MDP Algorithms
Part II

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Outline of this lecture

- Markov decision processes
- Planning via determinization
- Monte-Carlo methods
- Monte-Carlo Tree Search
- Heuristic Search
- Trial-based Heuristic Tree Search

Please ask questions at any time!
presented several algorithms for probabilistic planning:
  - Determinizations
  - Hindsight Optimization
  - Policy Sampling
  - Sparse Sampling

there are applications for all where they perform well

but all are suboptimal even if provided with unlimited resources
there is a lot of research in MCTS ⇒ I can only cover the basics

- definition of MCTS controversial in the literature
- I only consider algorithms as MCTS that incorporate concepts of Monte-Carlo and Tree Search

Browne et al.
A Survey of Monte Carlo Tree Search Methods
2012
perform iterations as long as resources (deliberation time, memory) allow:

- build a partial MDP tree, where nodes $n$ are annotated with
  - average reward $\hat{Q}_{MCTS}^k(n, \text{state}, a)$ for action $a$ after $k$ iterations
  - visit counter $N_k(n)$ and $N_k(n, a)$ for action $a$ after $k$ iterations

- initially, the tree contains only the root node
- each iteration adds one node to the tree

execute the action with the highest reward estimate
Each iteration consists of (up to) four phases:

- **selection**: traverse the tree by sampling the execution of the tree policy until
  - a terminal node is reached (skip next two phases and proceed with $r = 0$ in this case), or
  - a state $s$ is reached that is not yet in the tree

- **expansion**: add a node for $s$ to the tree

- **simulation**: from $s$, apply default policy until a terminal state is reached, yielding reward $r$

- **backpropagation**: if $a$ has been selected in $n$, update $n$:
  - increase visit counter $N_k(n)$ and $N_k(n, a)$
  - set $r \leftarrow r + R(n.\text{state}, a)$
  - update current average reward $\hat{Q}^{MCTS}_k(n, a)$ based on $r$
Iterations

Selection → Expansion → Simulation → Backpropagation

Tree Policy

Default Policy

Taken from Browne et al., “A Survey of Monte Carlo Tree Search Methods”, 2012
Selection Phase

apply tree policy to traverse tree
Selection Phase

apply tree policy to traverse tree
Selection Phase

apply tree policy to traverse tree
Expansion Phase

create a node for **first state** not in tree
Simulation Phase

apply **default policy** until terminal state is reached
Backpropagation Phase

update visited nodes
Backpropagation Phase

update visited nodes
MCTS Configurations

- MCTS is a framework of algorithms
- concrete algorithms are specified in terms of:
  - tree policy
  - default policy
- for many probabilistic planning problems, there is a well-suited MCTS configuration
- However: there are also many poorly suited MCTS configurations
- and for every MCTS configuration that works well in one problem, there is another problem where it performs poorly

⇒ Are there properties we can analyse theoretically?
Asymptotic Optimality

An MCTS algorithm is asymptotically optimal if $Q_{k}^{MCTS}(n)$ converges to optimal action-value $Q^*(n\.state)$ for all $n \in \text{succ}(n_0)$ with $k \to \infty$. Note: there are MCTS instantiations that act optimally although the values do not converge in this way (e.g., if all $Q_{k}^{MCTS}(n)$ converge to $\ell \cdot Q^*(n\.state)$ for a constant $\ell > 0$).
Asymptotic Optimality

An MCTS algorithm is asymptotically optimal if $Q_{k}^{MCTS}(n)$ converges to optimal action-value $Q^{*}(n\cdot \text{state})$ for all $n \in \text{succ}(n_0)$ with $k \rightarrow \infty$.

Note: there are MCTS instantiations that act optimally although the values do not converge in this way (e.g., if all $Q_{k}^{MCTS}(n)$ converge to $\ell \cdot Q^{*}(n\cdot \text{state})$ for a constant $\ell > 0$)
A tree policy is **asymptotically optimal** if

- it **explores forever**:
  - every position is expanded **eventually and visited infinitely often**

- and it is **greedy in the limit**:
  - the probability that an optimal move action selected converges to 1

\[ \implies \text{in the limit, backups based on iterations where only an optimal policy is followed dominate suboptimal backups} \]
Tree Policy: Objective

tree policies have two contradictory objectives:

- **explore** parts of the game tree that have not been investigated thoroughly
- **exploit** knowledge about good moves to focus search on promising areas

central challenge: **balance** exploration and exploitation
**ε-greedy: Idea**

- tree policy with constant parameter $\varepsilon$
- with probability $1 - \varepsilon$, pick a greedy move (i.e., one that leads to a successor node with the best action-value estimate)
- otherwise, pick a non-greedy successor uniformly at random
$\epsilon$-greedy: Example

$\epsilon = 0.2$

$P(n_1) = 0.1 \quad P(n_2) = 0.8 \quad P(n_3) = 0.1$
\( \varepsilon \)-greedy: Asymptotic Optimality

Asymptotic Optimality of \( \varepsilon \)-greedy

- explores forever
- not greedy in the limit

\( \varepsilon = 0.2 \)

- not asymptotically optimal
\( \varepsilon \)-greedy: Asymptotic Optimality

Asymptotic Optimality of \( \varepsilon \)-greedy

- explores forever
- not greedy in the limit
  \[ \implies \text{not asymptotically optimal} \]

Asymptotically optimal variant: use \textit{decaying} \( \varepsilon \), e.g. \( \varepsilon = \frac{1}{k} \)
\(\varepsilon\)-greedy: Weakness

Problem:
when \(\varepsilon\)-greedy explores, all non-greedy moves are treated equally

\[ \ell \text{ nodes} \]

\[ \begin{align*}
50 & \quad 49 & \quad 0 & \quad \ldots & \quad 0 \\
\end{align*} \]

\( e.g., \ \varepsilon = 0.2, \ \ell = 9: \mathbb{P}(n_1) = 0.8, \mathbb{P}(n_2) = 0.02 \)
Softmax: Idea

- tree policy with constant parameter $\tau$
- select moves proportionally to their action-value estimate
- Boltzmann exploration selects moves proportionally to
  $$\mathbb{P}(n) \propto e \frac{\hat{Q}^{\text{MCTS}}_k(n)}{\tau}$$
Softmax: Example

\[ \ell \text{ nodes} \]

\[ \text{e.g., } \tau = 10, \ell = 9: \mathbb{P}(n_1) \approx 0.51, \mathbb{P}(n_2) \approx 0.46 \]
Boltzmann Exploration: Asymptotic Optimality

Asymptotic Optimality of Boltzmann Exploration

- explores forever
- not greedy in the limit
  (probabilities converge to positive constant)
  ⇨ not asymptotically optimal

asymptotically optimal variants: use decaying $\tau$

**careful:** $\tau$ must not decay faster than logarithmically
  (i.e., must have $\tau \geq \frac{\text{const}}{\log k}$) to explore infinitely
Boltzmann Exploration: Weakness

- Boltzmann exploration only considers **mean** of sampled action-values for the given moves.
- As we sample the same node many times, we can also gather information about variance (how **reliable** the information is).
- Boltzmann exploration ignores the variance, treating the two scenarios equally.
Upper Confidence Bounds: Idea

balance **exploration** and **exploitation** by preferring moves that
- have been **successful in earlier iterations** (exploit)
- have been **selected rarely** (explore)
Upper Confidence Bounds: Idea

- select successor $n'$ of $n$ that maximizes $\hat{Q}_{k}^{MCTS}(n') + B(n')$
- based on action-value estimate $\hat{Q}^{MCTS}(n')$
- and a bonus term $B(n')$
- select $B(n')$ such that $Q^*(n'.state) \leq \hat{Q}_{k}^{MCTS}(n') + B(n')$ with high probability
- idea: $\hat{Q}_{k}^{MCTS}(n') + B(n')$ is an upper confidence bound on $Q^*(n')$ under the collected information
Upper Confidence Bounds: UCB1

- use $B(a) = \sqrt{\frac{2 \cdot \ln N_k(n)}{N_k(n',a)}}$ as bonus term

- bonus term is derived from Chernoff-Hoeffding bound:
  - gives the probability that a sampled value (here: $\hat{Q}^\text{MCTS}_k(n')$)
  - is far from its true expected value (here: $Q^*(n'.\text{state})$)
  - in dependence of the number of samples (here: $N_k(n',n'.\text{action})$)

- picks the optimal move exponentially more often
Upper Confidence Bounds: Asymptotic Optimality

<table>
<thead>
<tr>
<th>Asymptotic Optimality of UCB1</th>
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<tbody>
<tr>
<td>- explores forever</td>
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<tr>
<td>- greedy in the limit</td>
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<tr>
<td>⇔ asymptotically optimal</td>
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</table>
Upper Confidence Bounds: Asymptotic Optimality

Asymptotic Optimality of UCB1

- explores forever
- greedy in the limit
- asymptotically optimal

However:

- no theoretical justification to use UCB1 in trees or planning scenarios
- development of tree policies active research topic
Tree Policy: Asymmetric Game Tree

full tree up to depth 4
Tree Policy: Asymmetric Game Tree

UCT tree (equal number of search nodes)
Default Policy

- Most often used: Monte-Carlo random walk
- Very successful: learned default policies, (e.g., for Go) Requires large amounts of data and/or computational power
AO*: Idea

AO* for acyclic MDPs (Nilsson, 1971)

- add $s_0$ to open list and to greedy policy graph
- repeat until greedy policy graph has no fringe
  - expand best state $s$ on the fringe of the greedy graph
  - initialize all new states with heuristic
  - backup all states from where $s$ is reachable
  - recompute the greedy graph
- output the greedy graph as the final policy
AO* Tree Search

- perform iterations as long as resources (deliberation time, memory) allow:
- build a partial MDP tree, where nodes $n$ are annotated with
  - average reward
  - a solve label
- initially, the tree contains only the root node
- each iteration expands one node in the tree
AO* Tree Search: Iterations

Iterations proceed as follows:

- starting from the root node, select a successor node with maximum action-value estimate
- until a node is reached without successors
- expand that node and add all children to the tree
- initialize action-value estimate of all children with heuristic
- if a child is a terminal node, set its solve label to true
- if $a$ has been selected in $n$, update $n$:
  - derive successor $n'$ with maximum action value
  - set $\hat{Q}_k(n) = \hat{Q}_k(n') + R(n\text{.state}, n'\text{.action})$
  - set the solve label of $n$ to the value of the solve label of $n'$
| AO* Tree Search very similar to (Trial-based) Real-Time Dynamic Programming (Barto, Bradtke, and Singh 1995) |
| Difference: RTDP expands states until a terminal state is reached |
asymptotically optimal MDP algorithms:
  - Monte-Carlo Tree Search (e.g., UCT)
  - Dynamic Programming (e.g., RTDP)
  - Heuristic Search (e.g., AO*)

all have complementary strengths
common framework that allows to describe them all Trial-based Heuristic Tree Search (THTS)
Trial-based Heuristic Tree Search

- initialize search tree with initial state
- extend search tree iteratively in trials
Trial-based Heuristic Tree Search

- initialize search tree with initial state
- extend search tree iteratively in trials
- 6 variable ingredients:
  - action selection
  - outcome selection
Trial-based Heuristic Tree Search

- initialize search tree with initial state
- extend search tree iteratively in trials
- 6 variable ingredients:
  - action selection
  - outcome selection
  - initialization
  - trial length
Trial-based Heuristic Tree Search

- initialize **search tree** with initial state
- extend search tree iteratively in **trials**
- 6 variable ingredients:
  - action selection
  - outcome selection
  - initialization
  - trial length
  - backup function
Trial-based Heuristic Tree Search

- initialize search tree with initial state
- extend search tree iteratively in trials

6 variable ingredients:
- action selection
- outcome selection
- initialization
- trial length
- backup function
- recommendation function
MCTS in the THTS Framework

- trial length: terminate trial once node is added to tree
- action selection: tree policy (e.g., UCB1 for MCTS)
- outcome selection: sample
- initialization: add single node to the tree and initialize with heuristic that simulates the default policy
- backup function: Monte-Carlo backups
- recommendation function: expected best arm
AO* in the THTS Framework

- **trial length**: terminate trial once node is added to tree
- **action selection**: greedy
- **outcome selection**: sample (or whatever is done in your version of AO*)
- **initialization**: add all successors, including all outcomes, and initialize with admissible heuristic
- **backup function**: Bellman backups
- **recommendation function**: expected best arm
RTDP in the THTS Framework

- trial length: finish trials only in terminal states
- action selection: greedy
- outcome selection: sample
- initialization: add all successors, including all outcomes, and initialize with admissible heuristic
- backup function: Bellman backups
- recommendation function: expected best arm
Other Ingredients

- recommendation function:
  - most played arm (MCTS variants)

- initialization:
  - tree expansion: add all (action) successors (UCT*)
  - state-action heuristic, e.g., IDS-based lookahead heuristic of PROST (UCT*)
Other Ingredients: backup functions

- Temporal Differences
- Q-Learning
- MaxMonte-Carlo (DP-UCT)
- Partial Bellman (UCT*)
Considered ingredients in my dissertation

- 1 trial length, 1 outcome selection, 1 initialization
- 2 different recommendation functions
- 9 different backup functions
- 9 different action selections

⇒ 162 different THTS algorithms

115 asymptotically optimal
Experimental Evaluation

- most played arm recommendation function often better than same configuration with expected best arm

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most played arm recommendation function often better than same configuration with expected best arm

Boltzmann exploration and root-valued UCB1 perform best in most domains
Experimental Evaluation

- most played arm recommendation function often better than same configuration with expected best arm
- Boltzmann exploration and root-valued UCB1 perform best in most domains
- Monte-Carlo and Partial Bellman backups perform best in most domains
Experimental Evaluation

- most played arm recommendation function often better than same configuration with expected best arm
- Boltzmann exploration and root-valued UCB1 perform best in most domains
- Monte-Carlo and Partial Bellman backups perform best in most domains
- almost all action selections and backup functions perform best in at least one domain
The PROST planner is an implementation of the MCTS framework.

- Mixing and matching of ingredients very simple.
- To add new ingredients, just inherit from the corresponding class.

https://bitbucket.org/tkeller/prost/
Summary

- MCTS asymptotically optimal with right components
- AO* and RTDP have complementary strength
- THTS allows to combine ideas from MCTS, DP and Heuristic Search
- almost all ingredients perform well in at least one domain