

Lecture 15: MCTS ¹

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CS234 Reinforcement Learning.

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¹With many slides from or derived from David Silver

Refresh Your Understanding: Batch RL

- Select all that are true:
 - ① Batch RL refers to when we have many agents acting in a batch
 - ② In batch RL we generally care more about sample efficiency than computational efficiency
 - ③ Importance sampling can be used to get an unbiased estimate of policy performance
 - ④ Q-learning can be used in batch RL and will generally provide a better estimate than importance sampling in Markov environments for any function approximator used for the Q
 - ⑤ Not sure

Refresh Your Understanding: Batch RL Solutions

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 - ⑤ Not sure
- **Answer. F. T. T. F.**

Class Structure

- Last time: Professor Doshi-Velez guest lecture
- **This Time: MCTS**
- Next time: Last lecture

- AlphaGo video

Monte Carlo Tree Search

- Why choose to have this as well?
- Responsible in part for one of the greatest achievements in AI in the last decade— becoming a better Go player than any human
- Brings in ideas of model-based RL and the benefits of planning

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2 Model-Based Reinforcement Learning

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Introduction: Model-Based Reinforcement Learning

- *Previous lectures*: For online learning, learn value function or policy directly from experience
- *This lecture*: For online learning, learn **model** directly from experience
- and use **planning** to construct a value function or policy
- Integrate learning and planning into a single architecture

$$p(s'/s, a) \quad r(s, a)$$

Model-Based and Model-Free RL

- Model-Free RL
 - No model
 - **Learn** value function (and/or policy) from experience

DQN
Q
policy gradient

Model-Based and Model-Free RL

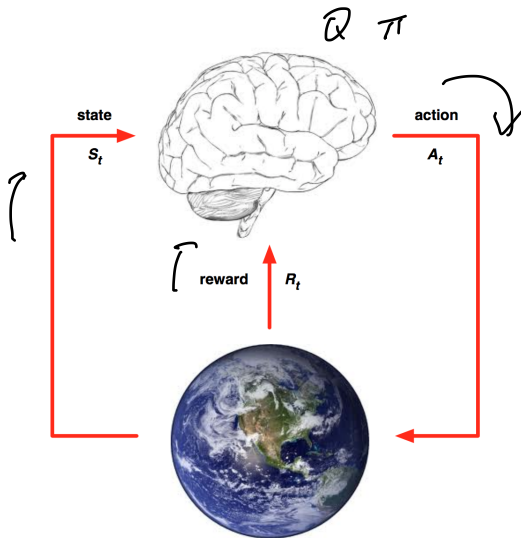
- Model-Free RL

- No model
- **Learn** value function (and/or policy) from experience

- Model-Based RL

- Learn a model from experience $p(s'/s, a)$ and/or $r(s, a)$
- **Plan** value function (and/or policy) from model

Model-Free RL



Model-Based RL

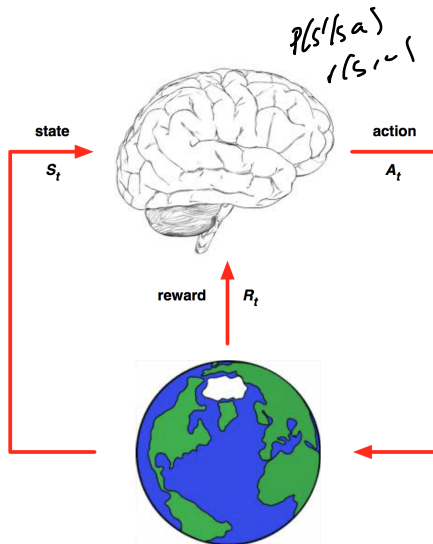
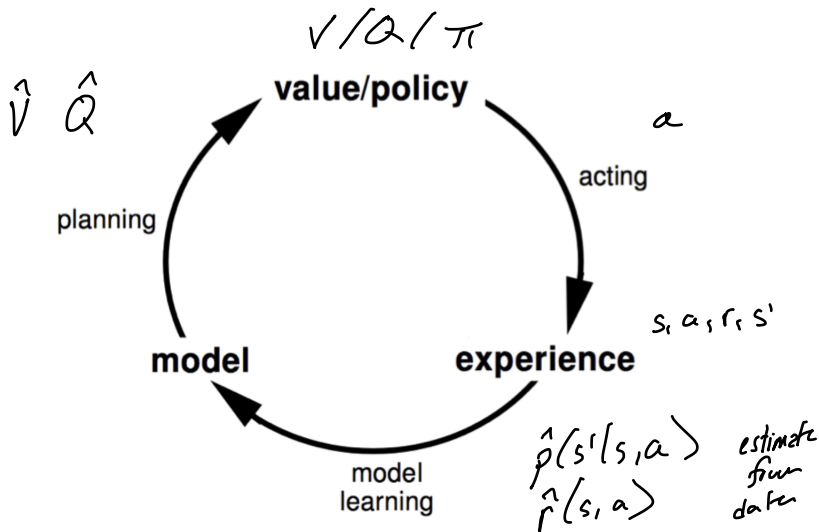


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Model-Based RL



Advantages of Model-Based RL

- Advantages:

- Can efficiently learn model by supervised learning methods
- Can **reason about model uncertainty** (like in upper confidence bound methods for exploration/exploitation trade offs)

UCB or MBIE-EB

- Disadvantages

- First learn a model, then construct a value function
⇒ two sources of approximation error

- model error (limited data and/or model misspec)
- value func error due to approx planning & model error

MDP Model Refresher

- A model $\mathcal{M}$ is a representation of an MDP $\langle S, \mathcal{A}, \mathcal{P}, \mathcal{R} \rangle$, parametrized by η *set of parameters* *↖ dynamics*
- We will assume state space S and action space $\mathcal{A}$ are known
- So a model $\mathcal{M} = \langle \mathcal{P}_\eta, \mathcal{R}_\eta \rangle$ represents state transitions $\mathcal{P}_\eta \approx \mathcal{P}$ and rewards $\mathcal{R}_\eta \approx \mathcal{R}$

$$S_{t+1} \sim \underbrace{\mathcal{P}_\eta}_{\text{dynamics}}(S_{t+1} \mid S_t, A_t)$$

$$R_t = \underbrace{\mathcal{R}_\eta}_{\text{reward}}(R_t \mid S_t, A_t)$$

- Typically assume conditional independence between state transitions and rewards $S, a, r, S' \quad r(S, a) \quad p(R_t \mid S_t, A_t) \propto R(S_t, a_t)$

$$\mathbb{P}[S_{t+1}, R_t \mid S_t, A_t] = \underbrace{\mathbb{P}[S_{t+1} \mid S_t, A_t]}_{\text{dynamics}} \underbrace{\mathbb{P}[R_t \mid S_t, A_t]}_{\text{reward}}$$

Model Learning

- Goal: estimate model $\mathcal{M}_\eta$ from experience $\{S_1, A_1, R_2, \dots, S_T\}$
- This is a supervised learning problem

$$S_1, A_1 \rightarrow R_1, S_2$$

$$S_2, A_2 \rightarrow R_2, S_3$$

$$\vdots$$

$$S_{T-1}, A_{T-1} \rightarrow R_{T-1}, S_T$$

- Learning $s, a \rightarrow r$ is a regression problem *$r(s,a)$*
- Learning $s, a \rightarrow s'$ is a density estimation problem *prob model*
- Pick loss function, e.g. mean-squared error, KL divergence, ...
- Find parameters η that minimize empirical loss *(not always ideal)*
max predic accuracy
ultimate goal is max reward

Examples of Models

- Table Lookup Model
- Linear Expectation Model
- Linear Gaussian Model
- Gaussian Process Model
- Deep Belief Network Model
- ... Bayesian DNN

} function capacity
- how expressive

how easy is it to
express uncertainty

Table Lookup Model

certainty RL
equiv in tabular
spaces

- Model is an explicit MDP, $\hat{P}, \hat{R}$
- Count visits $N(s, a)$ to each state action pair

$$\hat{P}_{s,s'}^a = \frac{1}{N(s, a)} \sum_{t=1}^T \mathbb{1}(S_t, A_t, S_{t+1} = s, a, s')$$

MLE

$$\hat{R}_s^a = \frac{1}{N(s, a)} \sum_{t=1}^T \mathbb{1}(S_t, A_t = s, a)$$

- Alternatively
 - At each time-step t , record experience tuple $\langle S_t, A_t, R_{t+1}, S_{t+1} \rangle$
 - To sample model, randomly pick tuple matching $\langle s, a, \cdot, \cdot \rangle$

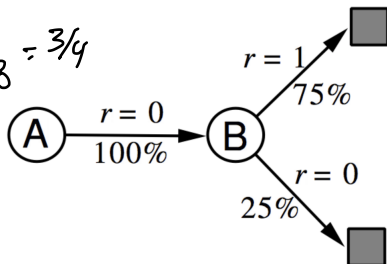
AB Example & Check Your Memory

- Two states A,B; no discounting ($\gamma=1$); 8 episodes of experience

→ A, 0, B, 0

{
B, 1
B, 1
B, 1
B, 1
B, 1
B, 1
B, 1
→ B, 0

$$r(B) = 6/8 = 3/4$$
$$V(B) = 3/4$$
$$V(A) = 3/4$$



- We have constructed a **table lookup model** from the experience
- Recall: For a particular policy, TD with a tabular representation with infinite experience replay will converge to the same value as computed if construct a MLE model and do planning (like calculating q_{π} for a given π)
- Check Your Memory: Will MC methods converge to the same solution?

AB Example & Check Your Memory Solution

- Two states A,B; no discounting; 8 episodes of experience

A, 0, B, 0

B, 1

B, 1

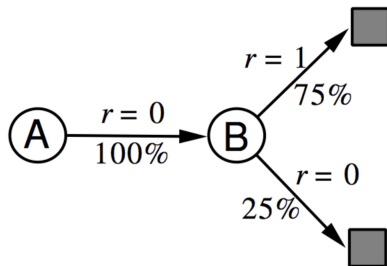
B, 1

B, 1

B, 1

B, 1

B, 0



- We have constructed a **table lookup model** from the experience
- Recall: For a particular policy, TD with a tabular representation with infinite experience replay will converge to the same value as computed if construct a MLE model and do planning
- Check Your Memory: Will MC methods converge to the same solution?
 $V^{\pi^0}(A) = 3/4$ $V^{MC}(A) = 0$
- Solution: Not necessary. MC methods will converge to solution which minimizes the MSE of the value and the observed returns**

Planning with a Model

- Given a model $\mathcal{M}_\eta = \langle \mathcal{P}_\eta, \mathcal{R}_\eta \rangle$
- Solve the MDP $\langle \mathcal{S}, \mathcal{A}, \mathcal{P}_\eta, \mathcal{R}_\eta \rangle \rightarrow \text{compute } Q^\pi \pi^\pi$
- Using favourite planning algorithm
 - Value iteration
 - Policy iteration
 - Tree search
 - ...

easy in course

Sample-Based Planning

- A simple but powerful approach to planning
- Use the model **only** to generate samples
- **Sample** experience from model

$$S_{t+1} \sim \mathcal{P}_\eta(S_{t+1} | S_t, A_t)$$

$$R_{t+1} = \mathcal{R}_\eta(R_{t+1} | S_t, A_t)$$

- Apply **model-free** RL to samples, e.g.:
 - Monte-Carlo control
 - Sarsa
 - Q-learning

given model & a π
a start state s_0
so $\pi(s_0)$
sample
 $s' \sim p(s' | s_0, \pi(s_0))$
↑
under
our
model

have a simulator to
take place of real
experience

Planning with an Inaccurate Model

- Given an imperfect model $\langle \mathcal{P}_\eta, \mathcal{R}_\eta \rangle \neq \langle \mathcal{P}, \mathcal{R} \rangle$
- Performance of model-based RL is limited to optimal policy for approximate MDP $\langle \mathcal{S}, \mathcal{A}, \mathcal{P}_\eta, \mathcal{R}_\eta \rangle$
- i.e. Model-based RL is only as good as the estimated model
- When the model is inaccurate, planning process will compute a sub-optimal policy

generally

Back to the AB Example

- Construct a table-lookup model from real experience
- Apply model-free RL to sampled experience

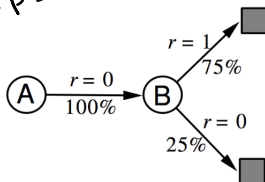
Real experience

→ A, 0, B, 0

→ B, 1

→ B, 1

3 episodes



model estimates here converge

$$\hat{V}(A) = 0$$
$$\hat{V}(B) = 2/3$$

- What values will TD with estimated model converge to assuming $\gamma = 1$?

$$\hat{V}(A) = 2/3$$

- Is this correct? No should be 3/4

Back to the AB Example

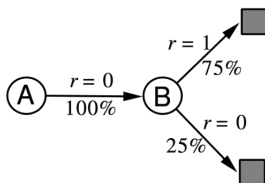
- Construct a table-lookup model from real experience
- Apply model-free RL to sampled experience

Real experience

A, 0, B, 0

B, 1

B, 1



- What values will TD with estimated model converge to assuming $\gamma = 1$?
- $V(B) = 2/3$, $V(A) = V(B) = 2/3$
- Is this correct? **No**

Planning with an Inaccurate Model

- Given an imperfect model $\langle \mathcal{P}_\eta, \mathcal{R}_\eta \rangle \neq \langle \mathcal{P}, \mathcal{R} \rangle$
- Performance of model-based RL is limited to optimal policy for approximate MDP $\langle \mathcal{S}, \mathcal{A}, \mathcal{P}_\eta, \mathcal{R}_\eta \rangle$
- i.e. Model-based RL is only as good as the estimated model
- When the model is inaccurate, planning process will compute a sub-optimal policy
- Solution 1: when model is wrong, use model-free RL
- Solution 2: reason explicitly about model uncertainty (see Lectures on Exploration / Exploitation)

fast RL, bandits

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Computing Action for Current State Only

- Previously would compute a policy for whole state space

$$Q(s, a) \quad \forall s, \forall a \quad \pi(s) \rightarrow a$$

Alternative is to only try to compute $\pi^*(s)$ for current state

Simulation-Based Search

- **Simulate** episodes of experience from **now** with the model starting from **current state** S_t

↓ current state of agent

✓ put diff actions

$$\{S_t^k, A_t^k, R_{t+1}^k, \dots, S_T^k\}_{k=1}^K \sim \mathcal{M}_v$$

simul
tree

- Apply **model-free** RL to simulated episodes
 - Monte-Carlo control → Monte-Carlo search
 - Sarsa → TD search

tabular
or func approx

Simple Monte-Carlo Search

- Given a model $\mathcal{M}_v$ and a **simulation policy** π
- For each action $a \in \mathcal{A}$
 - Simulate K episodes from current (real) state s_t

$$\{s_t, a, R_{t+1}^k, \dots, S_T^k\}_{k=1}^K \sim \mathcal{M}_v(\pi)$$

simulate using π

- Evaluate actions by mean return (**Monte-Carlo evaluation**)

$$Q(s_t, a) = \frac{1}{K} \sum_{k=1}^K G_t \xrightarrow{P} q_\pi(s_t, a)$$

disc. Σ of rewards

true Q^π estimate (1)

- Select current (real) action with maximum value

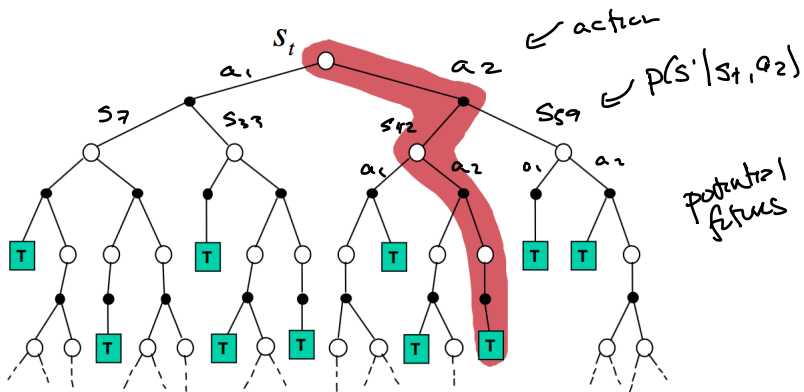
take in real world

$$a_t = \operatorname{argmax}_{a \in \mathcal{A}} Q(s_t, a) \approx Q^\pi(s_t, a)$$

- This is essentially doing 1 step of policy improvement over π

Simulation-Based Search

- Simulate episodes of experience from now with the model
- Apply model-free RL to simulated episodes



Expectimax Tree

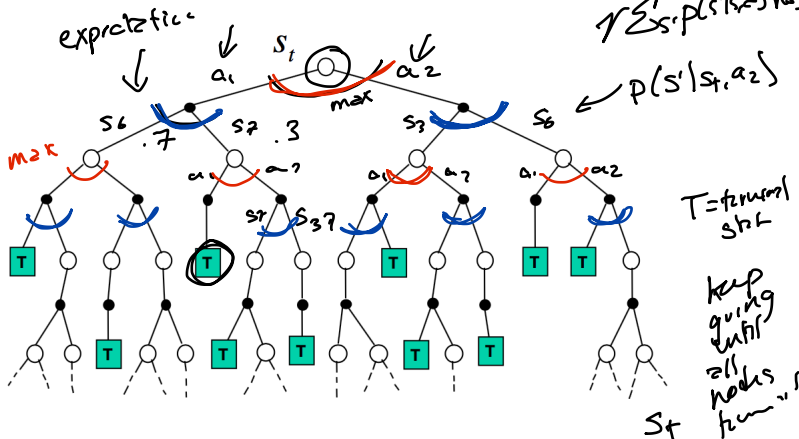
- Can we do better than 1 step of policy improvement?
- If have a MDP model $\mathcal{M}_v$
- Can compute optimal $q(s, a)$ values for current state by constructing an expectimax tree

Forward Search Expectimax Tree

- **Forward search** algorithms select the best action by **lookahead**
- They build a **search tree** with the current state s_t at the root
- Using a **model** of the MDP to look ahead

$$Q^*(s_t, a_t) = R(s_t, a_t) + \gamma \sum_{s'} p(s'|s_t, a_t) V(s')$$

$\cup$ = expect
 $\cup$ = max



- No need to solve whole MDP, just sub-MDP starting from now

Expectimax Tree

- Can we do better than 1 step of policy improvement?
- If have a MDP model $\mathcal{M}_v$
- Can compute optimal $q(s, a)$ values for current state s by constructing an expectimax tree
- Limitations: Size of tree scales as: *Try to work out yourself*

Expectimax Tree

- Can we do better than 1 step of policy improvement?
- If have a MDP model $\mathcal{M}_v$
- Can compute optimal $q(s, a)$ values for current state by constructing an expectimax tree
- Limitations: Size of tree scales as $(|S||A|)^H$ *expon in H*

Monte-Carlo Tree Search (MCTS)

*doesn't build the whole
expectimax tree*

- Given a model $\mathcal{M}_v$
- Build a search tree rooted at the current state s_t
- Samples actions and next states
- Iteratively construct and update tree by performing K simulation episodes starting from the root state
- After search is finished, select current (real) action with maximum value in search tree

*strategically
expand the
tree*

$$a_t = \operatorname{argmax}_{a \in A} Q(s_t, a) \quad \text{at root node}$$

Monte-Carlo Tree Search

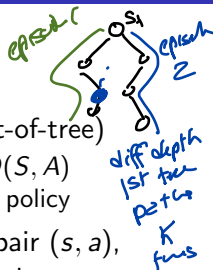
much full forward search w/ much less computation

- Goal: Compute optimal action for current state
- Simulating an episode involves two phases (in-tree, out-of-tree)
 - **Tree policy**: pick actions for tree nodes to maximize $Q(S, A)$
 - **Roll out policy**: e.g. pick actions randomly, or another policy



Monte-Carlo Tree Search

- Goal: Compute optimal action for current state
- Simulating an episode involves two phases (in-tree, out-of-tree)
 - **Tree policy**: pick actions for tree nodes to maximize $Q(S, A)$
 - **Roll out policy**: e.g. pick actions randomly, or another policy
- To evaluate the value of a tree node i at state action pair (s, a) , average over all rewards received from that node onwards across simulated episodes in which this tree node was reached



$$Q(i) = \frac{1}{N(i)} \sum_{k=1}^K \sum_{u=t}^T \mathbb{1}(i \in \text{epi}.k) G_k(i) \xrightarrow{P} q(s, a)$$

- Under mild conditions, converges to the optimal search tree, $Q(S, A) \rightarrow q^*(S, A)$

Check Your Understanding: MCTS

- MCTS involves deciding on an action to take by doing tree search where it picks actions to maximize $Q(S, A)$ and samples states.
Select all
 - ① Given a MDP, MCTS may be a good choice for short horizon problems with a small number of states and actions.
 - ② Given a MDP, MCTS may be a good choice for long horizon problems with a large action space and a small state space
 - ③ Given a MDP, MCTS may be a good choice for long horizon problems with a large state space and small action space
 - ④ Not sure

Check Your Understanding: MCTS

- MCTS involves deciding on an action to take by doing tree search where it picks actions to maximize $Q(S, A)$ and samples states.

Select all

*value iteration or policy
iteration*

- ☐ ① Given a MDP, MCTS may be a good choice for short horizon problems with a small number of states and actions.
- ☐ ② Given a MDP, MCTS may be a good choice for long horizon problems with a large action space and a small state space *enormous action branching*
- ☒ ③ Given a MDP, MCTS may be a good choice for long horizon problems with a large state space and small action space
- ☐ ④ Not sure

- **Solutions: F F T**

Upper Confidence Tree (UCT) Search

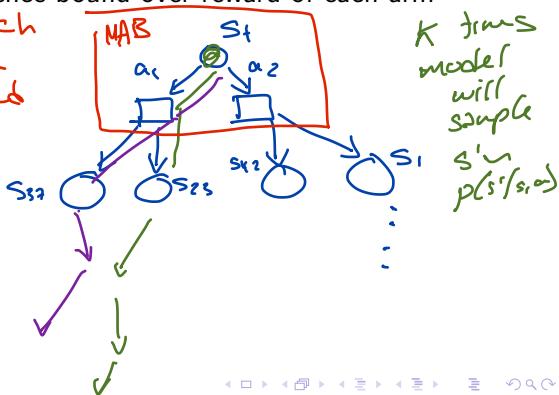
(variant of MCTS)

- How to select what action to take during a simulated episode?

Upper Confidence Tree (UCT) Search

- How to select what action to take during a simulated episode?
- UCT: borrow idea from bandit literature and treat each node where can select actions as a multi-armed bandit (MAB) problem
- Maintain an upper confidence bound over reward of each arm

use to decide which action to choose during a simulated episode / traj through the forward search tree



Case Study: the Game of Go

- Go is 2500 years old
- Hardest classic board game
- Grand challenge task (John McCarthy) for AI
- Traditional game-tree search has failed in Go
- Check your understanding: does playing Go involve learning to make decisions in a world where dynamics and reward model are unknown?

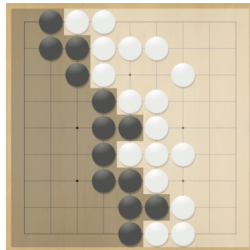
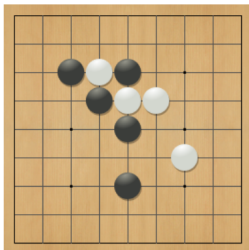


adversarial not stochastic
reward known
dynamics

minmax tree vs
expectimax

Rules of Go

- Usually played on 19x19, also 13x13 or 9x9 board
- Simple rules, complex strategy
- Black and white place down stones alternately
- Surrounded stones are captured and removed
- The player with more territory wins the game



Position Evaluation in Go

- How good is a position s
- Reward function (undiscounted):

$R_t = 0$ for all non-terminal steps $t < T$

$$R_T = \begin{cases} 1, & \text{if Black wins.} \\ 0, & \text{if White wins.} \end{cases}$$

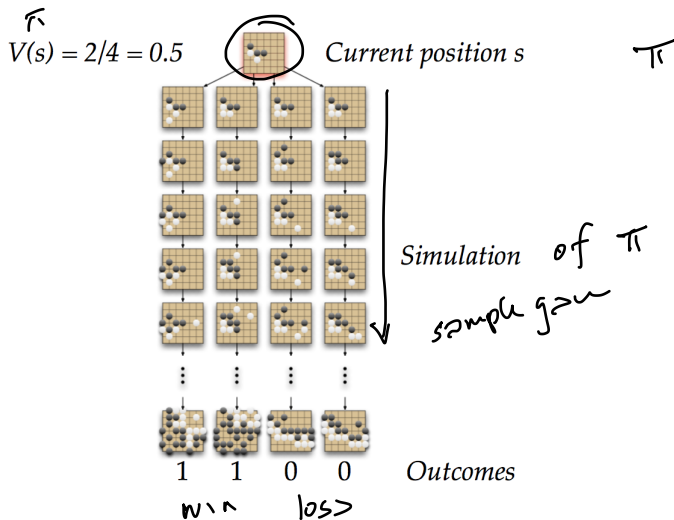
*extremely
hard credit
assignment*

- Policy $\pi = \langle \pi_B, \pi_W \rangle$ selects moves for both players
- Value function (how good is position s):

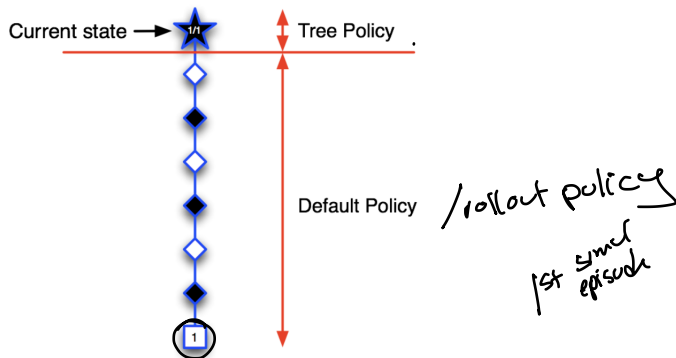
$$v_\pi(s) = \mathbb{E}_\pi[R_T \mid S = s] = \mathbb{P}[\text{Black wins} \mid S = s]$$

$$v^*(s) = \max_{\pi_B} \min_{\pi_W} v_\pi(s)$$

Monte-Carlo Evaluation in Go

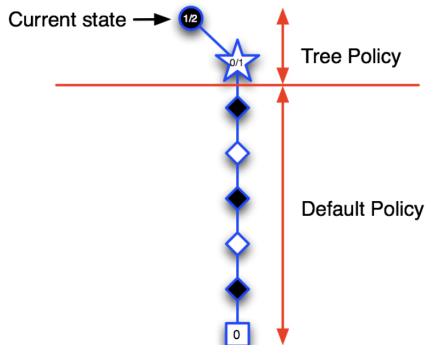


Applying Monte-Carlo Tree Search (1)

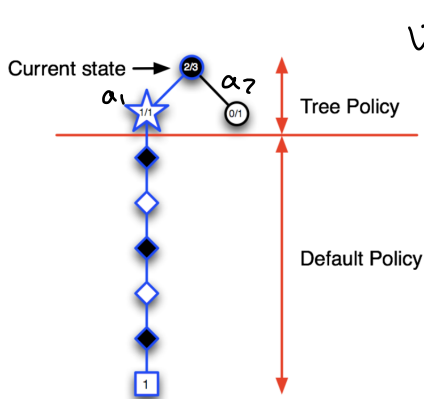


- Go is a 2 player game so tree is a minimax tree instead of expectimax
- White minimizes future reward and Black maximizes future reward when computing action to simulate

Applying Monte-Carlo Tree Search (2)



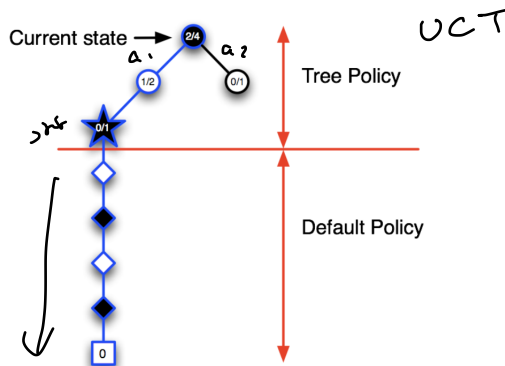
Applying Monte-Carlo Tree Search (3)



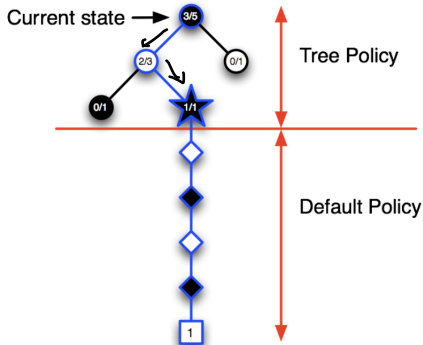
VCT

in general Go
has a very
large
action
space

Applying Monte-Carlo Tree Search (4)



Applying Monte-Carlo Tree Search (5)



*selectively
constructs
for
tree*

Advantages of MC Tree Search

- Highly selective best-first search
- Evaluates states dynamically (unlike e.g. DP)
- Uses sampling to break curse of dimensionality
- Works for “black-box” models (only requires samples)
- Computationally efficient, anytime, parallelisable

sample s'

In more depth: Upper Confidence Tree (UCT) Search

- UCT: borrow idea from bandit literature and treat each tree node where can select actions as a multi-armed bandit (MAB) problem
- Maintain an upper confidence bound over reward of each arm and select the best arm
- Check your understanding: Why is this slightly strange? Hint: why were upper confidence bounds a good idea for exploration/ exploitation? Is there an exploration/ exploitation problem during simulated episodes?¹

¹Relates to metalevel reasoning (for an example related to Go see "Selecting Computations: Theory and Applications", Hay, Russell, Tolpin and Shimony 2012)

Check Your Understanding: UCT Search

- In Upper Confidence Tree (UCT) search we treat each tree node as a multi-armed bandit (MAB) problem, and use an upper confidence bound over the future value of each action to help select actions for later rollouts. Select all that are true
 - 1 This may be useful since it will prioritize actions that lead to later good rewards
 - 2 UCB minimizes regret. UCT is minimizing regret within rollouts of the tree. (If this is true, think about if this a good idea?)
 - 3 Not sure

Check Your Understanding: UCT Search Solutions

- In Upper Confidence Tree (UCT) search we treat each tree node as a multi-armed bandit (MAB) problem, and use an upper confidence bound over the future value of each action to help select actions for later rollouts. Select all that are true
 - ① This may be useful since it will prioritize actions that lead to later good rewards
 - ② UCB minimizes regret. UCT is minimizing regret within rollouts of the tree. (If this is true, think about if this a good idea?)
 - ③ Not sure
- **T. T (but not a good idea)**

↑
this is
just in
agent's
head,
not real
episodes in
the world

In more depth: Upper Confidence Tree (UCT) Search

- UCT: borrow idea from bandit literature and treat each tree node where can select actions as a multi-armed bandit (MAB) problem
- Maintain an upper confidence bound over reward of each arm and select the best arm
- Hint: why were upper confidence bounds a good idea for exploration/ exploitation? Is there an exploration/ exploitation problem during simulated episodes?²

²Relates to metalevel reasoning (for an example related to Go see "Selecting Computations: Theory and Applications", Hay, Russell, Tolpin and Shimony 2012)

▶ AlphaGo trailer link

- MCTS is part of what lead to success in Go
- A number of key additional choices
- There are an enormous number of possible moves. Prioritizing which actions to take when branching matters. In AlphaGo this was initially done by training a supervised learning NN to mimic moves made by humans. *imitation learning s, a labels train $\pi(s) \rightarrow a$*
- Instead of rolling all the way out to the leaves (game won or lost), one can bootstrap and substitute an estimate of the future value. They did this in alphaGo and this also made a big difference. *MC TD*
- For training this value estimate they used **self-play**. This was extremely useful. Self-play in games means that an agent will frequently win and lose because the other agent it is playing is of a similar difficulty level. This is very helpful for providing enough reward signal.

Beyond AlphaGo

- There have been several more impressive insights that don't rely on human knowledge:
- ▶ Mastering the game of Go without human knowledge. Silver et al. Nature 2017.
- ▶ A general RL algorithm that masters chess, shogi, and Go through self-play. Silver et al. Science 2018.

What You Should Know

- MCTS computes a decision only for the current state
- It is an alternative to value iteration or policy iteration and can be used in extremely large state spaces
- UCT uses optimism under uncertainty to choose to further expand action nodes that seem promising
- MCTS has been used with RL to create an AI Go player that exceeds the best human performance

Class Structure

- Last time: Quiz
- **This Time: MCTS**
- Next time: Last lecture