

# Planning and Optimization

## F8. Monte-Carlo Tree Search Algorithms (Part I)

Malte Helmert and Gabriele Röger

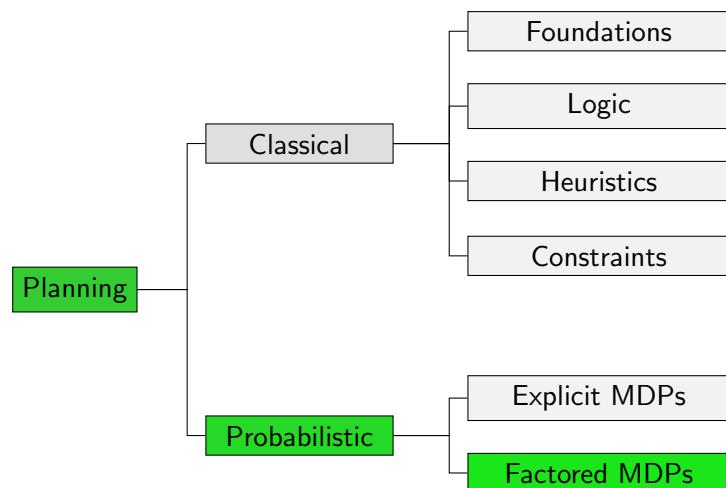
Universität Basel

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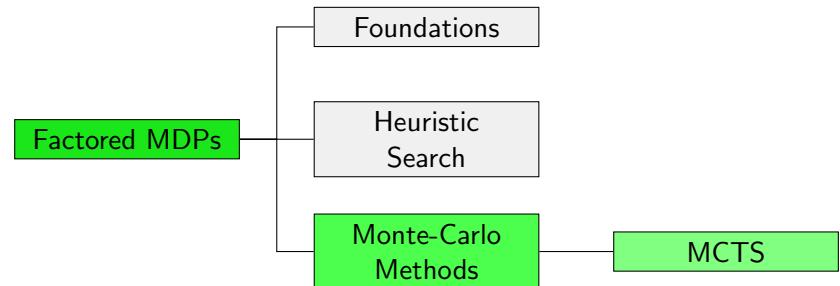
## — F8. Monte-Carlo Tree Search Algorithms (Part I)

- F8.1 Introduction
- F8.2 Default Policy
- F8.3 Asymptotic Optimality
- F8.4 Multi-armed Bandit Problem
- F8.5 Summary

## Content of this Course



## Content of this Course: Factored MDPs

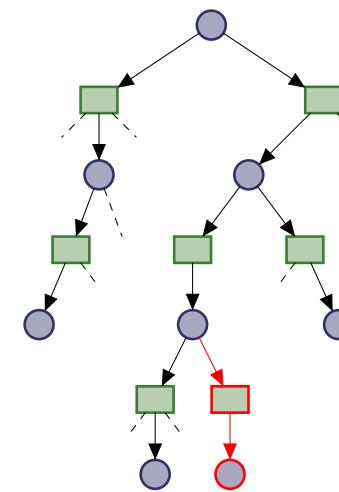


## F8.1 Introduction

## Monte-Carlo Tree Search: Reminder

Performs iterations with 4 phases:

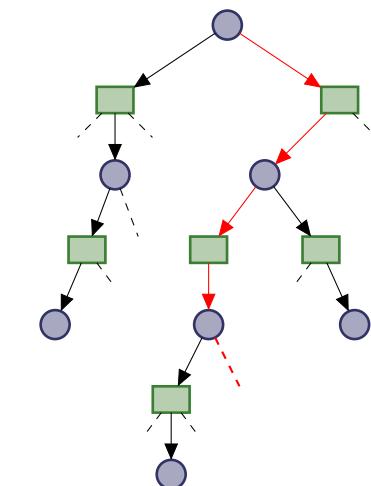
- ▶ **selection**: use **given tree policy** to traverse explicated tree
- ▶ **expansion**: add node(s) to the tree
- ▶ **simulation**: use **given default policy** to simulate run
- ▶ **backpropagation**: update visited nodes with Monte-Carlo backups



## Monte-Carlo Tree Search: Reminder

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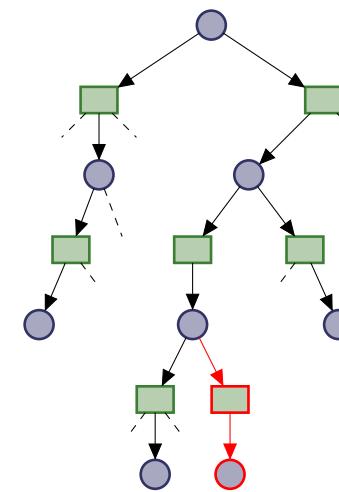
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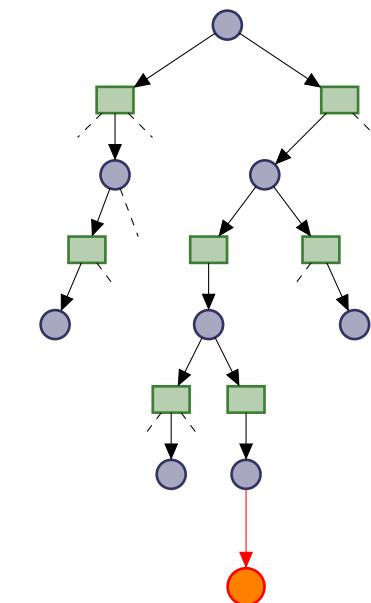
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## Monte-Carlo Tree Search: Reminder

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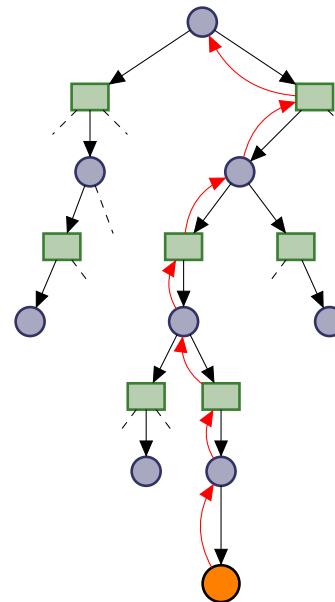
- ▶ **selection**: use **given tree policy** to traverse explicated tree
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## Monte-Carlo Tree Search: Reminder

Performs iterations with 4 phases:

- ▶ **selection**: use **given tree policy** to traverse **exploited tree**
- ▶ **expansion**: add node(s) to the tree
- ▶ **simulation**: use **given default policy** to simulate run
- ▶ **backpropagation**: update visited nodes with Monte-Carlo backups



## Role of Tree Policy

- ▶ used to **traverse exploited tree** from root node to a leaf
- ▶ maps **decision nodes** to a probability distribution over actions (usually as a function over a decision node and its children)
- ▶ **exploits** information from search tree
  - ▶ able to **learn over time**
  - ▶ requires MCTS tree to **memorize** collected information

## Motivation

- ▶ Monte-Carlo Tree Search is a **framework** of algorithms
- ▶ concrete MCTS algorithms are specified in terms of
  - ▶ a tree policy;
  - ▶ and a default policy
- ▶ for most tasks, a **well-suited** MCTS configuration exists
- ▶ but for each task, many MCTS configurations **perform poorly**
- ▶ and every MCTS configuration that **works well** in one problem **performs poorly** in another problem

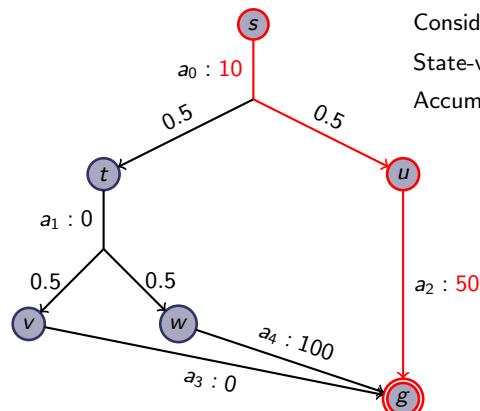
⇒ There is no “Swiss army knife” configuration for MCTS

## Role of Default Policy

- ▶ used to **simulate run** from some state to a goal
- ▶ maps **states** to a probability distribution over actions
- ▶ **independent** from MCTS tree
  - ▶ does not improve over time
  - ▶ can be **computed quickly**
  - ▶ **constant memory** requirements
- ▶ **accumulated cost of simulated run** used to **initialize** state-value estimate of decision node

## F8.2 Default Policy

### Default Policy: Example



### MCTS Simulation

MCTS simulation with default policy  $\pi$  from state  $s$

```
cost := 0
while  $s \notin S_*$ :
     $a := \pi(s)$ 
    cost := cost +  $c(a)$ 
     $s := \text{succ}(s, a)$ 
return cost
```

Default policy must be **proper**

- ▶ to guarantee **termination** of the procedure
- ▶ and a **finite cost**

### Default Policy Realizations

- ▶ Early MCTS implementations used **random default policy**:

$$\pi(a | s) = \begin{cases} \frac{1}{|A(s)|} & \text{if } a \in A(s) \\ 0 & \text{otherwise} \end{cases}$$

- ▶ only **proper** if goal can be reached from each state
- ▶ **poor** guidance, and due to high variance even **misguidance**

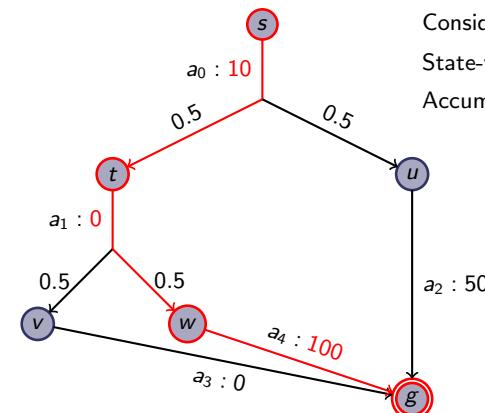
## Default Policy Realizations

There are only **few alternatives** to random default policy, e.g.,

- ▶ heuristic-based policy
- ▶ domain-specific policy

**Reason:** No matter how good the policy, result of simulation can be arbitrarily poor

## Default Policy: Example (2)



Consider deterministic default policy  $\pi$

State-value of  $s$  under  $\pi$ : 60

Accumulated cost of run: 110

## Default Policy Realizations

Possible **solution** to overcome this weakness:

- ▶ **average** over multiple random walks
- ▶ **converges** to true action-values of policy
- ▶ computationally **often very expensive**

Cheaper and more **successful** alternative:

- ▶ skip **simulation** step of MCTS
- ▶ use heuristic **directly for initialization** of state-value estimates
- ▶ instead of simulating execution of heuristic-guided policy
- ▶ much more successful (e.g. neural networks of **AlphaGo**)

## F8.3 Asymptotic Optimality

## Optimal Search

Heuristic search algorithms (like RTDP) achieve optimality by combining

- ▶ greedy search
- ▶ admissible heuristic
- ▶ Bellman backups

In Monte-Carlo Tree Search

- ▶ search behavior defined by a **tree policy**
- ▶ **admissibility** of default policy / heuristic **irrelevant** (and usually **not given**)
- ▶ **Monte-Carlo backups**

MCTS requires a different idea for **optimal behavior in the limit**.

## Asymptotically Optimal Tree Policy

An MCTS algorithm is **asymptotically optimal** if

- ➊ its tree policy **explores forever**:
  - ▶ the (infinite) sum of the probabilities that a decision node is visited must diverge
  - ▶  $\Rightarrow$  every search node is **explored eventually** and **visited infinitely often**
- ➋ its tree policy is **greedy in the limit**:
  - ▶ probability that optimal action is selected converges to 1
  - ▶  $\Rightarrow$  in the limit, backups based on iterations where only an **optimal policy** is followed dominate suboptimal backups
- ➌ its default policy initializes decision nodes with **finite values**

## Asymptotic Optimality

### Asymptotic Optimality

Let an MCTS algorithm build an MCTS tree  $\mathcal{G} = \langle d_0, D, C, E \rangle$ . The MCTS algorithm is **asymptotically optimal** if

$$\lim_{k \rightarrow \infty} \hat{Q}^k(c) = Q_*(s(c), a(c)) \text{ for all } c \in C^k,$$

where  $k$  is the number of trials.

- ▶ this is just one special form of asymptotic optimality
- ▶ some optimal MCTS algorithms are not asymptotically optimal by this definition (e.g.,  $\lim_{k \rightarrow \infty} \hat{Q}^k(c) = \ell \cdot Q_*(s(c), a(c))$  for some  $\ell \in \mathbb{R}^+$ )
- ▶ all **practically relevant** optimal MCTS algorithms are asymptotically optimal by this definition

## Example: Random Tree Policy

### Example

Consider the **random tree policy** for decision node  $d$  where:

$$\pi(a | d) = \begin{cases} \frac{1}{|A(s(d))|} & \text{if } a \in A(s(d)) \\ 0 & \text{otherwise} \end{cases}$$

The random tree policy **explores forever**:

Let  $\langle d_0, c_0, \dots, d_n, c_n, d \rangle$  be a sequence of connected nodes in  $\mathcal{G}^k$  and let  $p := \min_{0 < i < n-1} T(s(d_i), a(c_i), s(d_{i+1}))$ .

Let  $\mathbb{P}^k$  be the probability that  $d$  is visited in trial  $k$ . With  $\mathbb{P}^k \geq (\frac{1}{|A|} \cdot p)^n$ , we have that

$$\lim_{k \rightarrow \infty} \sum_{i=1}^k \mathbb{P}^k \geq k \cdot \left(\frac{1}{|A|} \cdot p\right)^n = \infty$$

## Example: Random Tree Policy

### Example

Consider the **random tree policy** for decision node  $d$  where:

$$\pi(a | d) = \begin{cases} \frac{1}{|A(s(d))|} & \text{if } a \in A(s(d)) \\ 0 & \text{otherwise} \end{cases}$$

The random tree policy is **not greedy in the limit** unless all actions are always optimal:

The probability that an optimal action  $a$  is selected in decision node  $d$  is

$$\lim_{k \rightarrow \infty} 1 - \sum_{\{a' \notin \pi_{V^*}(s)\}} \frac{1}{|A(s(d))|} < 1.$$

⇒ MCTS with random tree policy **not asymptotically optimal**

## Example: Greedy Tree Policy

### Example

Consider the **greedy tree policy** for decision node  $d$  where:

$$\pi(a | d) = \begin{cases} \frac{1}{|A_*^k(d)|} & \text{if } a \in A_*^k(d) \\ 0 & \text{otherwise,} \end{cases}$$

with  $A_*^k(d) = \{a(c) \in A(s(d)) \mid c \in \arg \min_{c' \in \text{children}(d)} \hat{Q}^k(c')\}$ .

- ▶ Greedy tree policy is **greedy in the limit**
- ▶ Greedy tree policy does **not explore forever**
- ⇒ MCTS with greedy tree policy **not asymptotically optimal**

## Tree Policy: Objective

To satisfy **both** requirements, MCTS tree policies have two contradictory objectives:

- ▶ **explore** parts of the search space that have not been investigated thoroughly
- ▶ **exploit** knowledge about good actions to focus search on promising areas of the search space

central challenge: **balance** exploration and exploitation

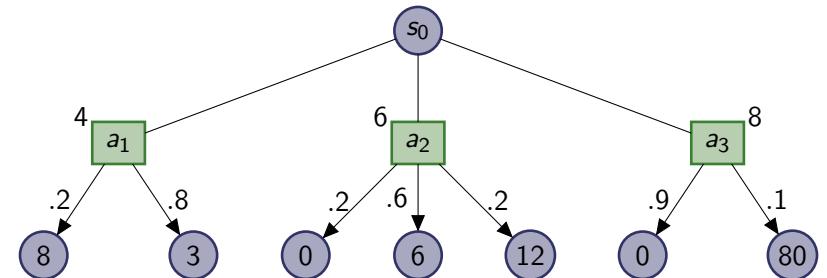
⇒ borrow ideas from related **multi-armed bandit** problem

## F8.4 Multi-armed Bandit Problem

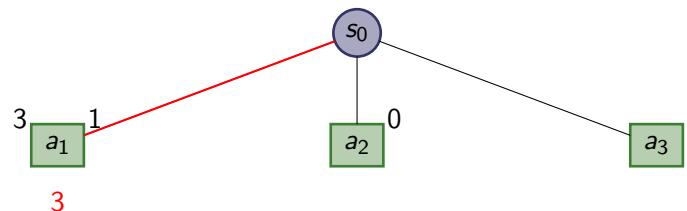
## Multi-armed Bandit Problem

- most commonly used tree policies are **inspired** from research on the multi-armed bandit problem (MAB)
- MAB is a **learning** scenario (model not revealed to agent)
- agent repeatedly faces the same decision: to pull one of several arms of a **slot machine**
- pulling an arm yields **stochastic reward**  
⇒ in MABs, we have rewards rather than costs
- can be modeled as an MDP

## Multi-armed Bandit Problem: Planning Scenario

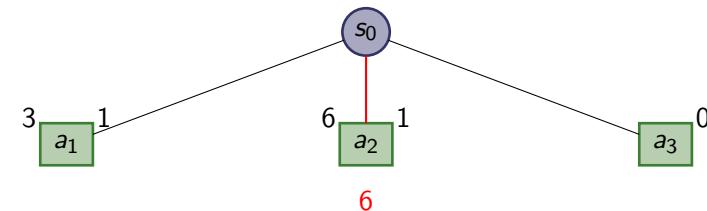


## Multi-armed Bandit Problem: Learning Scenario



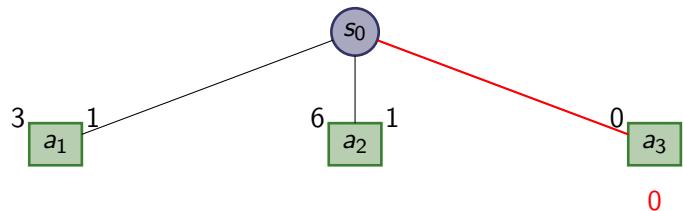
- Pull arms following **policy** to **explore** or **exploit**
- Update  $\hat{Q}$  and  $N$  based on observations
- Accumulated reward after 1 trial is 3

## Multi-armed Bandit Problem: Learning Scenario



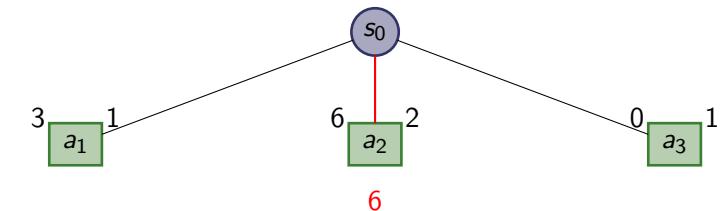
- Pull arms following **policy** to **explore** or **exploit**
- Update  $\hat{Q}$  and  $N$  based on observations
- Accumulated reward after 2 trials is  $3 + 6 = 9$

## Multi-armed Bandit Problem: Learning Scenario



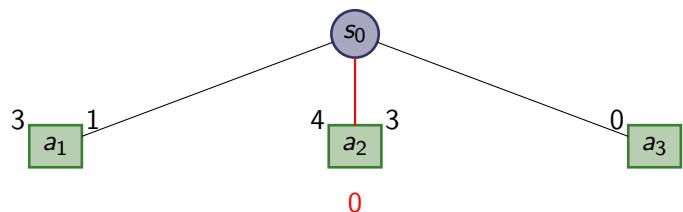
- ▶ Pull arms following **policy** to **explore** or **exploit**
- ▶ Update  $\hat{Q}$  and  $N$  based on observations
- ▶ Accumulated reward after 3 trials is  $3 + 6 + 0 = 9$

## Multi-armed Bandit Problem: Learning Scenario



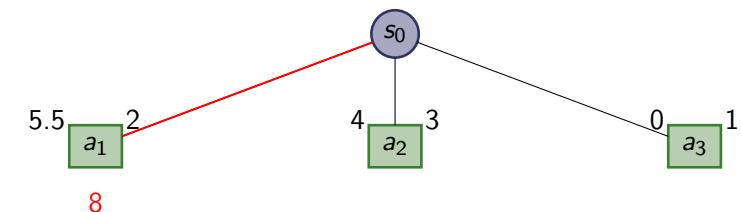
- ▶ Pull arms following **policy** to **explore** or **exploit**
- ▶ Update  $\hat{Q}$  and  $N$  based on observations
- ▶ Accumulated reward after 4 trials is  $3 + 6 + 0 + 6 = 15$

## Multi-armed Bandit Problem: Learning Scenario



- ▶ Pull arms following **policy** to **explore** or **exploit**
- ▶ Update  $\hat{Q}$  and  $N$  based on observations
- ▶ Accumulated reward after 5 trials is  $3 + 6 + 0 + 6 + 0 = 15$

## Multi-armed Bandit Problem: Learning Scenario



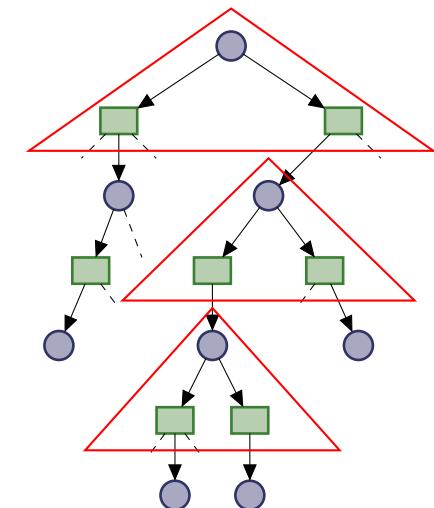
- ▶ Pull arms following **policy** to **explore** or **exploit**
- ▶ Update  $\hat{Q}$  and  $N$  based on observations
- ▶ Accumulated reward after 6 trials is  $3 + 6 + 0 + 6 + 0 + 8 = 23$

## Policy Quality

- ▶ Since model unknown to MAB agent, it cannot achieve accumulated reward of  $k \cdot V_*$  with  $V_* := \max_a Q_*(a)$  in  $k$  trials
- ▶ Quality of MAB policy  $\pi$  measured in terms of **regret**, i.e., the difference between  $k \cdot V_*$  and expected reward of  $\pi$  in  $k$  trials
- ▶ Regret cannot grow slower than **logarithmically** in the number of trials

## MABs in MCTS Tree

- ▶ many tree policies treat **each decision node as MAB**
- ▶ where each action yields a **stochastic reward**
- ▶ dependence of reward on future decision is **ignored**
- ▶ MCTS **planner** uses simulations to **learn reasonable behavior**
- ▶ SSP model is **not considered**



## F8.5 Summary

### Summary

- ▶ The simulation phase **simulates the execution** of the default policy
- ▶ MCTS algorithms are **optimal in the limit** if
  - ▶ the tree policy is **greedy in the limit**,
  - ▶ the tree policy **explores forever**, and
  - ▶ the default policy **initializes with finite value**
- ▶ Central challenge of most tree policies: **balance exploration and exploitation**
- ▶ each decision of an MCTS tree policy can be viewed as an **multi-armed bandit problem**.