

# Reinforcement Learning I: Theory

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- ▶ Reinforcement learning: rough overview
  - mainly following Sutton & Barto 1998
- ▶ Learning theory
  - classical & instrumental conditioning
- ▶ Dopamine
  - prediction errors and more
- ▶ Fitting behaviour with RL models
  - some applied tips & tricks

# Types of learning

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- ▶ Supervised
- ▶ Unsupervised
- ▶ Reinforcement learning

# Setup

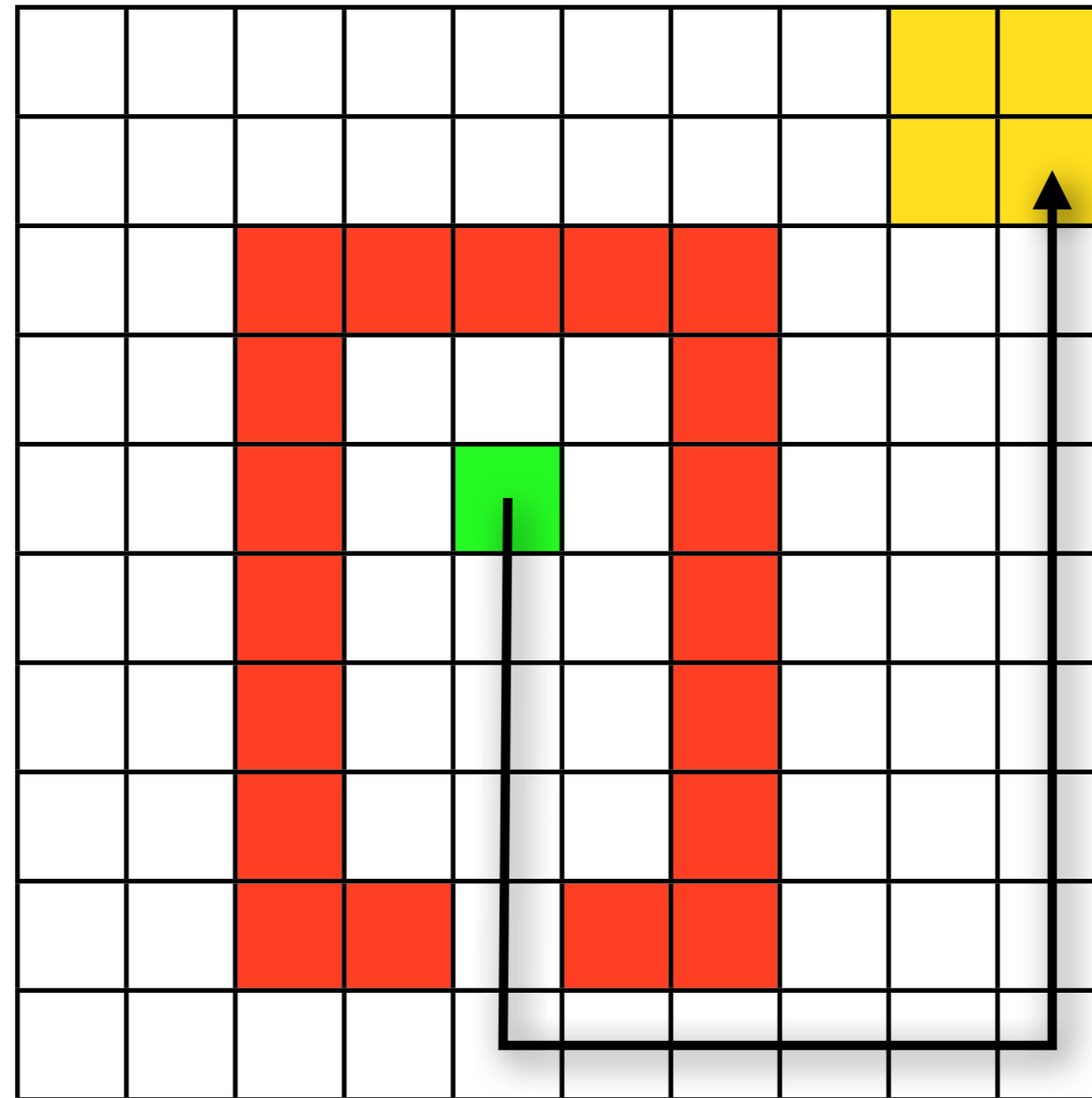


$$\{a_t\} \leftarrow \operatorname{argmax}_{\{a_t\}} \sum_{t=1}^{\infty} r_t$$

After Sutton and Barto 1998

# State space

Electric  
shocks  
-1



Gold  
+1

# A Markov Decision Problem

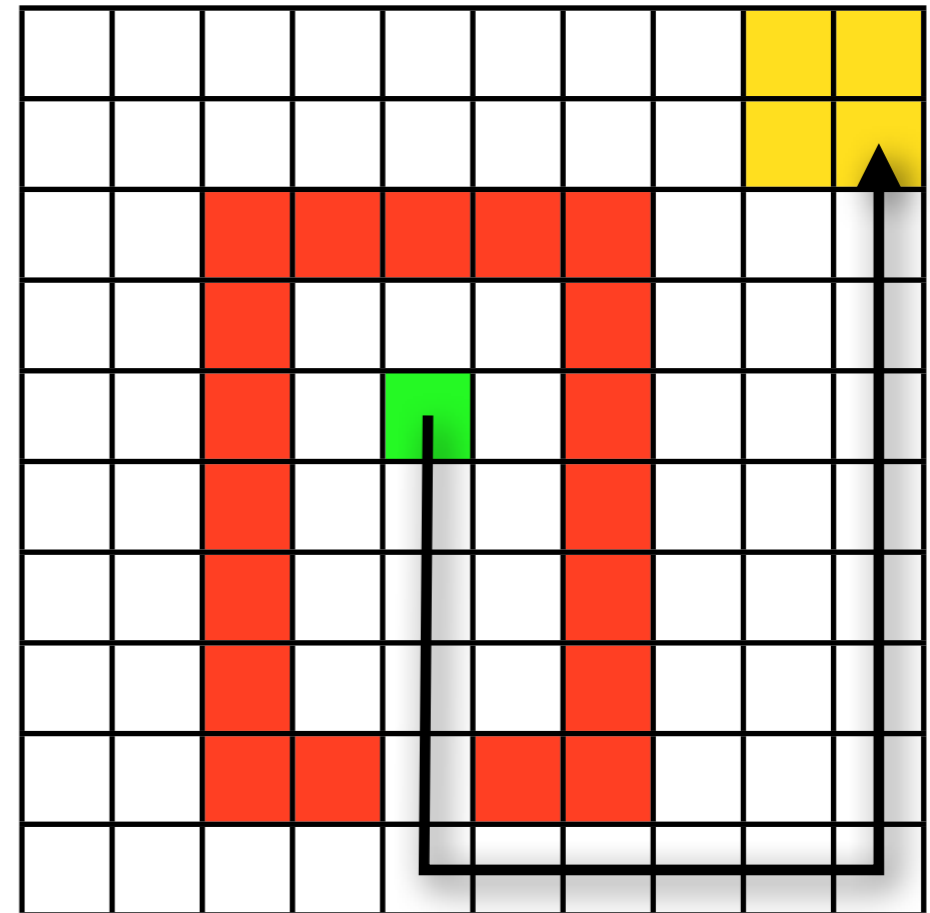
$$s_t \in \mathcal{S}$$

$$a_t \in \mathcal{A}$$

$$\mathcal{T}_{ss'}^a = p(s_{t+1} | s_t, a_t)$$

$$r_t \sim \mathcal{R}(s_{t+1}, a_t, s_t)$$

$$\pi(a|s) = p(a|s)$$



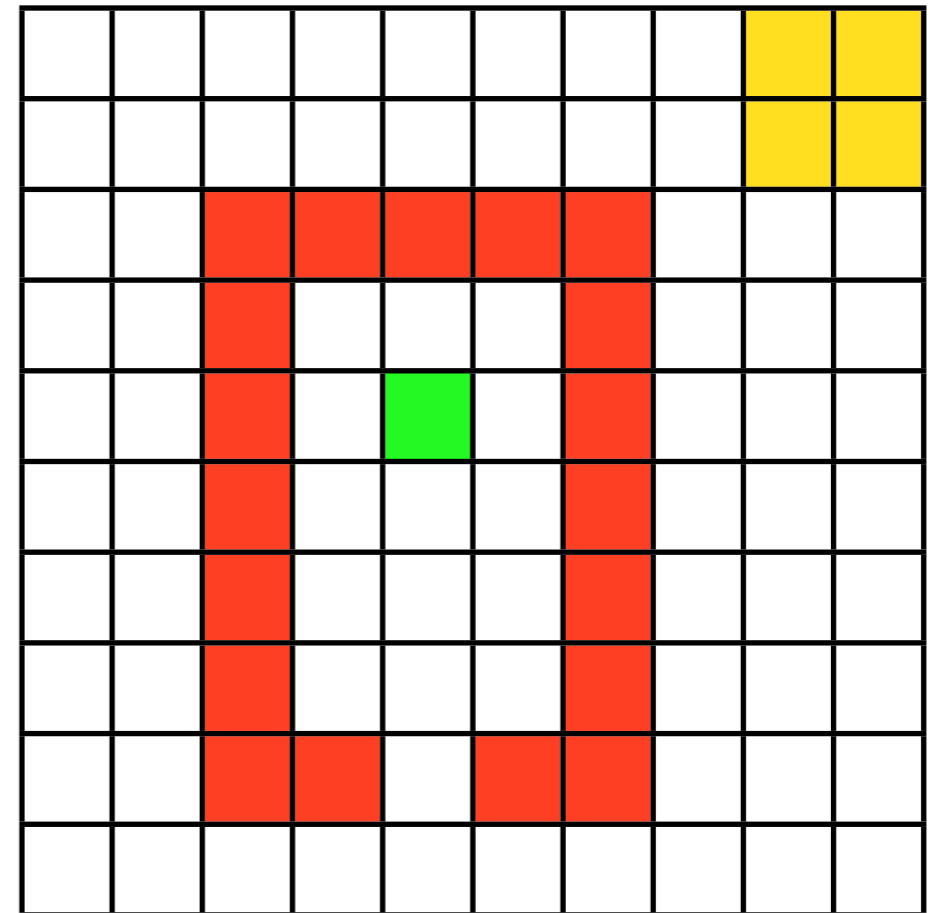
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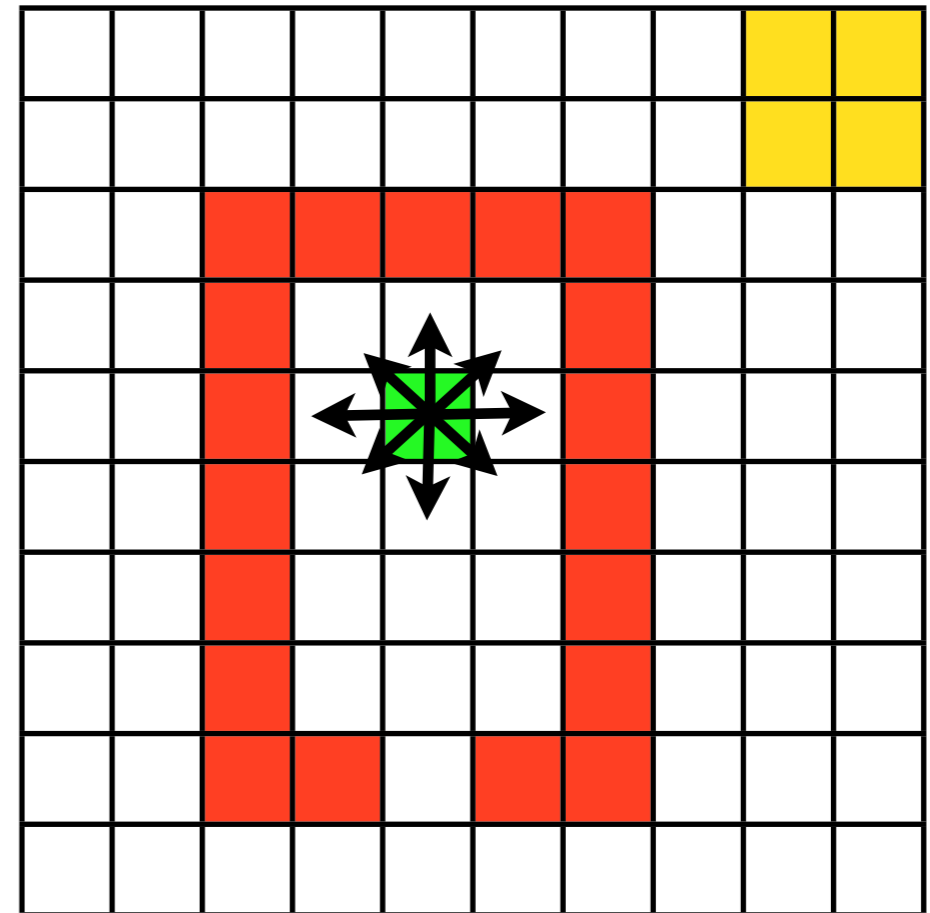
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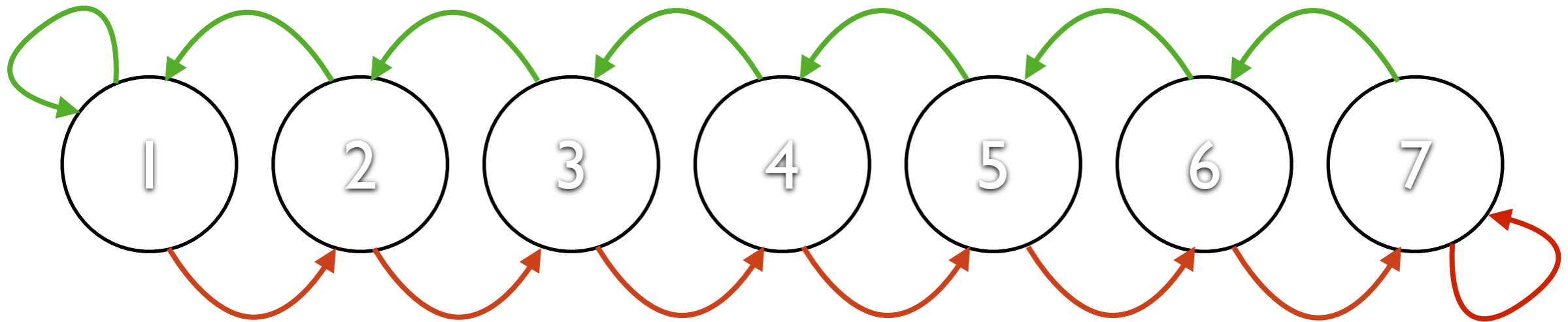
$$r_t \sim \mathcal{R}(s_{t+1}, a_t, s_t)$$

$$\pi(a|s) = p(a|s)$$



# Actions

Action left



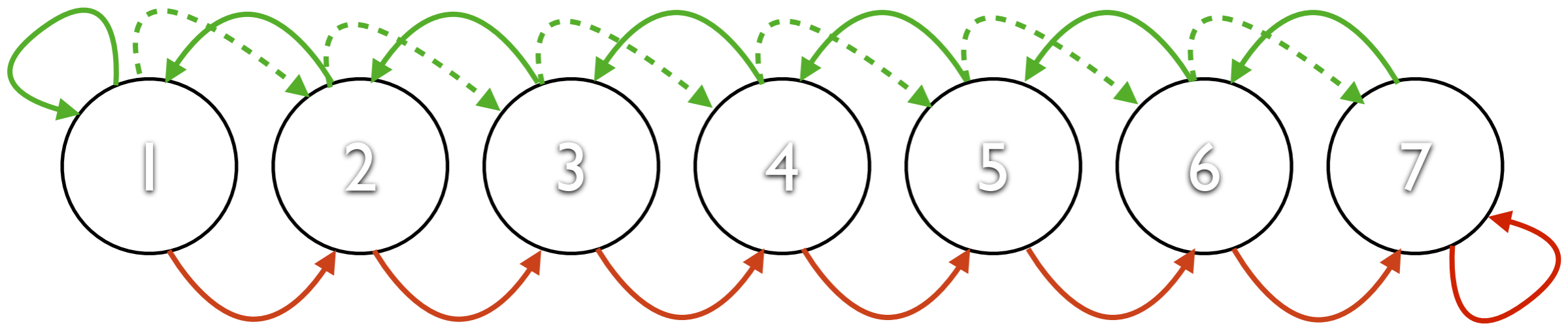
Action right

$$T^{\text{left}} = \begin{bmatrix} 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$T^{\text{right}} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 \end{bmatrix}$$

# Actions

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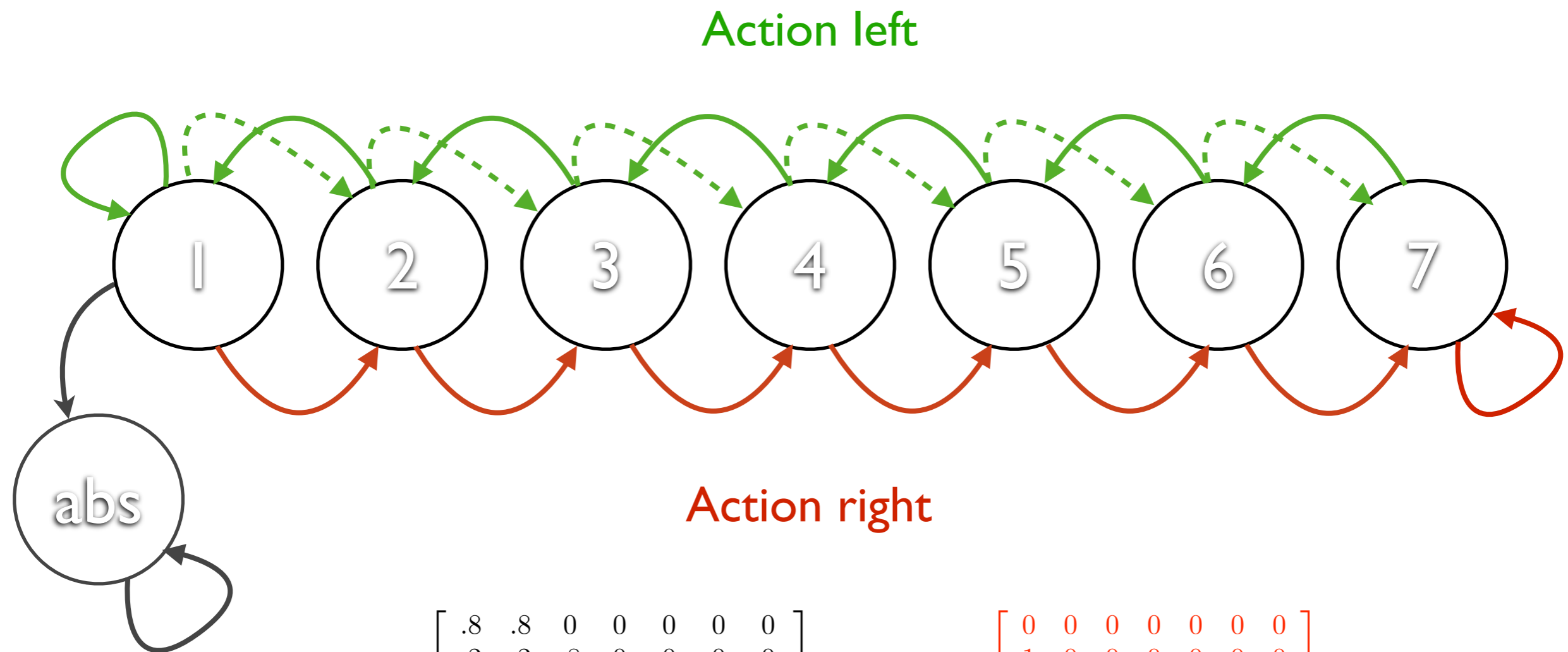
Action right

$$T^{\text{left}} = \begin{bmatrix} .8 & .8 & 0 & 0 & 0 & 0 & 0 \\ .2 & .2 & .8 & 0 & 0 & 0 & 0 \\ 0 & 0 & .2 & .8 & 0 & 0 & 0 \\ 0 & 0 & 0 & .2 & .8 & 0 & 0 \\ 0 & 0 & 0 & 0 & .2 & .8 & 0 \\ 0 & 0 & 0 & 0 & 0 & .2 & .8 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

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Noisy: plants, environments, agent

# Actions



$$T^{\text{left}} = \begin{bmatrix} .8 & .8 & 0 & 0 & 0 & 0 & 0 \\ .2 & .2 & .8 & 0 & 0 & 0 & 0 \\ 0 & 0 & .2 & .8 & 0 & 0 & 0 \\ 0 & 0 & 0 & .2 & .8 & 0 & 0 \\ 0 & 0 & 0 & 0 & .2 & .8 & 0 \\ 0 & 0 & 0 & 0 & 0 & .2 & .8 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

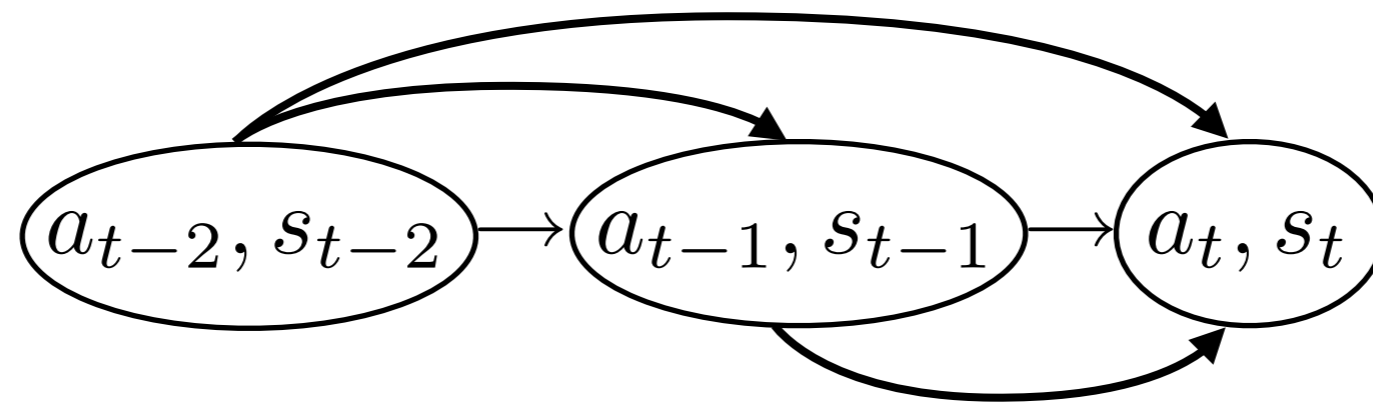
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Noisy: plants, environments, agent

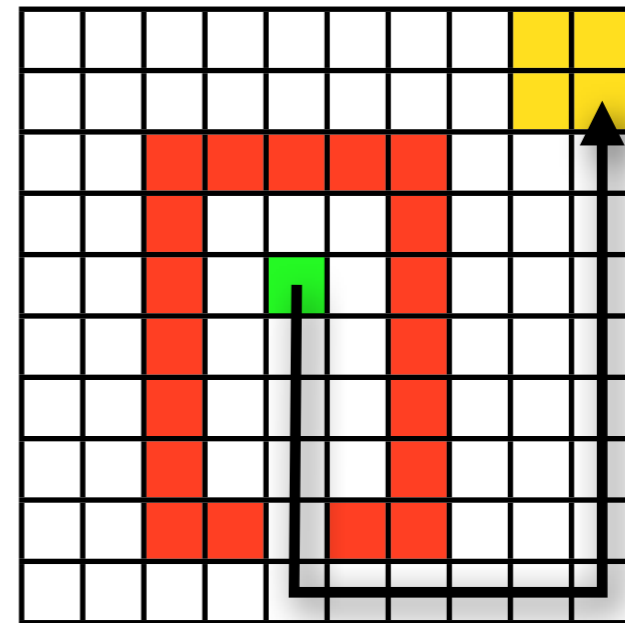
Absorbing state  $\rightarrow$  max eigenvalue  $< 1$

# Markovian dynamics

$$p(s_{t+1} | a_t, s_t, a_{t-1}, s_{t-1}, a_{t-2}, s_{t-2}, \dots) = p(s_{t+1} | a_t, s_t)$$

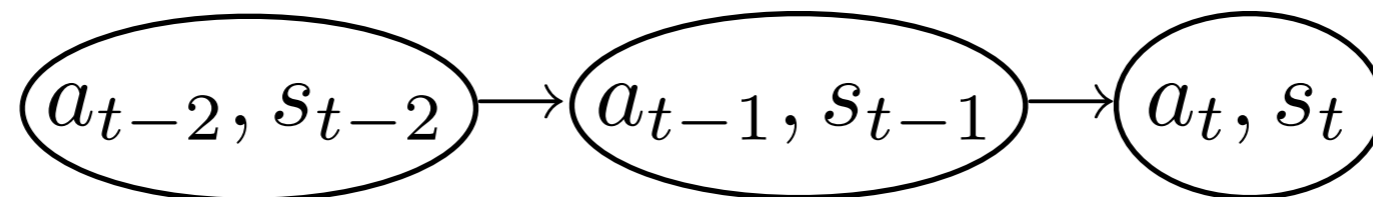


Velocity

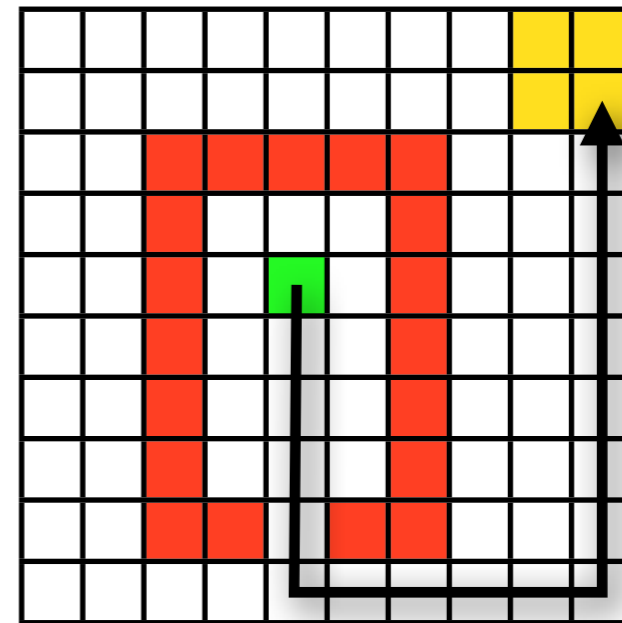


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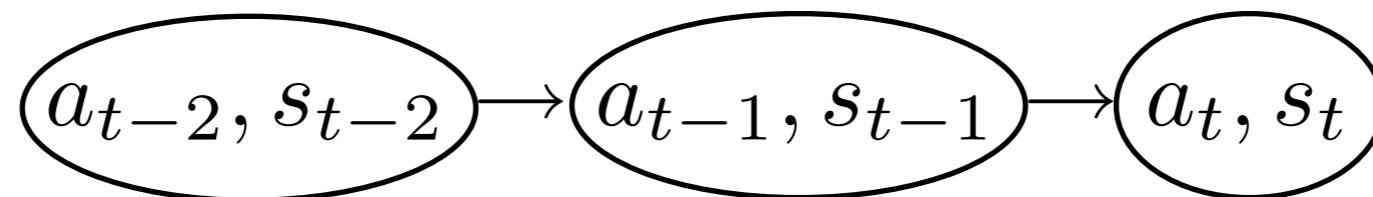


Velocity



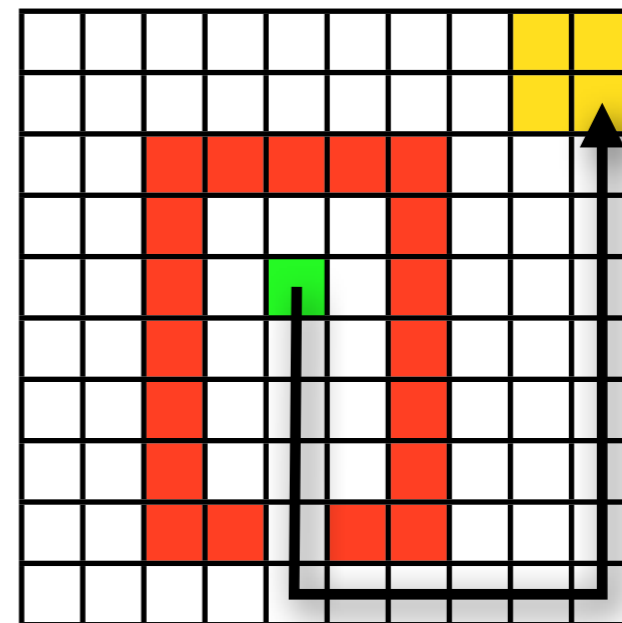
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Velocity

$$s' = [\text{position}] \rightarrow s' = \begin{bmatrix} \text{position} \\ \text{velocity} \end{bmatrix}$$



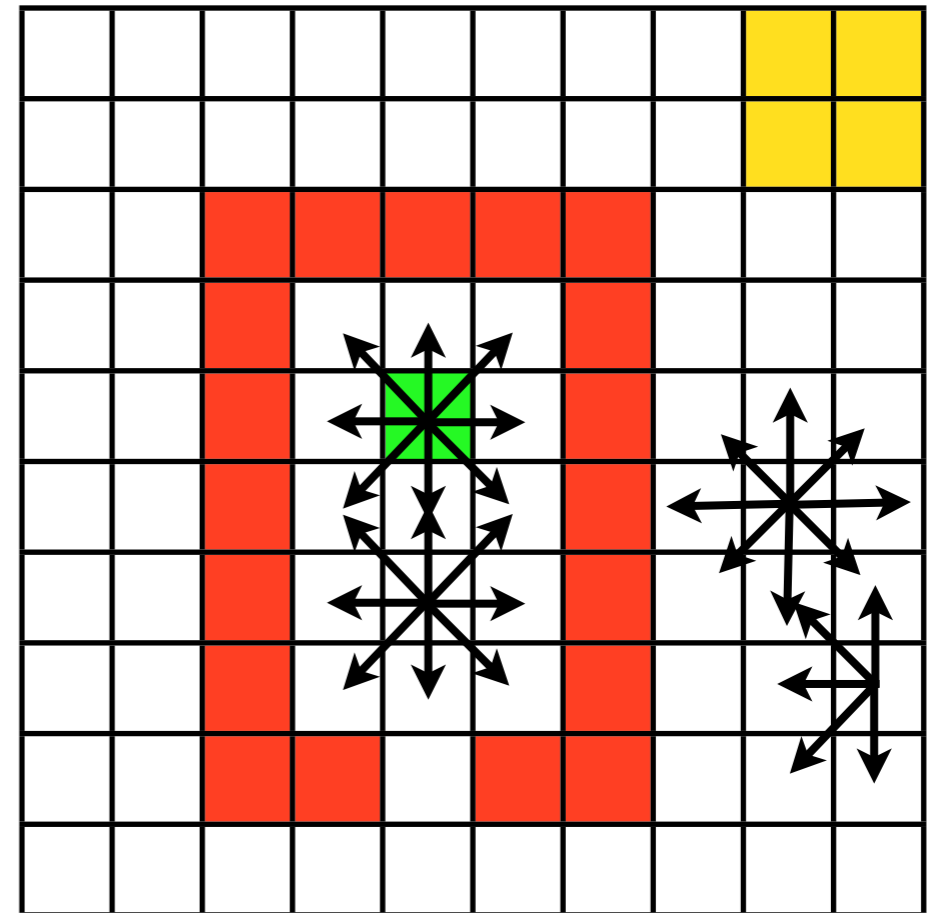
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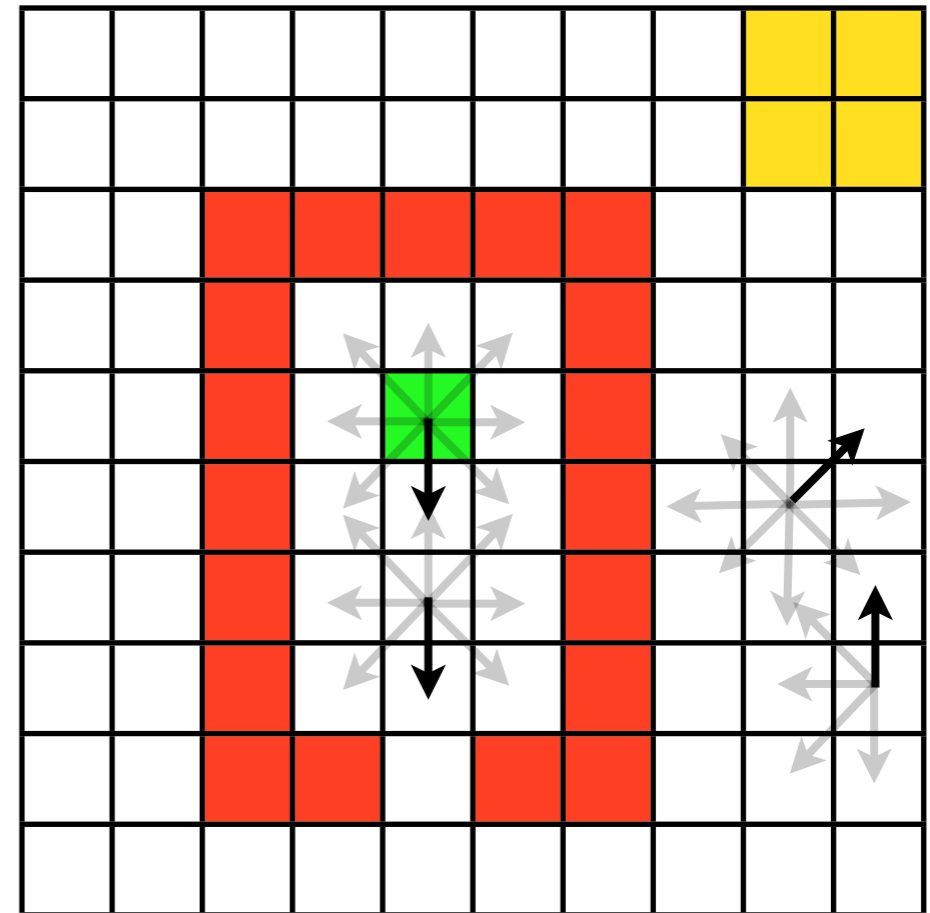
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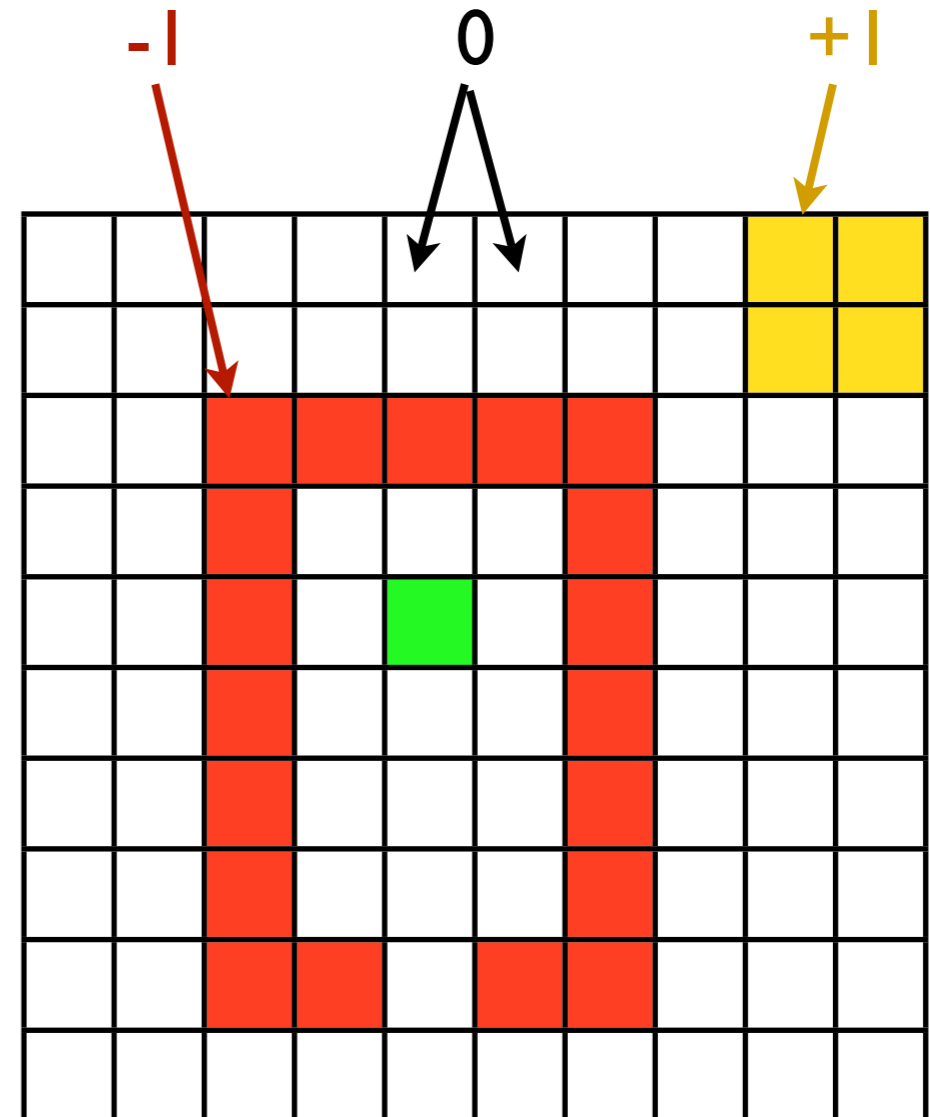
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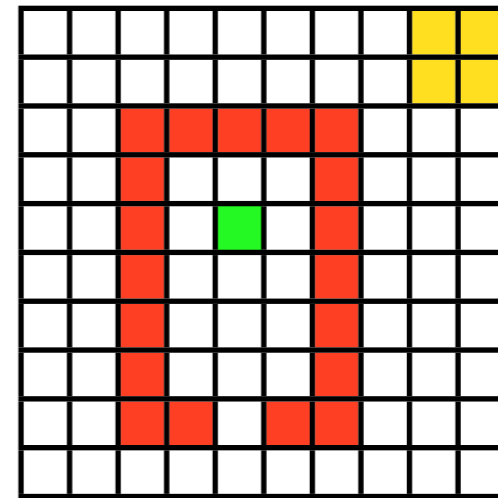
$$\pi(a|s) = p(a|s)$$



# Tall orders

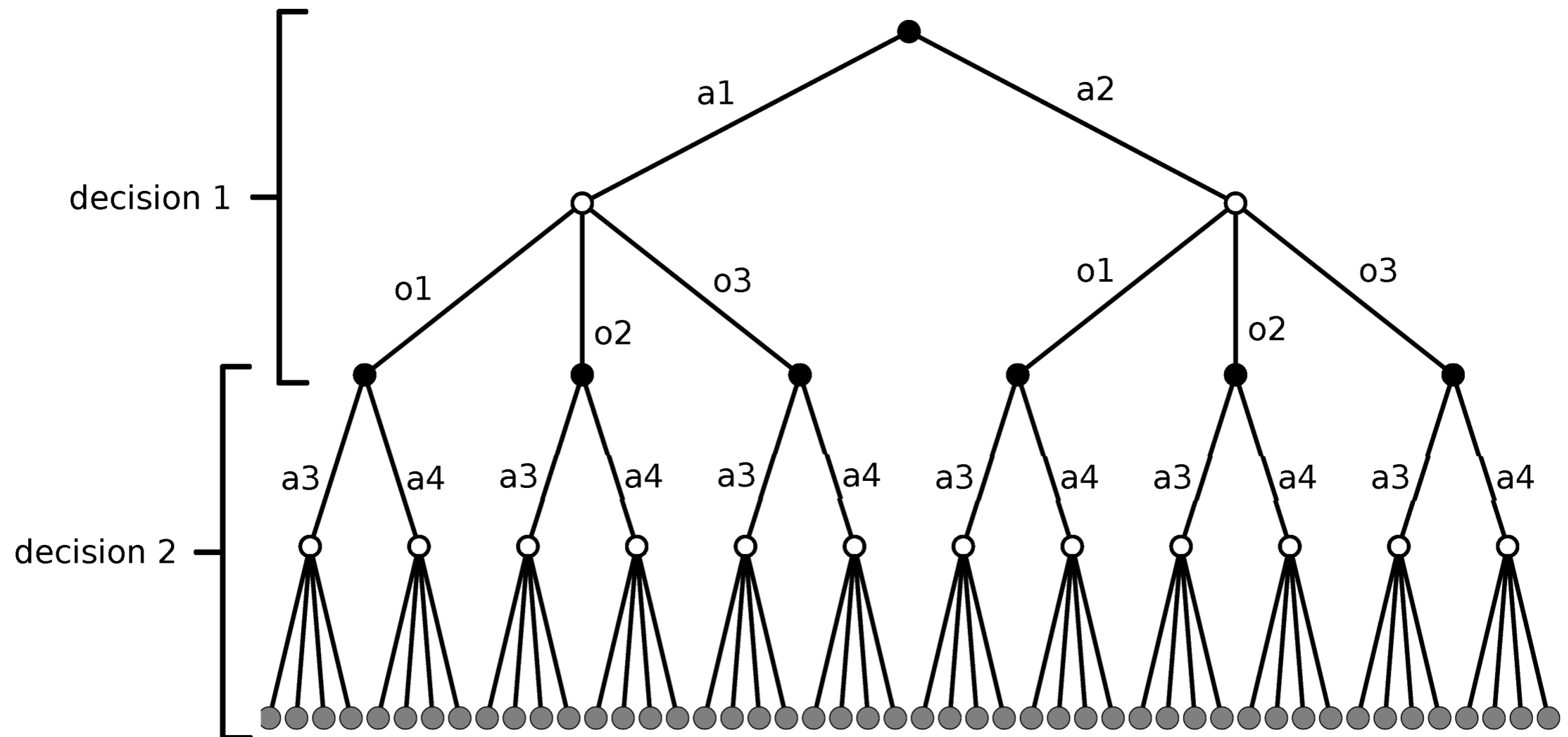
- Aim: maximise total future reward

$$\sum_{t=1}^{\infty} r_t$$

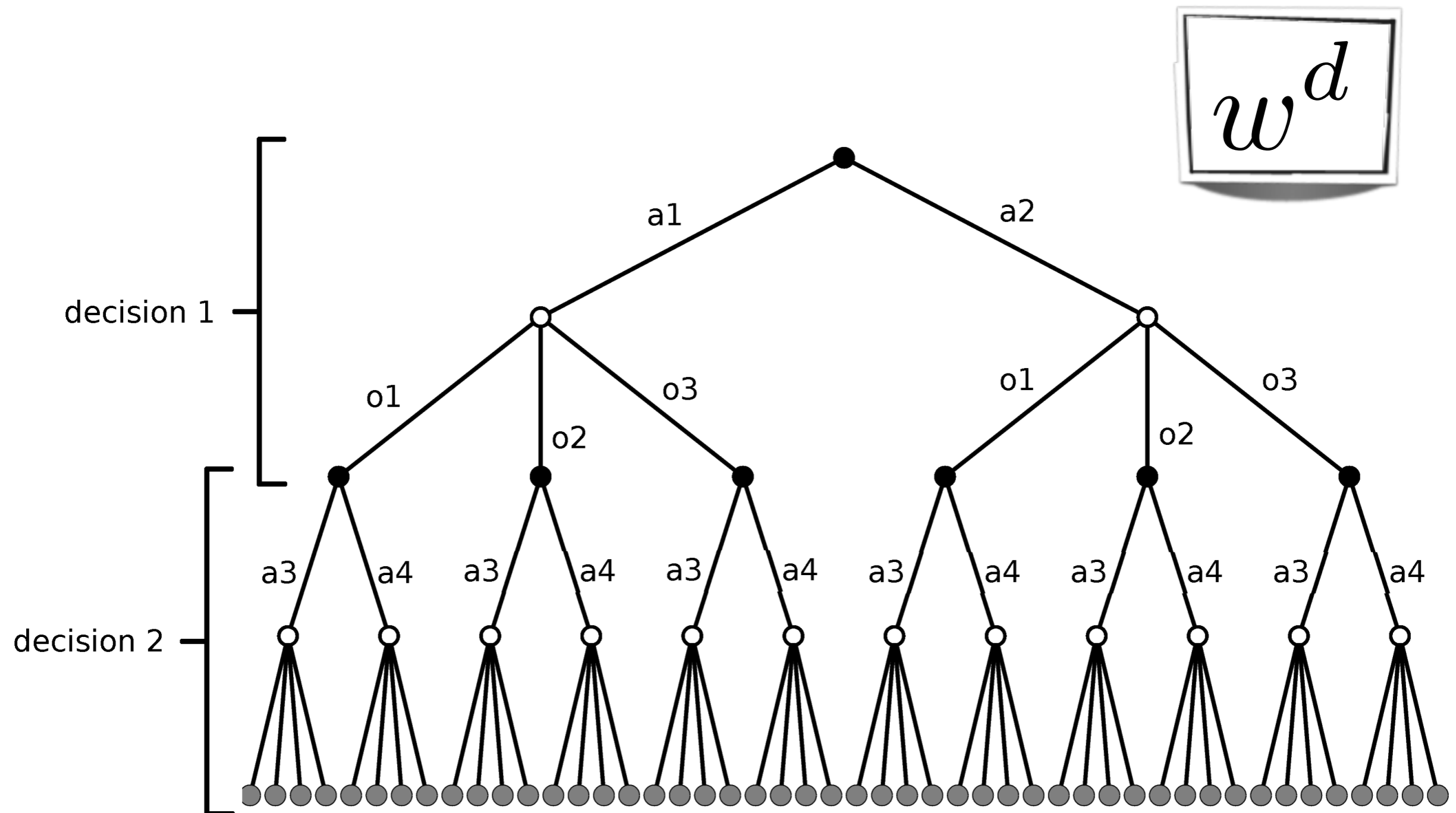


- ▶ i.e. we have to sum over paths through the future and weigh each by its probability
- ▶ Best policy achieves best long-term reward

# Exhaustive tree search

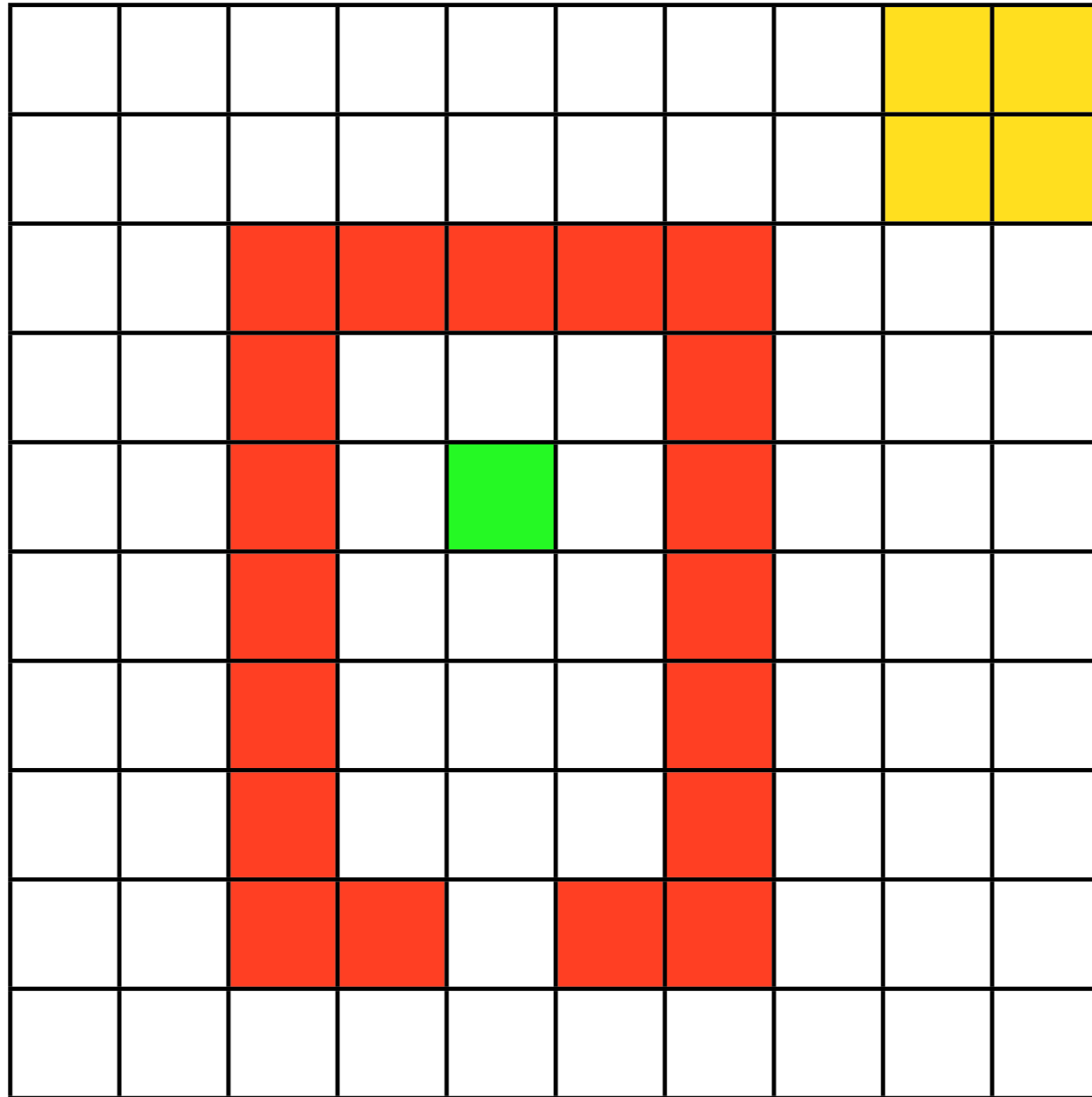


# Exhaustive tree search



# Decision tree

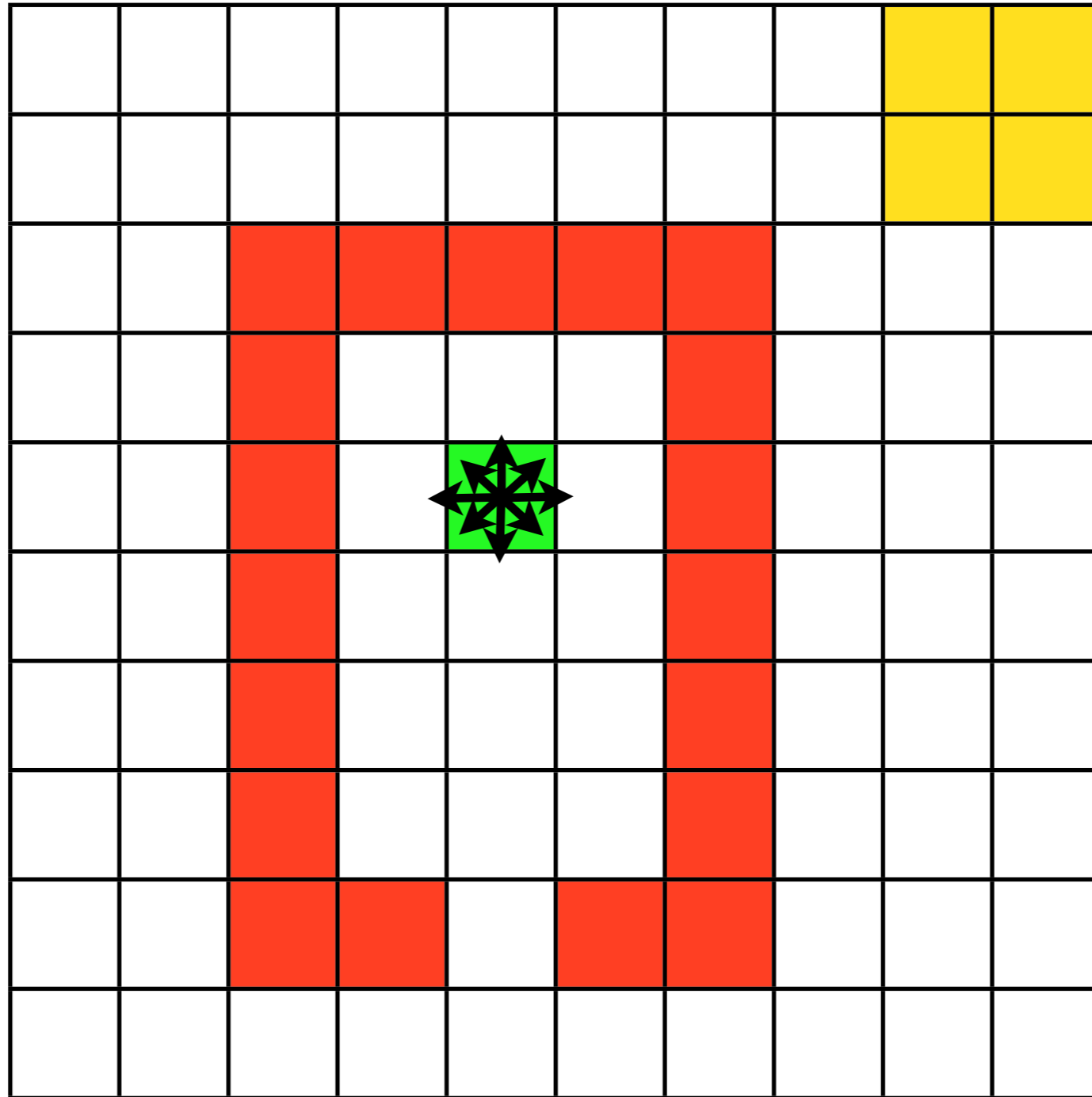
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# Decision tree

$$\sum_{t=1}^{\infty} r_t$$

8

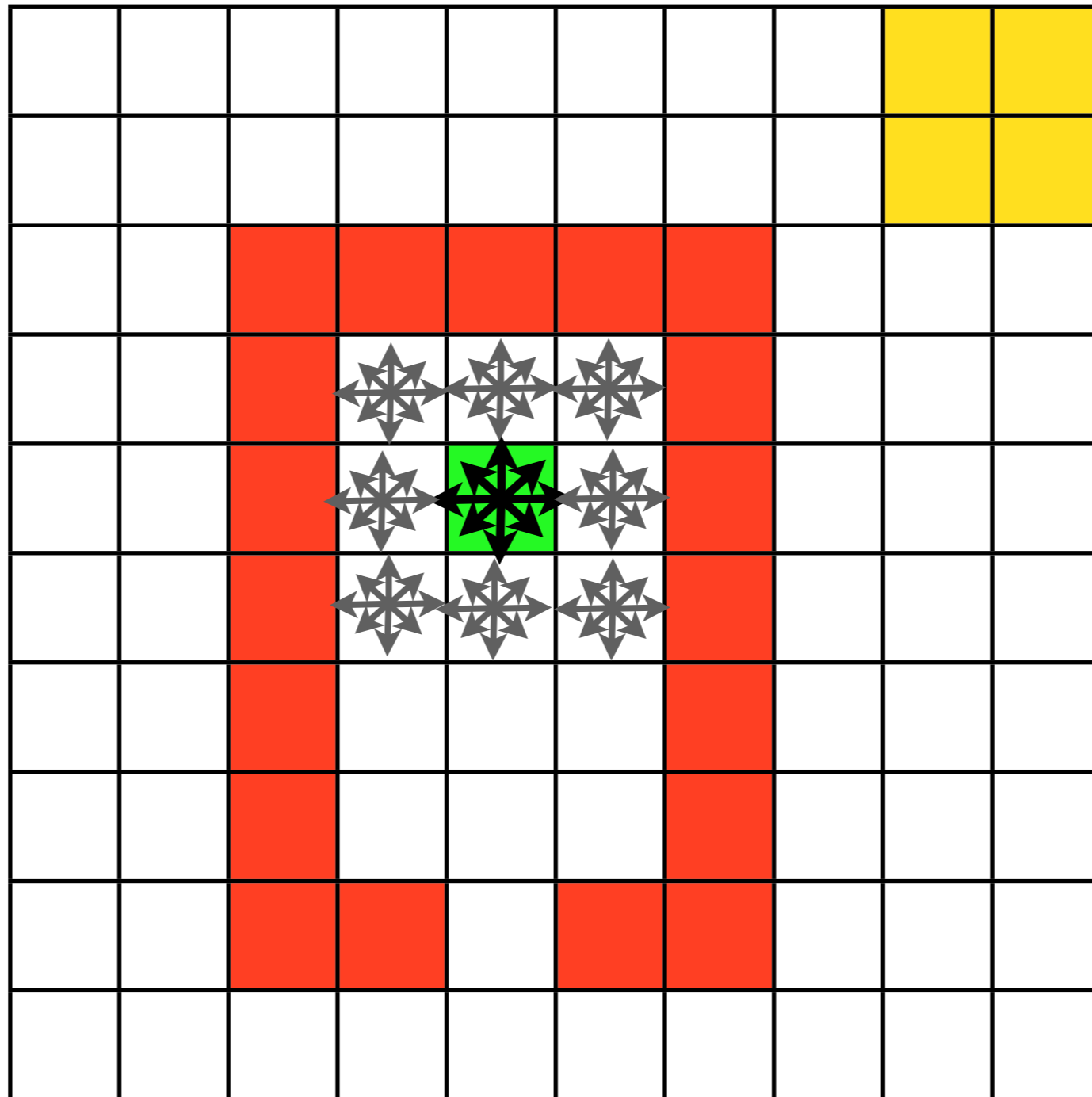


# Decision tree

$$\sum_{t=1}^{\infty} r_t$$

8

64



# Decision tree

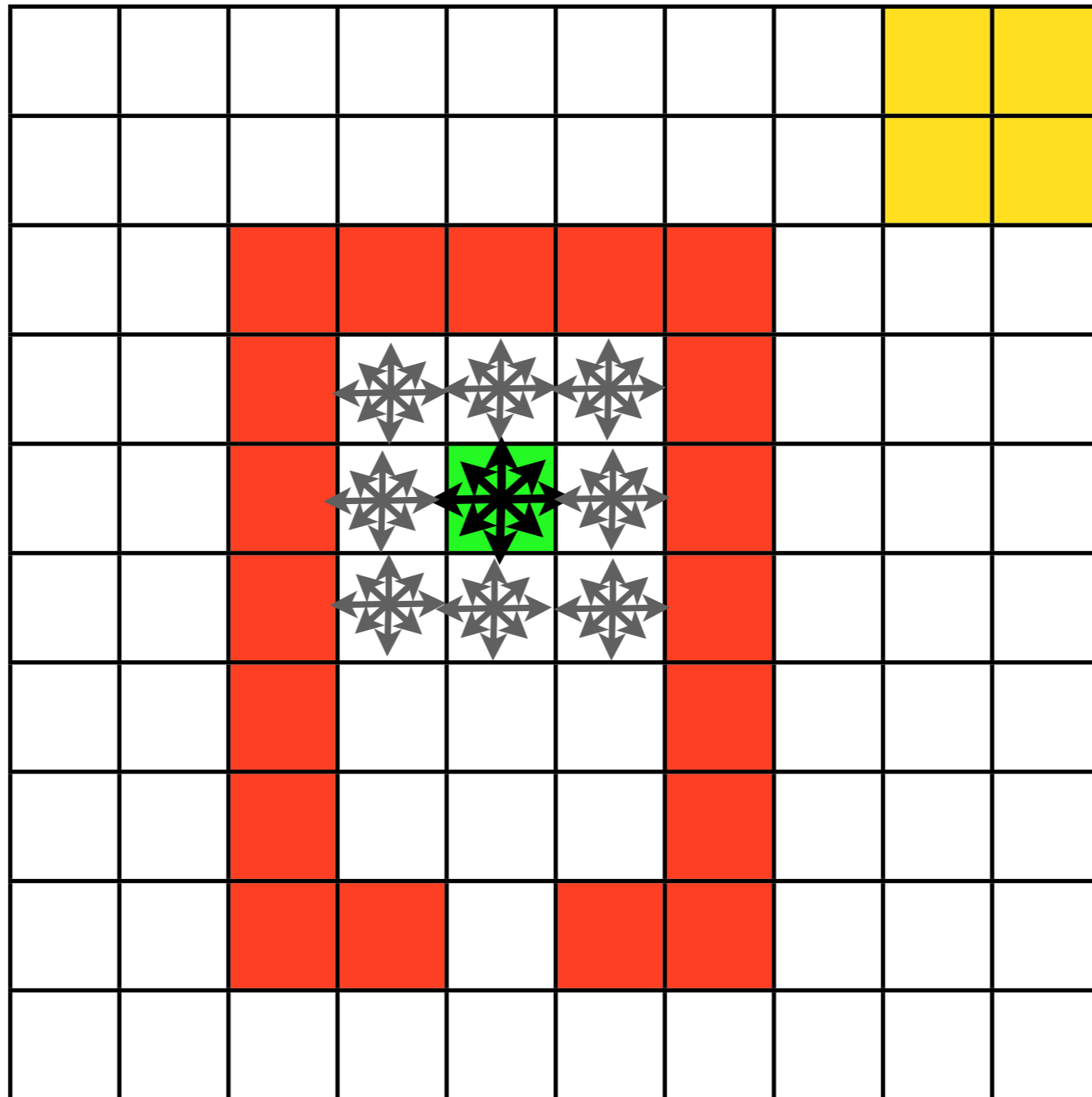
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8

64

512

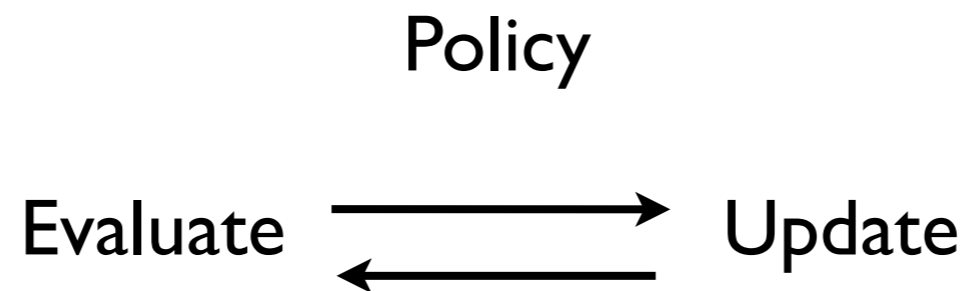
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# Policy for this talk

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- ▶ Pose the problem mathematically
- ▶ Policy evaluation
- ▶ Policy iteration
- ▶ Monte Carlo techniques: experience samples
- ▶ TD learning



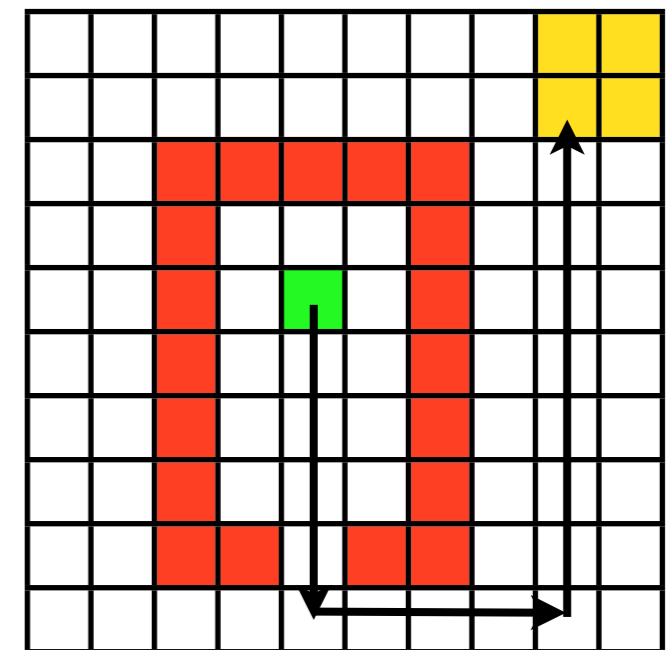
# Evaluating a policy

- ▶ Aim: maximise total future reward

$$\sum_{t=1}^{\infty} r_t$$

- ▶ To know which is best, evaluate it first
- ▶ The policy determines the expected reward from each state

$$\mathcal{V}^{\pi}(s_1) = \mathbb{E} \left[ \sum_{t=1}^{\infty} r_t \mid s_1 = 1, a_t \sim \pi \right]$$



# Discounting

- ▶ Given a policy, each state has an expected value

$$\mathcal{V}^{\pi}(s_1) = \mathbb{E} \left[ \sum_{t=1}^{\infty} r_t \mid s_1 = 1, a_t \sim \pi \right]$$

- ▶ But:  $\sum_{t=0}^{\infty} r_t = \infty$

- ▶ Episodic  $\sum_{t=0}^T r_t < \infty$

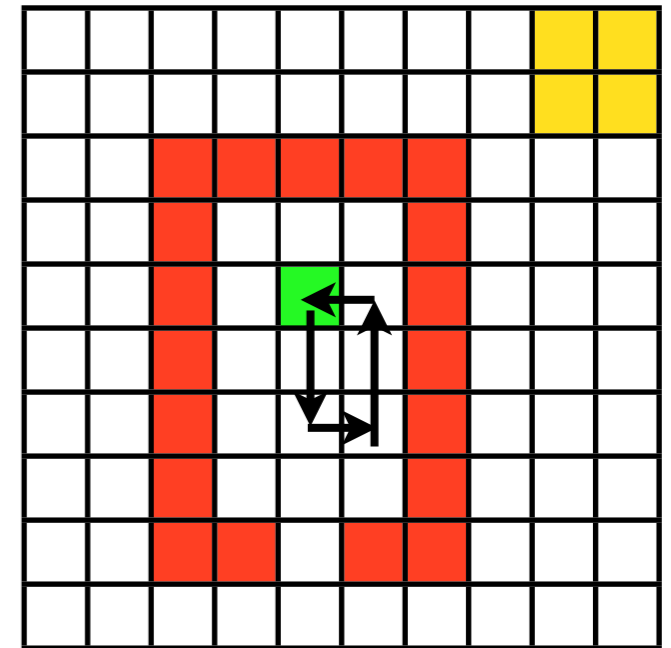
- ▶ Discounted

- infinite horizons  $\sum_{t=0}^{\infty} \gamma^t r_t < \infty$

- finite, exponentially distributed horizons

$$\sum_{t=0}^T \gamma^t r_t$$

$$T \sim \frac{1}{\tau} e^{t/\tau}$$



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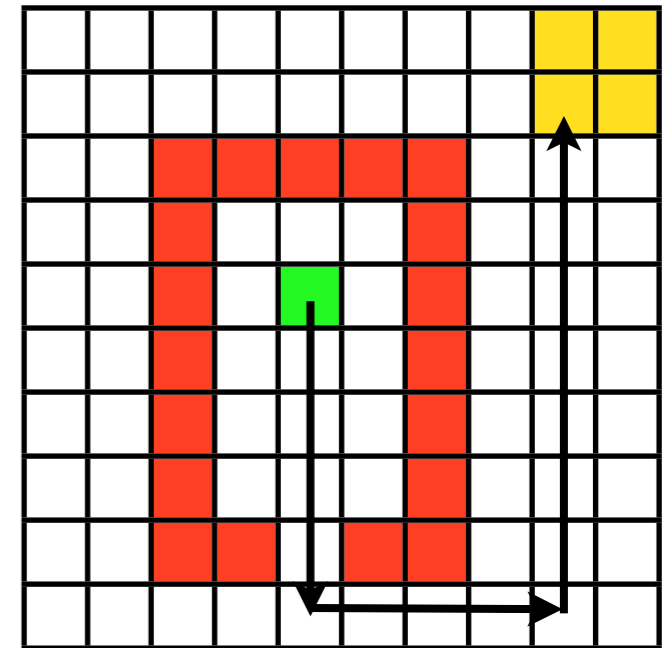
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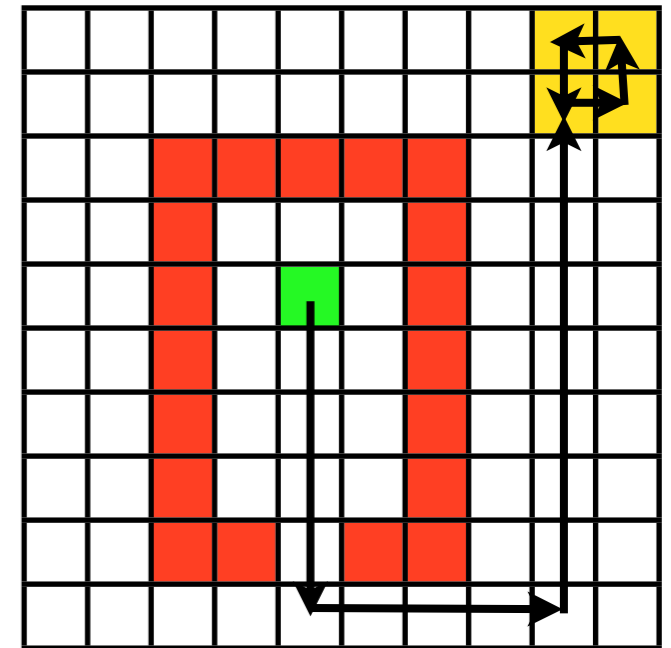
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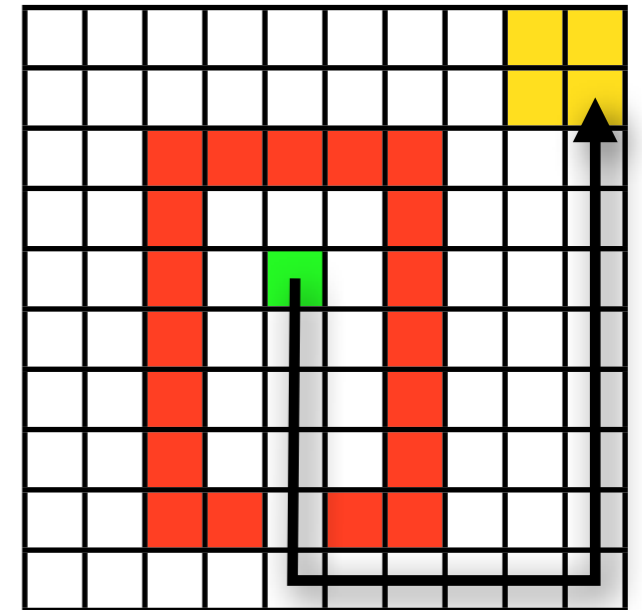


# Markov Decision Problems

$$V^{\pi}(s_t) = \mathbb{E} \left[ \sum_{t'=1}^{\infty} r_{t'} \mid s_t = s, \pi \right]$$

$$= \mathbb{E} [r_1 \mid s_t = s, \pi] + \mathbb{E} \left[ \sum_{t=2}^{\infty} r_t \mid s_t = s, \pi \right]$$

$$= \mathbb{E} [r_1 \mid s_t = s, \pi] + \mathbb{E} [V^{\pi}(s_{t+1}) \mid s_t = s, \pi]$$



This dynamic consistency is key to many solution approaches.  
It states that the value of a state  $s$  is related to  
the values of its successor states  $s'$ .

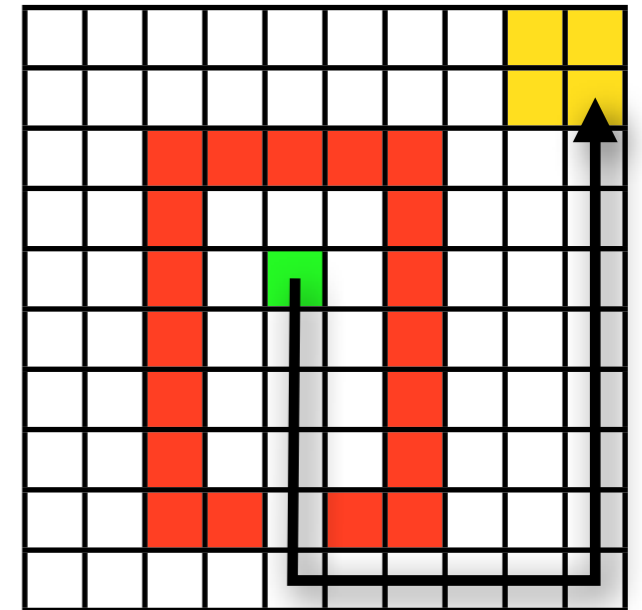
# Markov Decision Problems

$$V^\pi(s_t) = \mathbb{E}[r_1 | s_t = s, \pi] + \mathbb{E}[V(s_{t+1}), \pi]$$
$$r_1 \sim \mathcal{R}(s_2, a_1, s_1)$$

$$\mathbb{E}[r_1 | s_t = s, \pi] = \mathbb{E} \left[ \sum_{s_{t+1}} p(s_{t+1} | s_t, a_t) \mathcal{R}(s_{t+1}, a_t, s_t) \right]$$

$$= \sum_{a_t} p(a_t | s_t) \left[ \sum_{s_{t+1}} p(s_{t+1} | s_t, a_t) \mathcal{R}(s_{t+1}, a_t, s_t) \right]$$

$$= \sum_{a_t} \pi(a_t, s_t) \left[ \sum_{s_{t+1}} \mathcal{T}_{s_t s_{t+1}}^{a_t} \mathcal{R}(s_{t+1}, a_t, s_t) \right]$$

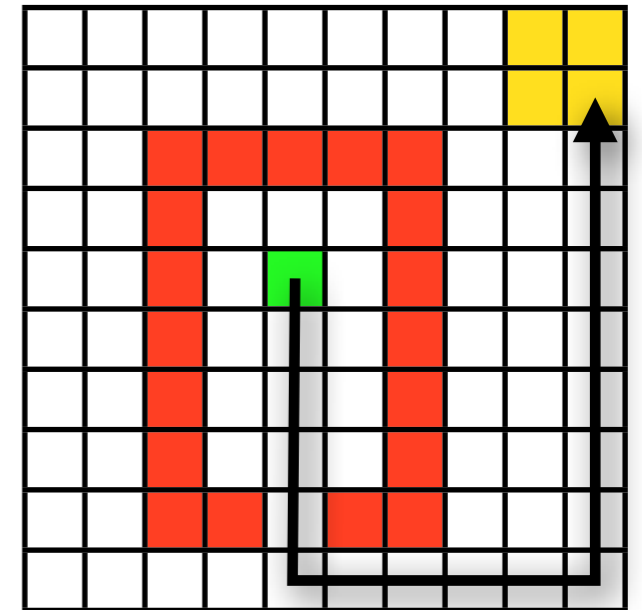


# Bellman equation

$$V^\pi(s_t) = \mathbb{E}[r_1 | s_t = s, \pi] + \mathbb{E}[V(s_{t+1}), \pi]$$

$$\mathbb{E}[r_1 | s_t, \pi] = \sum_a \pi(a, s_t) \left[ \sum_{s_{t+1}} \mathcal{T}_{s_t s_{t+1}}^a \mathcal{R}(s_{t+1}, a, s_t) \right]$$

$$\mathbb{E}[V^\pi(s_{t+1}), \pi, s_t] = \sum_a \pi(a, s_t) \left[ \sum_{s_{t+1}} \mathcal{T}_{s_t s_{t+1}}^a V^\pi(s_{t+1}) \right]$$



$$V^\pi(s) = \sum_a \pi(a|s) \left[ \sum_{s'} \mathcal{T}_{ss'}^a [\mathcal{R}(s', a, s) + V^\pi(s')] \right]$$

# Bellman Equation

---

$$V^{\pi}(s) = \sum_a \pi(a|s) \left[ \sum_{s'} \mathcal{T}_{ss'}^a [\mathcal{R}(s', a, s) + V^{\pi}(s')] \right]$$

# Bellman Equation

---

All future reward from state  $s$  = E [ Immediate reward + All future reward from next state  $s'$  ]

$$V^{\pi}(s) = \sum_a \pi(a|s) \left[ \sum_{s'} \mathcal{T}_{ss'}^a [\mathcal{R}(s', a, s) + V^{\pi}(s')] \right]$$

# Bellman Equation

---

$$V^{\pi}(s) = \sum_a \pi(a|s) \left[ \sum_{s'} \mathcal{T}_{ss'}^a [\mathcal{R}(s', a, s) + V^{\pi}(s')] \right]$$

$$\begin{array}{c} \text{All future} \\ \text{reward} \\ \text{from state } s \end{array} = \mathbb{E} \left[ \begin{array}{c} \text{Immediate} \\ \text{reward} \end{array} + \begin{array}{c} \text{All future} \\ \text{reward} \\ \text{from} \\ \text{next state } s' \end{array} \right]$$

# Q values = state-action values

---

$$V^{\pi}(s) = \sum_a \pi(a|s) \underbrace{\left[ \sum_{s'} \mathcal{T}_{ss'}^a [\mathcal{R}(s', a, s) + V^{\pi}(s')] \right]}_{Q^{\pi}(s, a)}$$

► so we can define state-action values as:

$$\begin{aligned} Q(s, a) &= \sum_{s'} \mathcal{T}_{ss'}^a [\mathcal{R}(s', a, s) + V(s')] \\ &= \mathbb{E} \left[ \sum_{t=1}^{\infty} r_t | s, a \right] \end{aligned}$$

► and state values are average state-action values:

$$V(s) = \sum_a \pi(a|s) Q(s, a)$$

# Bellman Equation

---

$$V^{\pi}(s) = \sum_a \pi(a|s) \left[ \sum_{s'} \mathcal{T}_{ss'}^a [\mathcal{R}(s', a, s) + V^{\pi}(s')] \right]$$

- ▶ to evaluate a policy, we need to solve the above equation, i.e. find the self-consistent state values
  
- ▶ options for policy evaluation
  - exhaustive tree search - outwards, inwards, depth-first
  - linear solution in 1 step
  - value iteration: iterative updates
  - experience sampling

# Solving the Bellman Equation

---

Option 1: turn it into update equation

Option 2: linear solution

(w/ absorbing states)

$$\begin{aligned} V(s) &= \sum_a \pi(a, s_t) \left[ \sum_{s'} \mathcal{T}_{ss'}^a [\mathcal{R}(s', a, s) + V(s')] \right] \\ \Rightarrow \mathbf{v} &= \mathbf{R}^\pi + \mathbf{T}^\pi \mathbf{v} \\ \Rightarrow \mathbf{v}^\pi &= (\mathbf{I} - \mathbf{T}^\pi)^{-1} \mathbf{R}^\pi \quad \mathcal{O}(|\mathcal{S}|^3) \end{aligned}$$

# Solving the Bellman Equation

---

Option 1: turn it into update equation

$$V^{k+1}(s) = \sum_a \pi(a, s_t) \left[ \sum_{s'} \mathcal{T}_{ss'}^a [\mathcal{R}(s', a, s) + V^k(s')] \right]$$

Option 2: linear solution

(w/ absorbing states)

$$V(s) = \sum_a \pi(a, s_t) \left[ \sum_{s'} \mathcal{T}_{ss'}^a [\mathcal{R}(s', a, s) + V(s')] \right]$$

$$\Rightarrow \mathbf{v} = \mathbf{R}^\pi + \mathbf{T}^\pi \mathbf{v}$$

$$\Rightarrow \mathbf{v}^\pi = (\mathbf{I} - \mathbf{T}^\pi)^{-1} \mathbf{R}^\pi \quad \mathcal{O}(|\mathcal{S}|^3)$$

# Policy update

---

Given the value function for a policy, say via linear solution

$$V^\pi(s) = \sum_a \pi(a|s) \underbrace{\left[ \sum_{s'} \mathcal{T}_{ss'}^a [\mathcal{R}(s', a, s) + V^\pi(s')] \right]}_{Q^\pi(s, a)}$$

Given the values  $V$  for the policy, we can improve the policy by always choosing the best action:

$$\pi'(a|s) = \begin{cases} 1 & \text{if } a = \operatorname{argmax}_a Q^\pi(s, a) \\ 0 & \text{else} \end{cases}$$

It is guaranteed to improve:

$$Q^\pi(s, \pi'(s)) = \max_a Q^\pi(s, a) \geq Q^\pi(s, \pi(s)) = \mathcal{V}^\pi(s)$$

← for deterministic policy

# Policy iteration

---

Policy evaluation

$$\mathbf{v}^{\pi} = (\mathbf{I} - \mathbf{T}^{\pi})^{-1} \mathbf{R}^{\pi}$$

$$\pi(a|s) = \begin{cases} 1 & \text{if } a = \operatorname{argmax}_a \sum_{s'} \mathcal{T}_{ss'}^a [\mathcal{R}_{ss}^a + V^{pi}(s')] \\ 0 & \text{else} \end{cases}$$

# Policy iteration

---

Policy evaluation

$$\mathbf{v}^{\pi} = (\mathbf{I} - \mathbf{T}^{\pi})^{-1} \mathbf{R}^{\pi}$$

greedy policy improvement

$$\pi(a|s) = \begin{cases} 1 & \text{if } a = \operatorname{argmax}_a \sum_{s'} \mathcal{T}_{ss'}^a [\mathcal{R}_{ss}^a + V^{pi}(s')] \\ 0 & \text{else} \end{cases}$$

# Policy iteration

Policy evaluation

$$\mathbf{v}^{\pi} = (\mathbf{I} - \mathbf{T}^{\pi})^{-1} \mathbf{R}^{\pi}$$

Value iteration

$$V^*(s) = \max_a \sum_{s'} \mathcal{T}_{ss'}^a [\mathcal{R}_{ss}^a + V^*(s')]$$

greedy policy improvement

$$\pi(a|s) = \begin{cases} 1 & \text{if } a = \operatorname{argmax}_a \sum_{s'} \mathcal{T}_{ss'}^a [\mathcal{R}_{ss}^a + V^{pi}(s')] \\ 0 & \text{else} \end{cases}$$

# Model-free solutions

---

- ▶ So far we have assumed knowledge of  $R$  and  $T$ 
  - $R$  and  $T$  are the ‘model’ of the world, so we assume full knowledge of the dynamics and rewards in the environment
- ▶ What if we don’t know them?
- ▶ We can still learn from state-action-reward samples
  - we can learn  $R$  and  $T$  from them, and use our estimates to solve as above
  - alternatively, we can directly estimate  $V$  or  $Q$

# Solving the Bellman Equation

---

## Option 3: sampling

$$V(s) = \sum_a \pi(a, s_t) \left[ \sum_{s'} \mathcal{T}_{ss'}^a [\mathcal{R}(s', a, s) + V(s')] \right]$$

So we can just draw some samples from the policy and the transitions and average over them:

$$a = \sum_k f(x_k) p(x_k)$$
$$x^{(i)} \sim p(x) \rightarrow \hat{a} = \frac{1}{N} \sum_i f(x^{(i)})$$

# Solving the Bellman Equation

---

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# Solving the Bellman Equation

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# Solving the Bellman Equation

---

## Option 3: sampling

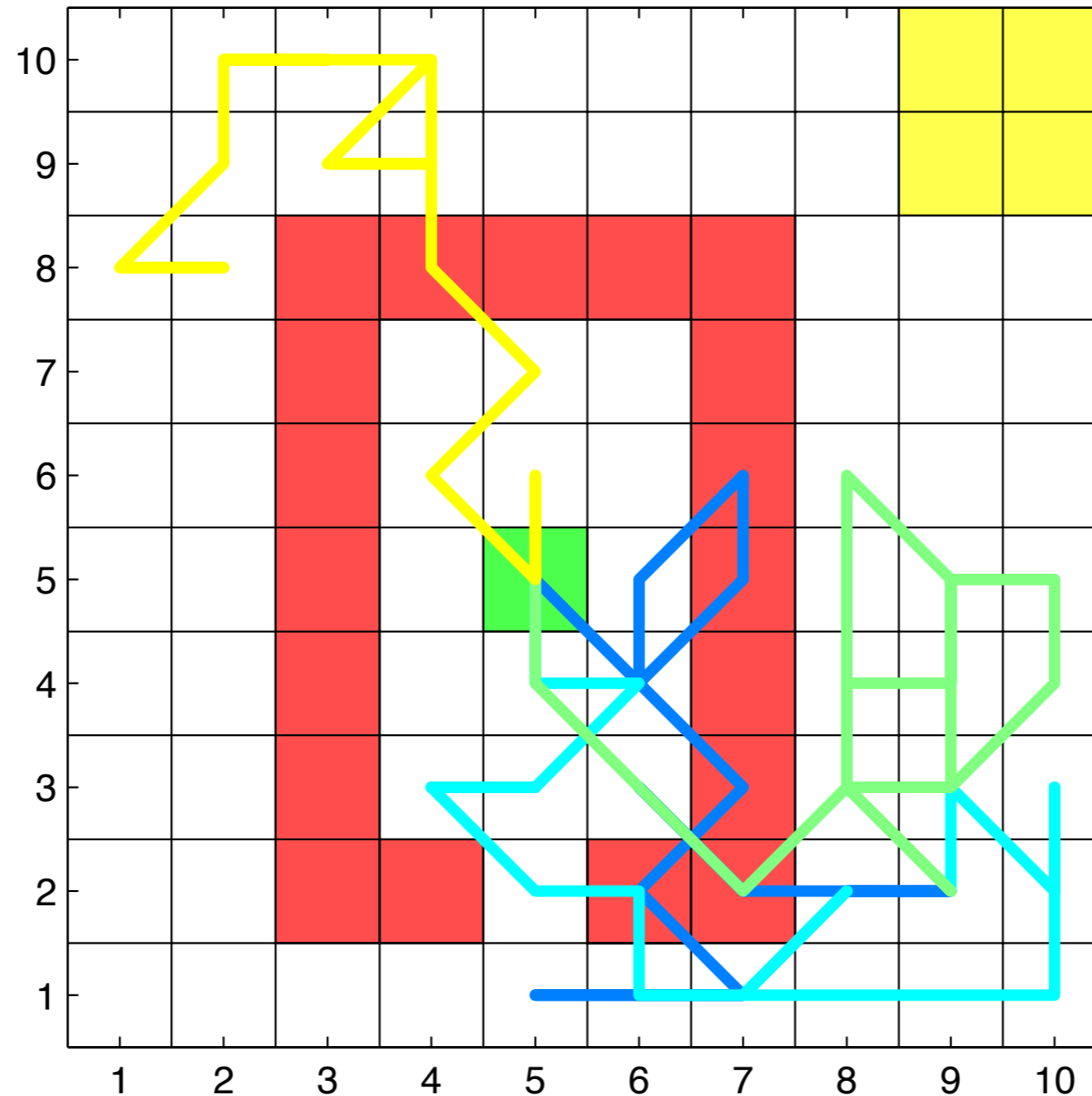
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more about this later...

# Learning from samples



A new problem: exploration versus exploitation

# Monte Carlo

## ► First visit MC

- randomly start in all states, generate paths, average for starting state only

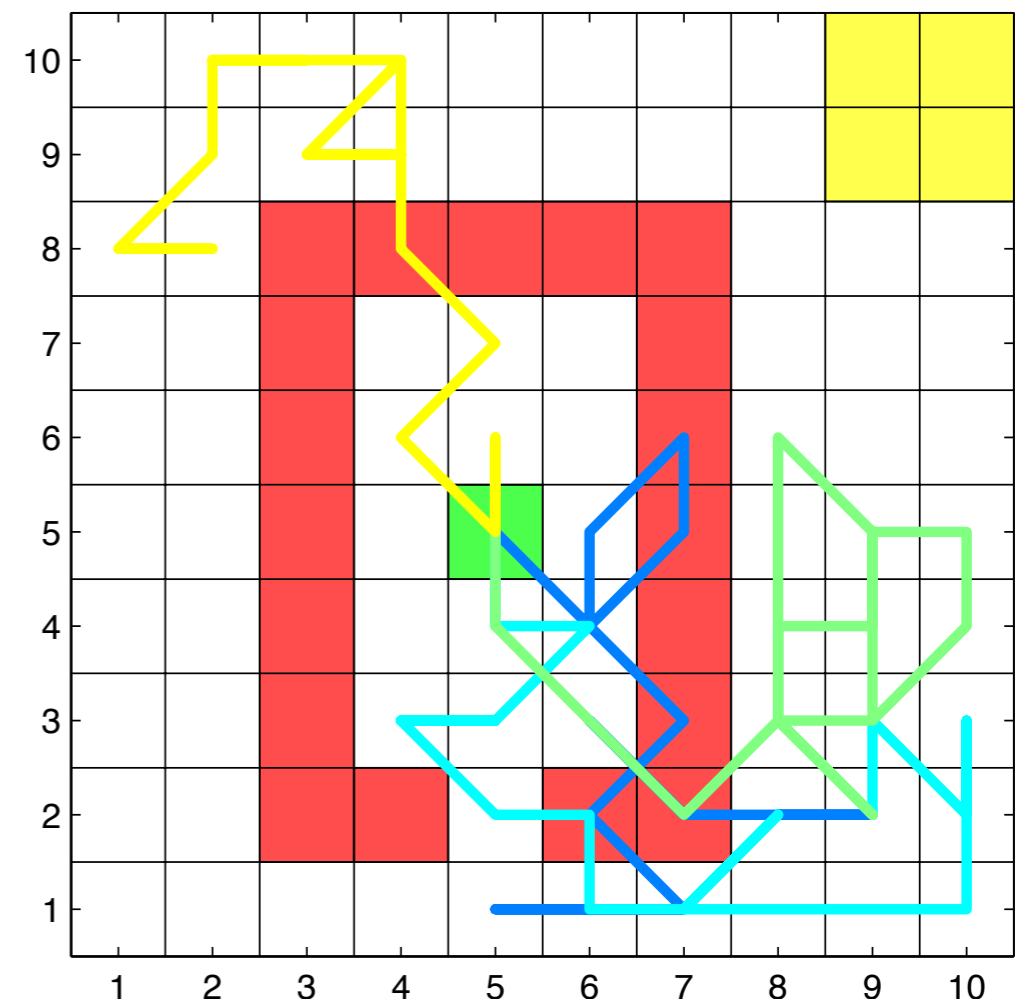
$$\mathcal{V}(s) = \frac{1}{N} \sum_i \left\{ \sum_{t'=1}^T r_{t'}^i \mid s_0 = s \right\}$$

## ► More efficient use of samples

- Every visit MC
- Bootstrap:TD
- Dyna

## ► Better samples

- on policy versus off policy
- Stochastic search, UCT...



# Update equation: towards TD

---

Bellman equation

$$V(s) = \sum_a \pi(a, s) \left[ \sum_{s'} \mathcal{T}_{ss'}^a [\mathcal{R}(s', a, s) + V(s')] \right]$$

Not yet converged, so it doesn't hold:

$$dV(s) = -V(s) + \sum_a \pi(a, s) \left[ \sum_{s'} \mathcal{T}_{ss'}^a [\mathcal{R}(s', a, s) + V(s')] \right]$$

And then use this to update

$$V^{i+1}(s) = V^i(s) + dV(s)$$

# TD learning

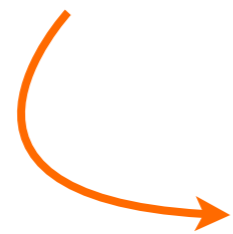
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$$dV(s) = -V(s) + \sum_a \pi(a, s) \left[ \sum_{s'} \mathcal{T}_{ss'}^a [\mathcal{R}(s', a, s) + V(s')] \right]$$

# TD learning

---

$$dV(s) = -V(s) + \sum_a \pi(a, s) \left[ \sum_{s'} \mathcal{T}_{ss'}^a [\mathcal{R}(s', a, s) + V(s')] \right]$$



Sample

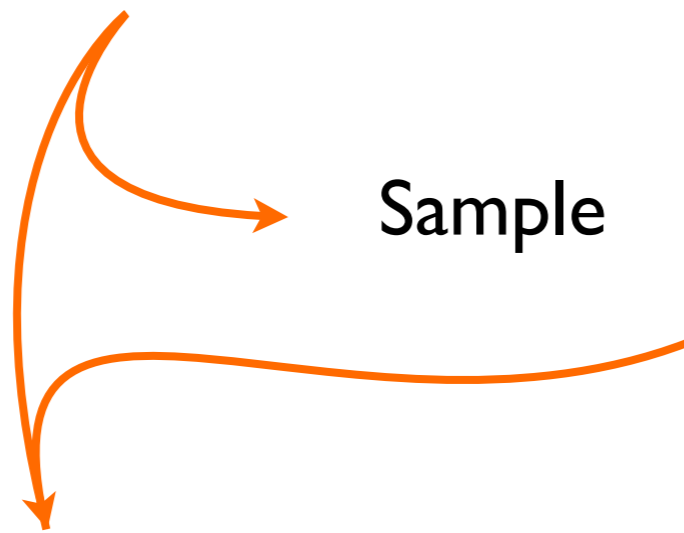
$$a_t \sim \pi(a|s_t)$$

$$s_{t+1} \sim \mathcal{T}_{s_t, s_{t+1}}^{a_t}$$

$$r_t = \mathcal{R}(s_{t+1}, a_t, s_t)$$

# TD learning

$$dV(s) = -V(s) + \sum_a \pi(a, s) \left[ \sum_{s'} \mathcal{T}_{ss'}^a [\mathcal{R}(s', a, s) + V(s')] \right]$$



$$a_t \sim \pi(a|s_t)$$

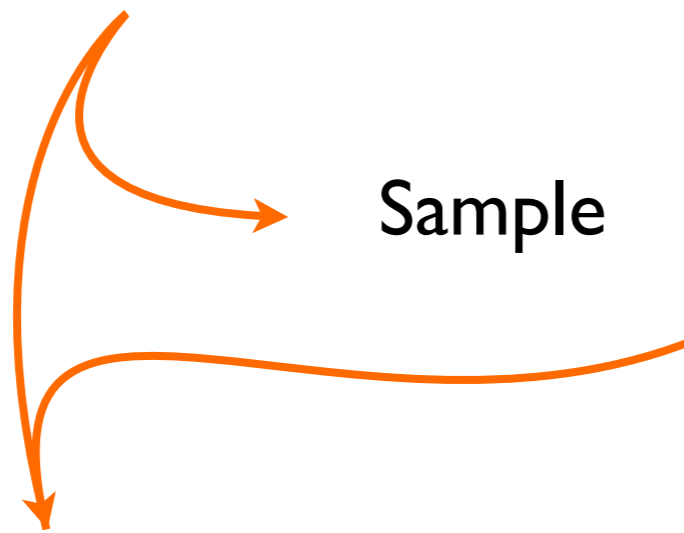
$$s_{t+1} \sim \mathcal{T}_{s_t, s_{t+1}}^{a_t}$$

$$r_t = \mathcal{R}(s_{t+1}, a_t, s_t)$$

$$\delta_t = -V_{t-1}(s_t) + r_t + V_{t-1}(s_{t+1})$$

# TD learning

$$dV(s) = -V(s) + \sum_a \pi(a, s) \left[ \sum_{s'} \mathcal{T}_{ss'}^a [\mathcal{R}(s', a, s) + V(s')] \right]$$



$$\begin{aligned} a_t &\sim \pi(a|s_t) \\ s_{t+1} &\sim \mathcal{T}_{s_t, s_{t+1}}^{a_t} \\ r_t &= \mathcal{R}(s_{t+1}, a_t, s_t) \end{aligned}$$

$$\delta_t = -V_{t-1}(s_t) + r_t + V_{t-1}(s_{t+1})$$

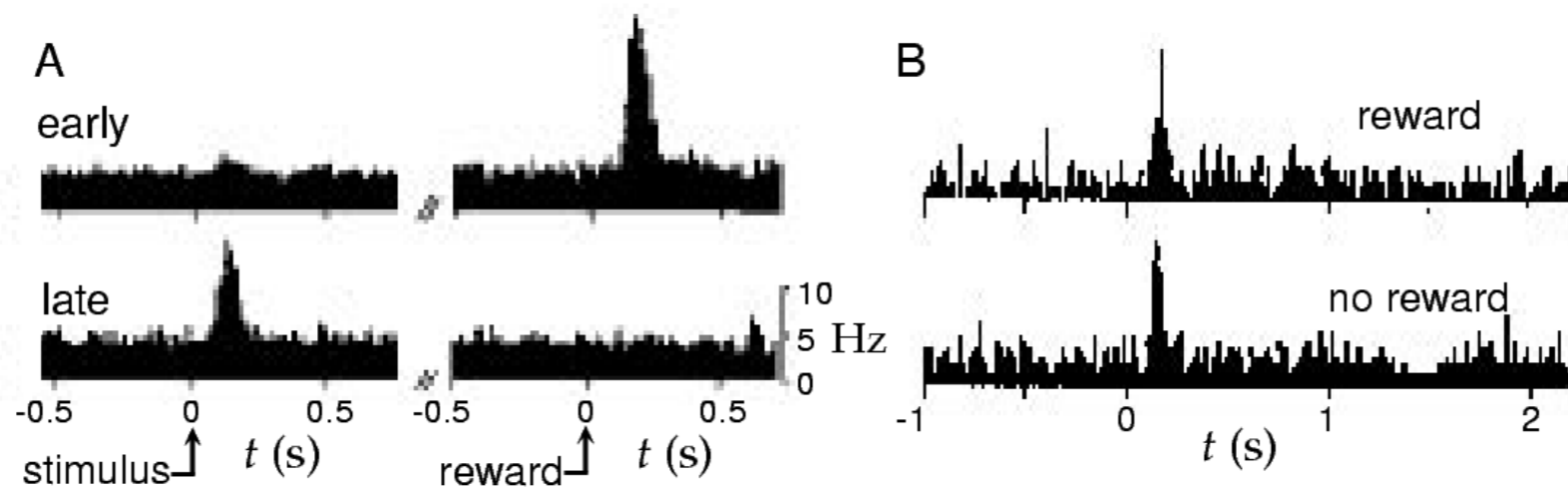
$$V^{i+1}(s) = V^i(s) + dV(s) \quad \xrightarrow{\hspace{1cm}} \quad V_t(s_t) = V_{t-1}(s_t) + \alpha \delta_t$$

# TD learning

---

$$\begin{aligned}a_t &\sim \pi(a|s_t) \\s_{t+1} &\sim \mathcal{T}_{s_t, s_{t+1}}^{a_t} \\r_t &= \mathcal{R}(s_{t+1}, a_t, s_t) \\\delta_t &= -V_t(s_t) + r_t + V_t(s_{t+1}) \\V_{t+1}(s_t) &= V_t(s_t) + \alpha \delta_t\end{aligned}$$

# Aside: what makes a TD error?

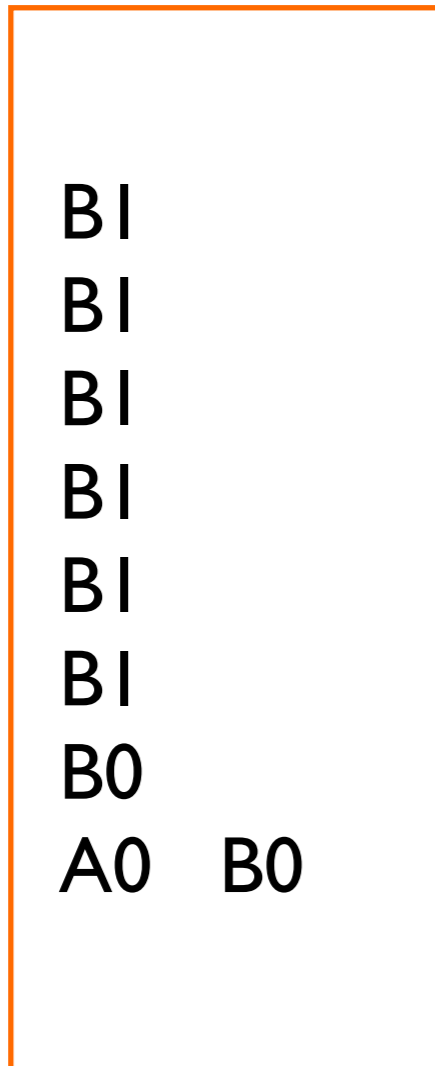


- ▶ unpredicted reward expectation change
- ▶ disappears with learning
- ▶ stays with probabilistic reinforcement
- ▶ sequentiality
  - TD error vs prediction error
- ▶ see Niv and Schoenbaum 2008

Schultz et al.

# The effect of bootstrapping

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Markov (every visit)

$$V(B)=3/4$$

$$V(A)=0$$

TD

$$V(B)=3/4$$

$$V(A)=\sim 3/4$$

► Average over various bootstrappings:  $TD(\lambda)$

after Sutton and Barto 1998

- policy and value separately parameterised

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

$$w(s, a) \leftarrow w(s, a) + \beta \delta_t$$

$$w(s, a) \leftarrow w(s, a) + \beta \delta_t (1 - \pi(s, a))$$

$$\pi(a|s) = \frac{e^{w(s,a)}}{\sum_{a'} e^{w(s,a')}}$$

- Do TD for state-action values instead:

$$Q(s_t, a_t) \leftarrow Q(s_t, a_t) + \alpha[r_t + \gamma Q(s_{t+1}, a_{t+1}) - Q(s_t, a_t)]$$

$$s_t, a_t, r_t, s_{t+1}, a_{t+1}$$

- convergence guarantees - will estimate  $Q^\pi(s, a)$

# Q learning: off-policy

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## ► Learn off-policy

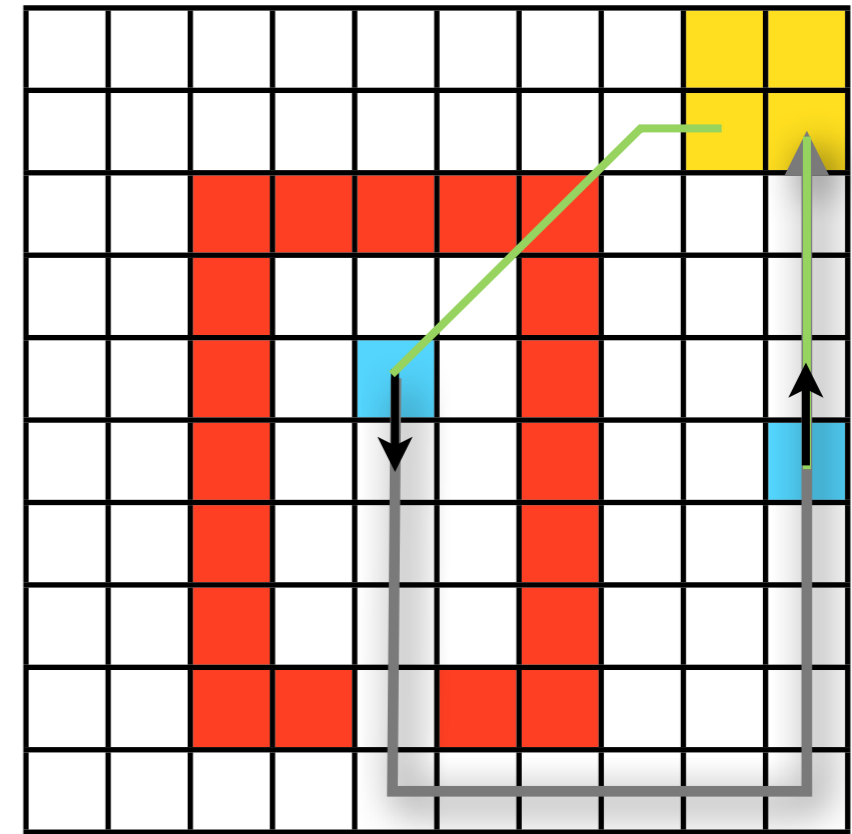
- draw from some policy
- “only” require extensive sampling

$$Q(s_t, a_t) \leftarrow Q(s_t, a_t) + \alpha \left[ \underbrace{r_t + \gamma \max_a Q(s_{t+1}, a)}_{\text{update towards optimum}} - Q(s_t, a_t) \right]$$

## ► will estimate $Q^*(s, a)$

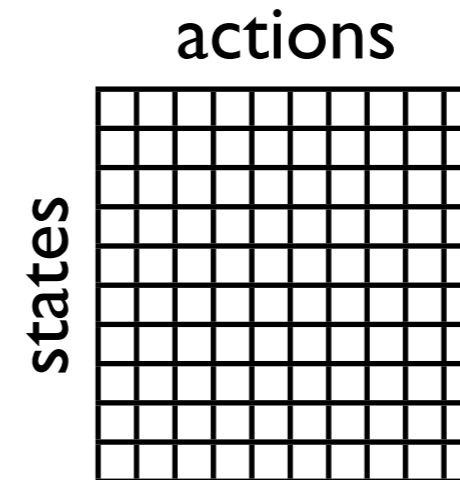
# Learning in the wrong state space

- ▶ states=distance from goal
- ▶ state-space choice crucial
  - too big -> curse of dimensionality
  - too small -> can't express good policies
  - unsolved problem
- ▶ humans in tasks have to infer state-space

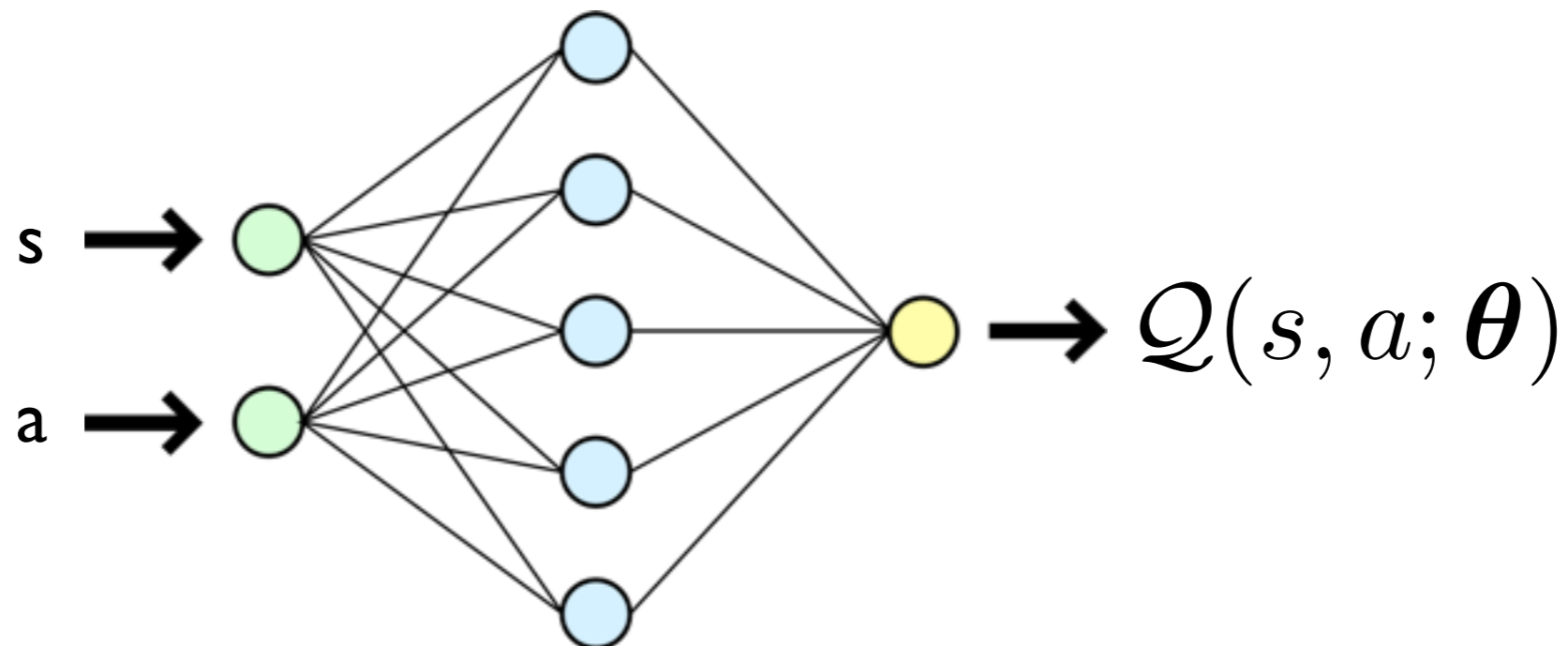


# Neural network approximations

- So far: look-up tables



- Parametric value functions



- Humans and animals generalize

# Hierarchical decompositions

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## ► Subtasks stay the same

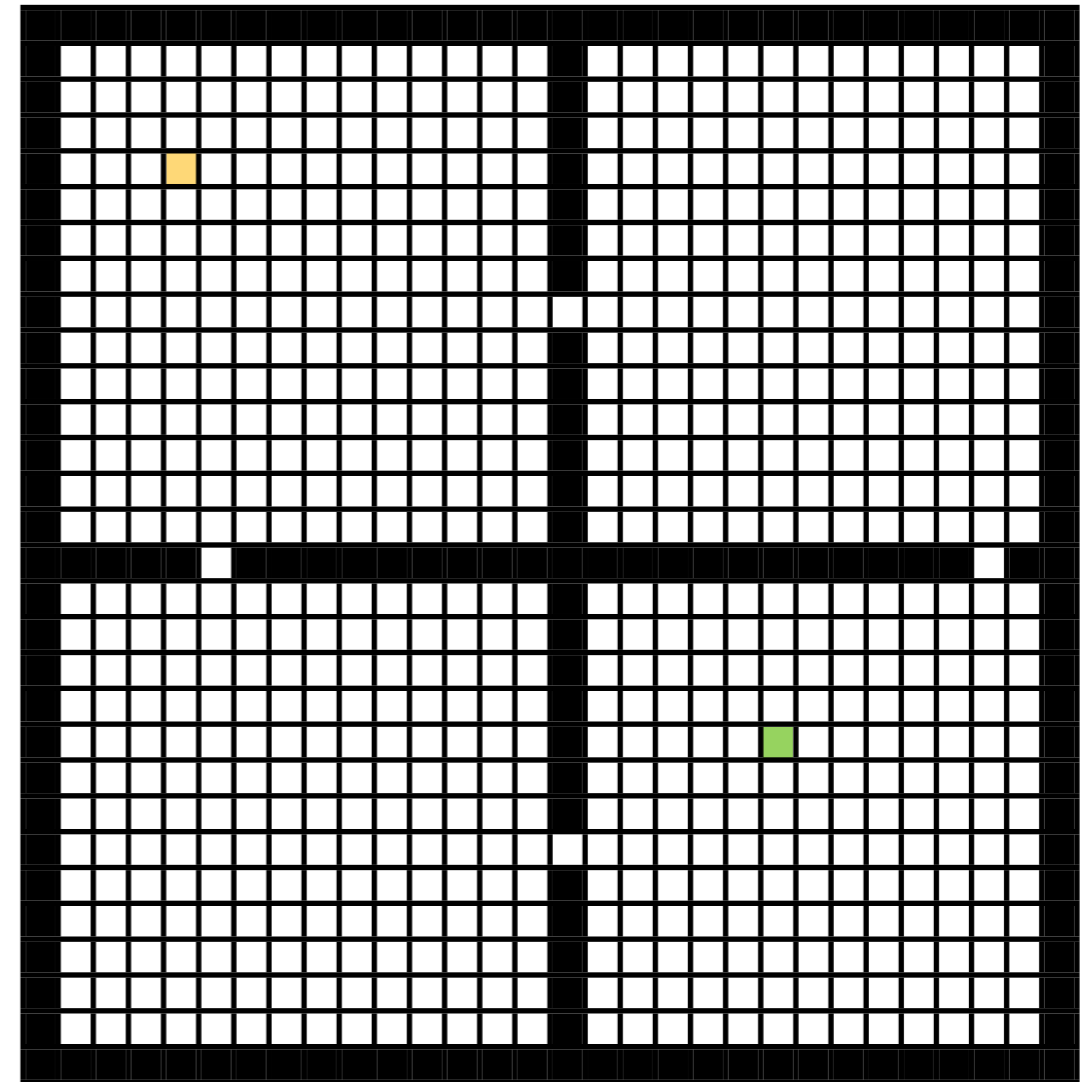
- Learn subtasks
- Learn how to use subtasks

## ► Macroactions

- ‘go to door’
- search goal

## ► Humans establish subgoals on-line

- how is not yet known



# Learning a model

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- ▶ So far we've concentrated on model-free learning
- ▶ What if we want to build some model of the environment?

$$V(s) = \sum_a \pi(a, s) \left[ \sum_{s'} \mathcal{T}_{ss'}^a [\mathcal{R}(s', a, s) + V(s')] \right]$$

- ▶ Count transitions

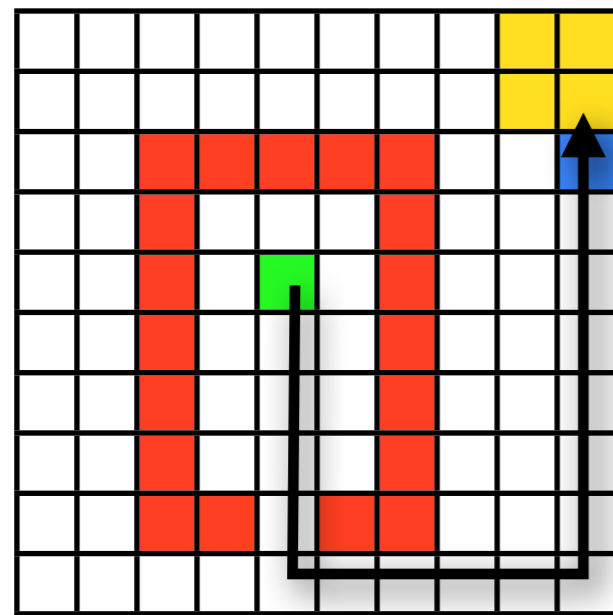
$$\hat{\mathcal{T}}_{ss'}^a = \frac{\sum_t \mathbf{1}(s_t = s, a_t = a, s_{t+1} = s')}{\sum_t \mathbf{1}(s_t = s, a_t = a)}$$

- ▶ Average rewards

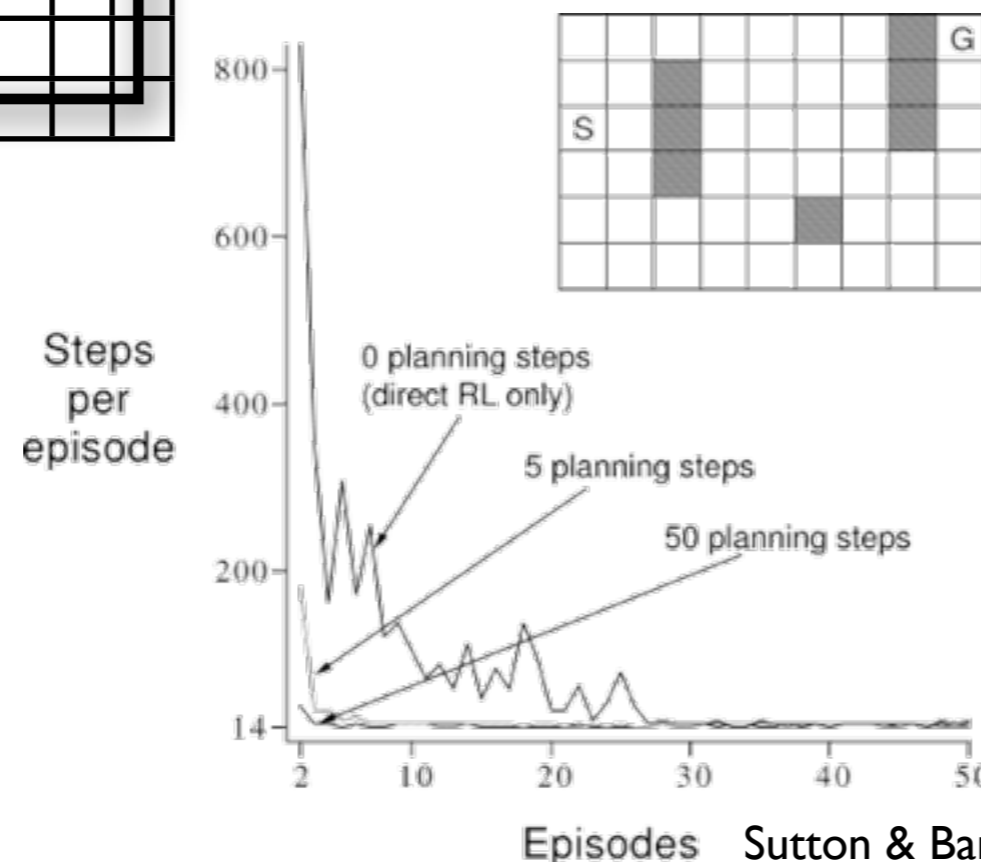
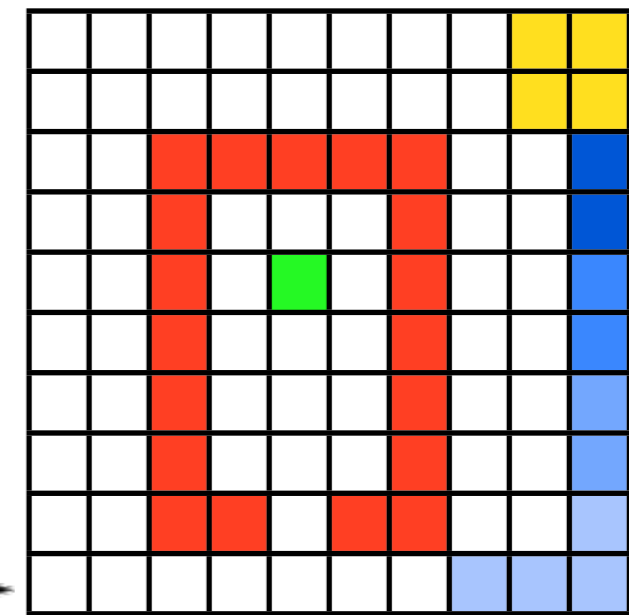
$$\hat{\mathcal{R}}_{ss'}^a = \frac{\sum_t r_t \mathbf{1}(s_t = s, a_t = a, s_{t+1} = s')}{\sum_t \mathbf{1}(s_t = s, a_t = a, s_{t+1} = s')}$$

## ► Combine model estimation with TD learning

$$V_{t+1}(s_t) = V_t(s_t) + \alpha \delta_t$$



Generate extra  
experience samples  
from estimated model



# Conclusion I

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- ▶ Long-term rewards have internal consistency
- ▶ This can be exploited for solution
- ▶ Exploration and exploitation trade off when sampling
- ▶ Clever use of samples can produce fast learning
  - Brain most likely does something like this