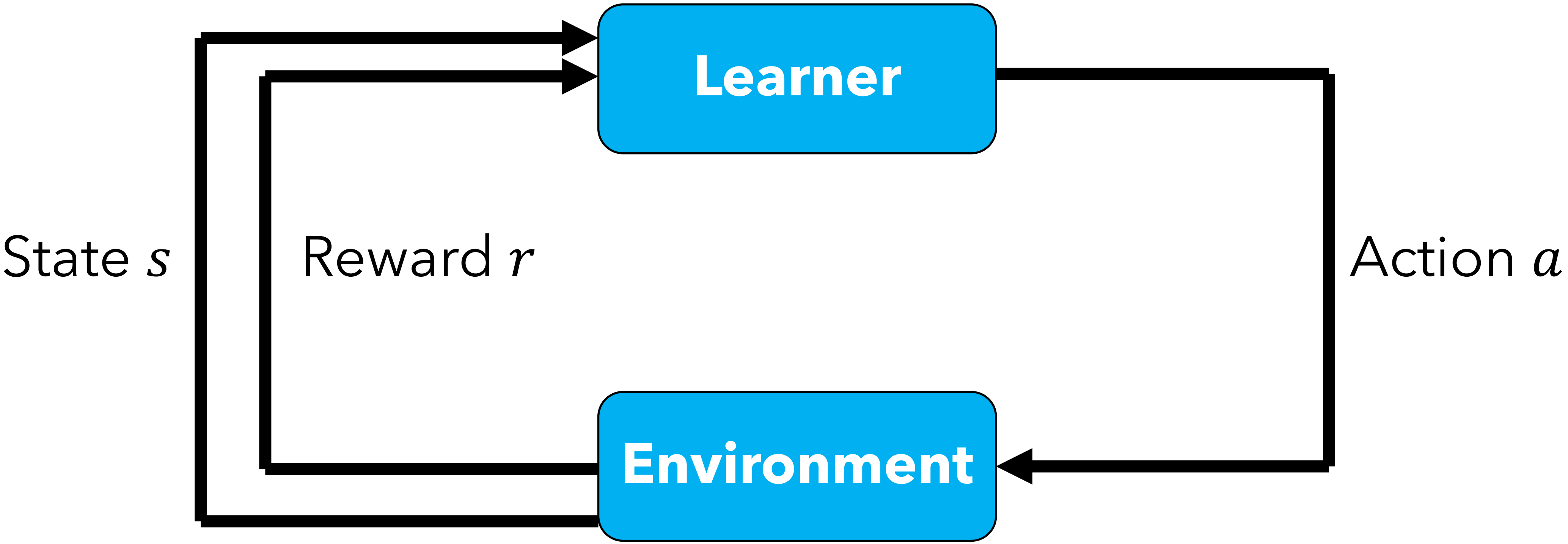
Reinforcement learning refresher

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 $P(s_{t+1} \mid s_t, a_t)$

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

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

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

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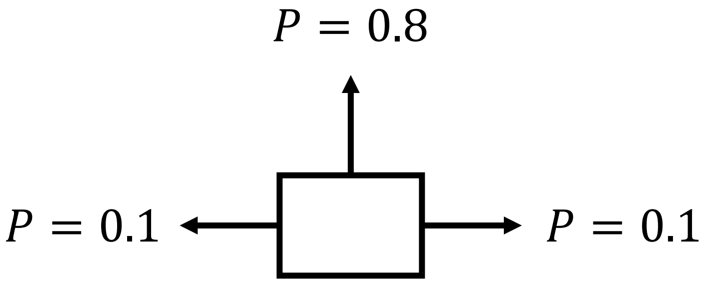
Gridworld domain

- Goal state with reward 2
- "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

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

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 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**

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Optimal policy and value function

Optimal policy achieves the highest value for every state

$$\pi^\star = \operatorname*{argmax}_{\pi} V^{\pi}(s)$$

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:

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

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

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Computing the optimal policy

Approach #1: value iteration

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:

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

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

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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

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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

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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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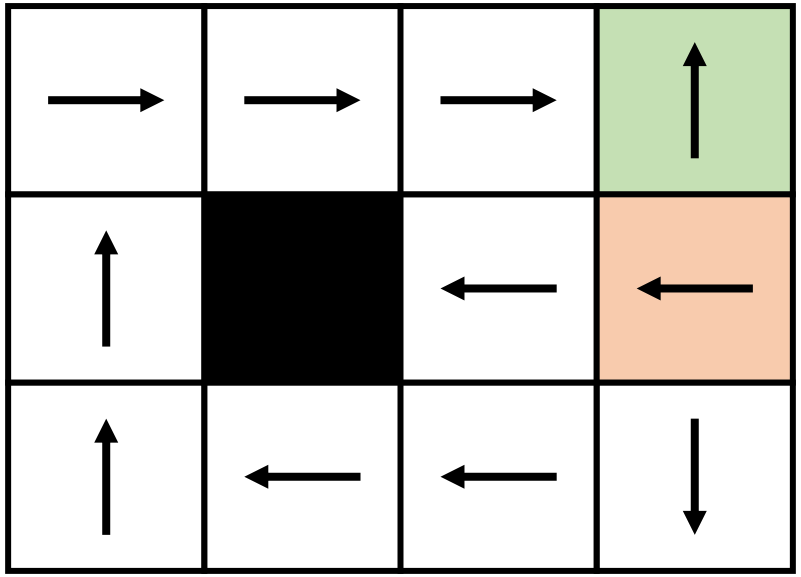
Illustration of value iteration

Running value iteration with $\gamma = 0.9$



Resulting policy after 1000 iterations

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Outline

1. Markov decision processes
   1. Computing the optimal policy
      1. Value iteration
      2. **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}
$$\pi(s) \leftarrow \operatorname*{argmax}_{a} \sum_{s' \in S} P(s' \mid s, a) V^{\pi}(s')$$
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

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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^{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

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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 $R : S \to \mathbb{R}$

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

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

- 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 $\left(S, A, \hat{P}, \hat{R}\right)$

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Model-based RL

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

How can we ensure we get the “right” samples?

Advantages (informally): makes “efficient” use of data

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^{π}

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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**

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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 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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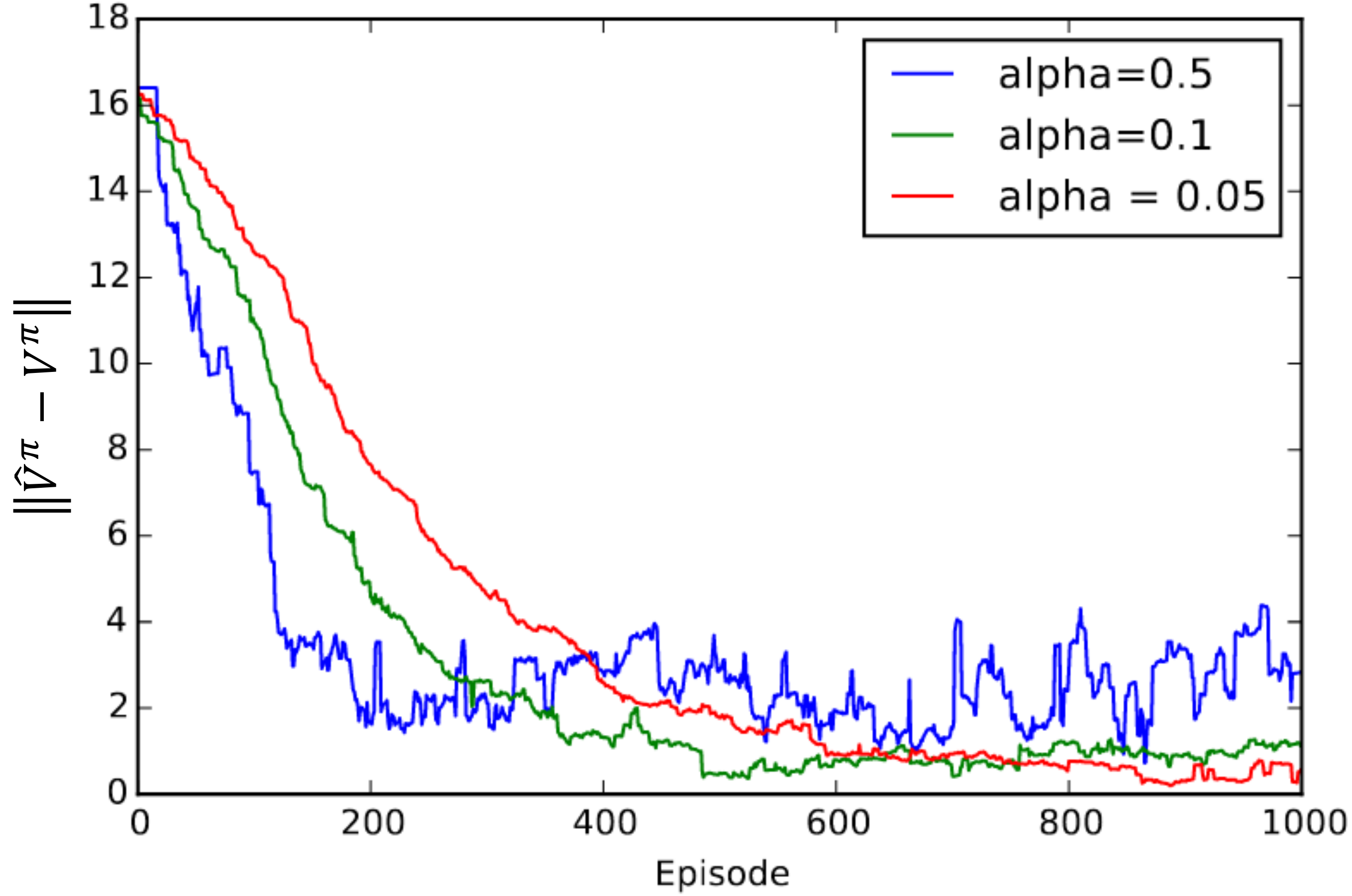
TD progress



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

$$\pi'(s) = \max_a \sum_{s'} T(s,a,s')\hat{V}^{\pi}(s')$$

We **need a model** anyway

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1. Markov decision processes
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    i. Model-free RL
        a. Temporal difference methods
        b. **Q-learning**
        c. Function approximation
    ii. Exploration vs exploitation
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Q-learning

Q functions:

Like value functions but defined over state-action pairs

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

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

1. Starting in state s
2. Taking action a
3. Then acting according to π

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Q-learning

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

$Q^\star$ 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

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

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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

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

with probability 0.9, else act randomly

0	0	0	1
0	■	0	-100
0	0	0	0

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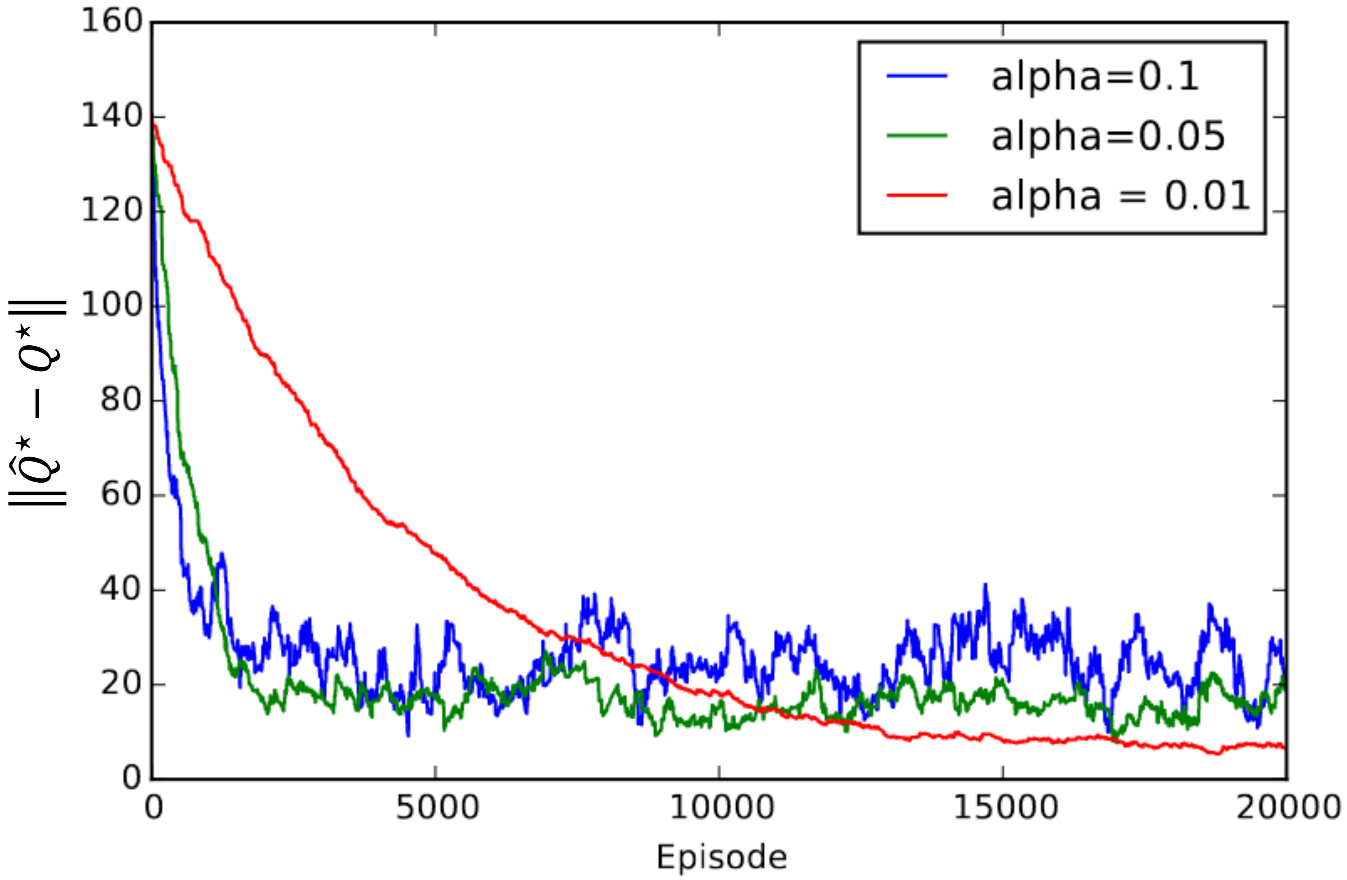
Q-learning progress



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Outline

1. Markov decision processes
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    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

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)

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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

Can use similar approximators for the Q function

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Outline

1. Markov decision processes
2. Reinforcement learning
   1. Model-free RL
   2. **Exploration vs exploitation**
3. Branch-and-bound as an MDP

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

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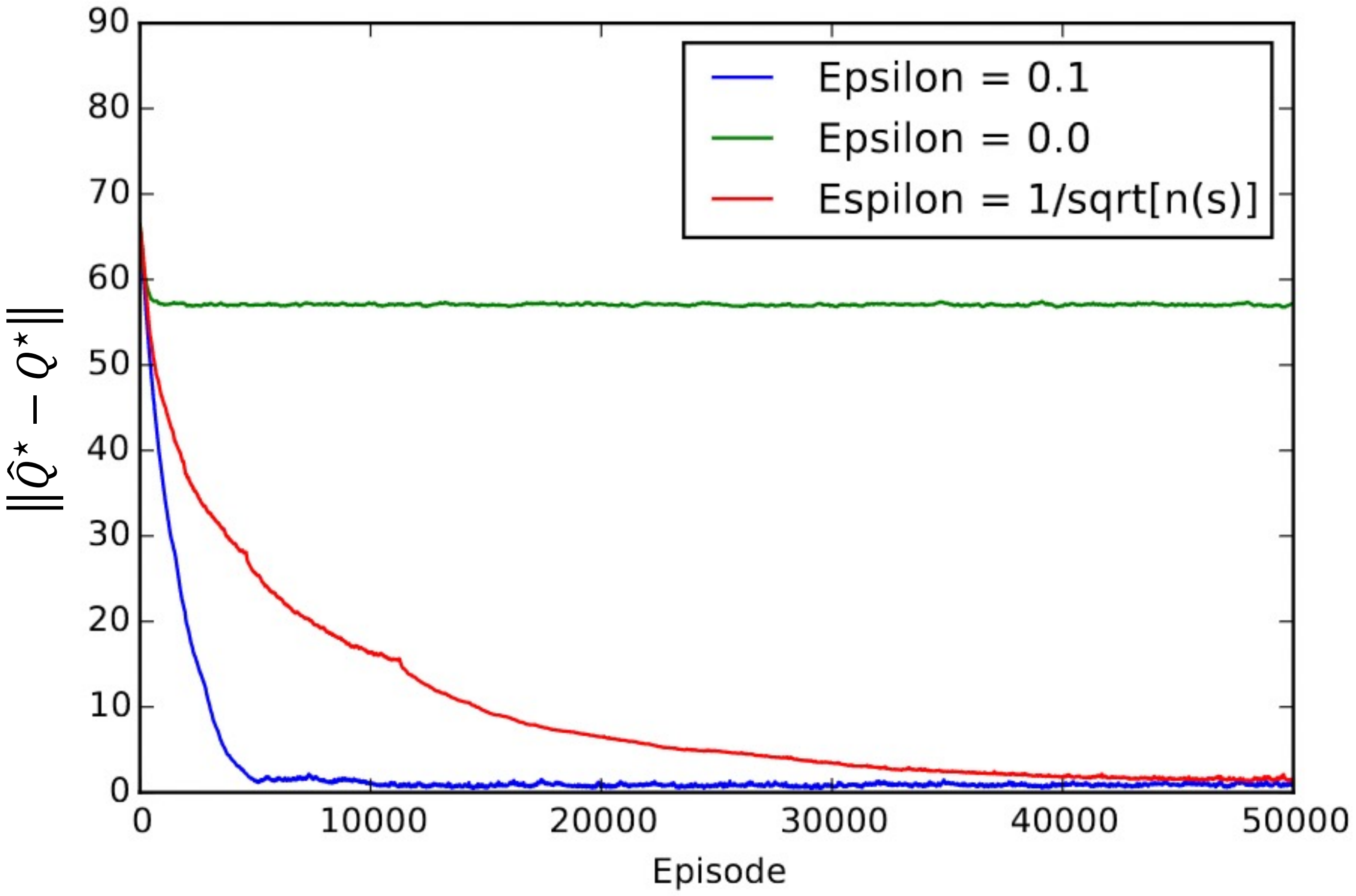
Exploration experiments



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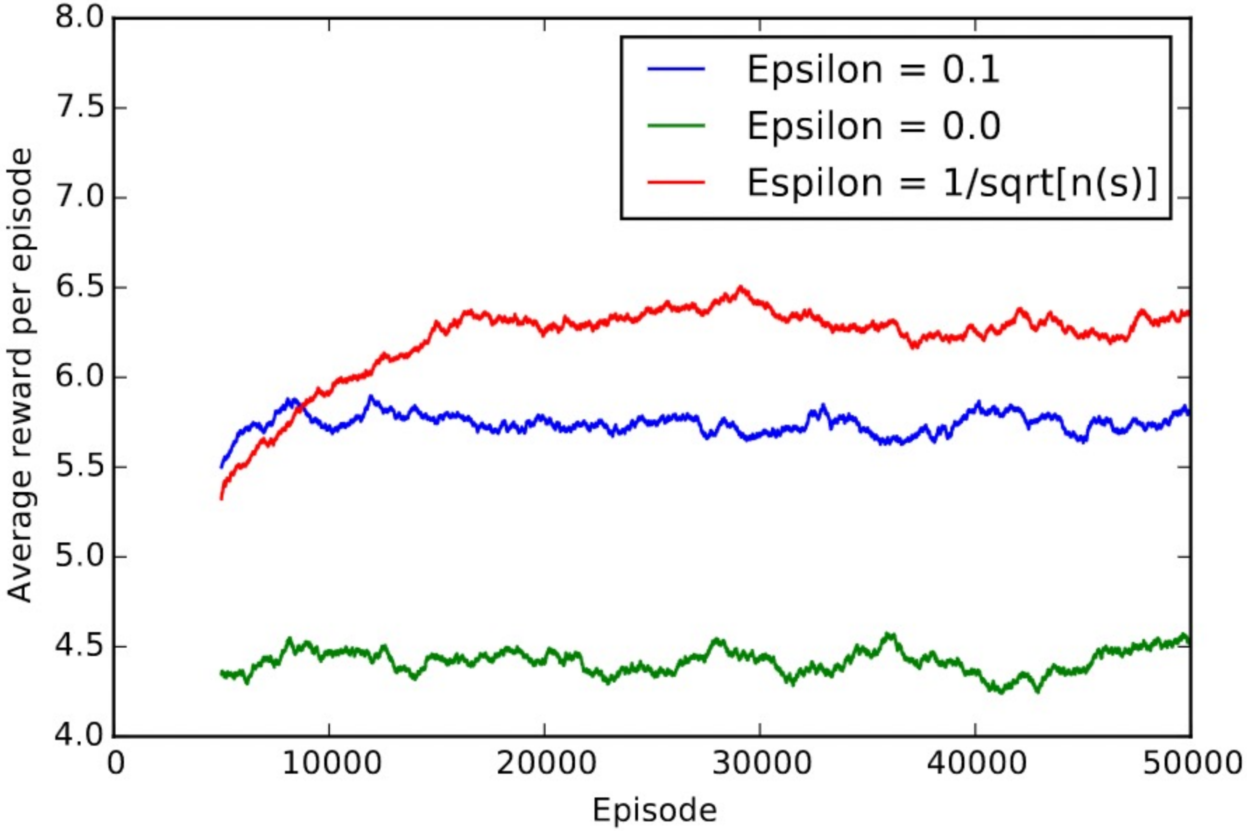
Exploration experiments



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

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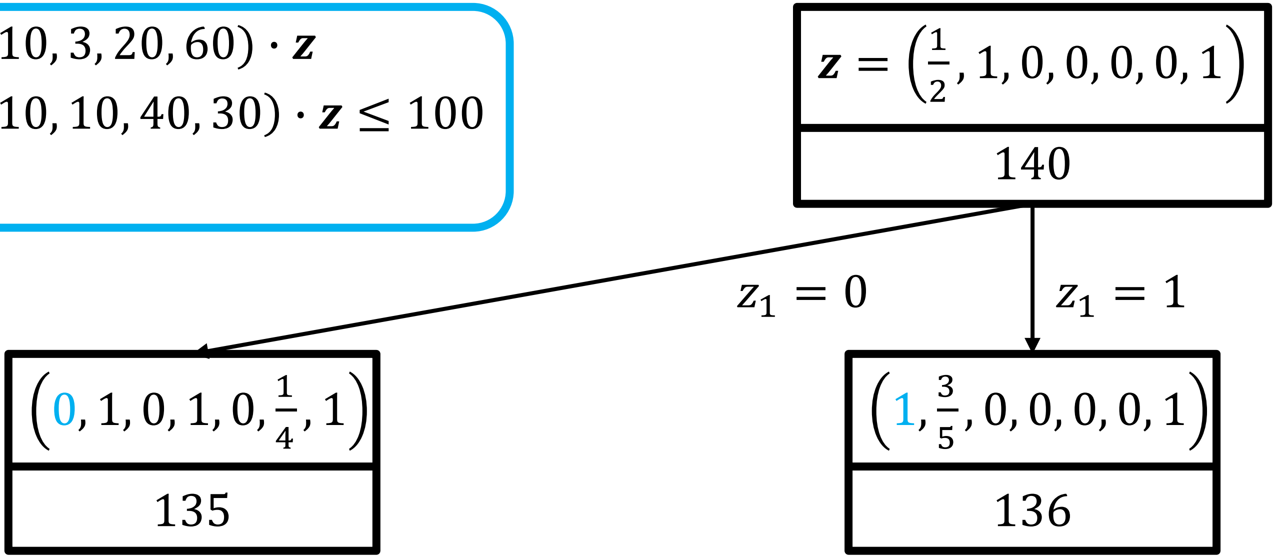
Outline

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

Branch and bound (B&B)

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



$\boldsymbol{z} = \left(\frac{1}{2}, 1, 0, 0, 0, 0, 1\right)$

140

$z_1 = 0$

$z_1 = 1$

$\left(0, 1, 0, 1, 0, \frac{1}{4}, 1\right)$

135

$\left(1, \frac{3}{5}, 0, 0, 0, 0, 1\right)$

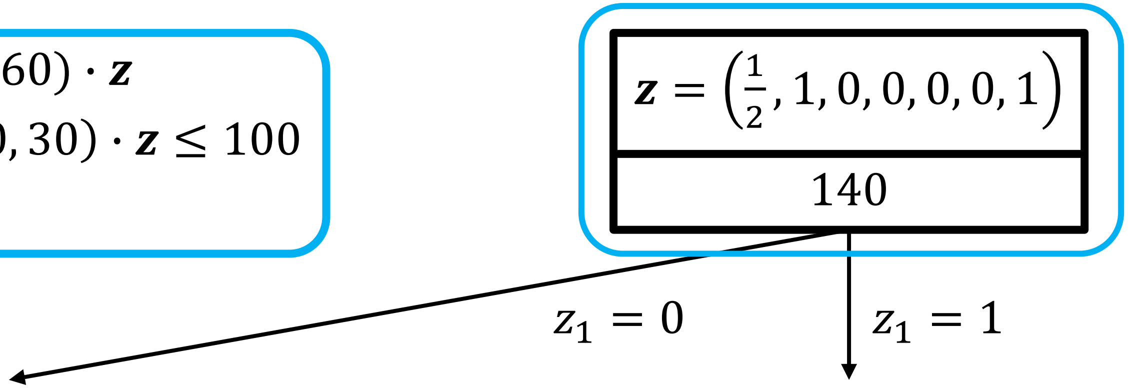
136

Branch and bound (B&B)

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

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

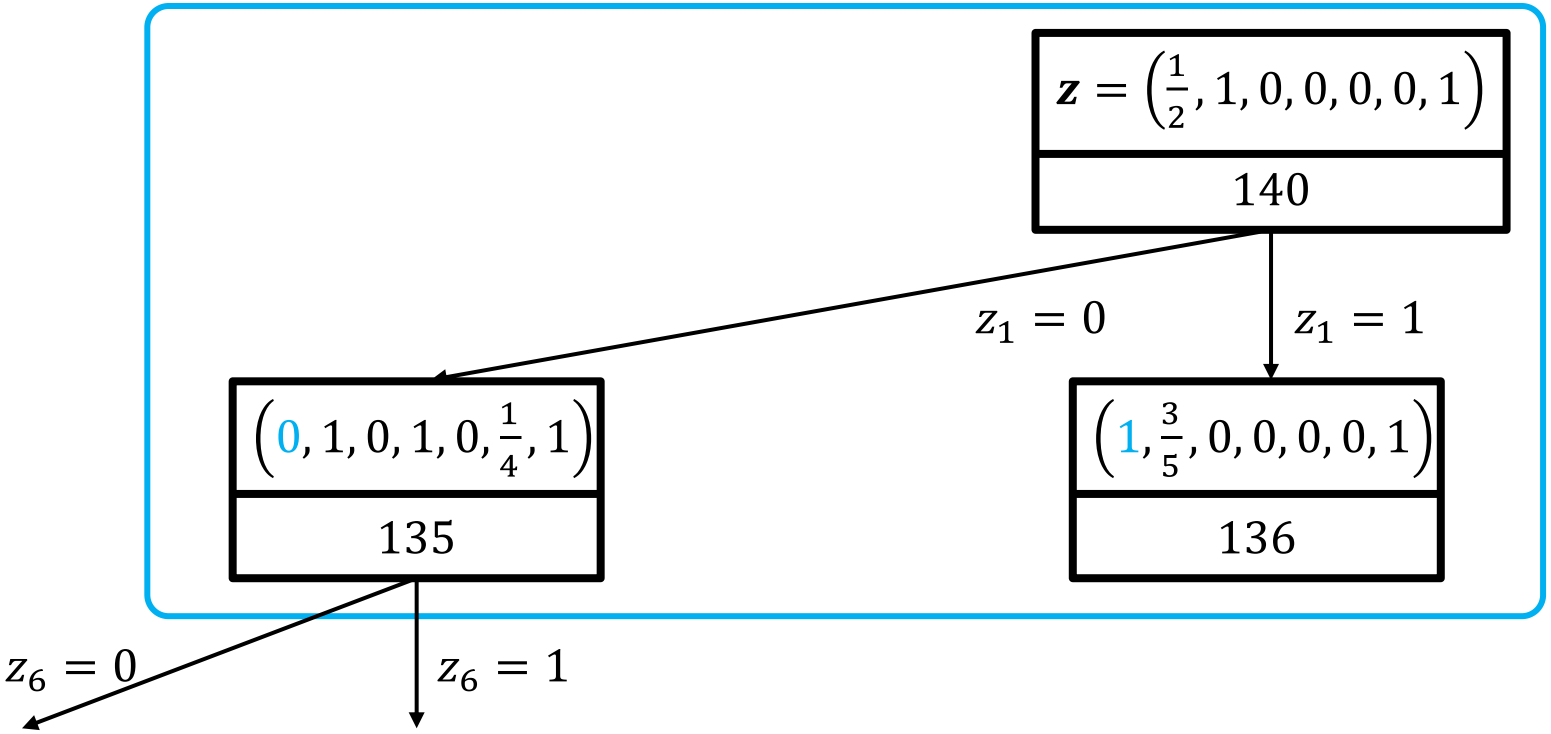
$\quad \boldsymbol{z} \in \{0,1\}^7$


$\boldsymbol{z} = \left(\frac{1}{2}, 1, 0, 0, 0, 0, 1\right)$
140
$z_1 = 0$
$z_1 = 1$

State s_0

Action a_0: Branch on z_1

Branch and bound (B&B)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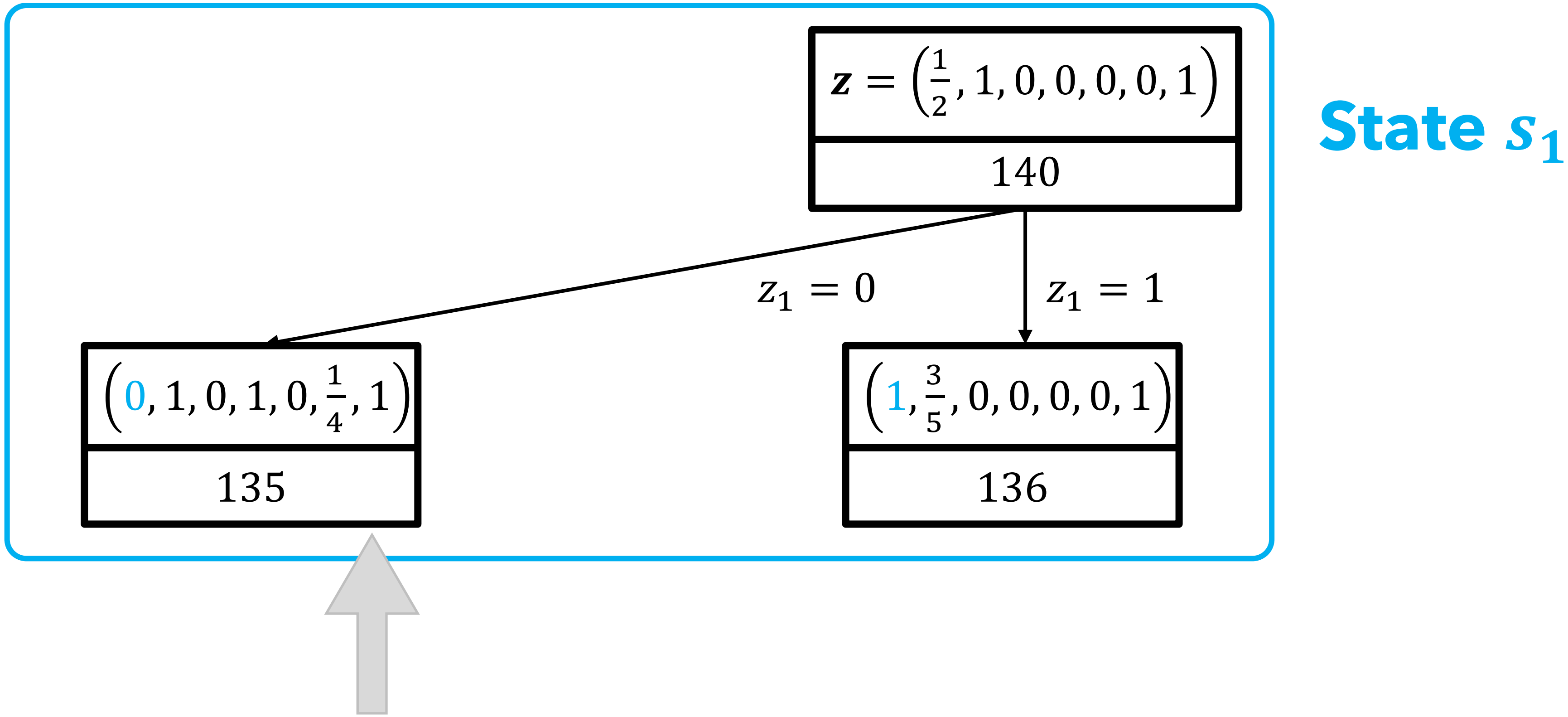
140
$z_1 = 0$
$z_1 = 1$
$\left(0, 1, 0, 1, 0, \frac{1}{4}, 1\right)$
135
$\left(1, \frac{3}{5}, 0, 0, 0, 0, 1\right)$
136
$z_6 = 0$
$z_6 = 1$

State s_1

Action a_1: Branch on z_6

Branch and bound (B&B)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140
$z_1 = 0$
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$\left(0, 1, 0, 1, 0, \frac{1}{4}, 1\right)$
135
$\left(1, \frac{3}{5}, 0, 0, 0, 0, 1\right)$
136
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**