Deep Learning

A course about theory & practice

UNIVERSITÀ DI PAVIA

Monte Carlo Tree Search (MCTS)

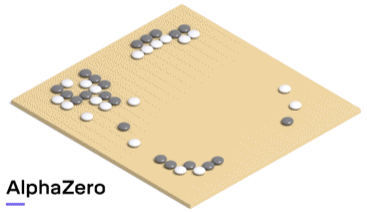
Marco Piastra

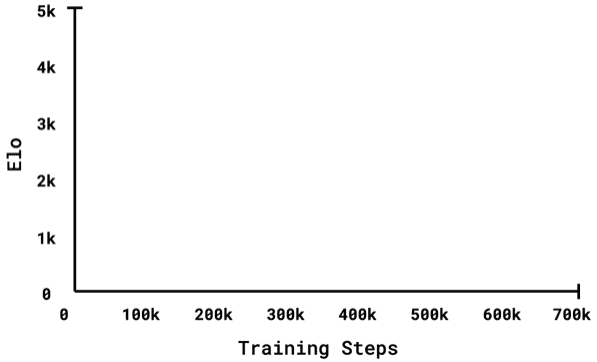
Prologue:
Playing Games better than Humans

Beyond Emulating Humans: AlphaZero (2018)

Image from: https://deepmind.com/blog/article/alphazero-shedding-new-light-grand-games-chess-shogi-and-go

AlphaGo is heavily reliant
on the experience of human players





- **AlphaZero learns by itself**
  [2018, D. Silver, et al. (13 authors), https://science.sciencemag.org/content/362/6419/1140.full]

Basic Knowledge Only

It just knows the basic rules of the games

Learning via Self-Play

It plays against a (frozen) copy of itself

MCTS and DCNN in a closed loop

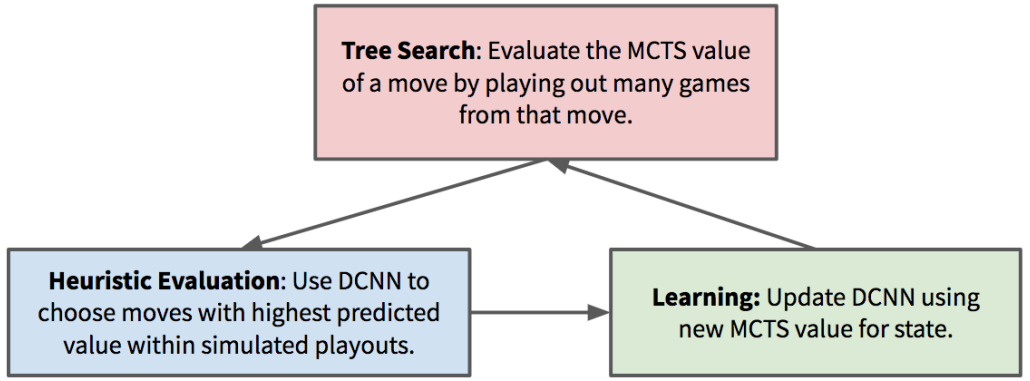


Image from: https://nikcheerla.github.io/deeplearningschool/2018/01/01/AlphaZero-Explained/

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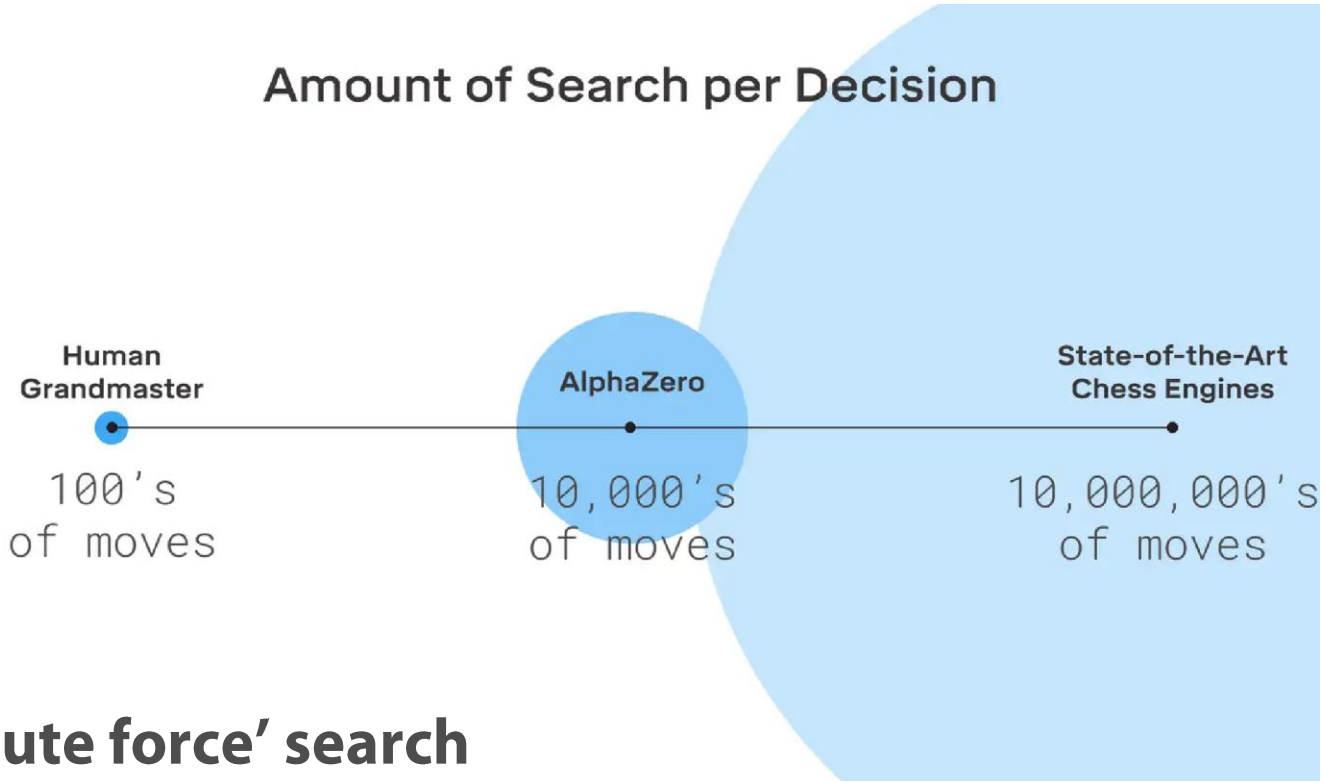
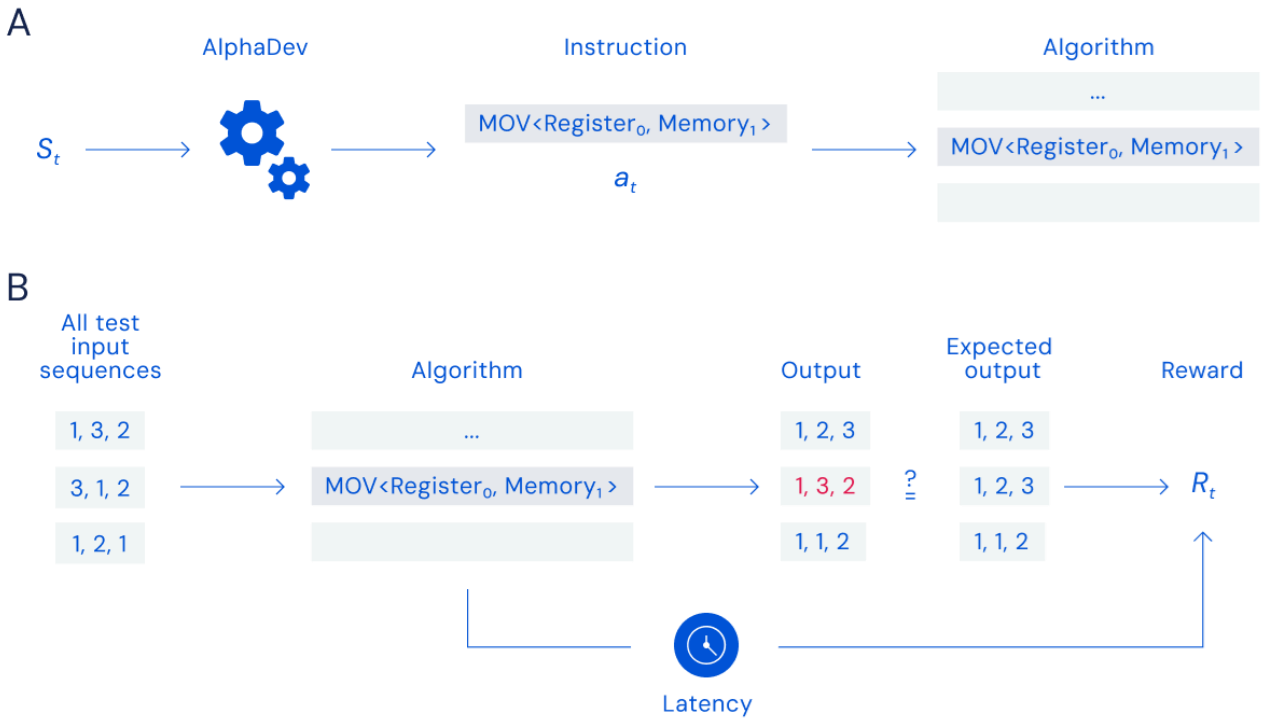


- **AlphaZero uses much less 'brute force' search**
  - When playing, the search process is driven by its neural network
    - *It acts like a memory of past experiences*
  - While training, it learns through a huge amount of self-playing
    - *But it is a faster learner than Alpha Go*

Discovering Better Algorithms: AlphaDev (2023)

https://deepmind.google/blog/alphadev-discovers-faster-sorting-algorithms/



AlphaDev uses reinforcement learning to discover *enhanced computer science algorithms* – surpassing those honed by scientists and engineers over decades

For instance, **AlphaDev** uncovered a faster algorithm for *sorting*, a method for ordering data
[see https://www.nature.com/articles/s41586-023-06004-9]

Playing Games with Trees

Tree representation

- **Game Tree (*simplest case*):**

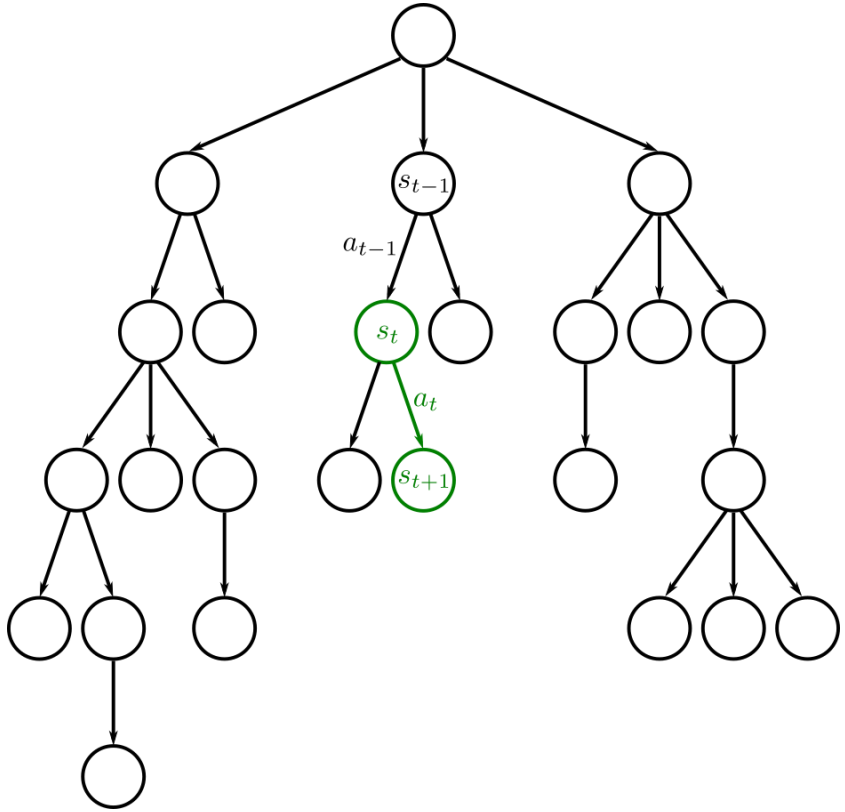
  The *current state* s_t at time t is a ***node*** with depth t

  Any admissible *action* a_t is an ***edge*** of the tree

  (branching factor = number of admissible actions in a state)

  State s_{t+1} obtained from s_t after executing a_t
  is determined by a *transition function*

$$\tau : \ (s_t, a_t) \mapsto s_{t+1}$$



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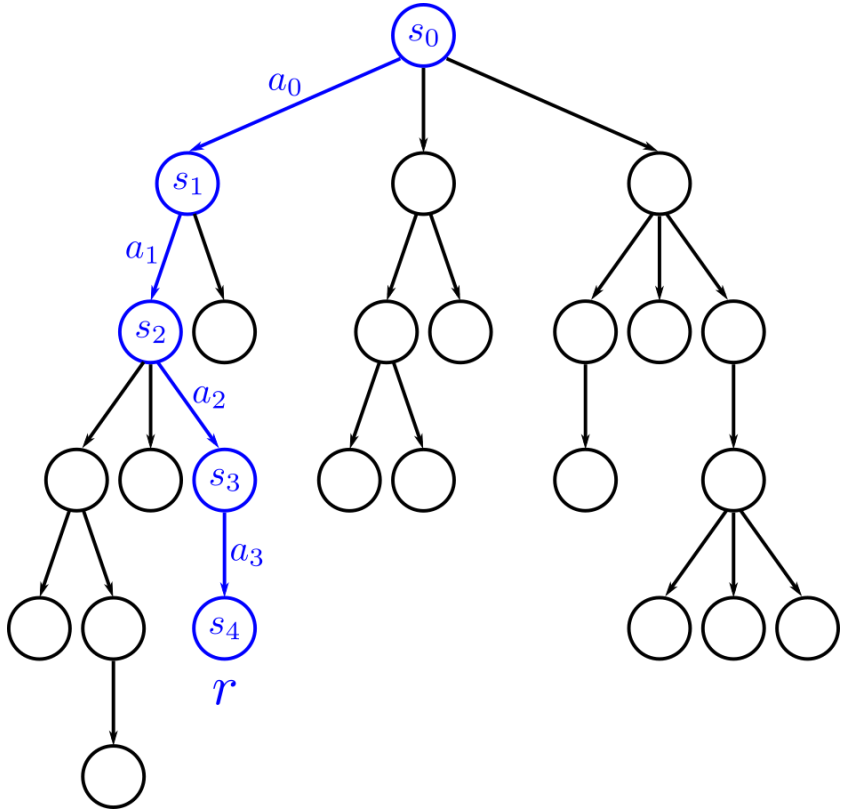

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A *playout* is a ***path*** $\langle s_0, a_0, s_1, \ldots, a_{T-1}, s_T \rangle$
from the *initial state* s_0 to a *terminal state* s_T

A *reward* r is the outcome of a playout

A *policy* is a map $\pi : \ s \mapsto a$ which selects action a to be executed in state s

Policy optimization

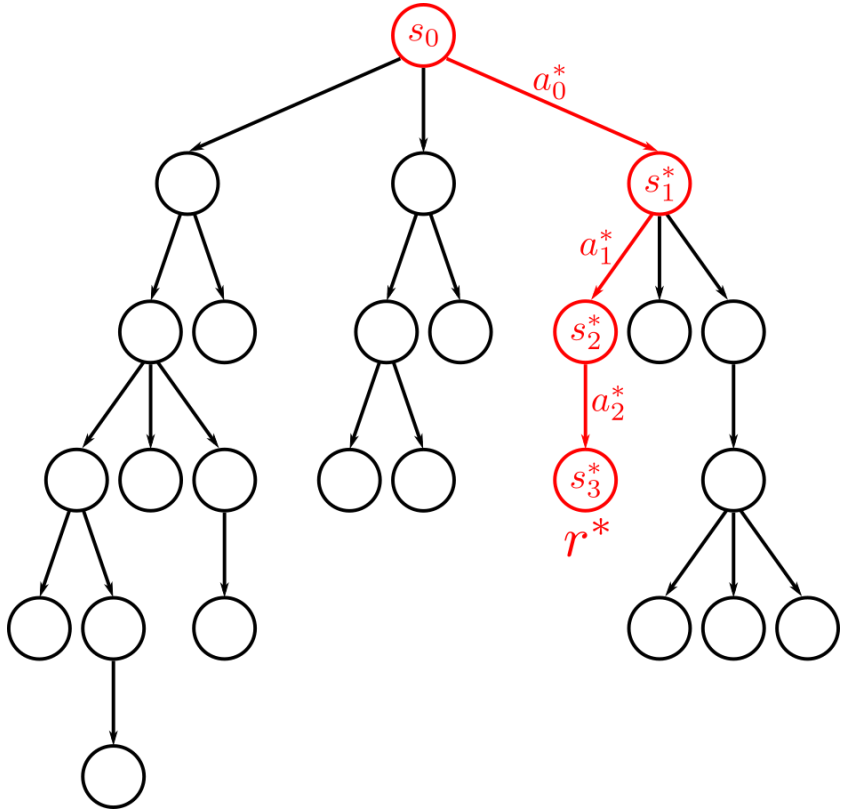
- Goal: finding the *best policy* π^*

  such that the reward r^* of playout

  $$\langle s_0, a_0^*, s_1^*, \ldots, a_{T-1}^*, s_T^* \rangle$$

  with $a_t^* := \pi^*(s_t^*)$ and $s_{t+1}^* := \tau(s_t^*, a_t^*)$

  is ***maximal***



"Brute Force": a simple (bad) policy optimization

- Goal: finding the *best policy* π^*

- ***"Brute Force"***:
  1. explore the entire tree by following **all** possible paths
  2. select the path(s) with the best outcome (and randomly choose one of them)
  3. play by following the policy associated with that path

  Possible problems:
  - ***Huge game tree*** making full exploration unfeasible
    (branching factor in Go is around 200)
  - Intrinsic ***stochasticity*** and/or ***uncertainty*** of transitions

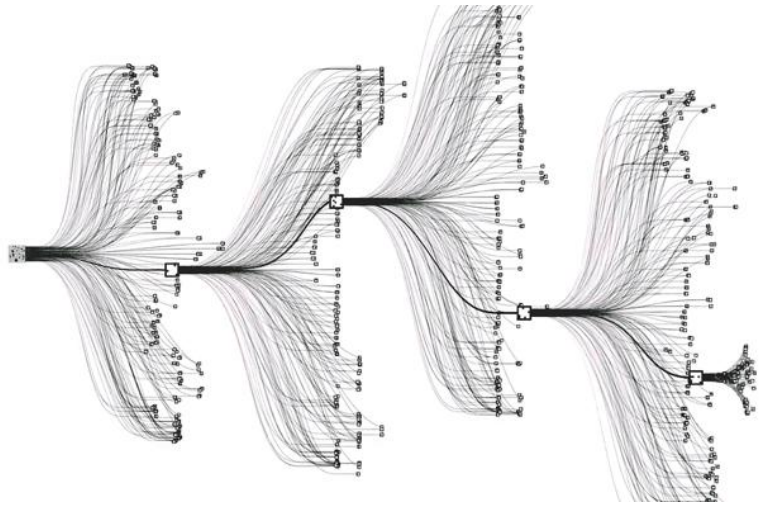


Image from https://thenewstack.io/google-ai-beats-human-champion-complex-game-ever-invented/

Stochasticity and Uncertainty: examples

- ***Multi-armed bandits***

  The reward after each action is *stochastic*

  i.e. which arm to play

  random variable

  probability of reward r for action a

$$Q(s,a) := \mathbb{E}[R \mid s,a] = \sum_r r\, P(r \mid s,a)$$

Q-value (expected reward of action a performed in state s)

- ***Games with two players (White and Black):***

  White plays action a_t in state s_t

  but the next state s_{t+1} depends on Black's next action

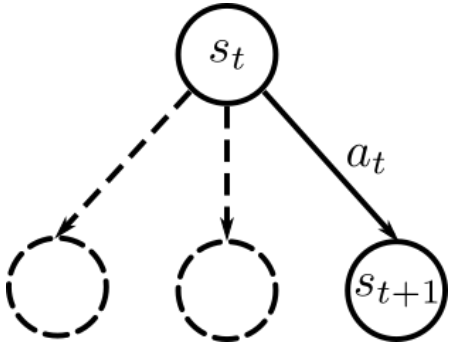
  Uncertainty of execution:
  nondeterministic $\tau : (s_t, a_t) \mapsto s_{t+1}$ as $P(s_{t+1} \mid s_t, a_t)$

  transition function

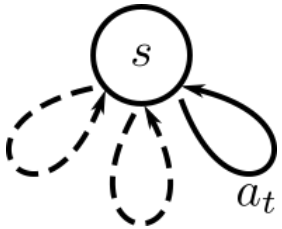
  probability transition distribution

Stochasticity and Uncertainty: tree representation

- ***Simplest case scenario***
  - deterministic transition
  - deterministic reward

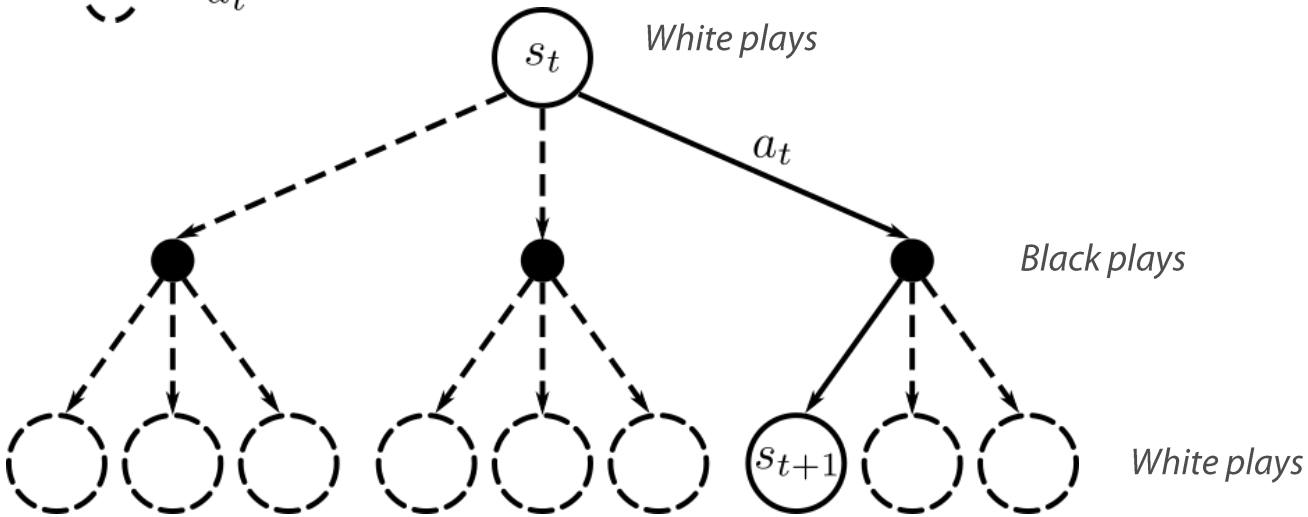


- ***Multi-armed bandits***
  - deterministic transition
  - stochastic reward



Actually, this is not a tree!
(but it can be expanded and became one)

- ***Uncertainty of next state***
  - stochastic transition
  - deterministic transition but with two or more players



Monte Carlo method: step-wise simulations

Monte Carlo (MC) step

- Goal: finding the *best policy* π^* *(avoiding brute-force approach)*

  It can be done iteratively, by focusing on the single best action $a^* =: \pi^*(s)$ in the current state s

- ***Monte Carlo (MC)** step:* [Abramson 1990]

repeat n times

1) perform a *random playout* from current state s
2) compute and save the reward r obtained at the end of the playout
3) for each admissible action a in state s compute the mean of the rewards

$$\hat{Q}(s,a) := \frac{1}{N(s,a)} \sum_{i=1}^{N(s,a)} r_{a,i}$$

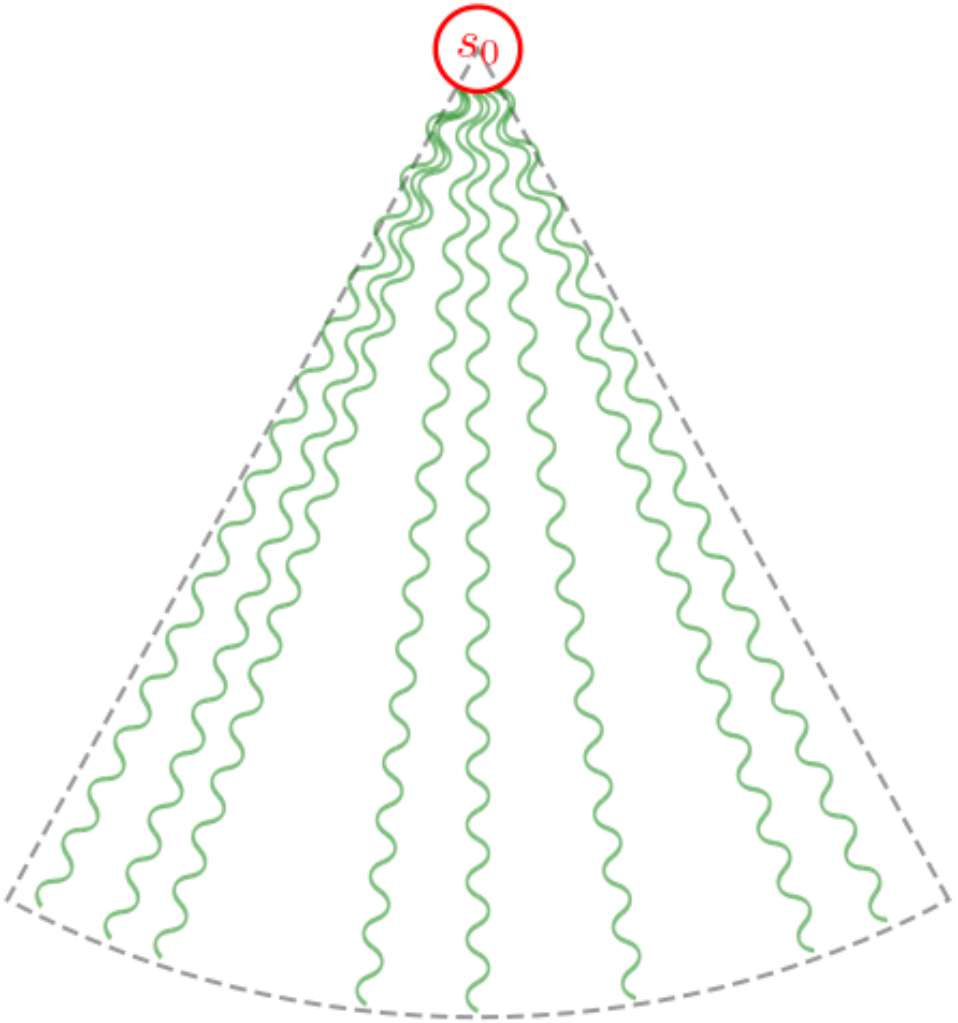
$N(s,a)$: number of playouts with first action a

$r_{a,i}$: reward of i^{th} playout with first action a

4) select $a^* := \text{argmax}_a \hat{Q}(s,a)$, *the action with the highest mean*

Monte Carlo episode

- ***Monte Carlo*** *episode:*
  1) set $t{:=}0$
  2) current state $s{:=}s_t$
  3) use *MC step* to decide a_t
  4) compute $s_{t+1} := \tau(s_t, a_t)$
  5) set $t{:=}t{+}1$
  6) repeat 2) to 5) until *end game*



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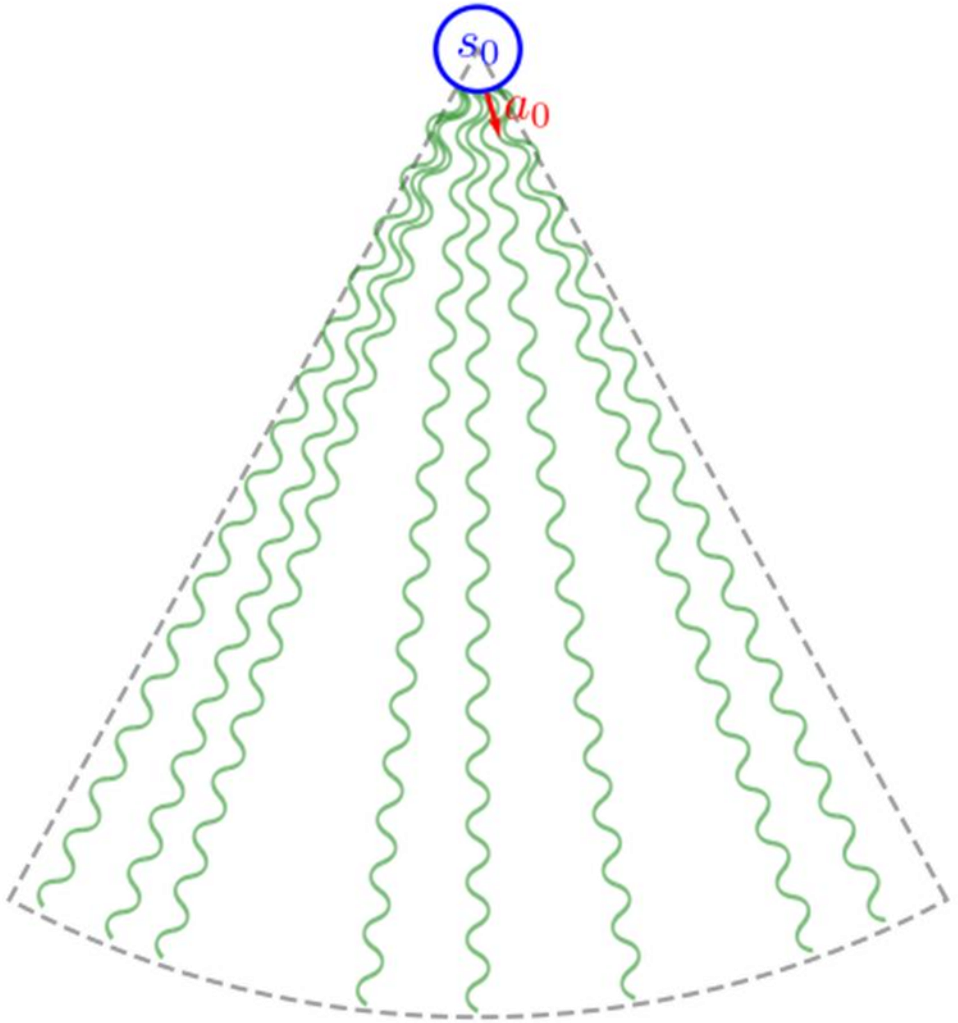

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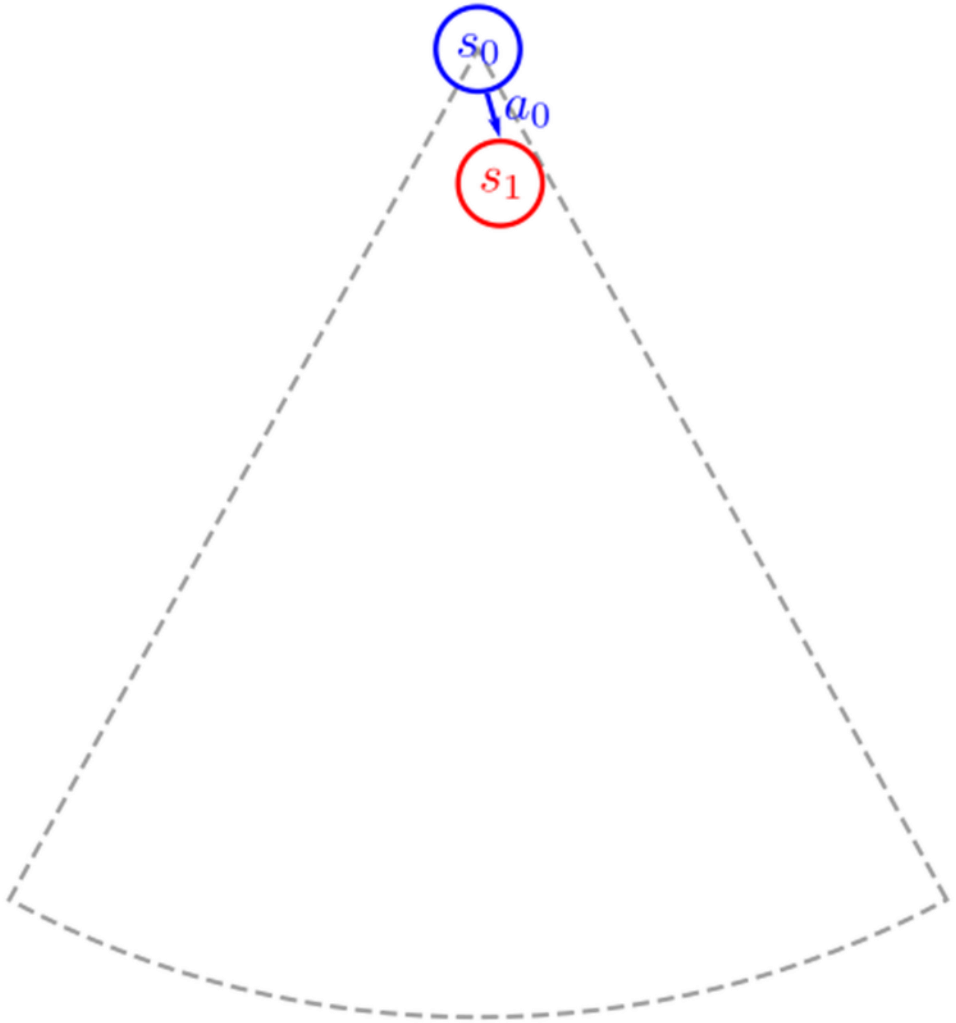

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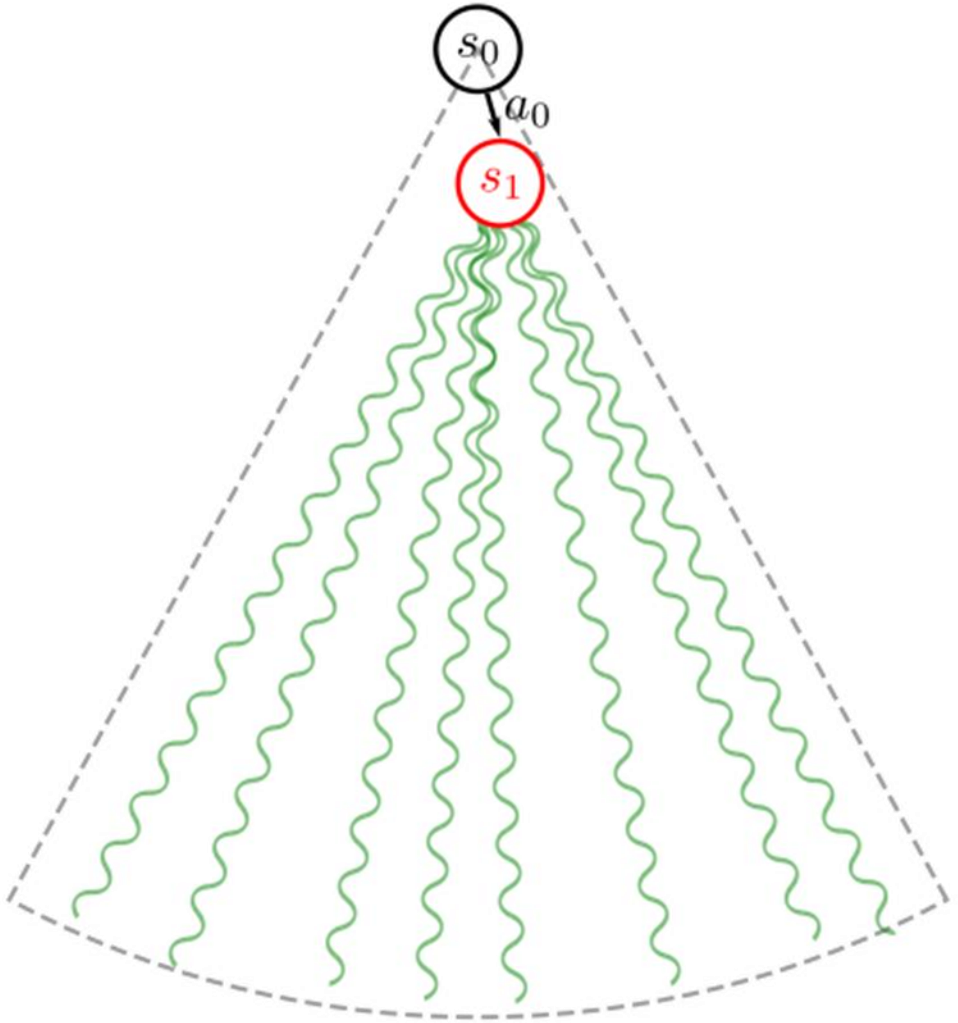

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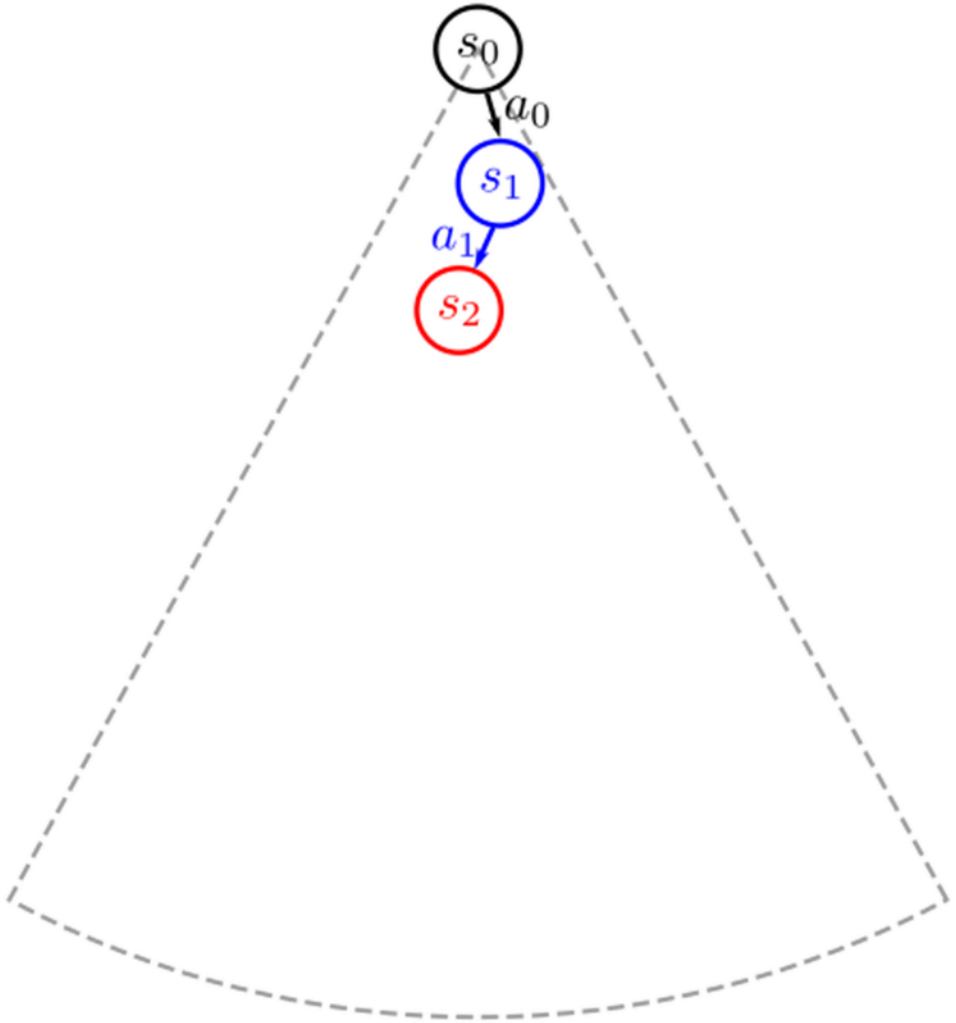

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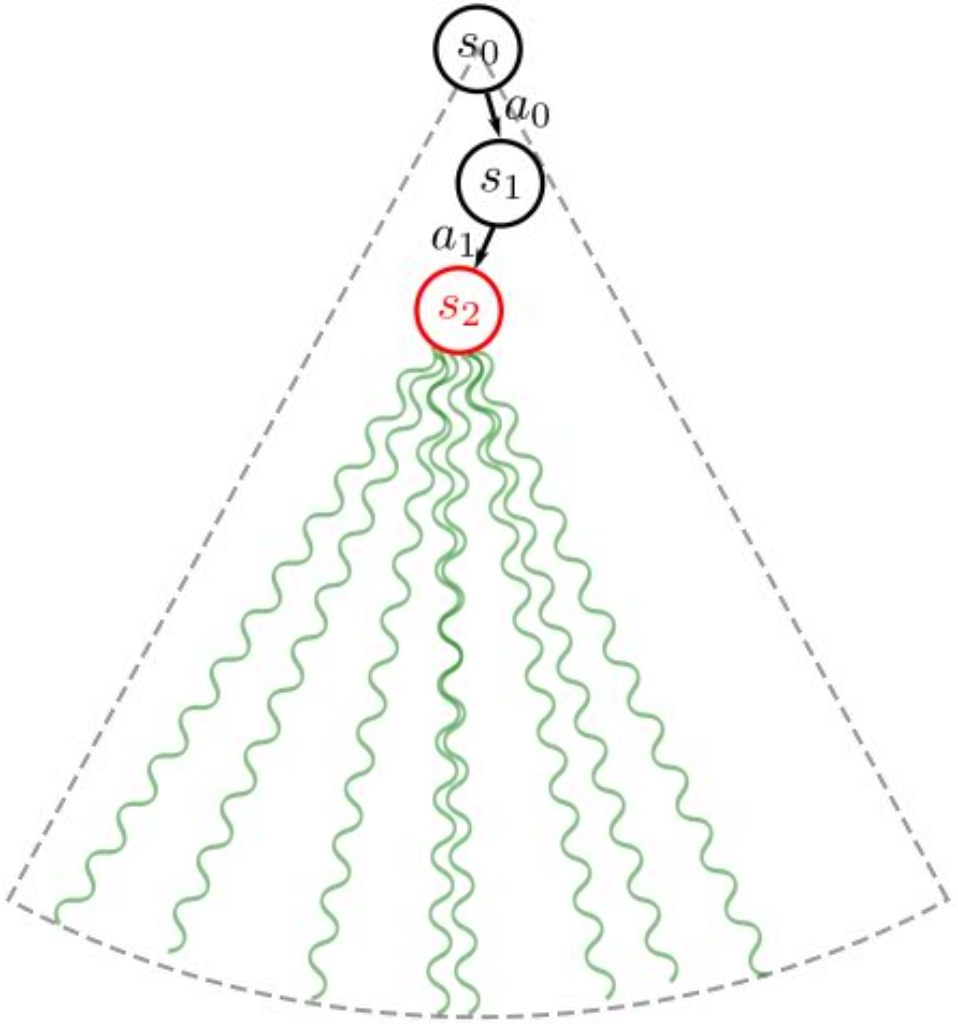
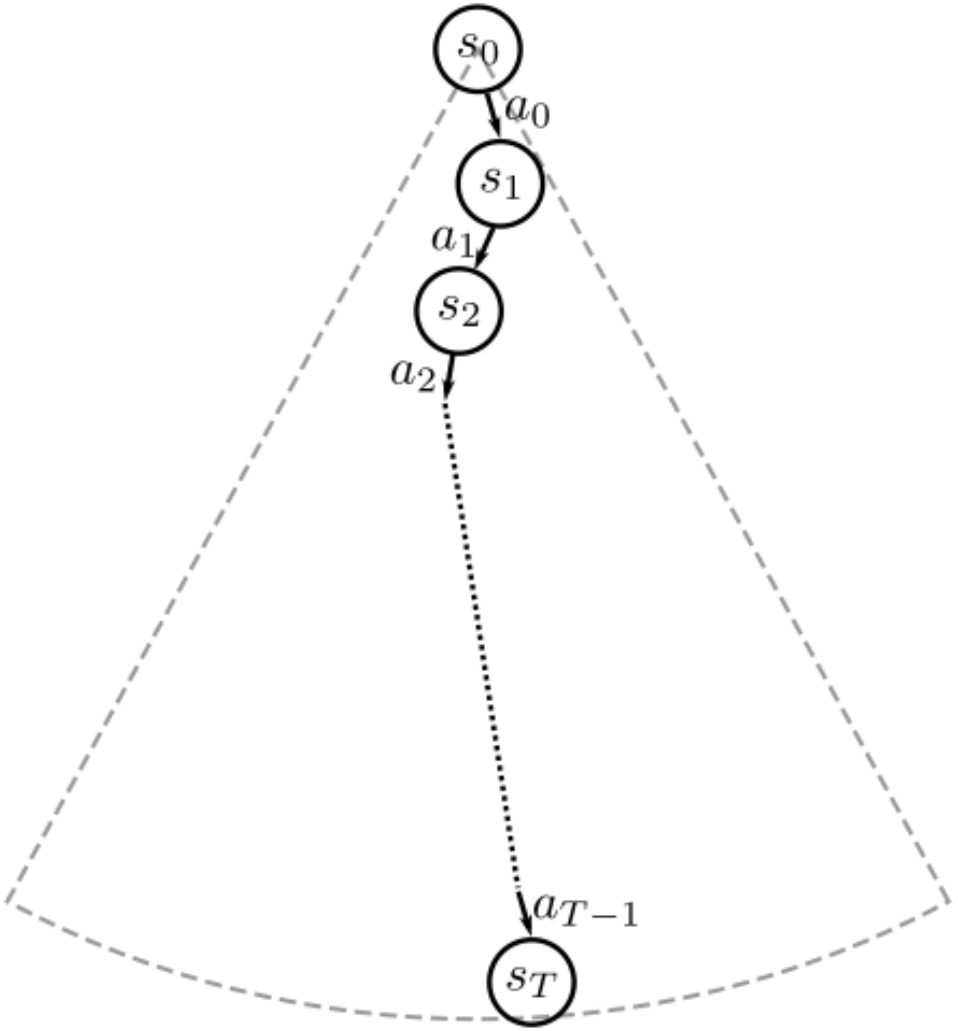


Monte Carlo method

- ***Monte Carlo*** *method:*
  - *no memory* of past playouts in a single *MC step*
    (only the reward is saved)
  - no *transfer knowledge* between *MC steps*
  - *no knowledge transfer* between *MC episodes*
  - optimal policy only *partially* identified
    (on visited states only)
  - *intrinsically stochastic* policy optimization
    (the same game state can yield different action choices)

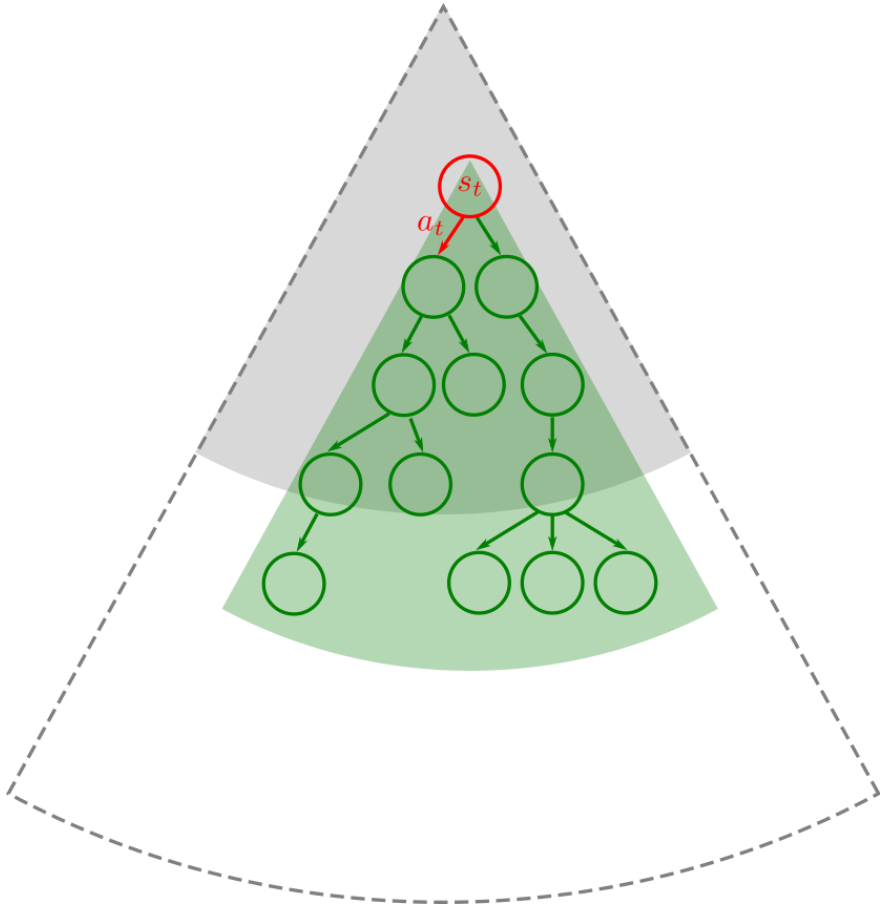


Monte Carlo Tree Search (MCTS):

simulation + incremental expansion

MCTS episode: basic idea

- *At each step (with current state s_t):*
  - a *subgraph* G_t with root s_t is created
  - *statistics* (*number of visits* and *estimate outcomes*) for states and actions in the subgraph are saved
  - best action a_t is decided *(accordingly to those statistics)*
  - next state $s_{t+1} := \tau(s_t, a_t)$ is computed



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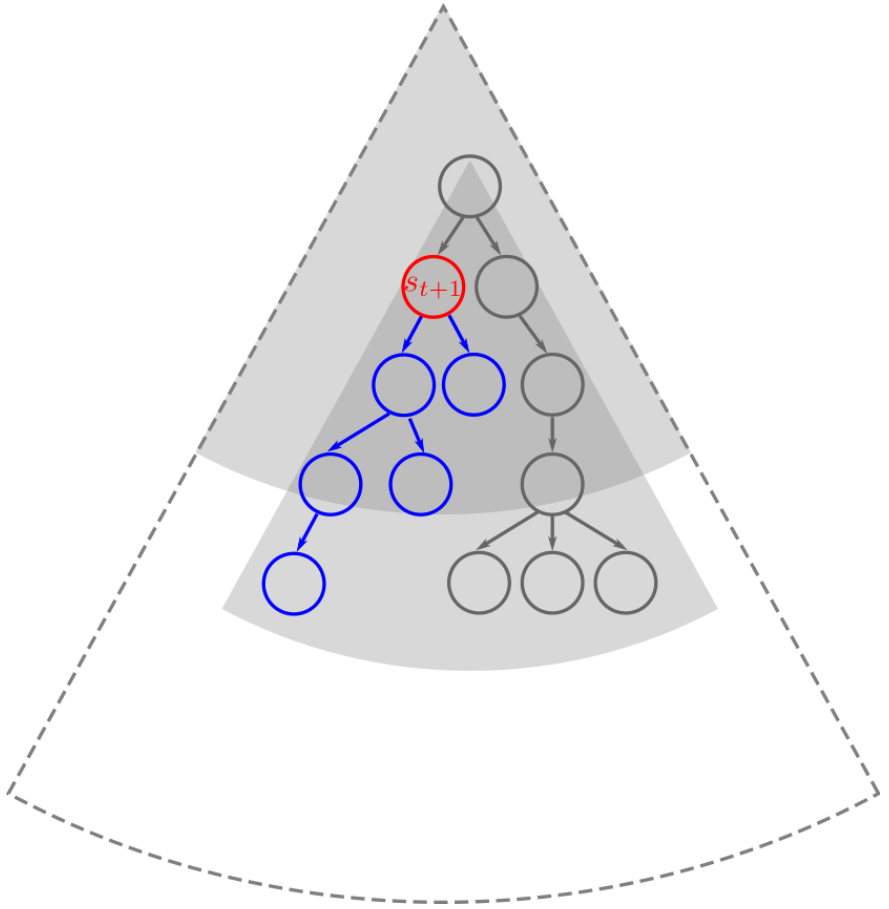
- *In the next step (with current state s_{t+1}):*
  - the subgraph of G_t with root s_{t+1} is *expanded* to create G_{t+1}
  - the statistics are *updated* and saved
  - best action a_{t+1} is decided
  - next state $s_{t+1} := \tau(s_t, a_t)$ is computed



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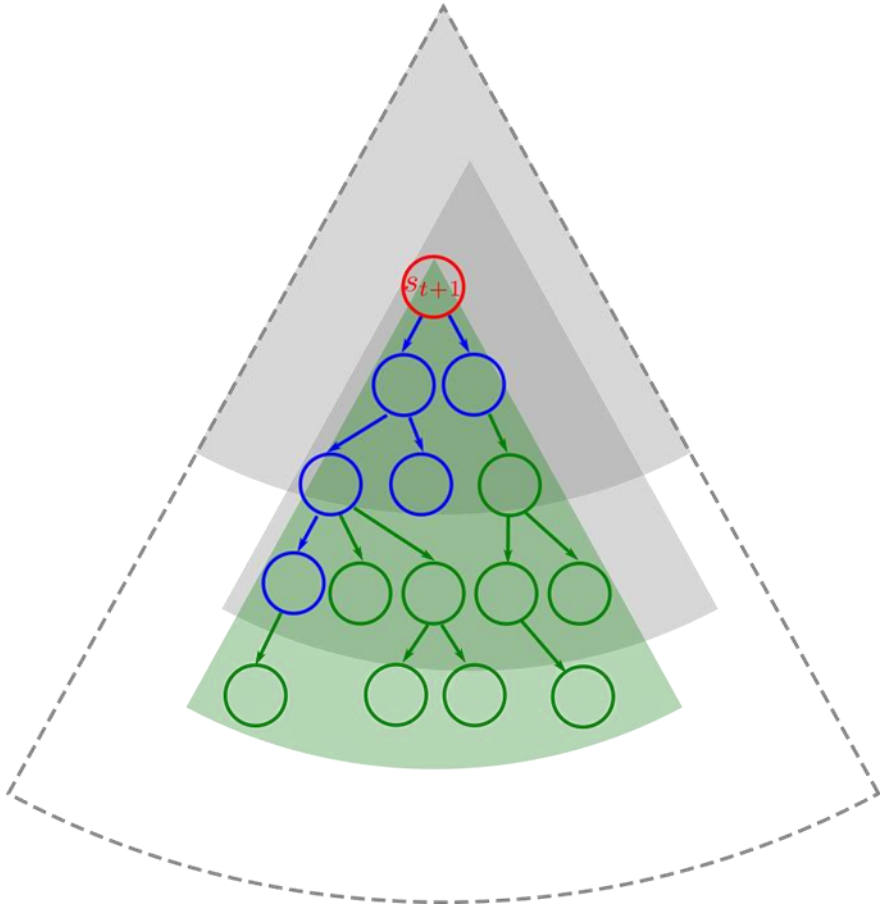
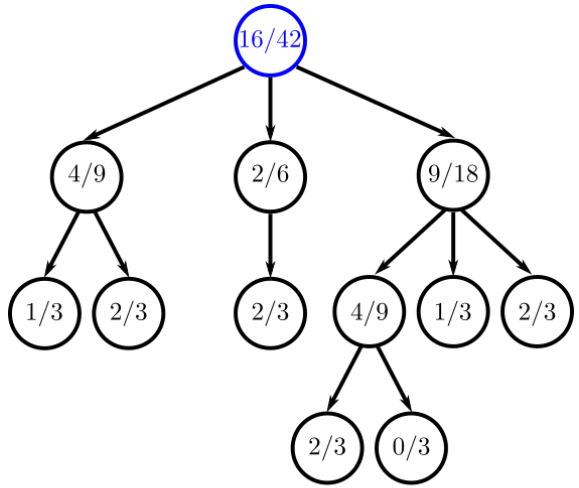


Monte Carlo Tree Search (MCTS) step

- ***Monte Carlo Tree Search (MCTS)*** *step:* [Coulom 2006]

  1) start from current state s *(and the –possibly empty– stored tree with root s)*



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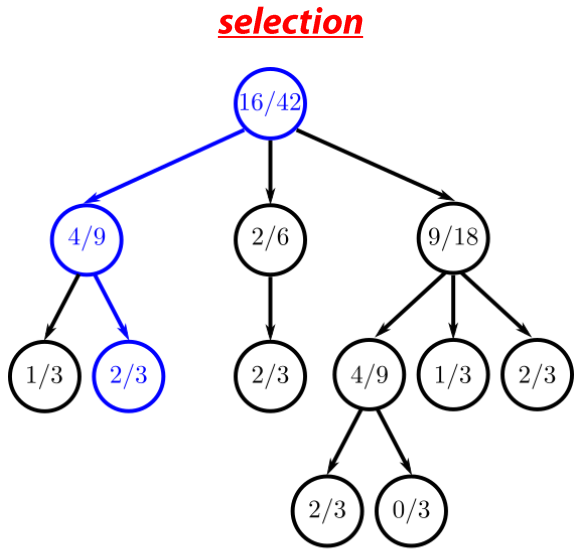
     $$\pi^{\text{sel}} : \; s_t \mapsto a_t$$

     until encountering a *leaf node* s_L (i.e. a state not stored in the tree)



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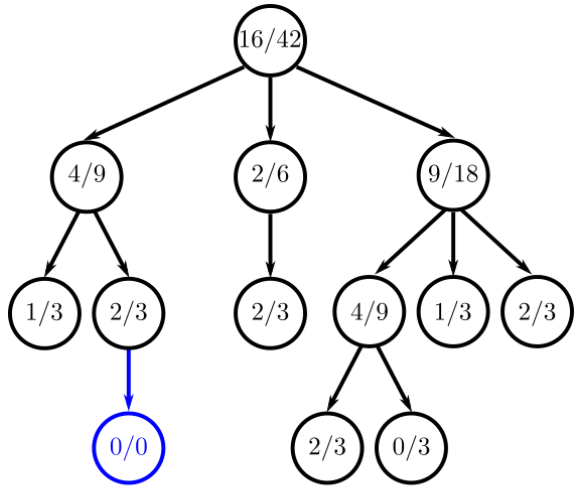
  3) *expand* the tree by adding s_L

expansion



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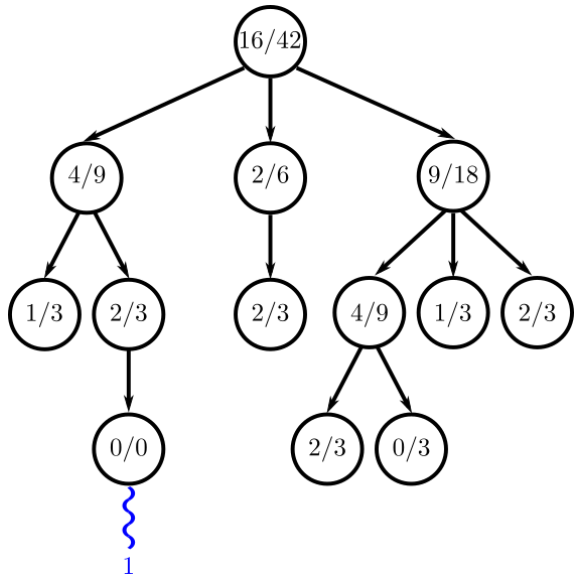
3) *expand* the tree by adding s_L

4) play one random playout from state s_L by following the *simulation policy*

$$\pi^{\text{sym}} : \; s_t \mapsto a_t$$

and obtain the reward r

simulation



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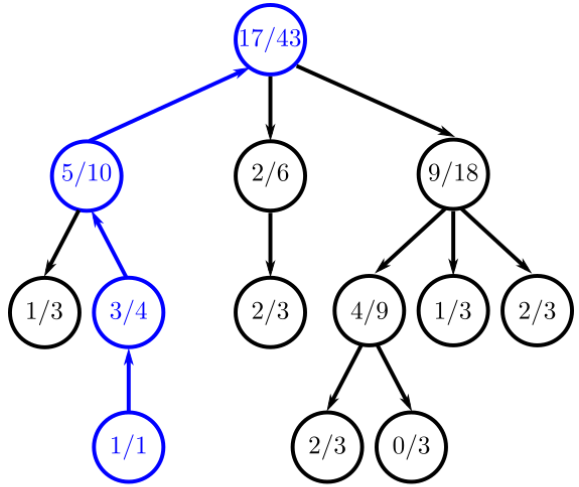
5) *backpropagate* r (and update the statistics of each encountered state and action)

backpropagation



Monte Carlo Tree Search (MCTS) step

- ***Monte Carlo Tree Search (MCTS)*** *step:* [Coulom 2006]

repeat m times

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2) traverse the tree by following the *selection policy*
$$\pi^{\text{sel}} : \; s_t \mapsto a_t$$
until encountering a *leaf node* s_L (i.e. a state not stored in the tree)
3) *expand* the tree by adding s_L

repeat n times

4) play one random playout from state s_L
by following the *simulation policy*
$$\pi^{\text{sym}} : \; s_t \mapsto a_t$$
and obtain the reward r
5) *backpropagate* r (and update the statistics of each encountered state and action)

6) decide the *best* action to be performed in s with the *greedy policy*
$$\pi^{\text{gre}} : \; s \mapsto a$$

MCTS statistics: expansion and backpropagation

- ***MCTS** statistics* for state s and action a:

  $N(s)$ = total number of times state s has been visited

  $N(s, a)$ = number of times action a has been selected in state s

  $\hat{Q}(s, a)$ = estimated outcome of action a when selected in state s

- *Expansion initialization:* $N(s) := 0, \quad N(s, a) := 0, \quad \hat{Q}(s, a) := 0$

- *Backpropagation update* after a single playout with reward r:

$$N(s) := N(s) + 1$$
$$N(s, a) := N(s, a) + 1$$
$$\hat{Q}(s, a) := \hat{Q}(s, a) + \frac{r - \hat{Q}(s, a)}{N(s, a)}$$

MCTS: greedy, selection and simulation policies

- *Greedy* policy:

$$\pi^{\text{gre}}(s) := \underset{N(s,a)>0}{\text{argmax}}\, \hat{Q}(s,a)$$

- *Selection* policy: ***Upper Confidence Bound applied to Trees (UCT)***

$$\pi^{\text{sel}}(s) := \pi^{\text{UCT}}(s) := \underset{a}{\text{argmax}} \left\{ \hat{Q}(s,a) + c\sqrt{\frac{2\log N(s)}{N(s,a)+\epsilon}} \right\}$$

parameter (default=1)

exploitation of actions that look currently the best

exploration of currently suboptimal-looking actions (no good alternatives are missed because of early estimation errors)

Convergence [Kocsis 2006]: for the first state s of a single *MCTS* episode

$$\pi^{\text{UCT}}(s) \to a^* := \pi^*(s) \quad \text{for } n \to +\infty$$

MCTS: greedy, selection and simulation policies

- *Greedy* policy:

$$\pi^{\mathrm{gre}}(s) := \operatorname*{argmax}_{N(s,a)>0} \hat{Q}(s,a)$$

- *Selection* policy: ***Upper Confidence Bound applied to Trees (UCT)***

$$\pi^{\mathrm{sel}}(s) := \pi^{\mathrm{UCT}}(s) := \operatorname*{argmax}_{a} \left\{ \hat{Q}(s,a) + c\sqrt{\frac{2\log N(s)}{N(s,a)+\epsilon}} \right\}$$

- *Simulation* policy: ***Random Uniform Policy***

$$\pi^{\mathrm{sym}}(s) := a \qquad \text{with } P(a \mid s) = \frac{1}{|\mathcal{A}(s)|}$$

$\mathcal{A}(s)$: set of admissible actions in state s