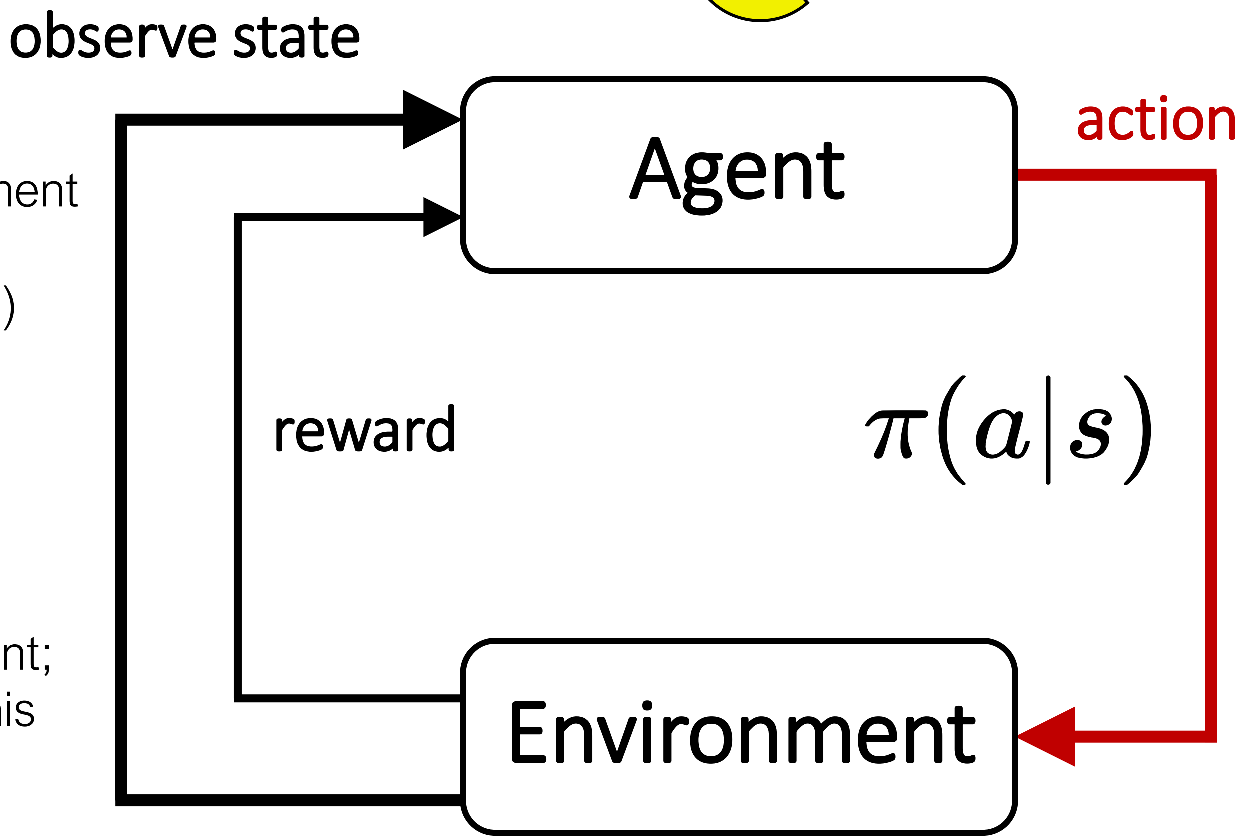
Basic RL: problem formulation



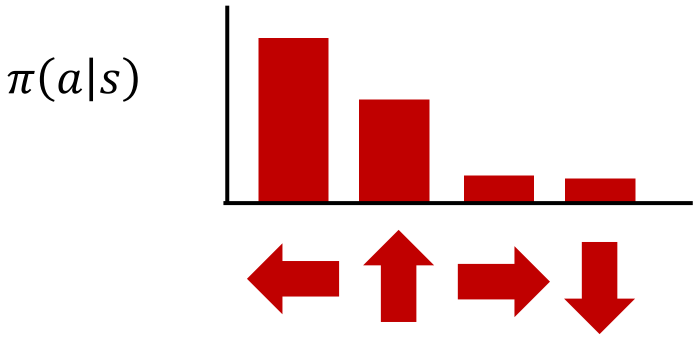
how an agent **interacts** with its environment

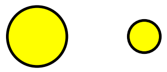


State:
current status of environment (e.g., location of agent or obstacles, "internal state")



Policy:
the probability of taking each action in a given state

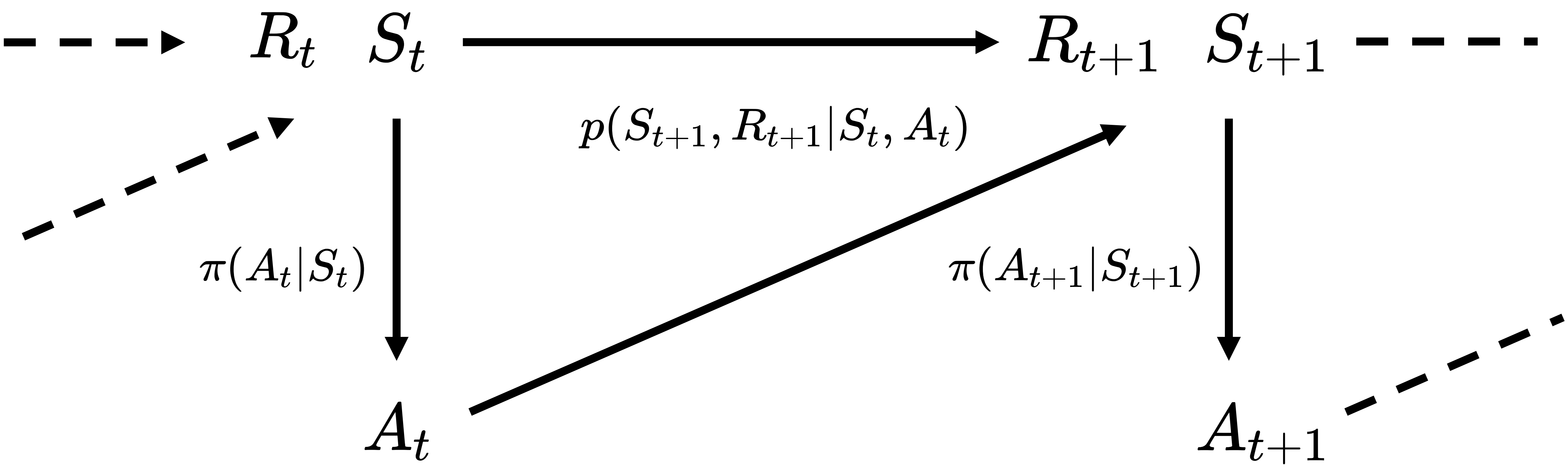


Reward:


feedback from environment; agent tries to maximize this

Model of environment (optional) :
knowledge of how your actions will bring you to rewards and other states (as opposed to just treating each state independently)

The math setting of RL: Markov decision processes



Key assumption: what you do, and what happens next, only depends on the current state, and not on previous ones.

The goal of RL: maximize expected (discounted) future reward

- **Return**: discounted future reward

$$G_t := R_{t+1} + \gamma R_{t+2} + \gamma^2 R_{t+3} + \cdots = \sum_{k=t+1}^{T} \gamma^{k-t-1} R_k$$

- **State value:** expected return, given a specific starting state and policy

$$v_\pi(s) := \mathbb{E}_\pi[G_t | S_t = s]$$

Value function

- **Action value:** expected return, given a specific starting state, action, and policy

$$q_\pi(s, a) := \mathbb{E}_\pi[G_t | S_t = s, A_t = a]$$

Q-value function

The goal of RL: maximize expected (discounted) future reward

- **Return**: discounted future reward

$$G_t := R_{t+1} + \gamma R_{t+2} + \gamma^2 R_{t+3} + \cdots = \sum_{k=t+1}^{T} \gamma^{k-t-1} R_k$$

- Prediction problem: How much reward will we get if we follow a given policy?

Target: $v_\pi(s) := \mathbb{E}_\pi[G_t | S_t = s]$

- Control problem: What's the 'best' policy?

Target: $\pi_*(a|s)$ $v_{\pi_*}(s) \geq v_\pi(s)$

not unique in general

Basic RL: solving the prediction problem

The Bellman equation and dynamic programming

- Prediction problem: How much reward will we get if we follow a given policy?
- Useful fact: the value function satisfies the **Bellman equation**:

$$v_\pi(s) = \sum_{s',r,a} p(s',r|s,a)\pi(a|s)\left[\, r + \gamma v_\pi(s')\,\right]$$

$$q_\pi(s,a) = \sum_{s',r} p(s',r|s,a)\left[\, r + \gamma \max_{a'} q_\pi(s',a')\,\right]$$

- This equation is the basis of an iterative approach to evaluating a policy.

$$V_\pi(s) \leftarrow \sum_{s',r,a} p(s',r|s,a)\pi(a|s)\left[\, r + \gamma V_\pi(s')\,\right]$$

The TD algorithm for evaluating the goodness of a policy

- Dynamic programming requires knowing environment's dynamics… generally not the case.

- But it inspires an online, model-free prediction algorithm:
  temporal difference (TD) learning!

- The TD algorithm lets you evaluate a policy in real time, by trial and error.

The TD algorithm for evaluating the goodness of a policy

In state S, take action A according to policy π(A | S).

Transition to S' and collect reward R.

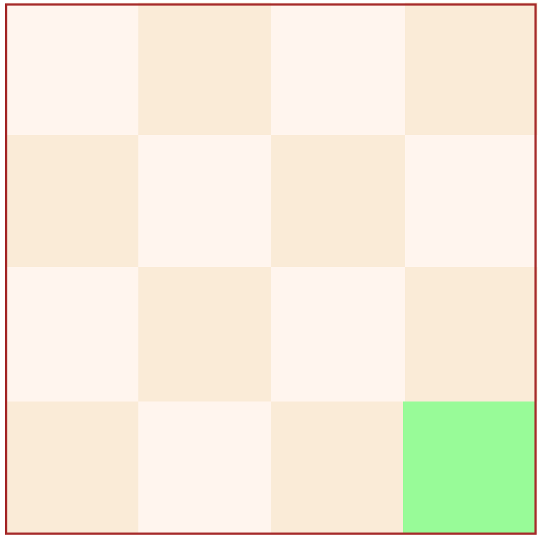
$$S \leftarrow S'$$

$$\delta := R + \gamma\, V_\pi(S') - V_\pi(S)$$ Prediction error

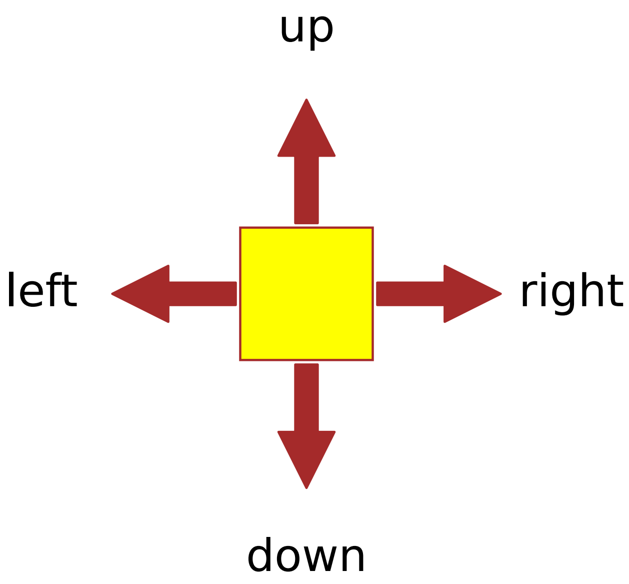
$$V_\pi(S) \leftarrow V_\pi(S) + \alpha\, \delta$$ Value update

A gridworld example

Environment



Possible actions



Possible rewards

Reach non-goal square:

$R = -1$

Reach goal square:

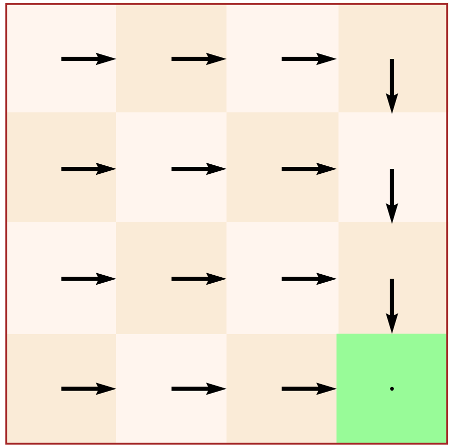
$R = 10 - 1$

Initial grid location is random

A gridworld example: evaluating the ‘down-right’ policy

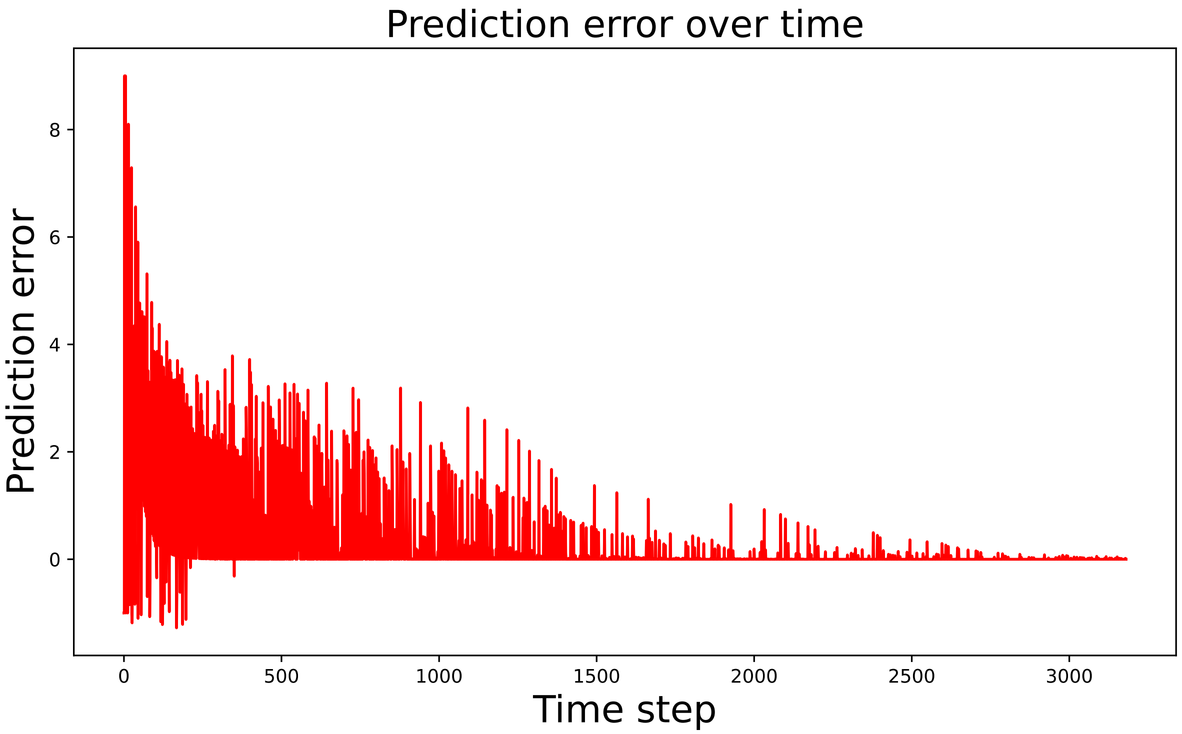
Using the TD algorithm (1000 episodes):

Policy



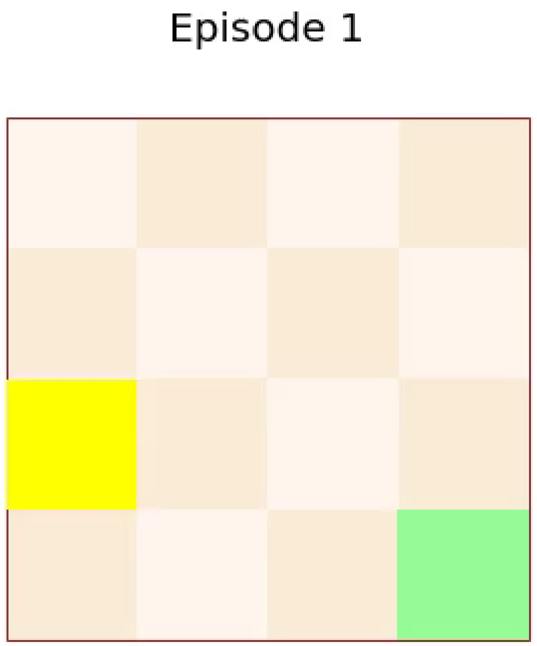
Value function

3.98	5.0	6.0	7.0
4.99	6.0	7.0	8.0
5.96	7.0	8.0	9.0
6.98	8.0	9.0	



A gridworld example: evaluating the ‘down-right’ policy

Using the TD algorithm (1000 episodes):



Basic RL: solving the control problem

Generalized policy iteration and the RL control problem

- Two things you don't know in general:

  (i) how much reward you're going to get given your current policy

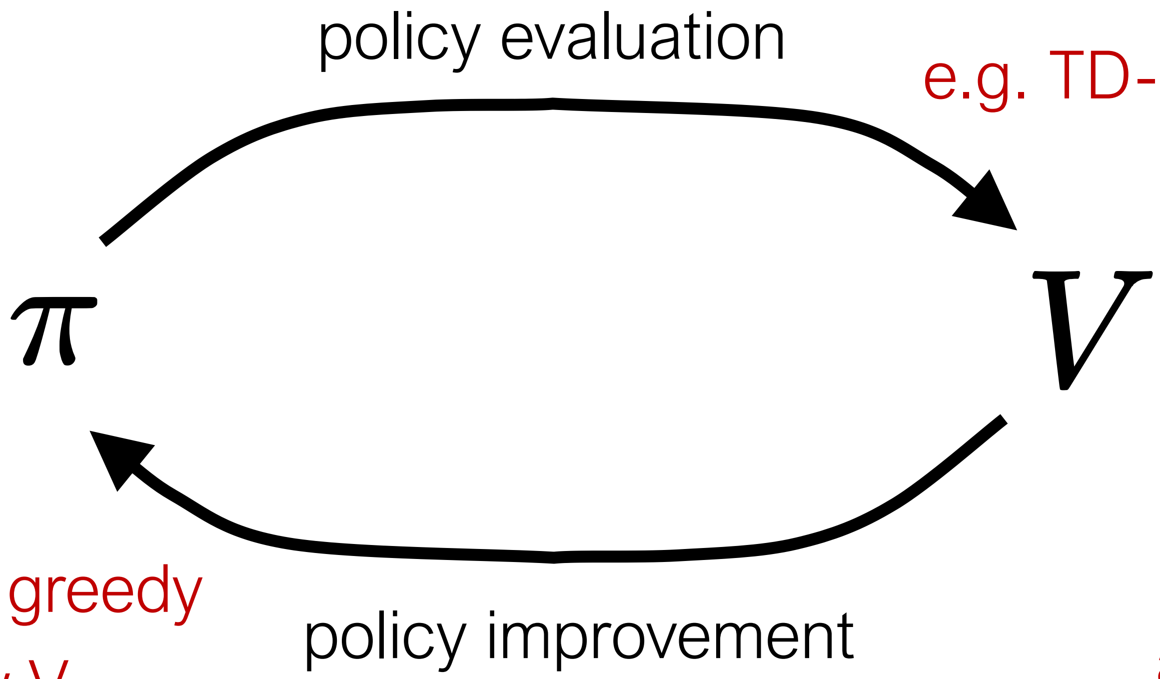
  (ii) what the best policy is.

- Idea of **generalized policy iteration**: switch between improving both by a little!

Generalized policy iteration and the RL control problem

- Idea of **generalized policy iteration**: switch between improving both by a little!

e.g. TD-like update



e.g. make π greedy
wrt new V

Hope to eventually
approach an **optimal**
policy / value function!

Two control strategy examples:
Q-learning and actor-critic

Q-learning: TD policy evaluation + greedy action selection

$$Q(s,a) \approx q_*(s,a) = \max_{\pi} \mathbb{E}_\pi[G_t | S_t = s, A_t = a]$$

- Suppose you know Q(s, a), an estimate of the optimal action-value function.
- Suppose you're in a state s. Could turn this into a control strategy by always picking the action a for which Q(s, a) is largest (with ties broken arbitrarily).

Q-learning: TD policy evaluation + greedy action selection

$$Q(s,a) \approx q_*(s,a) = \max_{\pi} \mathbb{E}_\pi[G_t | S_t = s, A_t = a]$$

- But if your Q estimate isn't perfect, may not truly know which actions are best.
- One possibility: couple a strategy like this with a **method for exploration.** Sometimes take actions you wouldn't normally take, and see if they give the expected reward. If so, great. If not, update Q!
- Epsilon-greedy: pick 'best' action with probability 1 – ε; otherwise random.

Q-learning: TD policy evaluation + greedy action selection

In state S, take action A according to policy π(A | S).

$$S \leftarrow S'$$

Transition to S' and collect reward R.

Update policy

e.g. ε-greedy wrt updated Q.

$$\delta := R + \gamma \max_a Q(S', a) - Q(S, A)$$

Prediction error

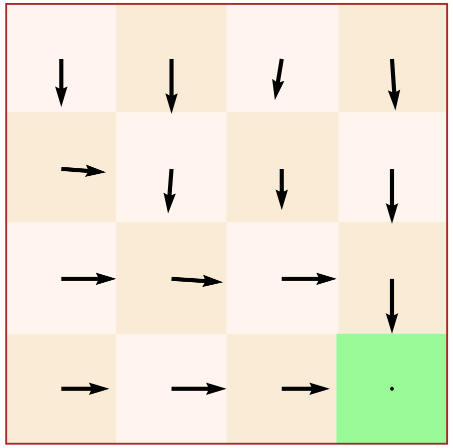
$$Q(S, A) \leftarrow Q(S, A) + \alpha\,\delta$$

Value update

A gridworld example: learning a good policy

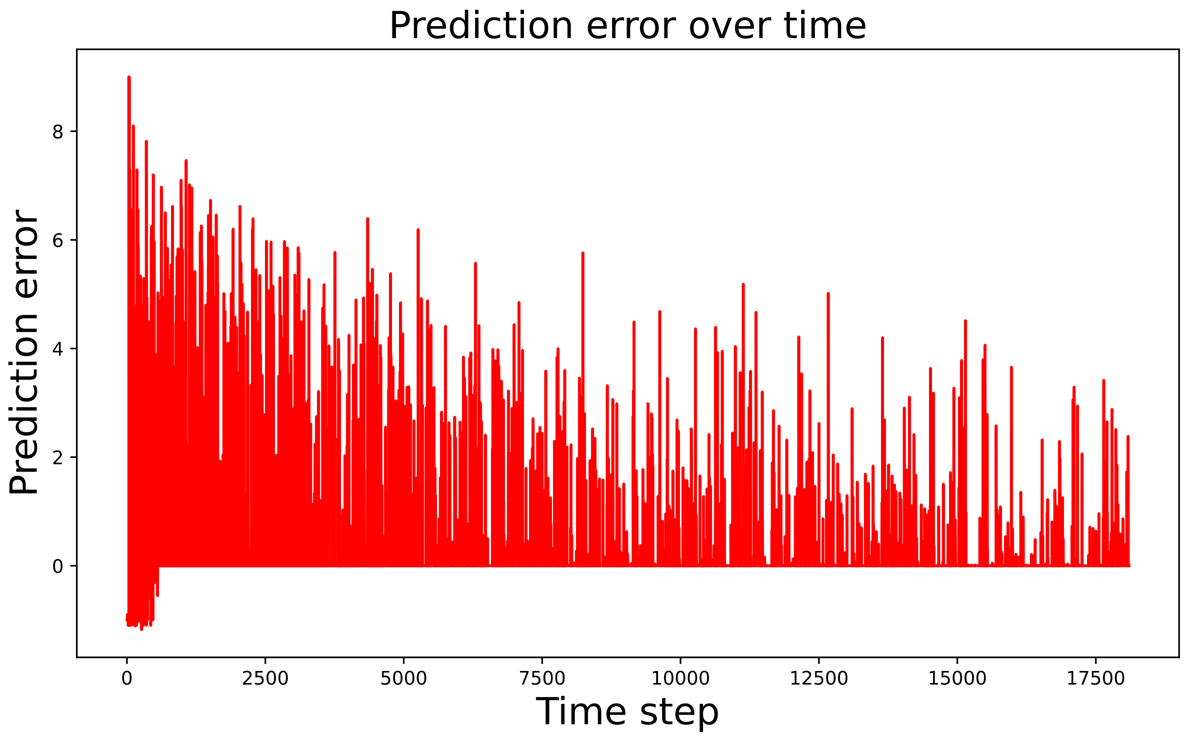
Using Q-learning (5000 episodes):

Policy



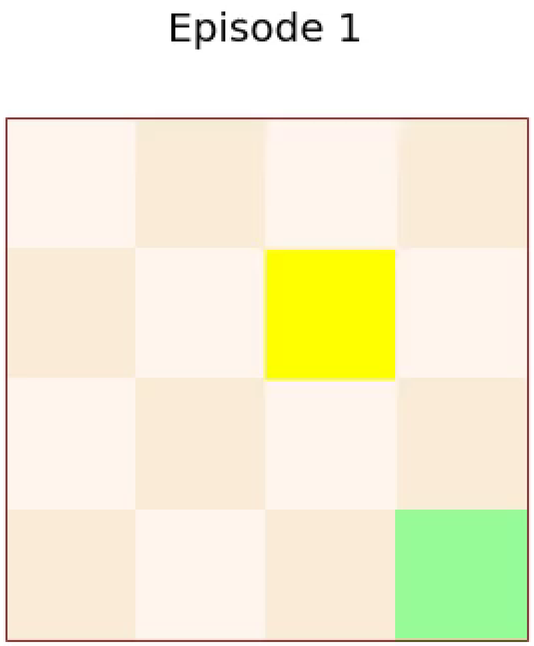
Value function

3.92	5.0	6.0	7.0
4.98	6.0	7.0	8.0
5.96	7.0	8.0	9.0
6.99	8.0	9.0	



A gridworld example: learning a good policy

Using Q-learning (5000 episodes):



Actor-critic: TD policy evaluation + action preferences

- One problem with Q-learning: policy (e.g. epsilon-greedy) closely linked to Q.
- Greedy is *eventually* optimal, but not while learning…
- Either have to accept randomly taking bad actions, or determining a (possibly complicated) schedule for reducing exploration over time.
- Idea for alternative: separate value and policy, and learn both simultaneously!

Actor-critic: TD policy evaluation + action preferences

- Idea: separate value and policy, and learn both simultaneously!

$$\pi(a|s) = \frac{e^{h(s,a)}}{\sum_b e^{h(s,b)}}$$

Want to learn "action preferences" $h(s, a)$ in addition to $V(s)$.

- How to update? **Gradient descent** (using value as objective function).
- Intuitive idea: if you took an action and things went better than expected, take that action more often!

Actor-critic: TD policy evaluation + action preferences

In state S, take action A according to policy π(A | S).

$$S \leftarrow S'$$

Transition to S' and collect reward R.

$$h(S, A) \leftarrow h(S, A) + \alpha\,\delta\,\frac{\nabla_{h(S)}\pi(A|S)}{\pi(A|S)}$$

$$\delta := R + \gamma\,V_\pi(S') - V_\pi(S)$$

Prediction error

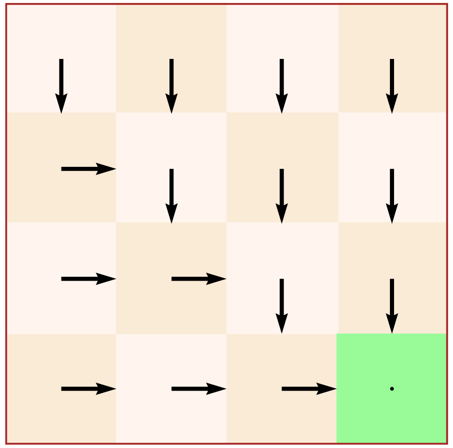
$$V_\pi(S) \leftarrow V_\pi(S) + \alpha\,\delta$$

Value update

A gridworld example: learning a good policy

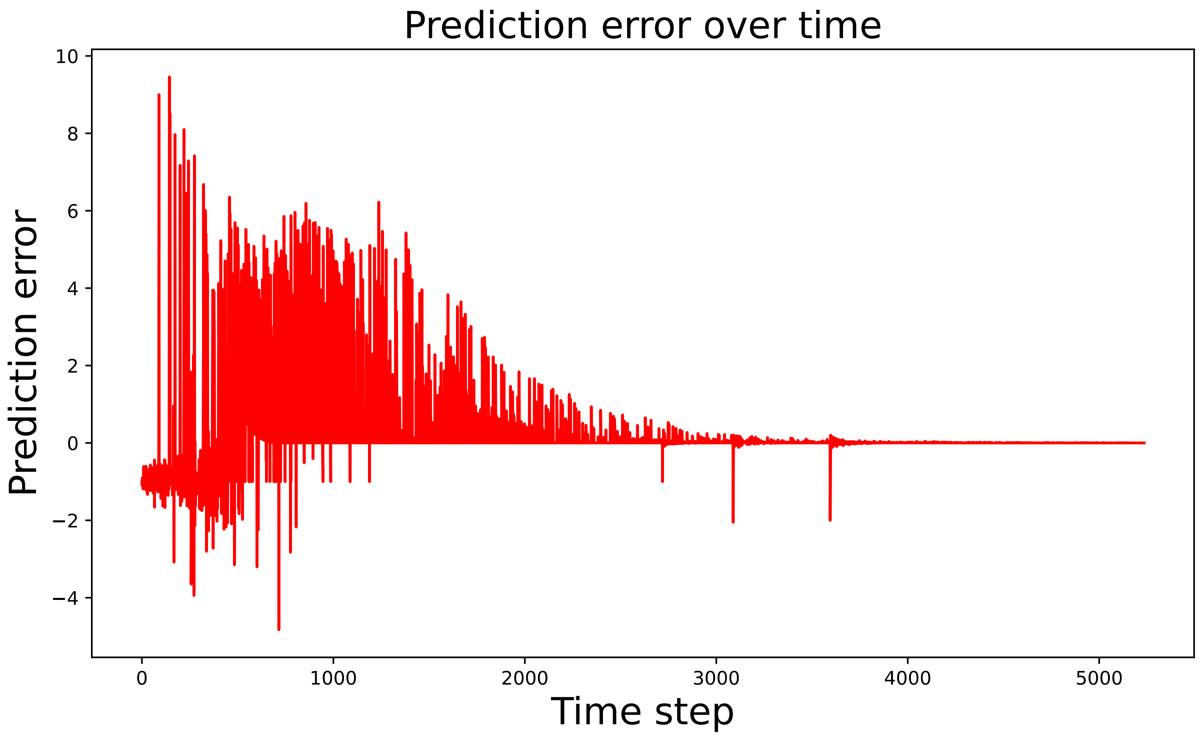
Using actor-critic (1500 episodes):

Policy



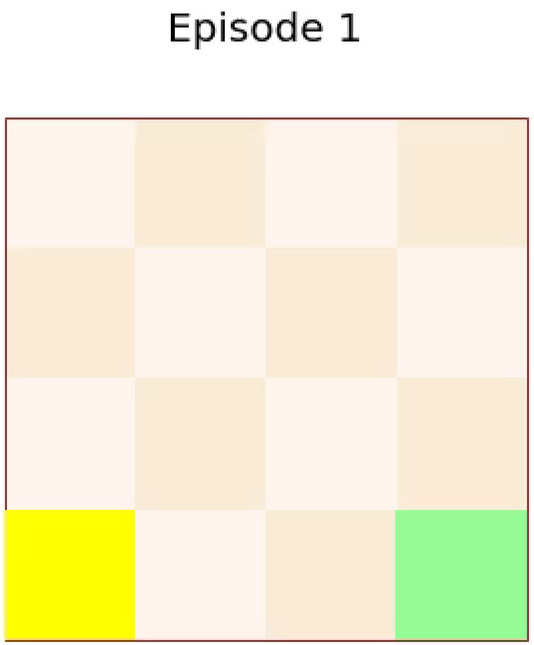
Value function

3.99	5.0	6.0	7.0
5.0	6.0	7.0	8.0
6.0	7.0	8.0	9.0
7.0	8.0	9.0	

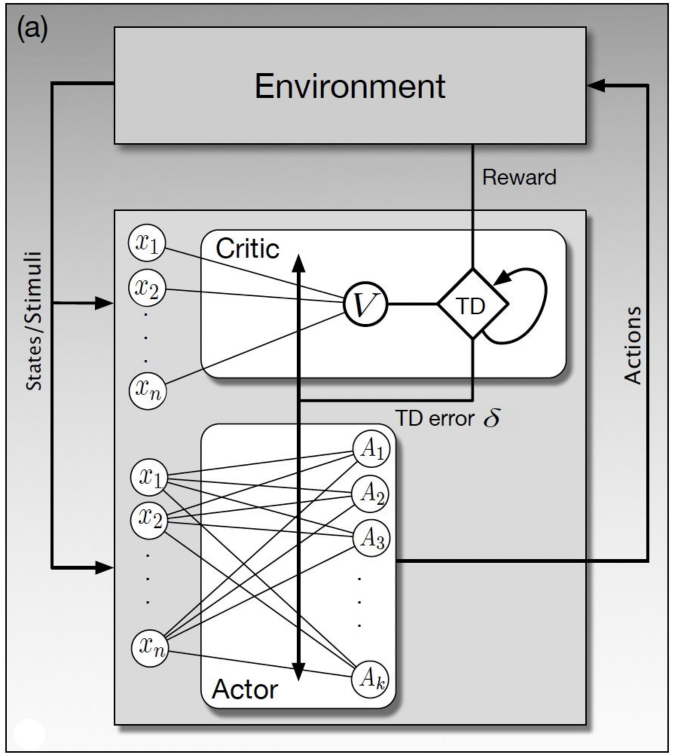


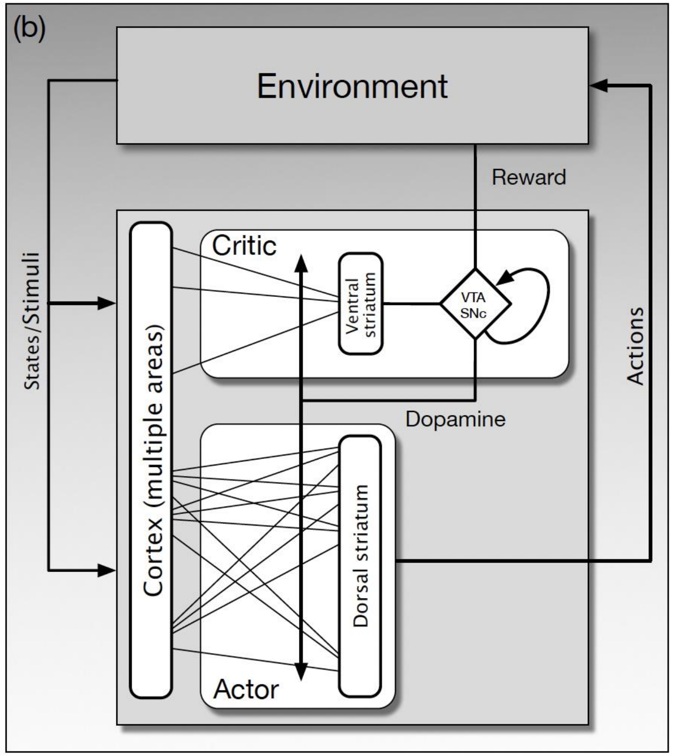
A gridworld example: learning a good policy

Using actor-critic (1500 episodes):



Actor-critic models





"Actor" learns policies (mappings from state to actions)

"Critic" evaluates whether the actions that the actor chose were high or low in value

TD error updates both state and action values

Dorsal striatum: implicated in influencing action selection

Ventral striatum: reward processing and assigning affective value to sensory input

Dopamine modulates synaptic plasticity in both the dorsal and ventral striatum

Deep RL: approximation as a way to address complexity

The curse of dimensionality

Earth ~ 10^{50} atoms

Chess ~ 10^{46} states

Go ~ 10^{170} states

~ 10^{84} photons produced in history of universe

Action space effectively continuous

Tabular RL requires separately keeping track of values/policies for every state/action…

Almost always <u>impossible</u>!

Function approximation as a way to accommodate complexity

- The way out is obvious: just don't use a table to track values/policies.
- This means coming up with a parameterized approximation to values/policies.
- E.g. A set of parameters w determine the value of V(s) for all states s.
- Function approximation can be used for…

$V(s) \rightarrow \hat{v}(s, \mathbf{w})$	Value function
$\pi(a \vert s) \rightarrow \hat{\pi}(a \vert s, \theta)$	Policy
$Q(s, a) \rightarrow \hat{q}(s, a, \mathbf{w})$	Q-value function

Function approximation as a way to accommodate complexity

- Can come up with analogues to all the important tabular RL algorithms, e.g.

TD prediction

$$\delta_t := R_{t+1} + \gamma\, \hat{v}(S_{t+1}, \mathbf{w}) - \hat{v}(S_t, \mathbf{w})$$

$$\mathbf{w} \leftarrow \mathbf{w} + \alpha\, \delta_t\, \nabla_{\mathbf{w}} \hat{v}(S_t, \mathbf{w})$$

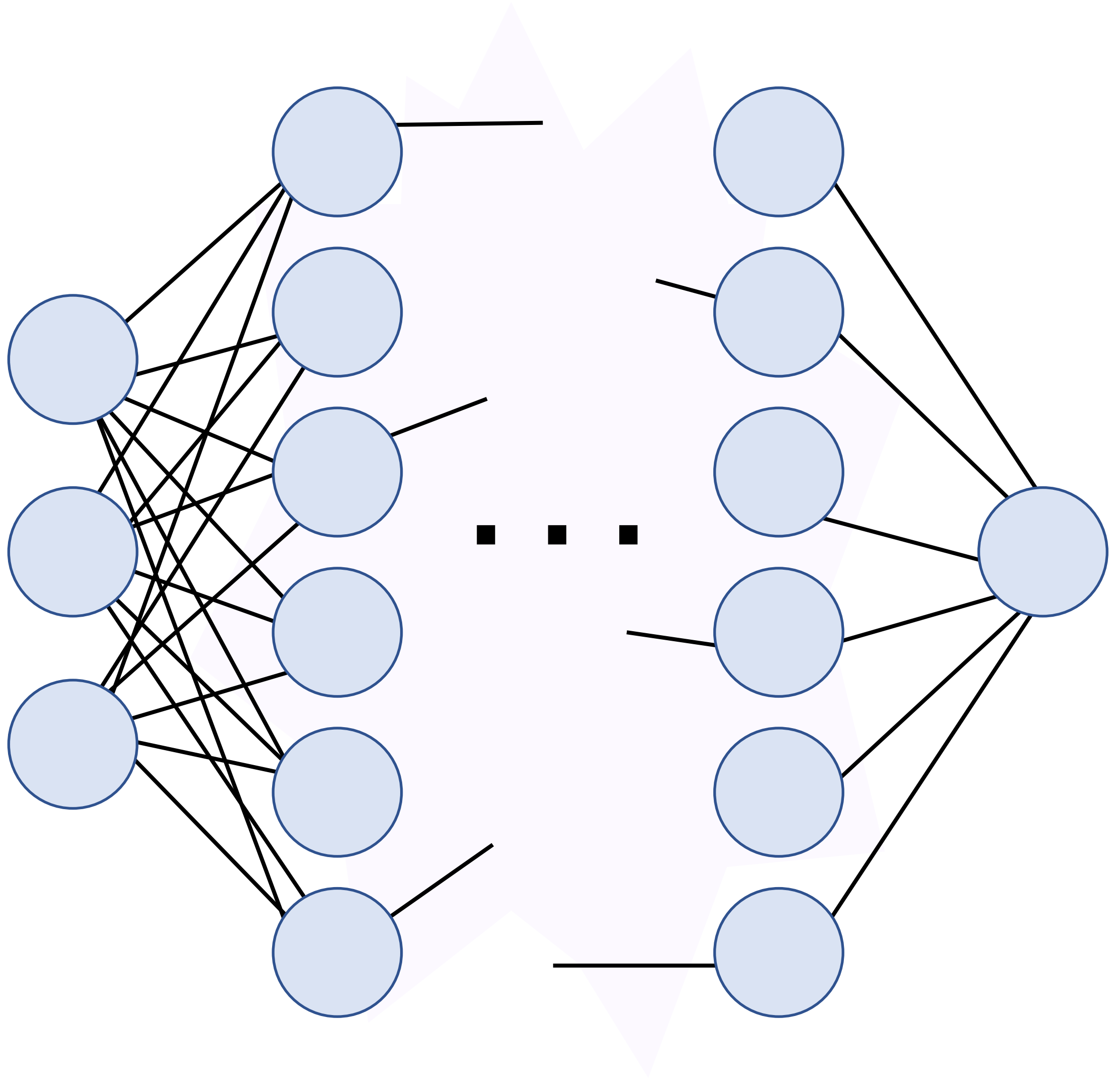
Q-learning control

$$\delta_t := R_{t+1} + \gamma\, \max_a \hat{q}(S_{t+1}, a, \mathbf{w}) - \hat{q}(S_t, A_t, \mathbf{w})$$

$$\mathbf{w} \leftarrow \mathbf{w} + \alpha\, \delta_t\, \nabla_{\mathbf{w}} \hat{q}(S_t, A_t, \mathbf{w})$$

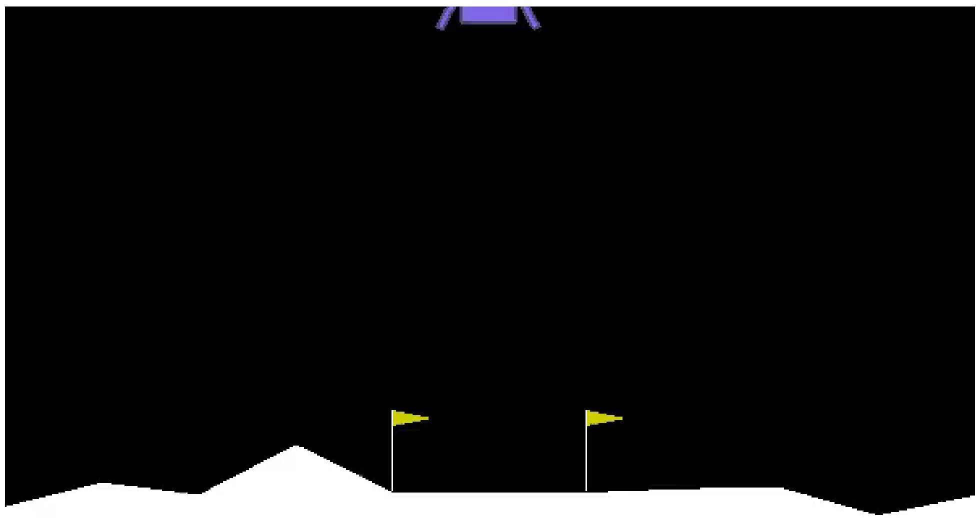
Deep RL: function approximation via deep neural networks

- Want function approximators good enough that closely approximating any (e.g.) V(s) is plausible.
- Neural networks are a natural and convenient choice.
- Despite being the workhorse of almost all practical RL…
  few theoretical guarantees so far!

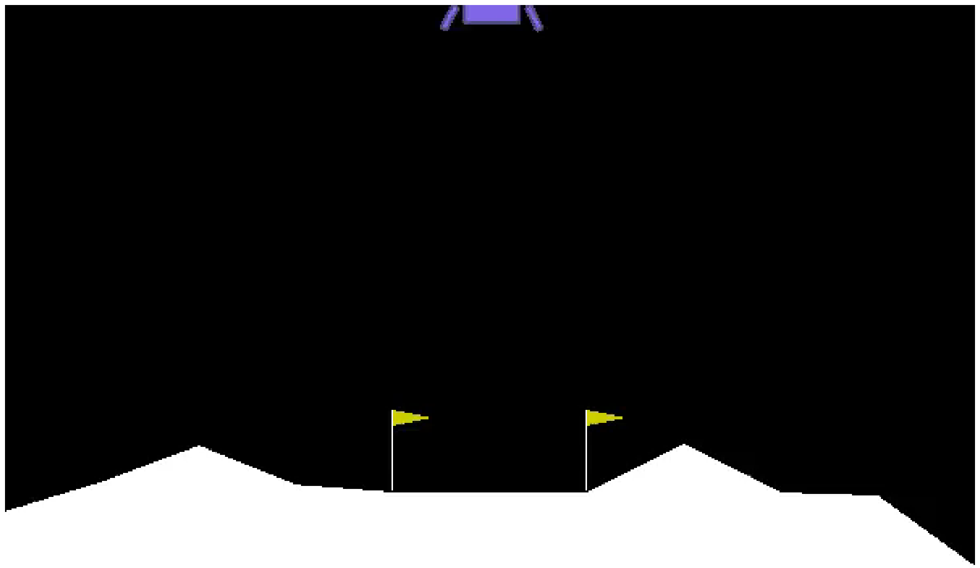


Deep RL: function approximation via deep neural networks

Before training:



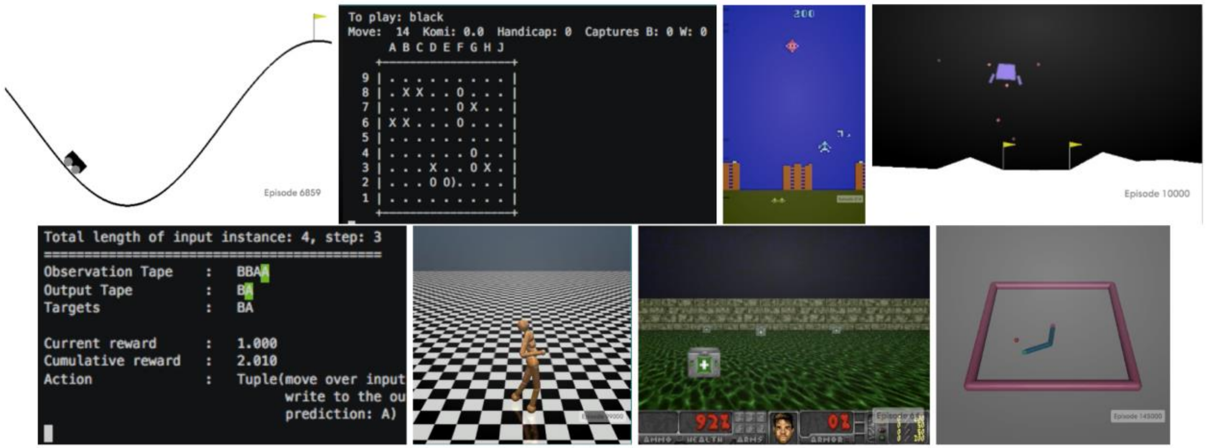
After training:



OpenAI Gym and Stable Baselines

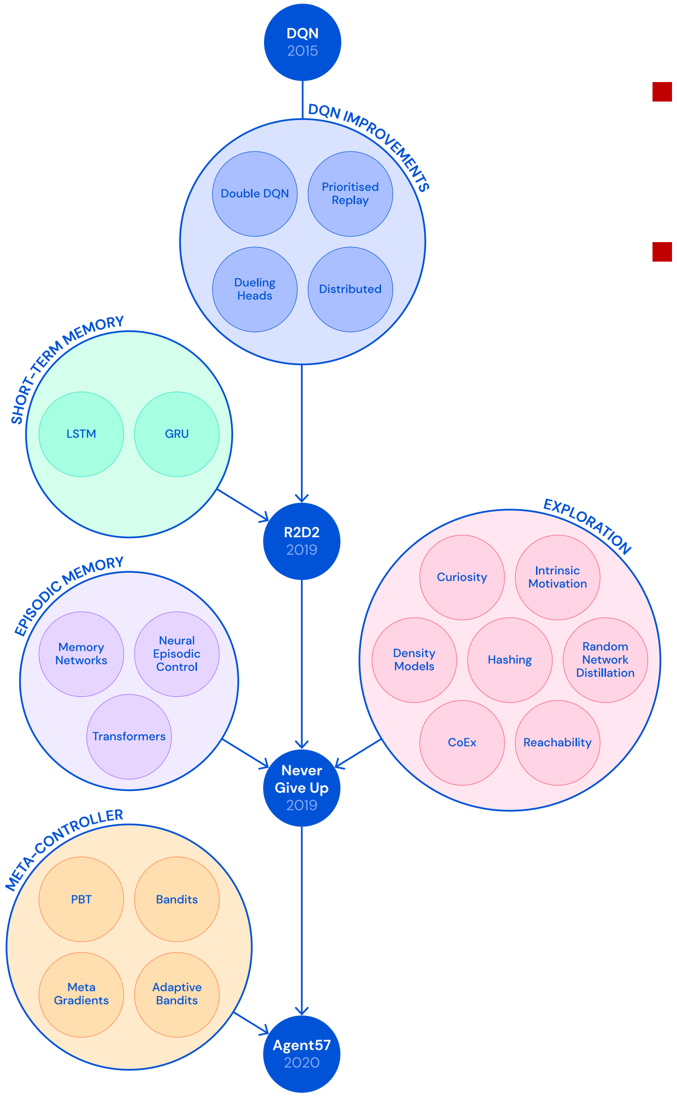
- Want to play around with RL yourself? Some recommended resources:

OpenAI Gym (gymlibrary.dev):
Environments to play around with + convenient API for constructing your own.



Stable Baselines (stable-baselines.readthedocs.io/en/master/):
Reference implementations of standard RL algorithms.
(e.g. Deep Q networks, actor-critic, etc.)

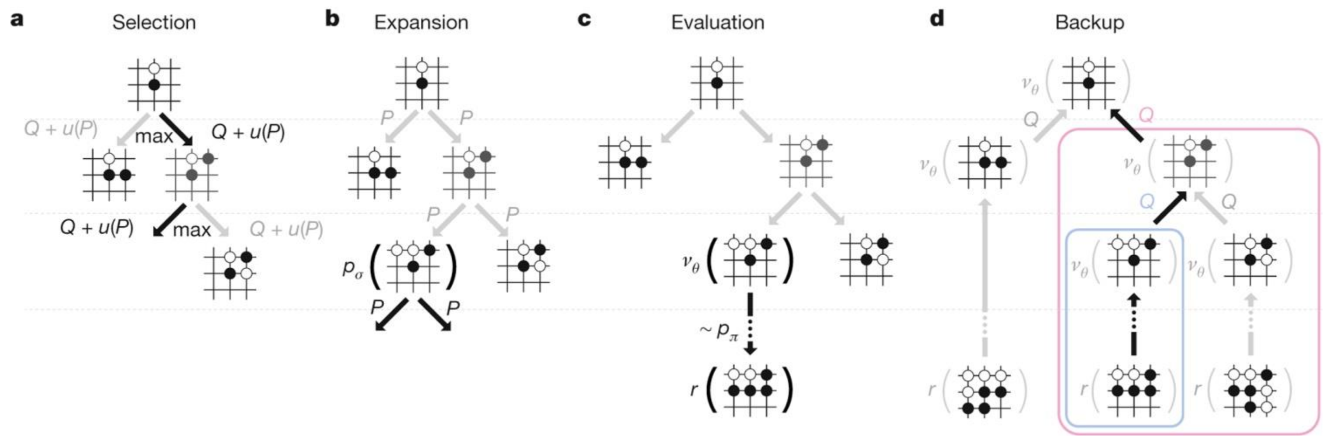
RL in practice: hacks, choices, and approximations



- Exploration (try new things) vs exploitation (use what works)
- Model-free vs model-based
    - On-policy learning vs off-policy learning
    - Memory mechanism
    - Attention and prioritization mechanisms
    - Hyperparameter tuning, expensive training using many GPUs…

On-policy vs off-policy learning

- Monte Carlo Tree Search (MCTS): a very successful off-policy learning technique, used to get e.g. Go AI from amateur to world-class level.



D Silver *et al. Nature* **529,** 484–489 (2016) doi:10.1038/nature16961

- Idea: With a model of the world, can mentally simulate how things might happen to reduce amount of trial and error necessary to learn.
- In a slogan: we don't need to walk into a wall to know that it's a bad idea!

Frontiers in RL

- Reinforcement learning is a huge field with many open questions!

Theoretical questions, e.g.

What kind of theoretical guarantees can we provide for typical RL implementations?

Scientific questions, e.g.

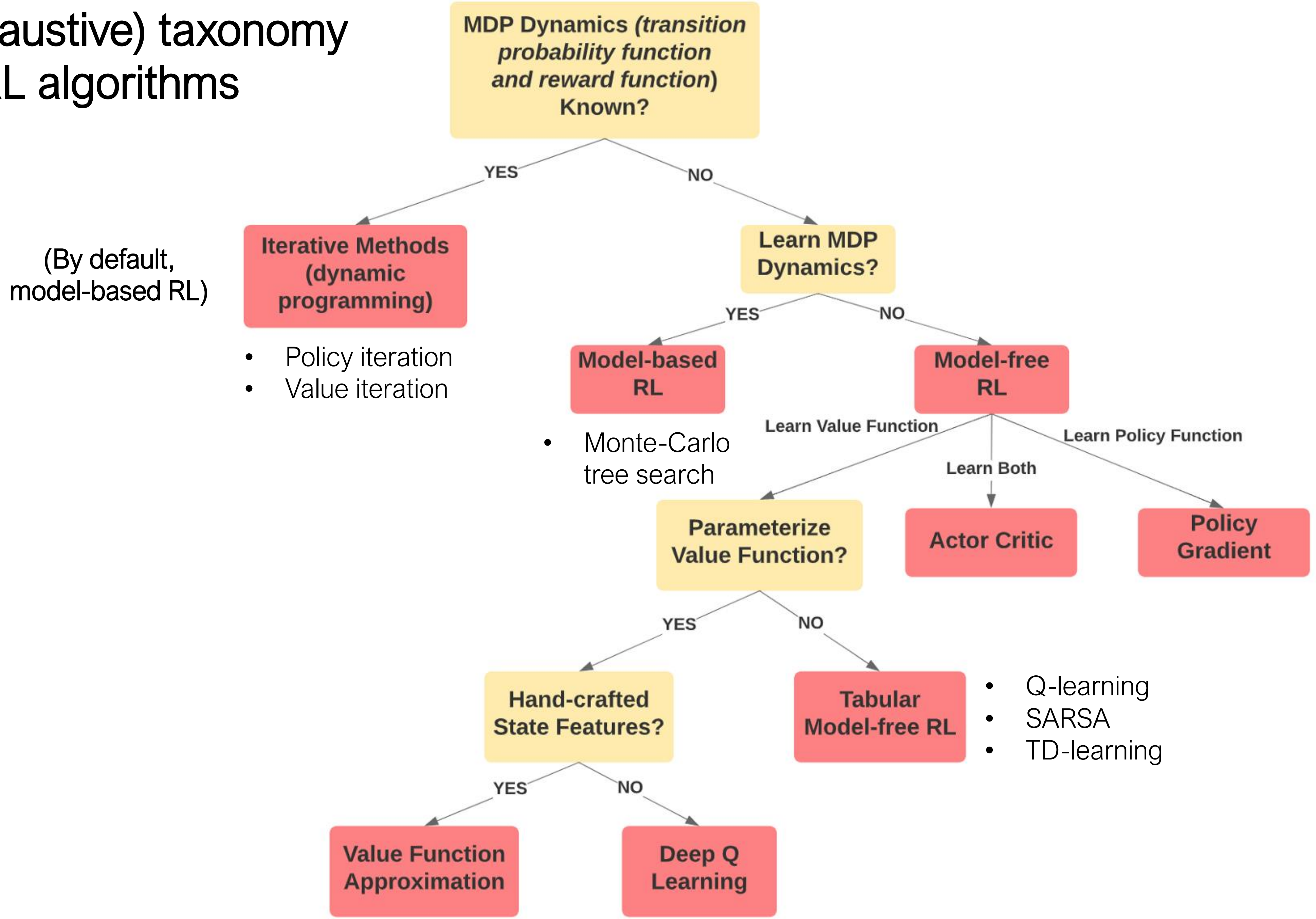
If the brain is doing something like RL, what do its RL algorithms look like? Also, what is dopamine doing???

Maybe *you* will figure it out!

Application questions, e.g.

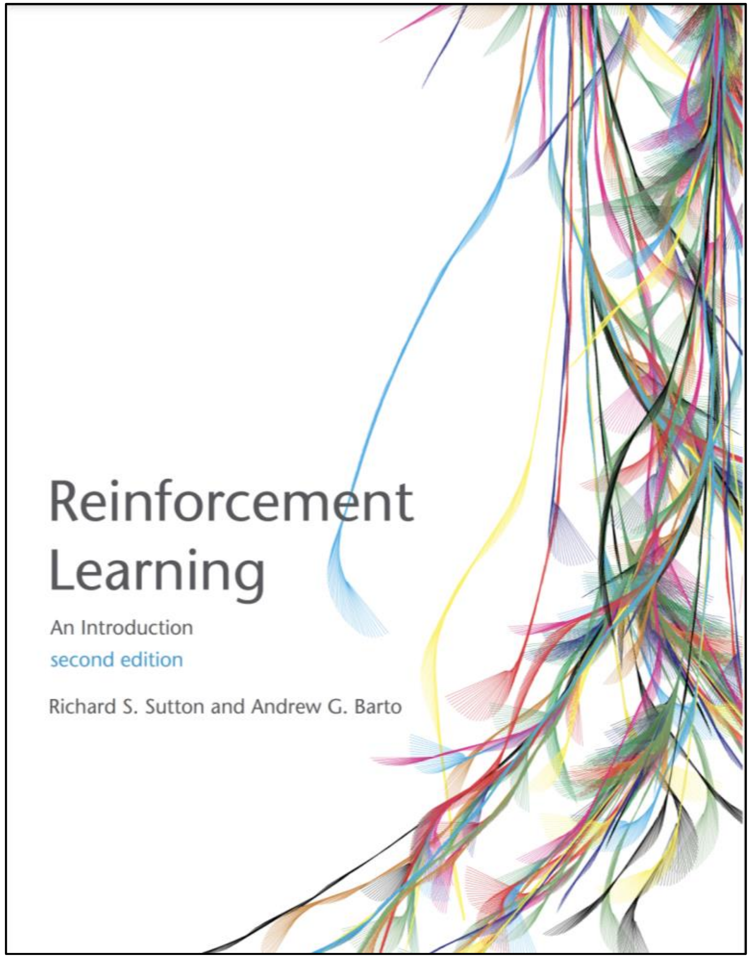
How do we use RL in robotics?
In public health? In self-driving cars? …

(Non-exhaustive) taxonomy of RL algorithms



Policy iteration A dynamic programming algorithm (model-based RL; used when the model of the environment is fully known) that finds the optimal policy by iteratively evaluating and improving the policy until convergence.	**Value iteration** A dynamic programming algorithm (model-based RL; used when the model of the environment is fully known) that finds the optimal state value function by iteratively looking ahead one step to find the maximum value action until convergence.
On-policy Agent evaluates or improves the policy that is used to make decisions. e.g., SARSA	**Off-policy** Agent evaluates or improves a policy different than the one used to act e.g., Q-learning
Model-based RL Learns a model of the world (the dynamics of the MDP, e.g., transition function $\mathrm{T}(s,a,s')$, reward function $R(s,a)$, etc.)	**Model-free RL** Does not learn a model of the world and treats states independently
Value learning Quantifying the value of every state-action pair and using that for action selection	**Policy learning** Directly inferring a policy that maximizes the reward in a specific environment
Actor-critic Dual architecture algorithm where actor learns policies and critic evaluates whether the actions chosen were high or low in value	

To learn more...



- Read this book by Sutton and Barto!

- **Companion Python notebook:**
github.com/john-vastola/RL-at-Harvard-tutorial-2022

- Conferences
  - Reinforcement Learning and Decision Making (RLDM) https://rldm.org/
  - From Neuroscience to Artificially Intelligent Systems (NAISys)
  - More ML/CS: ICLR, ICML, NeurIPS
  - More Psych/Neuro: CogSci,

- Labs at Harvard
  - See the people on the speaker list!