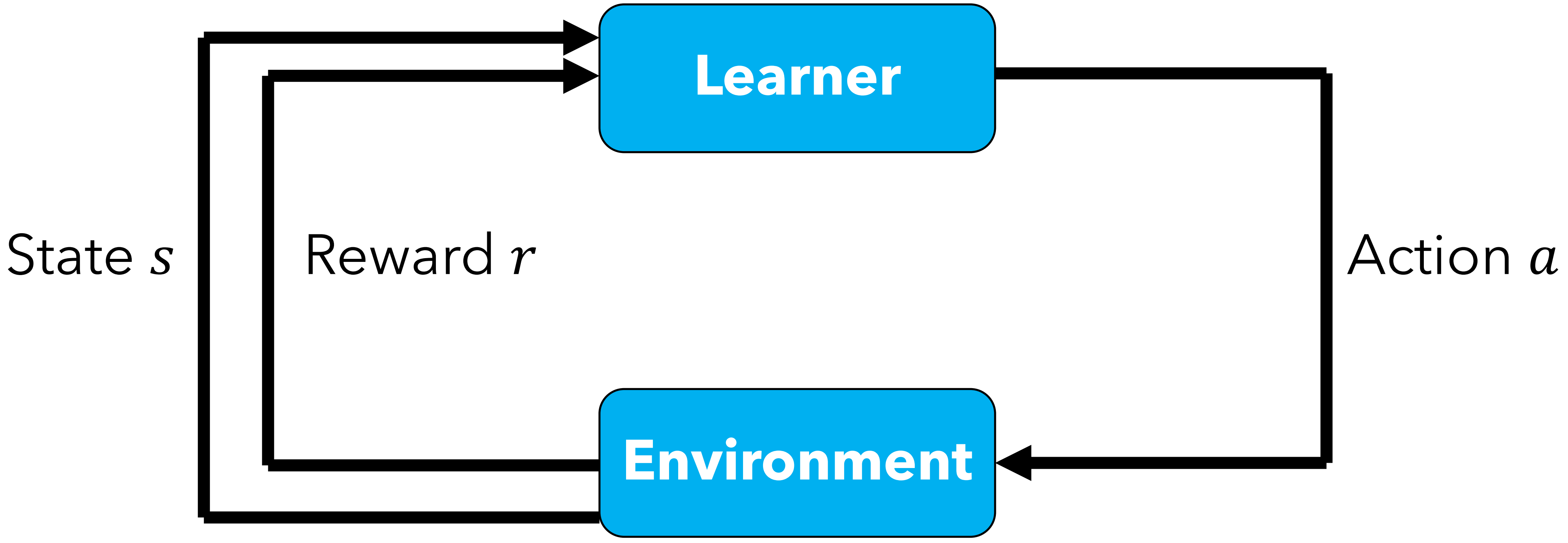
Reinforcement learning refresher

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

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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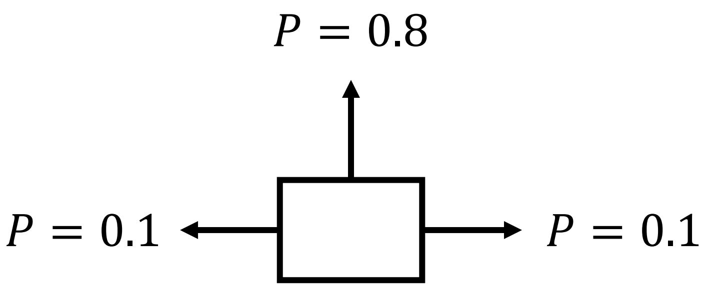
Gridworld domain

- 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 $\pi: S \to A$

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

Bellman equation

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

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

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 π

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

- **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**

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

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

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:

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

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

Computing the optimal policy

Approach #1: value iteration

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

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

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

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Illustration of value iteration

Running value iteration with $\gamma = 0.9$

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

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

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

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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

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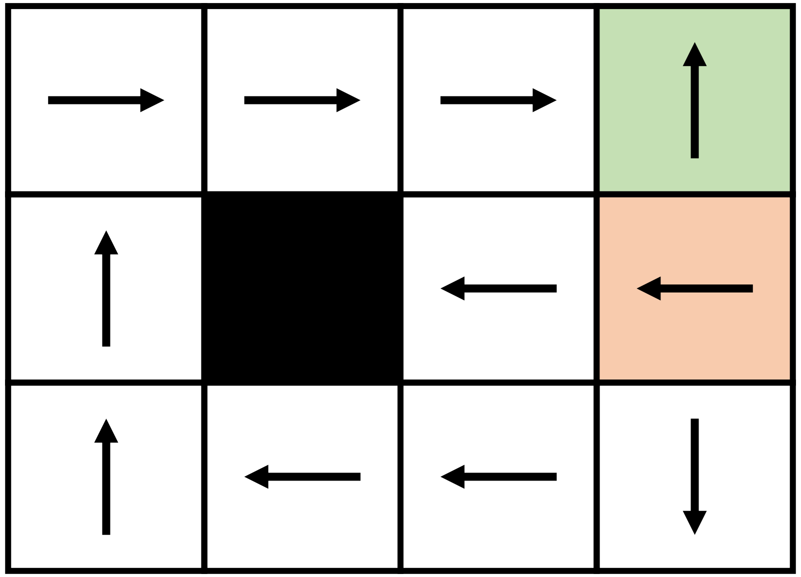
Illustration of value iteration

Running value iteration with $\gamma = 0.9$



Resulting policy after 1000 iterations

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 π randomly
2. Compute value of policy V^π (e.g., by solving linear system)
3. Update π to be greedy policy with respect to V^π

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

4. If policy π 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

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^{π} 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^{π} 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^{π} 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

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)
  - $\Rightarrow$ 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 $R: S \to \mathbb{R}$

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

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^π

Temporal difference (TD) methods

- Consider computing V^π 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**

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 $\hat{V}^{\pi}(s) \to V^{\pi}(s)$ (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 π
- Starting at a random state

Initialize with $\hat{V} = R$

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

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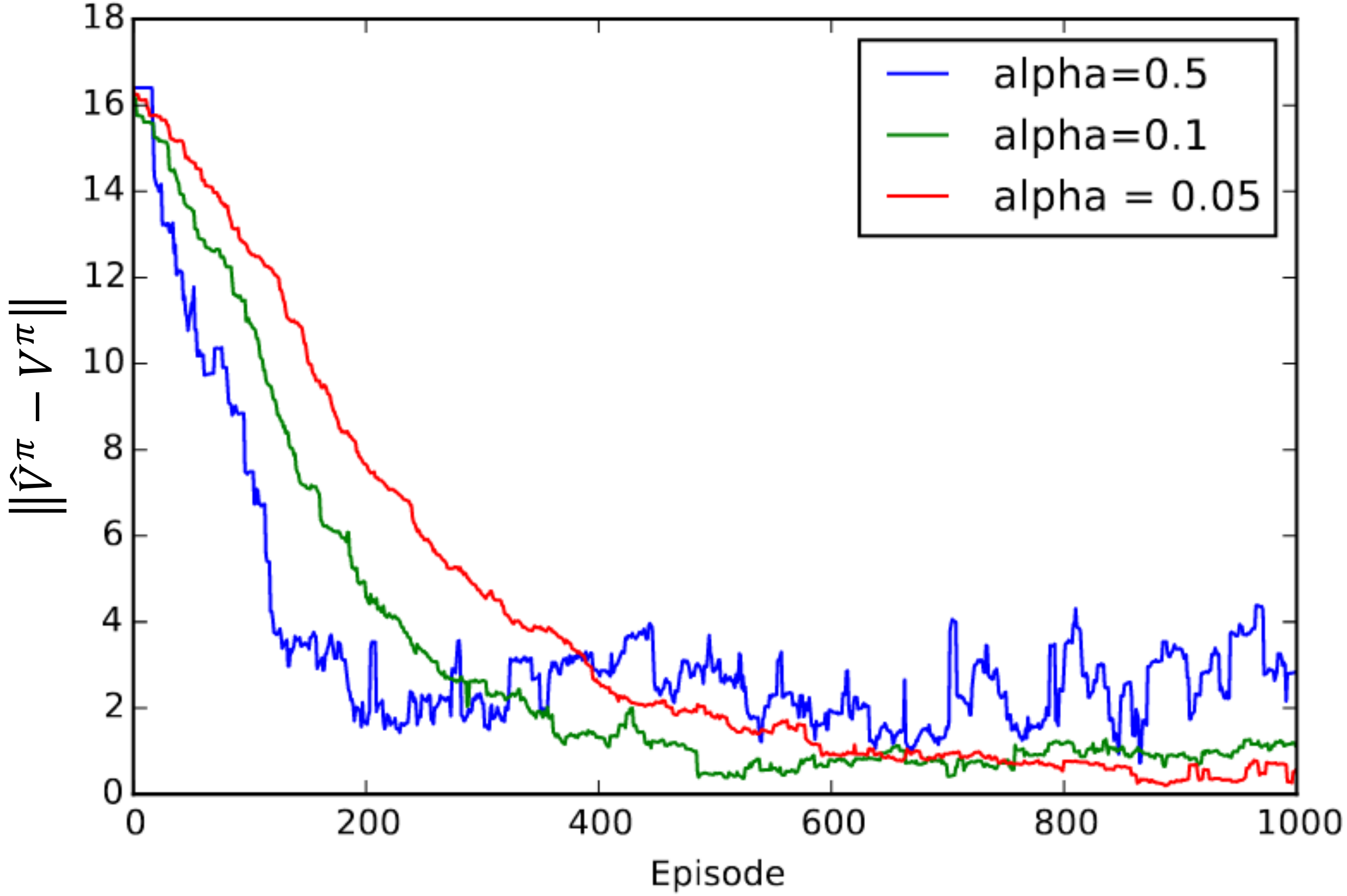
TD progress



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Temporal difference (TD) algorithm

TD lets us **learn the value function** of a policy π 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 $\hat{V}^{\pi}$

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

We **need a model** anyway

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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 π

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

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

$\hat{Q}^\star \rightarrow Q^\star$ 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

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

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

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

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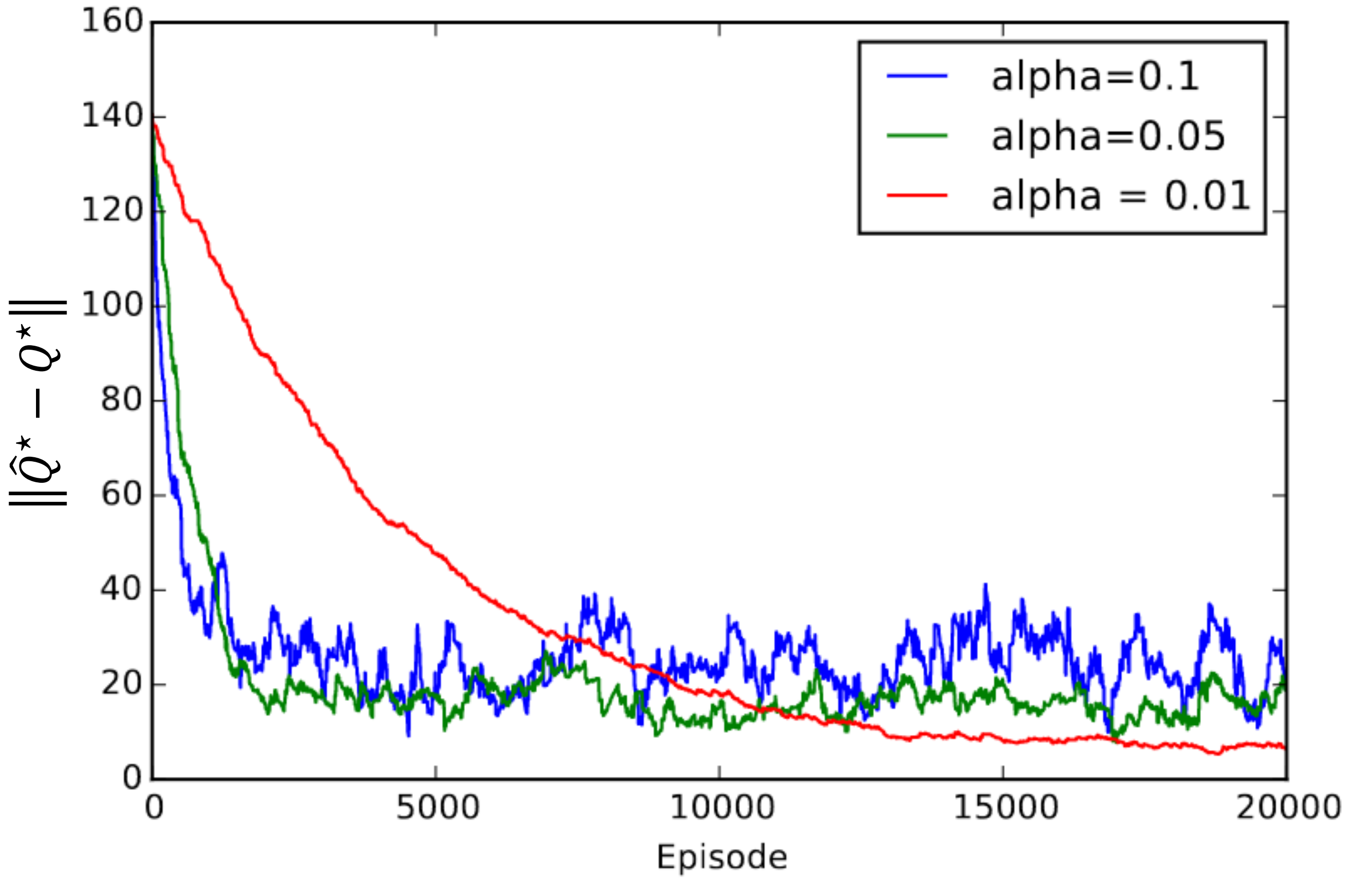
Q-learning progress



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1. Markov decision processes
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      c. **Function approximation**
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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 θ
- TD update: $\hat{V}^\pi(s) \leftarrow (1-\alpha)\hat{V}^\pi(s) + \alpha\left(r + \gamma \hat{V}^\pi(s')\right)$
- Update θ: ideally $\operatorname{argmin}_\theta \left(\hat{V}^\pi(s) - f_\theta(s)\right)^2$
- Instead, $\operatorname{argmin}_\theta \left((1-\alpha) f_\theta(s) + \alpha\left(r + \gamma f_\theta(s')\right) - f_\theta(s)\right)^2$
  (using gradient descent)

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 θ

Can use similar approximators for the Q function

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1. Markov decision processes
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   i. Model-free RL
   ii. **Exploration vs exploitation**
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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?

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 ϵ 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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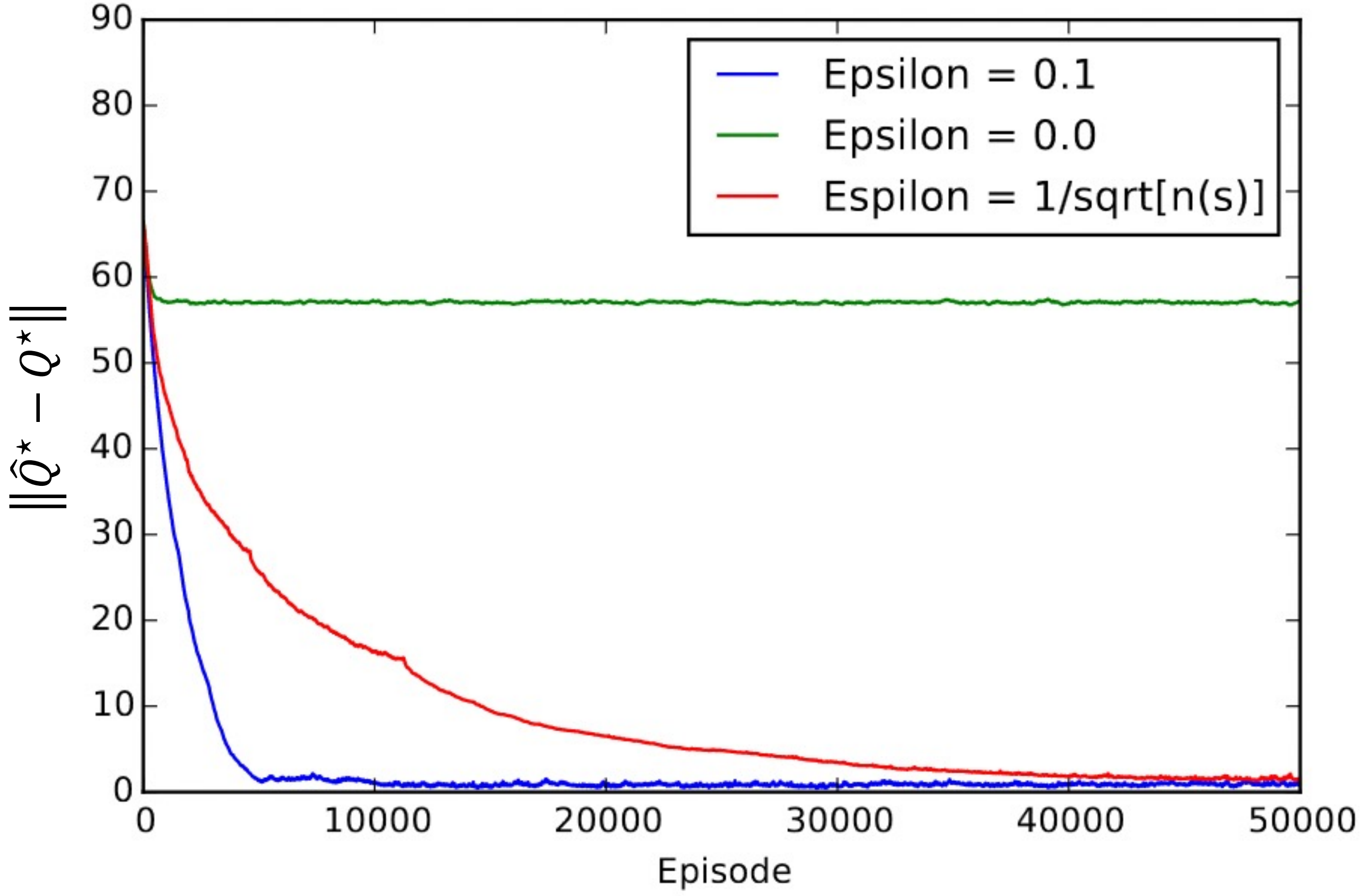
Exploration experiments

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

- 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), $\epsilon = \frac{1}{\sqrt{n(s)}}$

Exploration experiments



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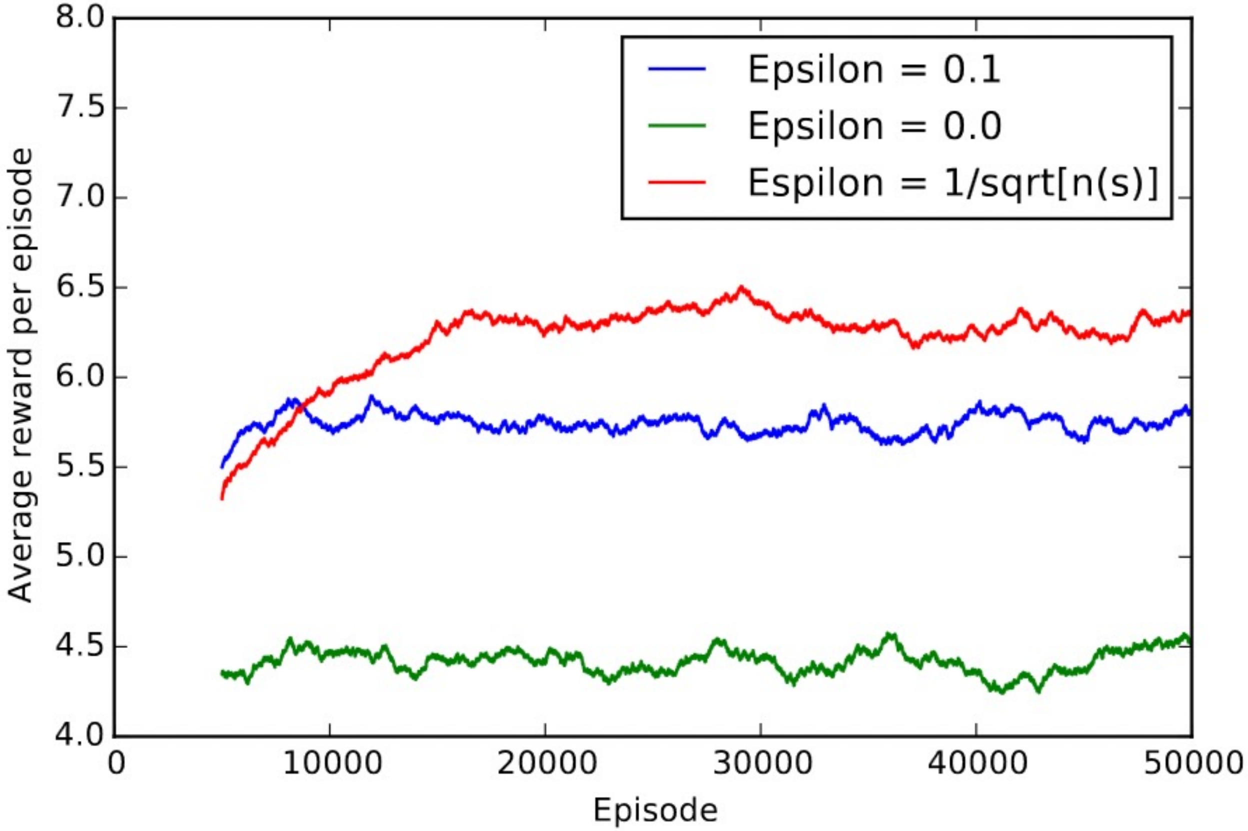
Exploration experiments



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

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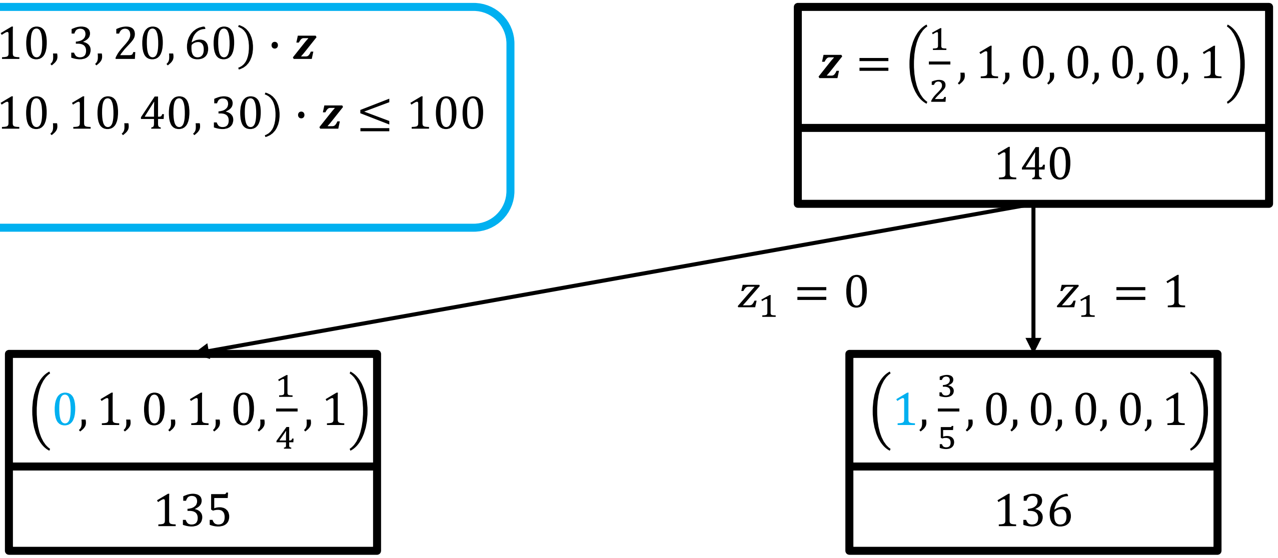
Outline

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

Branch and bound (B&B)

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

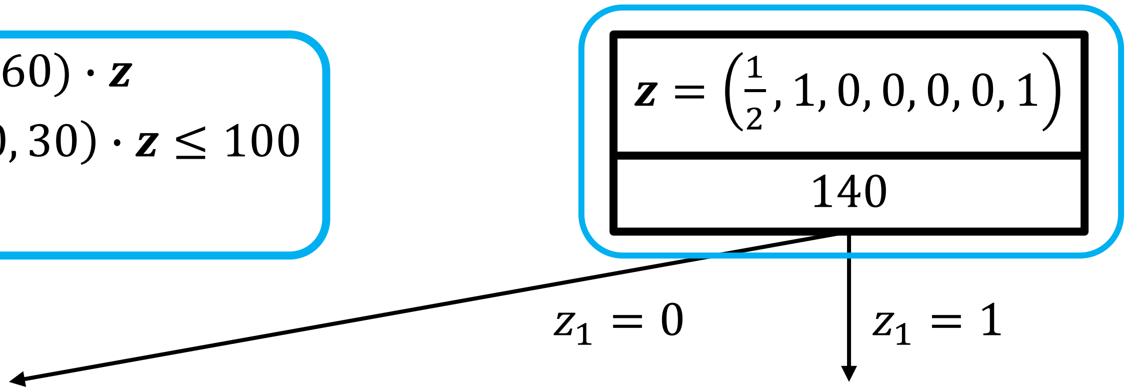


Branch and bound (B&B)

max $(40, 60, 10, 10, 3, 20, 60) \cdot \boldsymbol{z}$

s.t. $(40, 50, 30, 10, 10, 40, 30) \cdot \boldsymbol{z} \leq 100$

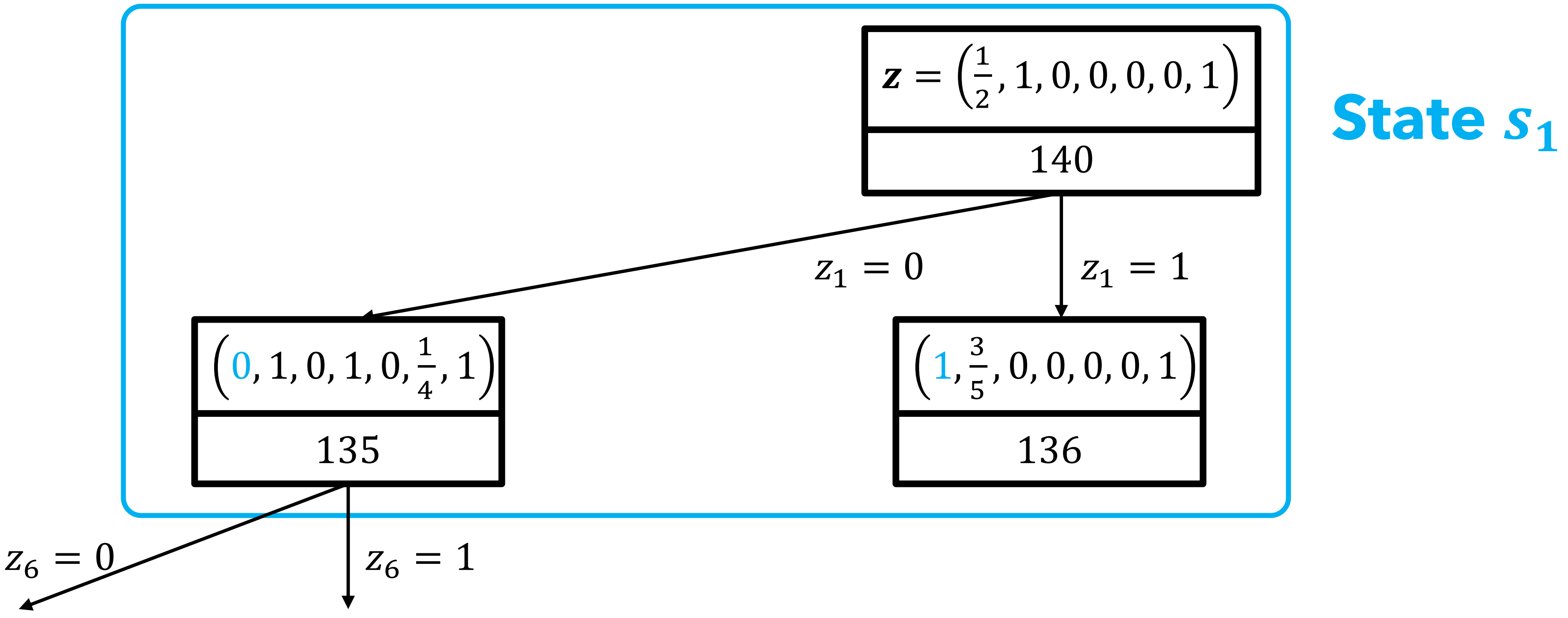
$\boldsymbol{z} \in \{0,1\}^7$



State s_0

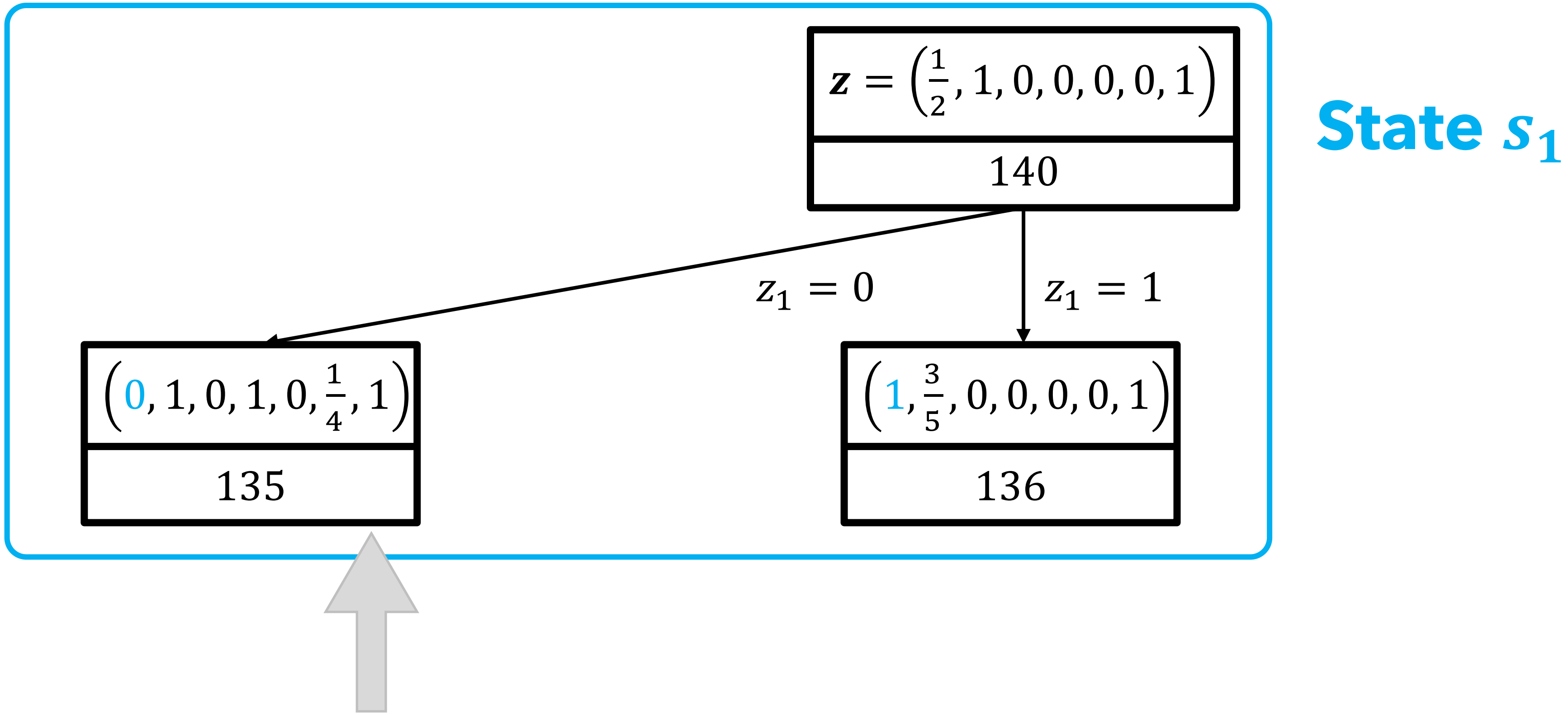
Action a_0: Branch on z_1

Branch and bound (B&B)



Action a_1: Branch on z_6

Branch and bound (B&B)



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**