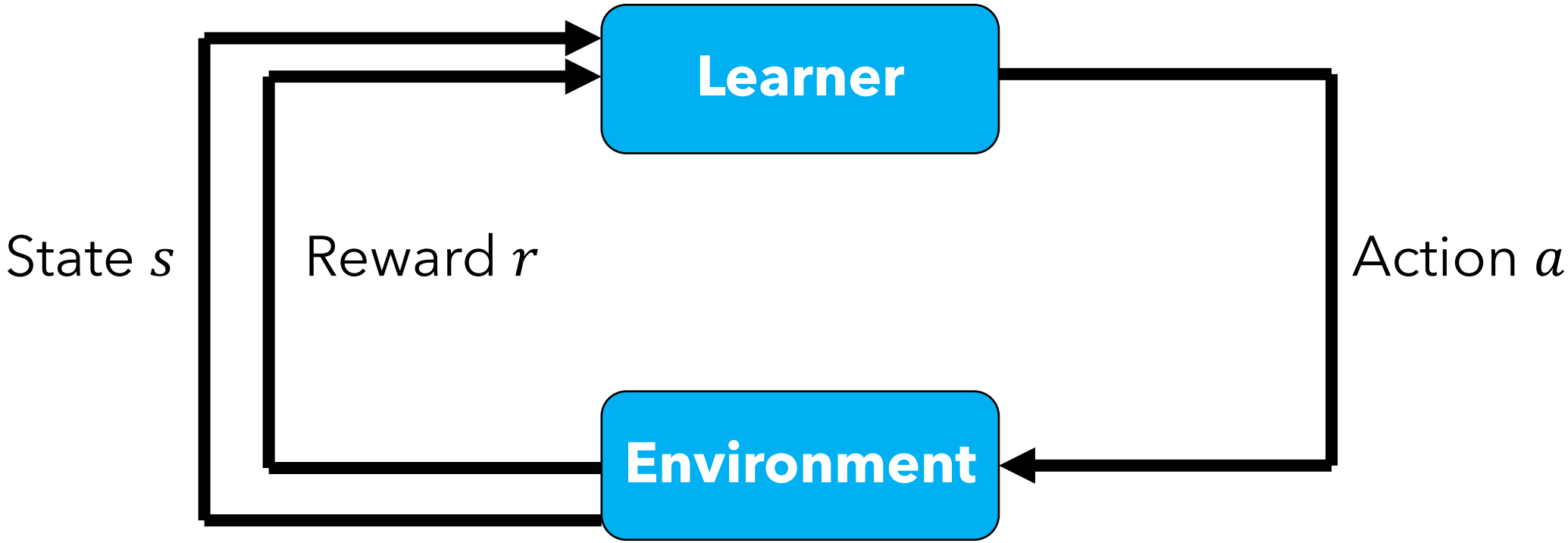
# Reinforcement learning refresher

Content draws on material by Zico Kolter

# Learner interaction with environment

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# Outline

1. **Markov decision processes**
2. Reinforcement learning
3. Branch-and-bound as an MDP

# Markov decision processes

- MDPs defined by:
  - States
  - Actions
  - Transition probabilities
  - Rewards
- **States**: encode how system will evolve when taking actions
- System governed by **transition probabilities** $P(s_{t+1} \mid s_t, a_t)$
  - Only depend on **current** state and action (Markov assumption)
- **Agent's goal**: take actions that maximize expected reward

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# Markov decision processes

$S$: set of states (assumed for now to be discrete)

$A$: set of actions

Transition probability distribution $P(s' \mid s, a)$

*Probability of entering state $s'$ from state $s$ after taking action $a$*

Reward function $R: S \rightarrow \mathbb{R}$

**Goal:** Policy $\pi: S \rightarrow A$ that maximizes total (discounted) reward

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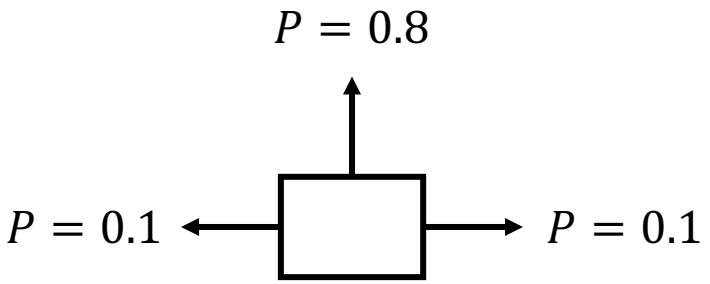
# Gridworld domain

- Goal state with reward 1
- “Bad state” with reward -100
- Actions move:
  - North with probably 0.8
  - East or west with probability 0.1
- Action that would bump into a wall leaves agent where it is

| | | | |
|---|---|---|---|
| 0 | 0 | 0 | 1 |
| 0 | | 0 | -100 |
| 0 | 0 | 0 | 0 |

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# Policies and value functions

Policy is a mapping from states to actions $\pi: S \rightarrow A$

**Value function for a policy:**

Expected sum of discounted rewards

$$V^{\pi}(s) = \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^{t} R(s_t) \mid s_0 = s, a_t = \pi(s_t), s_{t+1} | s_t, a_t \sim P\right]$$

Discount factor

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# Bellman equation

Can also define $V^{\pi}(s)$ recursively via the **Bellman equation**:

$$V^{\pi}(s) = R(s) + \gamma \sum_{s' \in S} P(\, s' \mid s, \pi(s)\,) V^{\pi}(s')$$

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# Computing the policy value

- $\boldsymbol{v}^\pi \in \mathbb{R}^{|S|}$ is a vector of **values** for each state
- $\boldsymbol{r} \in \mathbb{R}^{|S|}$ is a vector of **rewards** for each state
- $P^\pi \in \mathbb{R}^{|S| \times |S|}$ contains the **transition probabilities** under $\pi$

$$P^\pi_{ij} = P(\, s_{t+1} = i \mid s_t = j, a_t = \pi(s_t)\,)$$

- **Bellman equation** can be written in vector form as

$$\boldsymbol{v}^\pi = \boldsymbol{r} + \gamma P^\pi \boldsymbol{v}^\pi$$
$$\Rightarrow (I - \gamma P^\pi)\boldsymbol{v}^\pi = \boldsymbol{r}$$
$$\Rightarrow \boldsymbol{v}^\pi = (I - \gamma P^\pi)^{-1}\boldsymbol{r}$$

i.e., computing the policy value requires solving a **linear system**

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# Optimal policy and value function

**Optimal policy** $\pi^\star$ achieves the highest value for every state

$$V^{\pi^\star}(s) = \max_{\pi} V^{\pi}(s)$$

Value function is written $V^\star = V^{\pi^\star}$

There are an exponential number of policies

⇒ Formulation is not very useful

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# Optimal policy and value function

Instead, define $V^\star(s)$ using the **Bellman optimality equation**

$$V^\star(s) = R(s) + \gamma \max_{a \in \mathcal{A}} \sum_{s' \in S} P(s' \mid s, a) V^\star(s')$$

Optimal policy is simply the action that attains this max

$$\pi^\star(s) = \operatorname{argmax}_{a} \sum_{s' \in S} P(s' \mid s, a) V^\star(s')$$

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# Outline

1. Markov decision processes
    i. **Computing the optimal policy**
        a. **Value iteration**
        b. Policy iteration
2. Reinforcement learning
3. Branch-and-bound as an MDP

# Computing the optimal policy

**Approach #1: value iteration**

Repeatedly update estimate of the optimal value function (according to Bellman optimality equation)

1. $\hat{V}(s) \leftarrow 0, \forall s \in S$
2. Repeat:

$$\hat{V}(s) \leftarrow R(s) + \gamma \max_{a \in \mathcal{A}} \sum_{s' \in S} P(s' \mid s, a) \hat{V}(s')$$

$$V^{\star}(s) = R(s) + \gamma \max_{a \in \mathcal{A}} \sum_{s' \in S} P(s' \mid s, a) V^{\star}(s')$$

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# Computing the optimal policy

**Approach #1: value iteration**

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$$\hat{V}(s) \leftarrow R(s) + \gamma \max_{a \in \mathcal{A}} \sum_{s' \in S} P(s' \mid s, a) \hat{V}(s')$$

**Theorem:** Value iteration converges to optimal value: $\hat{V} \rightarrow V^{\star}$

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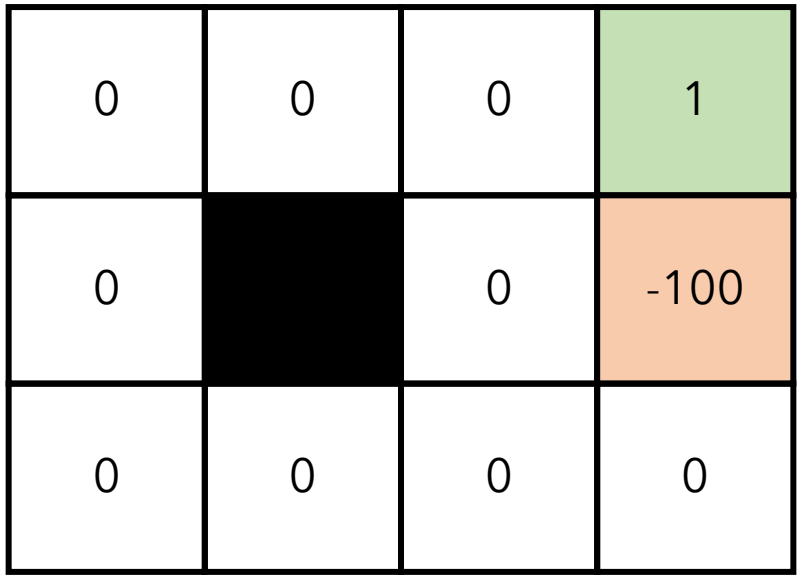
# Illustration of value iteration

Running value iteration with $\gamma = 0.9$




Original reward function

# Illustration of value iteration

Running value iteration with $\gamma = 0.9$

| | | | |
|---|---|---|---|
| 0 | 0 | 0.72 | 1.81 |
| 0 | | 0 | -99.91 |
| 0 | 0 | 0 | 0 |

$\hat{V}$ at 1 iteration

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# Illustration of value iteration

Running value iteration with $\gamma = 0.9$

| | | | |
|---|---|---|---|
| 0.809 | 1.598 | 2.475 | 3.745 |
| 0.268 | | 0.302 | -99.59 |
| 0 | 0.034 | 0.122 | 0.004 |

$\hat{V}$ at 5 iterations

# Illustration of value iteration

Running value iteration with $\gamma = 0.9$

| | | | |
|---|---|---|---|
| 2.686 | 3.527 | 4.402 | 5.812 |
| 2.021 | | 1.095 | -98.82 |
| 1.390 | 0.903 | 0.738 | 0.123 |

$\hat{V}$ at 10 iterations

# Illustration of value iteration

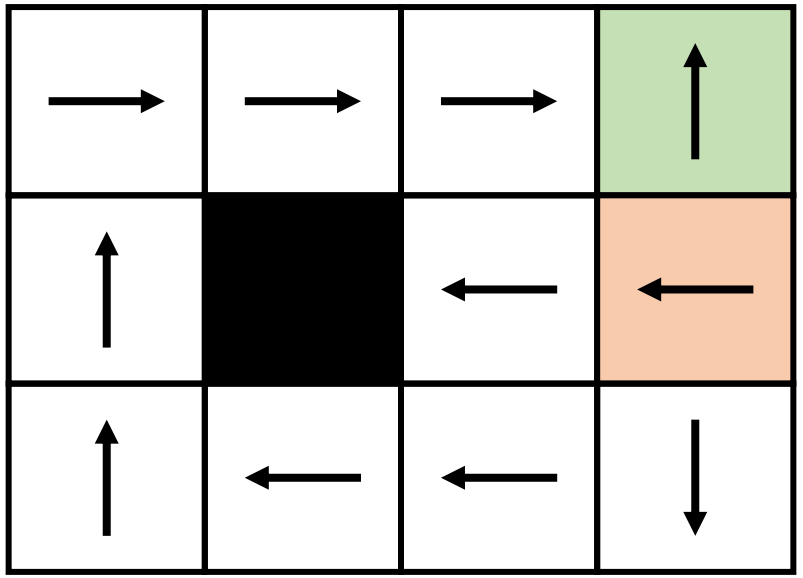
Running value iteration with $\gamma = 0.9$

| | | | |
|---|---|---|---|
| 5.470 | 6.313 | 7.190 | 8.669 |
| 4.802 | | 3.347 | -96.67 |
| 4.161 | 3.654 | 3.222 | 1.526 |

$\hat{V}$ at 1000 iterations

# Illustration of value iteration

Running value iteration with $\gamma = 0.9$



Resulting policy after 1000 iterations

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# Outline

1. Markov decision processes
    i. Computing the optimal policy
        a. Value iteration
        **b. Policy iteration**
2. Reinforcement learning
3. Branch-and-bound as an MDP

# Policy iteration

1. Initialize policy $\pi$ randomly
2. Compute value of policy $V^{\pi}$ (e.g., by solving linear system)
3. Update $\pi$ to be greedy policy with respect to $V^{\pi}$

$$\pi(s) \leftarrow \operatorname*{argmax}_{a} \sum_{s' \in S} P(\, s' \mid s, a \,) V^{\pi}(s')$$

4. If policy $\pi$ changed in last iteration, return to step 2

**Theorem:** Policy iteration converges to optimal policy: $\pi \rightarrow \pi^{\star}$

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# Illustration of policy iteration

Running policy iteration with $\gamma = 0.9$, initialize with $\pi(s)$ = North

| | | | |
|---|---|---|---|
| 0 | 0 | 0 | 1 |
| 0 | | 0 | -100 |
| 0 | 0 | 0 | 0 |

Original reward function

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# Illustration of policy iteration

Running policy iteration with $\gamma = 0.9$, initialize with $\pi(s)$ = North

| | | | |
|---|---|---|---|
| 0.418 | 0.884 | 2.331 | 6.367 |
| 0.367 | | -8.610 | -105.7 |
| -0.168 | -4.641 | -14.27 | -85.05 |

$V^{\pi}$ at iteration 1

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# Illustration of policy iteration

Running policy iteration with $\gamma = 0.9$, initialize with $\pi(s)$ = North

| | | | |
|---|---|---|---|
| 5.414 | 6.248 | 7.116 | 8.634 |
| 4.753 | | 2.881 | -102.7 |
| 2.251 | 1.977 | 1.849 | -8.701 |

$V^{\pi}$ at iteration 2

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# Illustration of policy iteration

Running policy iteration with $\gamma = 0.9$, initialize with $\pi(s)$ = North

| | | | |
|---|---|---|---|
| 5.470 | 6.313 | 7.190 | 8.669 |
| 4.803 | | 3.347 | -96.67 |
| 4.161 | 3.654 | 3.222 | 1.526 |

$V^{\pi}$ at iteration 3 (converged)

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# Gridworld results

## Approximation of value function

- Policy iteration: exact value function after three iterations
- Value iteration: after 100 iterations, $\|V - V^\star\|_2 = 7.1 \cdot 10^{-4}$

## Calculation of optimal policy

- Policy iteration: three iterations
- Value iteration: 12 iterations

VI converges to $\pi^\star$ long before it converges to $V^\star$ in this MDP

*But this property is highly MDP-specific*

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# Policy iteration or value iteration?

Policy iteration requires **fewer iterations** than value iteration

- But each iteration requires solving a linear system
- Only need to apply Bellman operator for **value iteration**

In practice, policy iteration is often **faster**

- Especially if the transition probabilities are structured (e.g., sparse)

  ⇒ Solving linear system is efficient

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# Outline

1. Markov decision processes
2. **Reinforcement learning**
3. Branch-and-bound as an MDP

# Challenge of RL

**MDP $(S, A, P, R)$:**

- $S$: set of states (assumed for now to be discrete)
- $A$: set of actions
- Transition probability distribution $P(s_{t+1} \mid s_t, a_t)$
- Reward function $R: S \rightarrow \mathbb{R}$

**RL twist:** We don't know $P$ or $R$, or too big to enumerate

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# Model-based RL

- A simple approach: just **estimate the MDP** from data
- Agent acts according to some policy, observes

$$s_1, r_1, a_1, s_2, r_2, a_2, \ldots, s_m, r_m, a_m$$

- We form the **empirical estimate** of the MDP:

$$\hat{P}(s' \mid s, a) = \frac{\sum_{i=1}^{m-1} \mathbf{1}\{s_i = s, a_i = a, s_{i+1} = s'\}}{\sum_{i=1}^{m-1} \mathbf{1}\{s_i = s, a_i = a\}}$$

$$\hat{R}(s) = \frac{\sum_{i=1}^{m} \mathbf{1}\{s_i = s\} r_i}{\sum_{i=1}^{m} \mathbf{1}\{s_i = s\}}$$

- Now solve the MDP $(S, A, \hat{P}, \hat{R})$

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# Model-based RL

Will **converge** to correct MDP (and hence correct policy)

**Disadvantages:**

- Requires we build the the actual MDP models
- State space may be too large

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# Outline

1. Markov decision processes
2. Reinforcement learning
    i. **Model-free RL**
        a. **Temporal difference methods**
        b. Q-learning
        c. Function approximation
    ii. Exploration vs exploitation
3. Branch-and-bound as an MDP

# Model-free RL

**Temporal difference methods** (TD, SARSA, Q-learning)**:**

Directly learn value function $V^{\pi}$

# Temporal difference (TD) methods

- Consider computing $V^\pi$ via the update

$$\hat{V}^\pi(s) \leftarrow R(s) + \gamma \sum_{s' \in S} P(\, s' \mid s, \pi(s)\,)\hat{V}^\pi(s')\,, \qquad \forall s \in S$$

- We're in state $s_t$, receive $r_t$, take action $a_t = \pi(s_t)$, end in $s_{t+1}$
- Can't update $\hat{V}^\pi$ for all $s$, but can we update **just for $s_t$**?

$$\hat{V}^\pi(s_t) \leftarrow r_t + \gamma \sum_{s' \in S} P(\, s' \mid s_t, a_t\,)\hat{V}^\pi(s')$$

- …No, still can't compute this sum

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# Temporal difference (TD) methods

But, $s_{t+1}$ is a sample from the distribution $P(\, s' \mid s_t, a_t \,)$

Could perform the update $\hat{V}^{\pi}(s_t) \leftarrow r_t + \gamma \hat{V}^{\pi}(s_{t+1})$

- Too "harsh" an assignment
- Assumes that $s_{t+1}$ is the only possible next state

Instead **"smooth"** the update using some $\alpha < 1$

$$\hat{V}^{\pi}(s_t) \leftarrow (1-\alpha)\hat{V}^{\pi}(s_t) + \alpha\left(r_t + \gamma \hat{V}^{\pi}(s_{t+1})\right)$$

This is the **temporal difference (TD) algorithm**

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# Temporal difference (TD) algorithm

**algorithm** $\hat{V}^{\pi} = \mathrm{TD}(\pi, \alpha, \gamma)$

**initialize** $\hat{V}^{\pi}(s) \leftarrow 0$

**repeat**

Observe state $s$ and reward $r$

Take action $a = \pi(s)$ and observe next state $s'$

$$\hat{V}^{\pi}(s) \leftarrow (1-\alpha)\hat{V}^{\pi}(s) + \alpha\left(r + \gamma\hat{V}^{\pi}(s')\right)$$

return $\hat{V}^{\pi}$

Will converge to $\hat{V}^{\pi}(s) \rightarrow V^{\pi}(s)$ (for all $s$ visited often enough)

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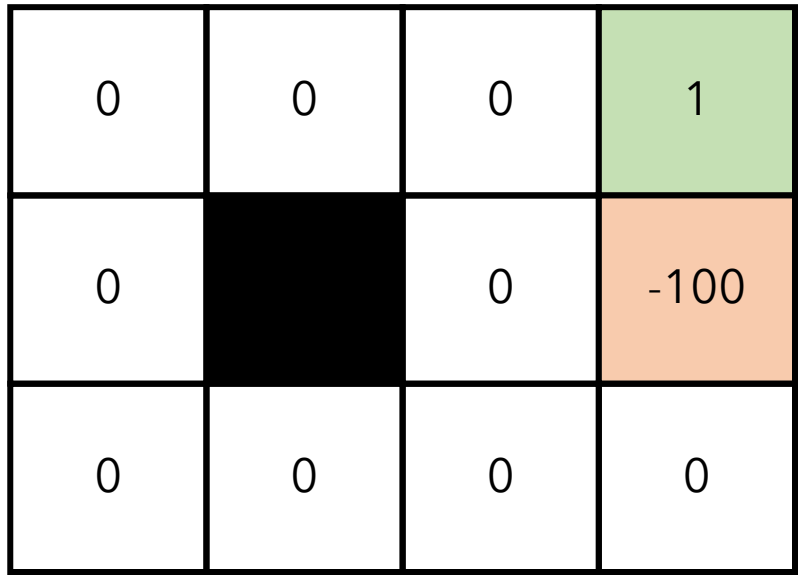
# TD experiments

Run TD on gridworld domain for 1000 episodes. Each episode:

- 10 steps
- Sampled according to policy $\pi$
- Starting at a random state

Initialize with $\hat{V} = R$

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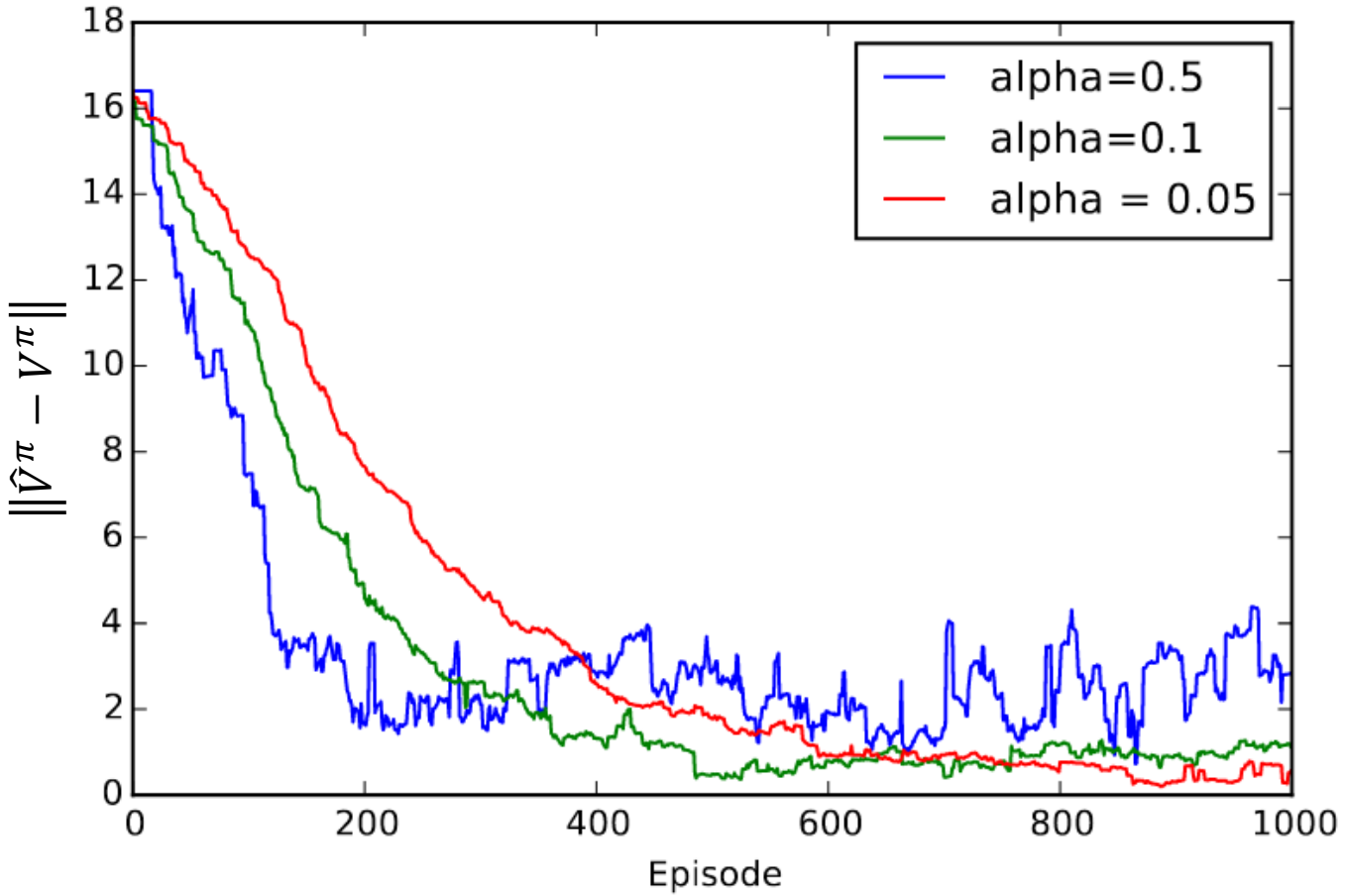
# TD progress

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# Temporal difference (TD) algorithm

TD lets us **learn the value function** of a policy $\pi$ directly

*Don't ever need to construct the MDP*

But is this really that helpful?

Consider trying to execute greedy policy w.r.t. estimated $\hat{V}^{\pi}$

$$\pi'(s) = \operatorname*{argmax}_{a} \sum_{s' \in S} T(s, a, s') \hat{V}^{\pi}(s')$$

We **need a model** anyway

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1. Markov decision processes
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        **b. Q-learning**
        c. Function approximation
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# Q-learning

**Q functions:**

Like value functions but defined over state-action pairs

$$Q^{\pi}(s,a) = R(s) + \gamma \sum_{s' \in S} P(\, s' \mid s, a\,) Q^{\pi}\big(s', \pi(s')\big)$$

I.e., Q function is the value of:

1. Starting in state $s$
2. Taking action $a$
3. Then acting according to $\pi$

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# Q-learning

$$Q^\star(s,a) = R(s) + \gamma \sum_{s' \in S} P(\, s' \mid s, a\,) \max_{a'} Q^\star(s', a')$$
$$= R(s) + \gamma \sum_{s' \in S} P(\, s' \mid s, a\,) V^\star(s')$$

$Q^\star$ is the value of:

1. Starting in state $s$
2. Taking action $a$
3. Then acting optimally

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# Q-learning

As with TD:

1. Observe $s$ and reward $r$
2. Take action $a$ (but not necessarily $a = \pi(s)$)
3. Observe next state $s'$

Estimate $Q^\star(s, a)$ as

$$\hat{Q}^\star(s, a) \leftarrow (1 - \alpha)\hat{Q}^\star(s, a) + \alpha\left(r + \gamma\hat{Q}^\star(s', a')\right)$$

$\hat{Q}^\star \rightarrow Q$ if all state-action pairs seen frequently enough

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# Q-learning

As with TD:

1. Observe $s$ and reward $r$
2. Take action a (but not necessarily $a = \pi(s)$)
3. Observe next state $s'$

Estimate $Q^\star(s, a)$ as

$$\hat{Q}^\star(s, a) \leftarrow (1 - \alpha)\hat{Q}^\star(s, a) + \alpha\left(r + \gamma\hat{Q}^\star(s', a')\right)$$

We can now learn an optimal policy without an MDP model

$$\hat{\pi}^\star(s) = \max \hat{Q}^\star(s, a)$$

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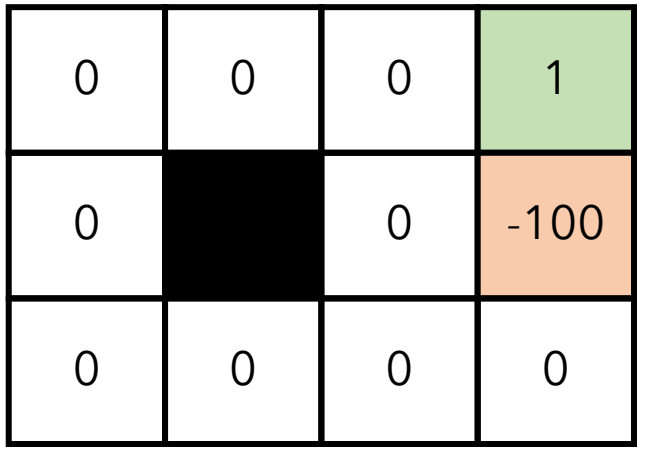
# Q-learning experiments

- Run Q-Learning on gridworld for 20000 episodes
  - 10 step per episode
- Initialize with $\hat{Q}^{\star}(s,a) = R(s)$
- Policy (epsilon-greedy): act according to current optimal

$$\hat{\pi}^{\star}(s) = \max \hat{Q}^{\star}(s,a)$$

with probability 0.9, else act randomly

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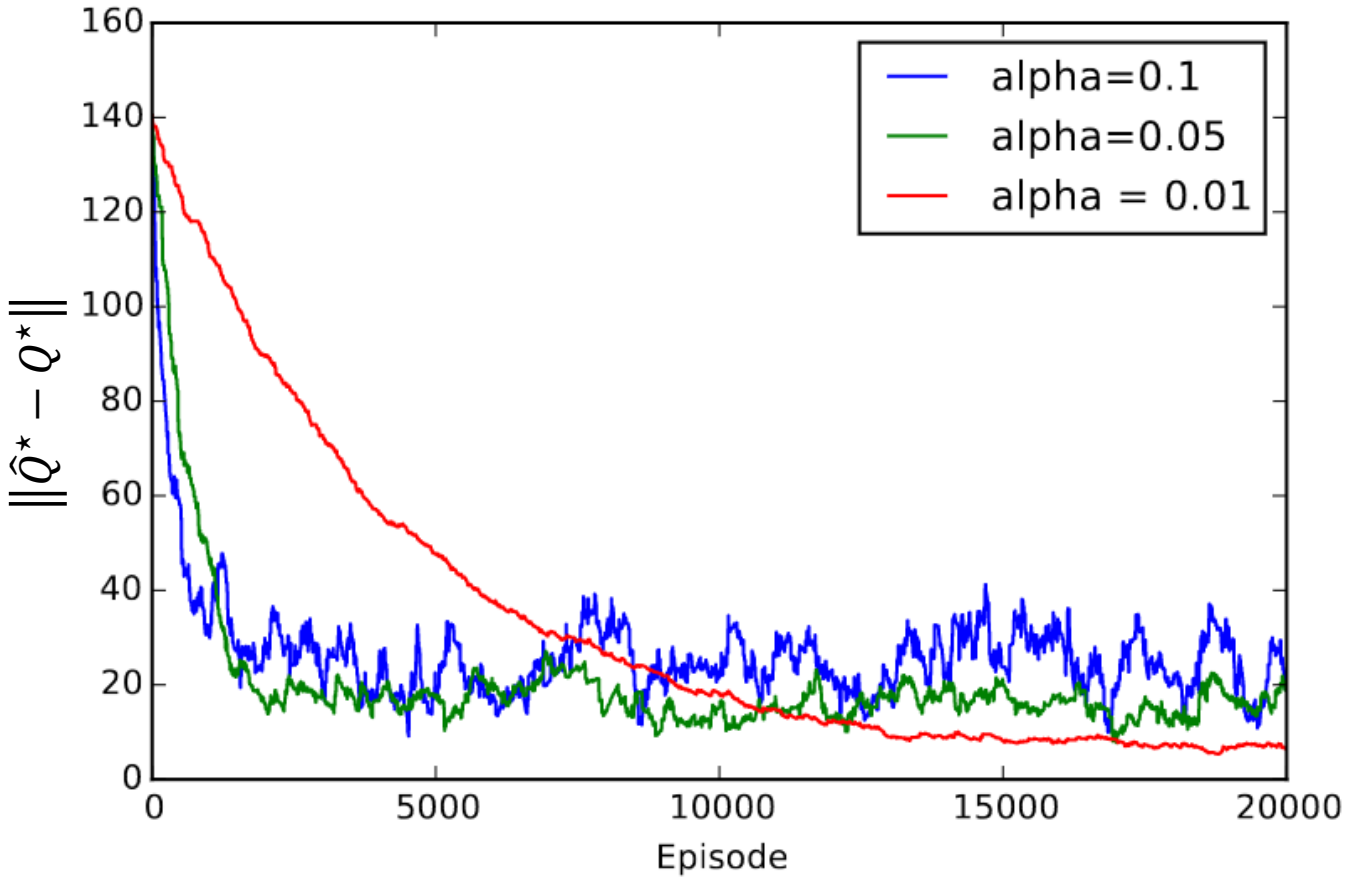
# Q-learning progress

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1. Markov decision processes
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        b. Q-learning
        **c. Function approximation**
    ii. Exploration vs exploitation
3. Branch-and-bound as an MDP

# Function approximation

- How to avoid keeping track of each state?
- Major advantage to model-free RL methods:
  Can use **function approximation** to represent $\hat{V}^{\pi}$ compactly
- Let $\hat{V}^{\pi}(s) = f_{\theta}(s)$ be our approximator parameterized by $\theta$
- TD update: $\hat{V}^{\pi}(s) \leftarrow (1-\alpha)\hat{V}^{\pi}(s) + \alpha\left(r + \gamma\hat{V}^{\pi}(s')\right)$
- Update $\theta$: ideally $\underset{\theta}{\text{argmin}}\left(\hat{V}^{\pi}(s) - f_{\theta}(s)\right)^2$
- Instead, $\underset{\theta}{\text{argmin}}\left((1-\alpha)f_{\theta}(s) + \alpha\left(r + \gamma f_{\theta}(s')\right) - f_{\theta}(s)\right)^2$

  (using gradient descent)

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# Function approximation

- How to avoid keeping track of each state?
- Major advantage to model-free RL methods:
  Can use **function approximation** to represent $\hat{V}^{\pi}$ compactly
- Let $\hat{V}^{\pi}(s) = f_{\theta}(s)$ be our approximator parameterized by $\theta$

Can use similar approximators for the $Q$ function

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# Exploration/exploitation problem

All the methods discussed so far had some condition like:

- "assuming we visit each state enough", or
- "taking actions according to some policy"

**Fundamental question:** should we

1. Take **exploratory** actions to get more information, or
2. **Exploit** current knowledge to perform as best we can?

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# Exploration/exploitation

**Epsilon-greedy policy:**

$$\pi(s) = \begin{cases} \max_a \hat{Q}^{\pi}(s,a) & \text{with probability } 1-\epsilon \\ \text{random action} & \text{otherwise} \end{cases}$$

Want to decrease $\epsilon$ as we see more examples, e.g.:

$\epsilon = \frac{1}{\sqrt{n(s)}}$ where $n(s)$ is the number of times we've visited state $s$

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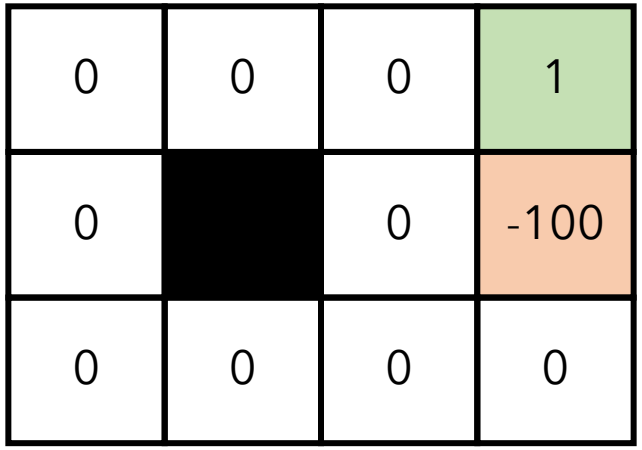
# Exploration experiments




- Gridworld but with U([0, 1]) rewards instead of rewards above
- Initialize Q function with $\hat{Q}(s, a) = 0$
- Run with $\alpha = 0.05, \epsilon = 0.1, \epsilon = 0$ (greedy), $\epsilon = \frac{1}{\sqrt{n(s)}}$

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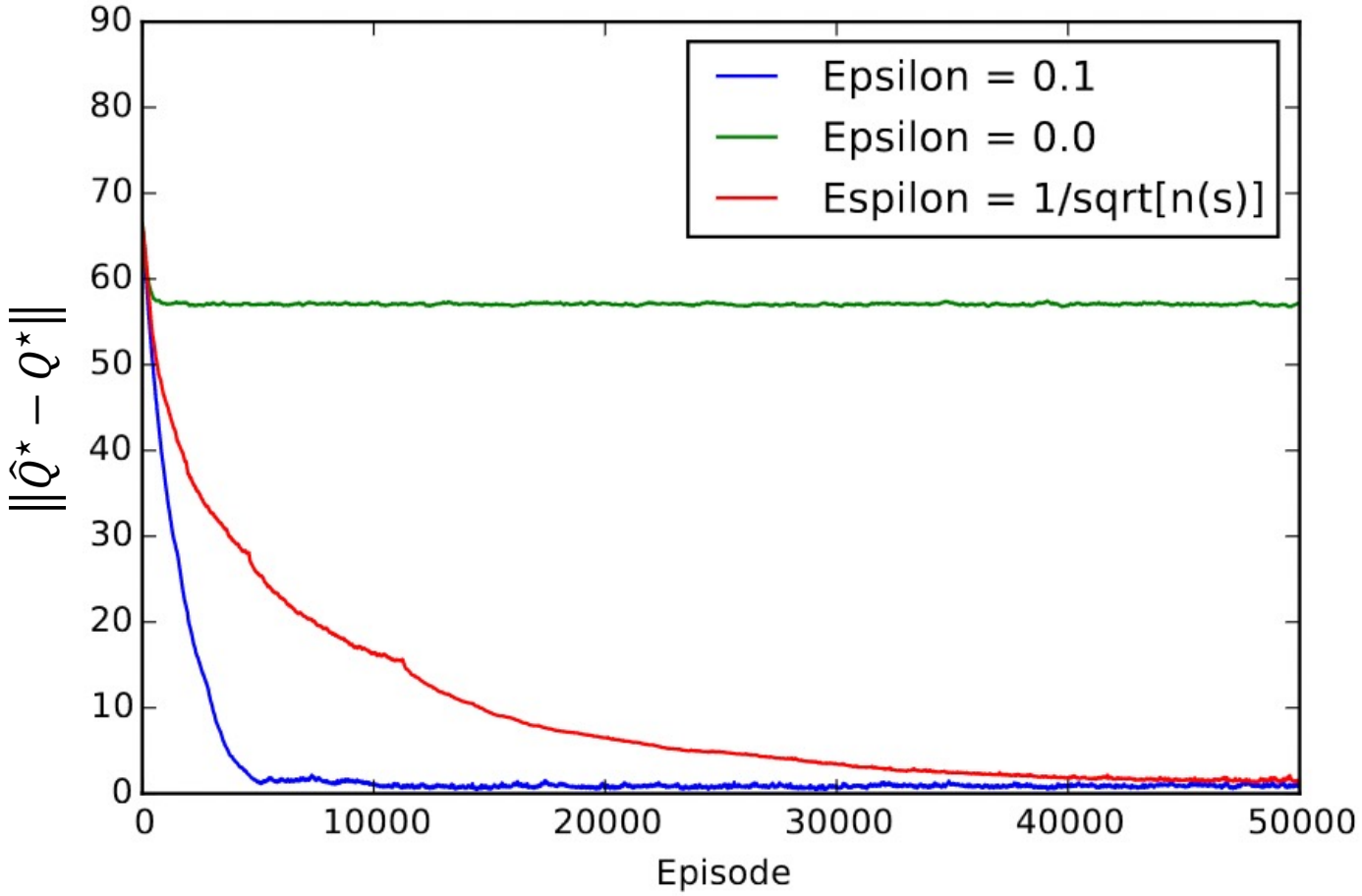
# Exploration experiments

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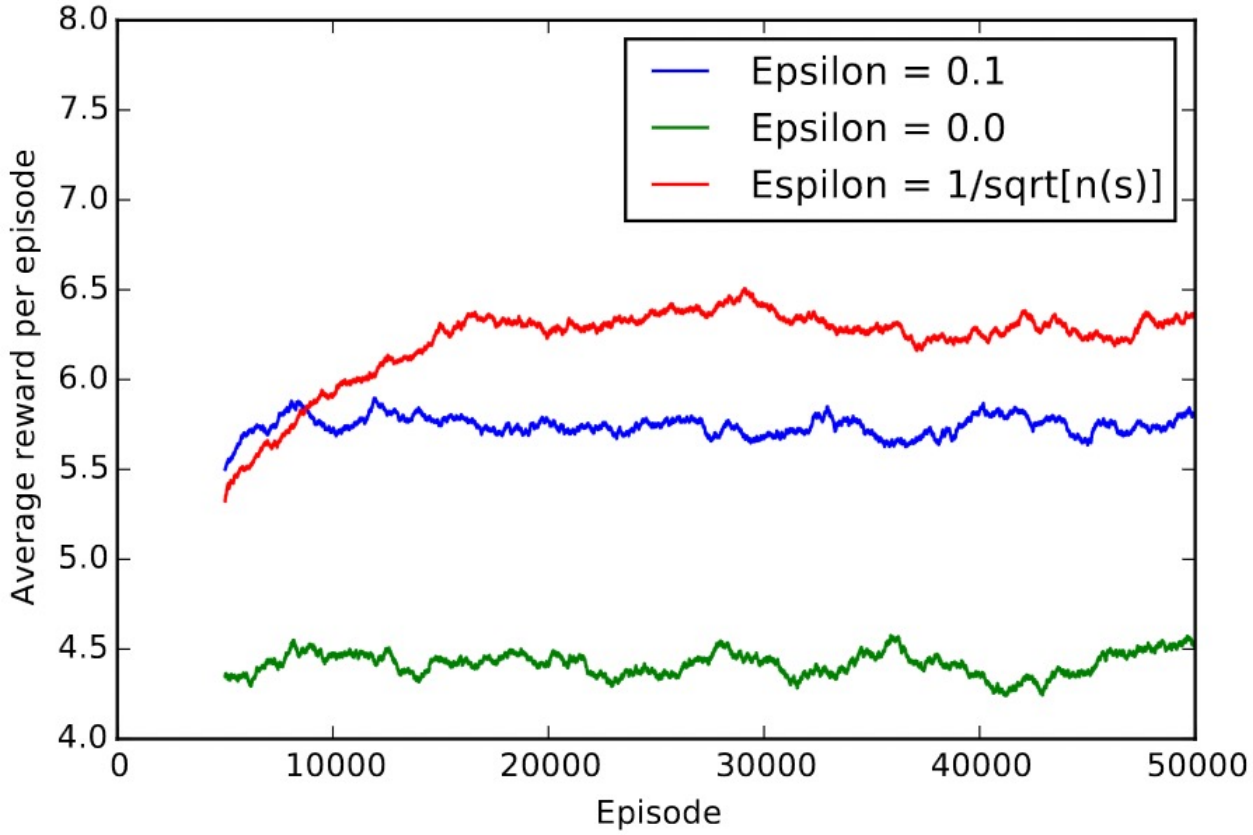
# Exploration experiments




Average reward (sliding average over past 5000 episodes) for different strategies

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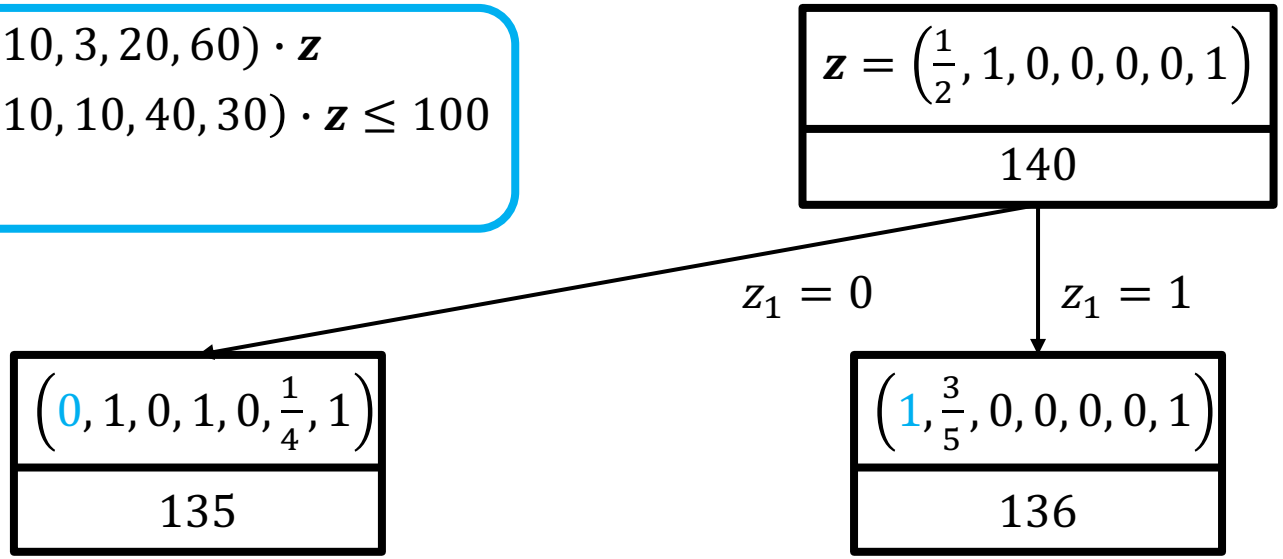
# Outline

1. Markov decision processes
2. Reinforcement learning
3. **Branch-and-bound as an MDP**

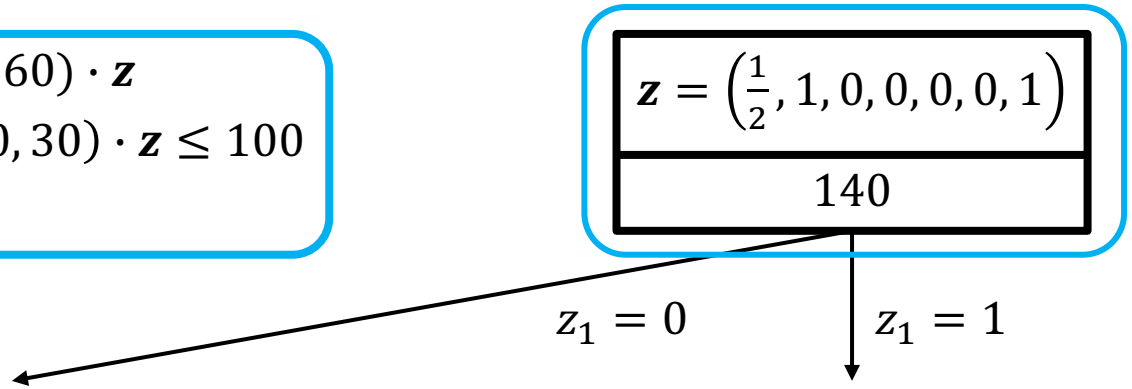
# Branch and bound (B&B)

$$\begin{aligned} \max \quad & (40, 60, 10, 10, 3, 20, 60) \cdot \boldsymbol{z} \\ \text{s.t.} \quad & (40, 50, 30, 10, 10, 40, 30) \cdot \boldsymbol{z} \leq 100 \\ & \boldsymbol{z} \in \{0,1\}^7 \end{aligned}$$



# Branch and bound (B&B)

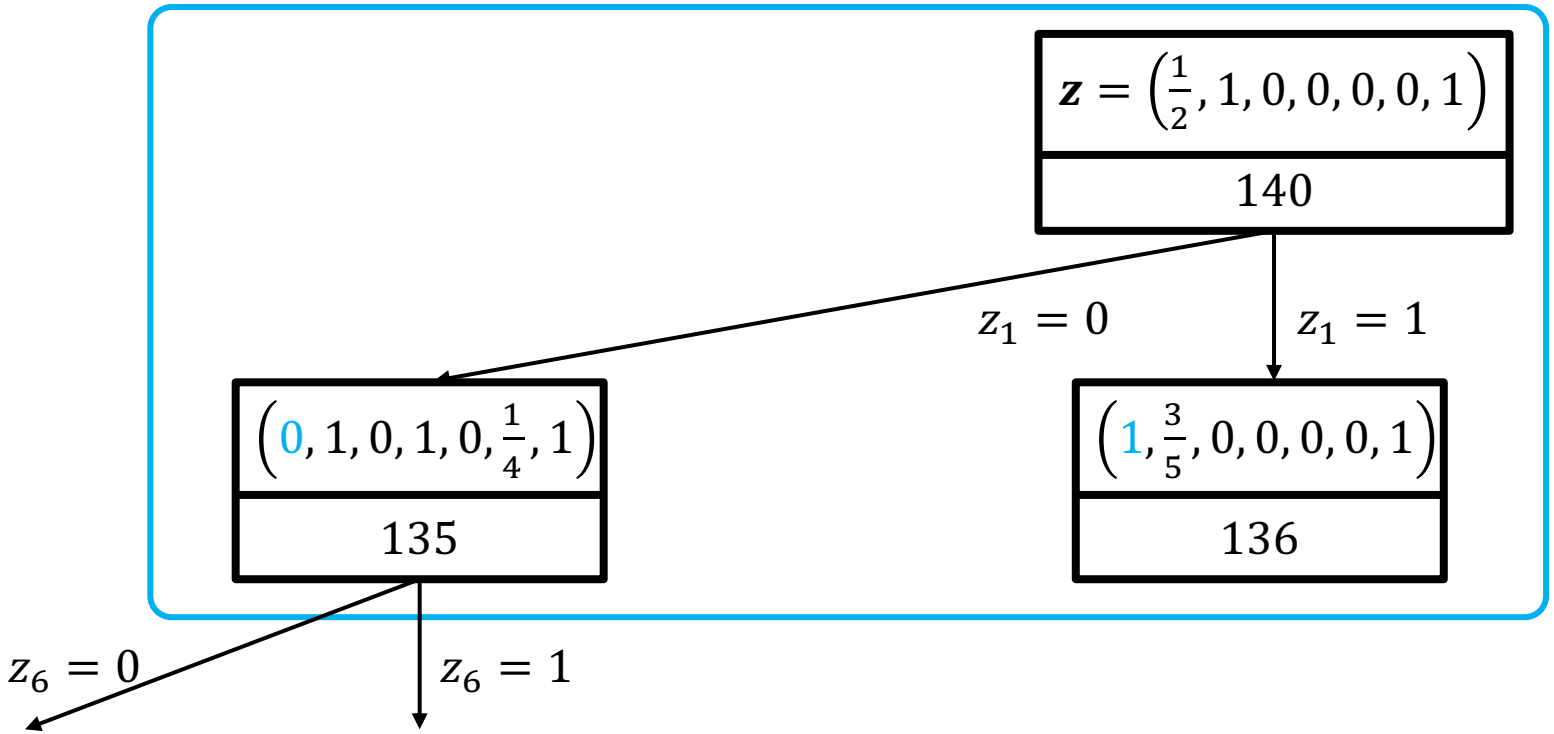
$$\begin{aligned} \max \quad & (40, 60, 10, 10, 3, 20, 60) \cdot \boldsymbol{z} \\ \text{s.t.} \quad & (40, 50, 30, 10, 10, 40, 30) \cdot \boldsymbol{z} \leq 100 \\ & \boldsymbol{z} \in \{0,1\}^7 \end{aligned}$$




**State $s_0$**

**Action $a_0$:** Branch on $z_1$

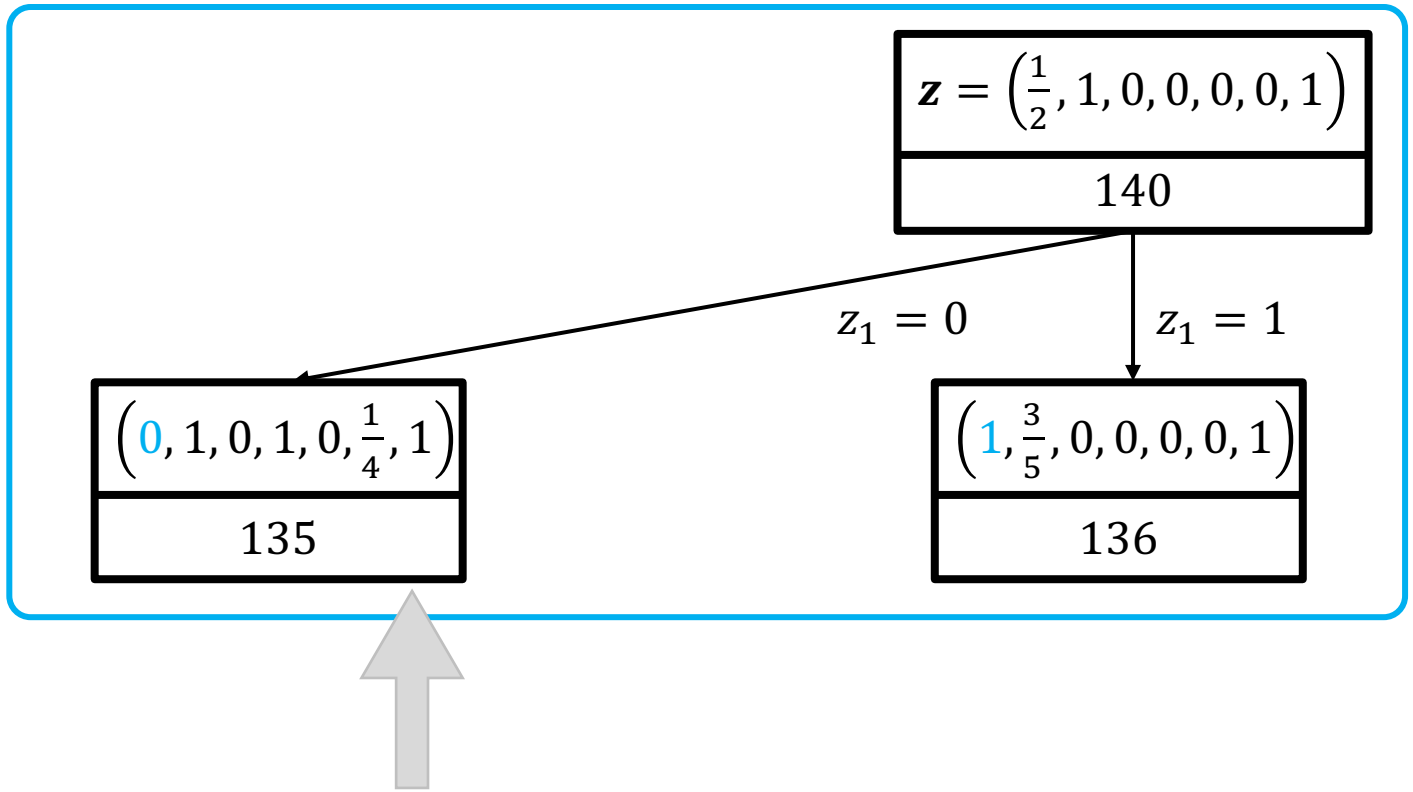
# Branch and bound (B&B)




**State $s_1$**

**Action $a_1$:** Branch on $z_6$

# Branch and bound (B&B)




**State $s_1$**

**Action $a_1$:** Explore this node

He et al., NeurIPS'14

# Papers we'll read

Gasse, Maxime, et al. "Exact combinatorial optimization with graph convolutional neural networks." *NeurIPS*. (2019).

- Frame B&B **variable selection** as an MDP
- Use **GNNs** to design variable selection policies

Dai, Hanjun, Khalil, Elias, et al. "Learning combinatorial optimization algorithms over graphs." *NeurIPS'17*.

- Develop **RL algorithms** for a variety of combinatorial problems
- Suggest RL could be used for **algorithm discovery**