Deep Learning

A course about theory & practice

Monte Carlo Tree Search (MCTS)

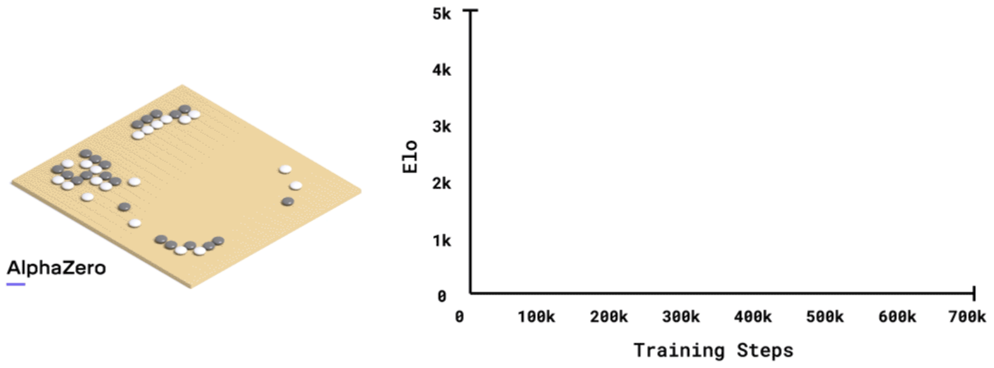
Marco Piastra

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

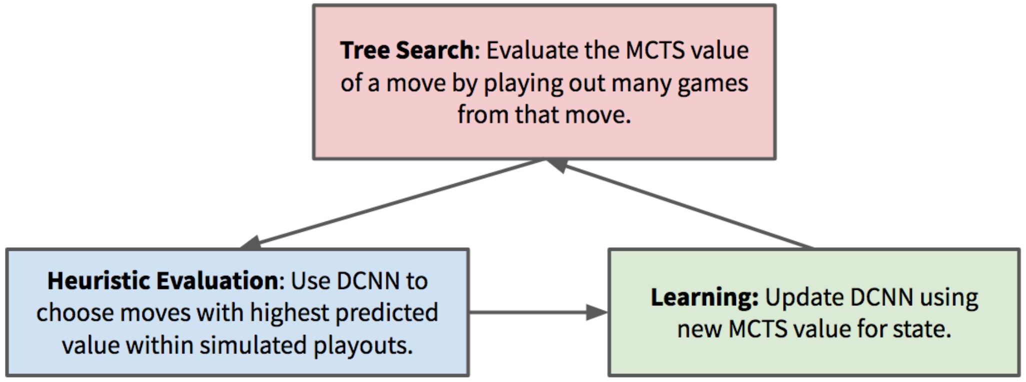


Image from: https://nikcheerla.github.io/deeplearningschool/2018/01/01/AlphaZero-Explained/

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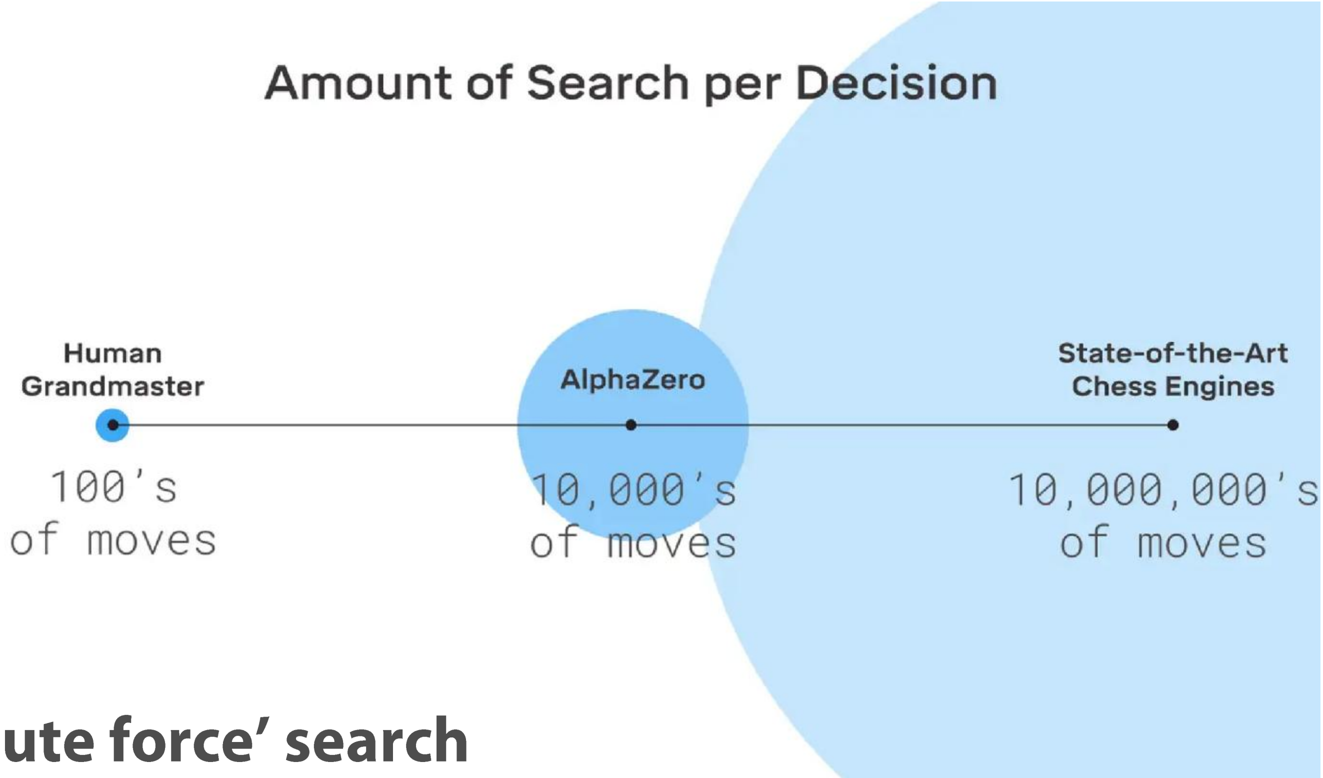


- **AlphaZero uses much less 'brute force' search**
  - When playing, the search process is driven by its neural network
    - *It acts like a memory of past experiences*
  - While training, it learns through a huge amount of self-playing
    - *But it is a faster learner than Alpha Go*

Playing Games with Trees

Tree representation

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

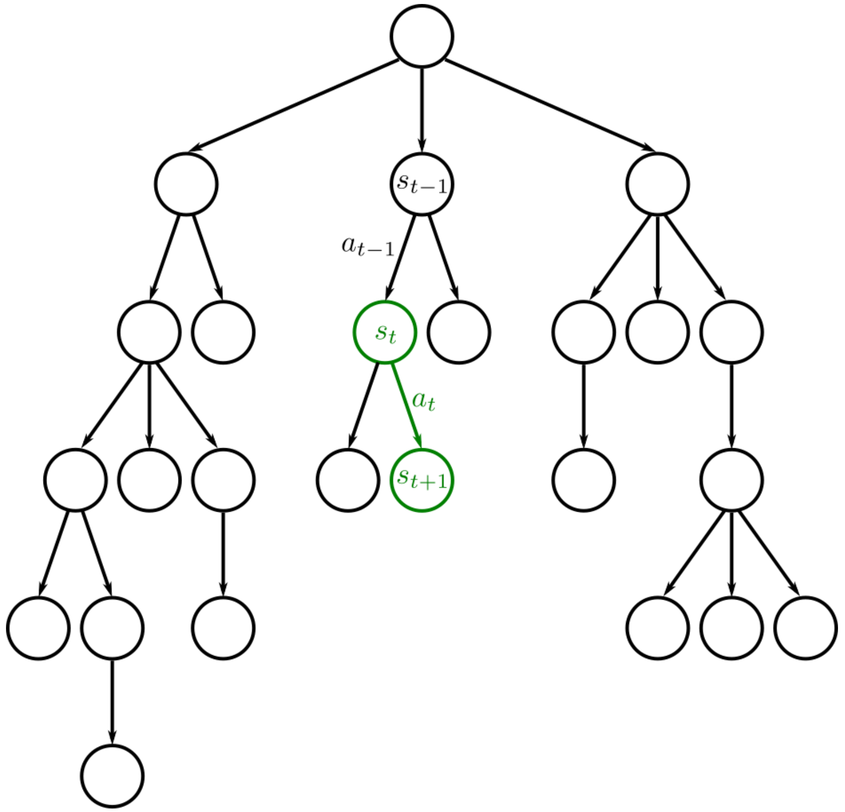
  The *current state* s_t at time t is a ***node*** with depth t

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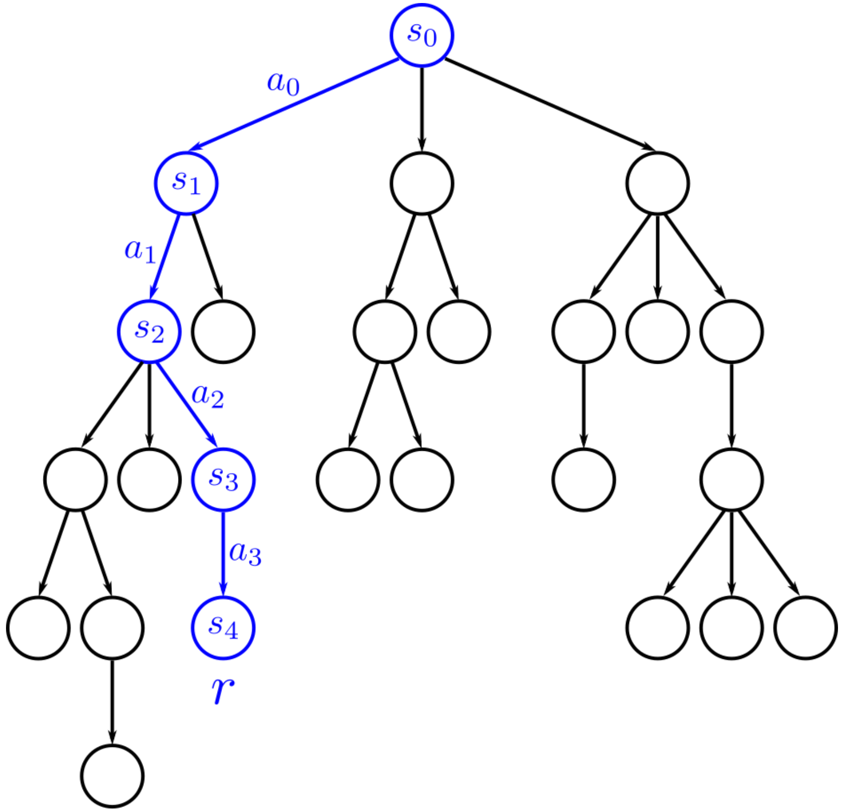
  A *playout* is a **path** $\langle s_0, a_0, s_1, \ldots, a_{T-1}, s_T \rangle$ from the *initial state* s_0 to a *terminal state* s_T

  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

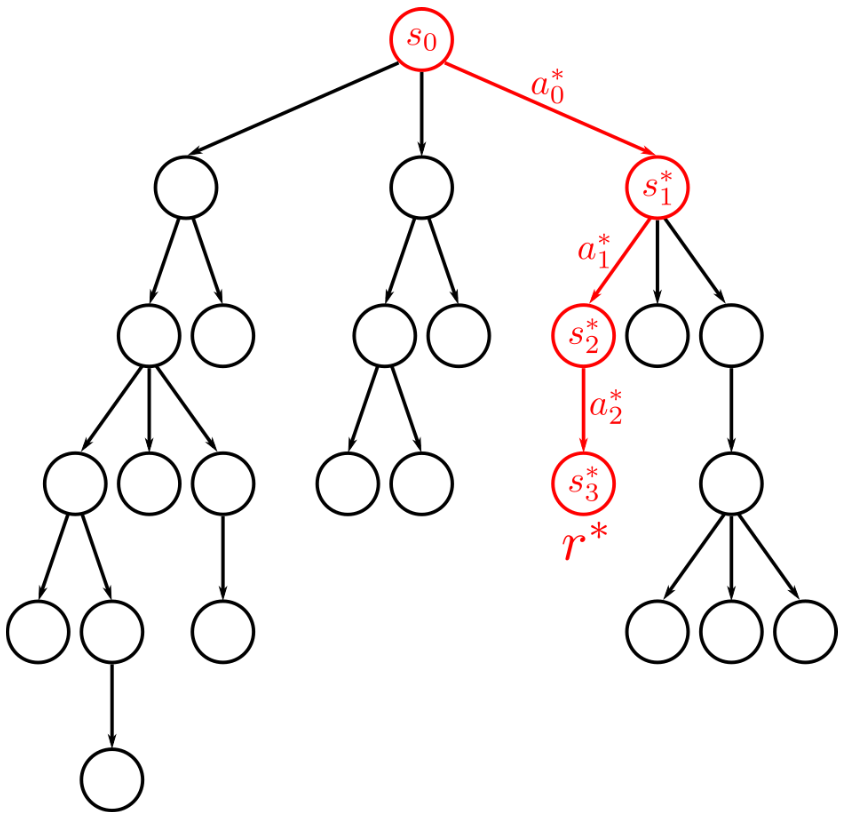
- Goal: finding the *best policy* π^*

  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

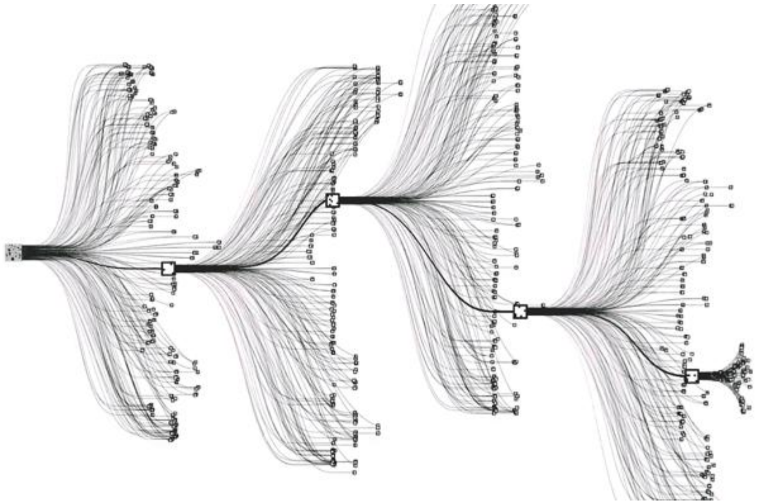


Image from https://thenewstack.io/google-ai-beats-human-champion-complex-game-ever-invented/

Stochasticity and Uncertainty: examples

- ***Multi-armed bandits***

  i.e. which arm to play

  The reward after each action is *stochastic*

  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):***

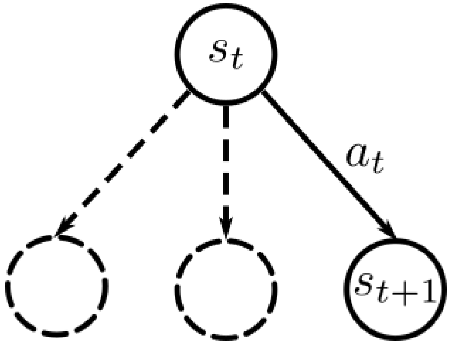
  White plays action a_t in state s_t
  but the next state s_{t+1} depends on Black's next action

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

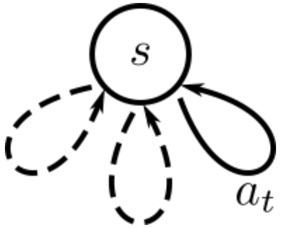
  transition function *probability transition distribution*

Stochasticity and Uncertainty: tree representation

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

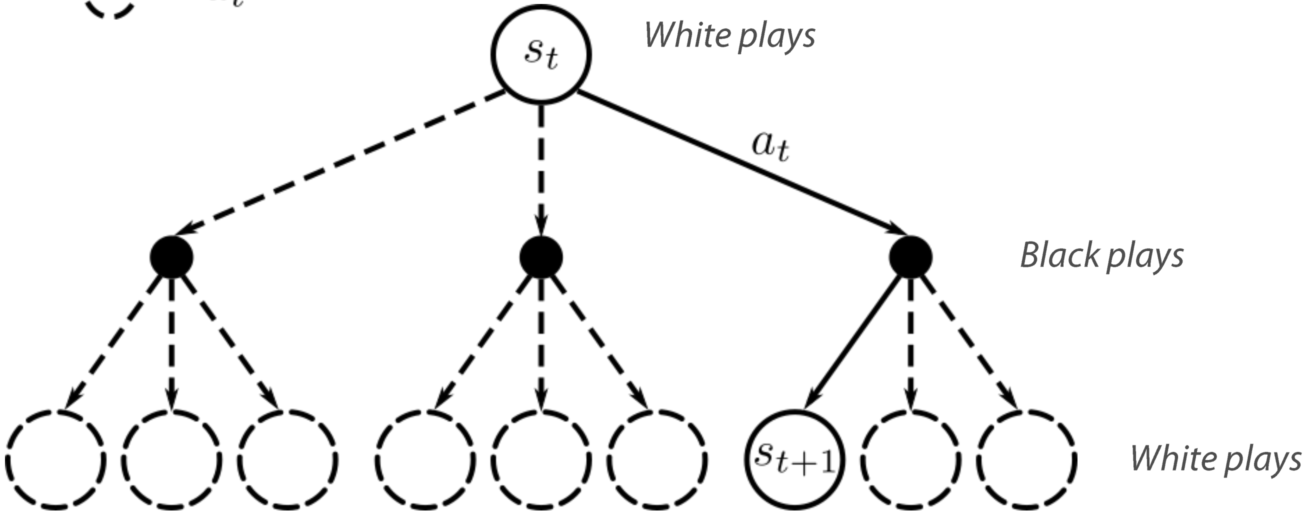


- ***Multi-armed bandits***
  - deterministic transition
  - stochastic reward



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 <u>*best policy*</u> 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 <u>*random*</u> *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

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

estimates $Q(s,a)$

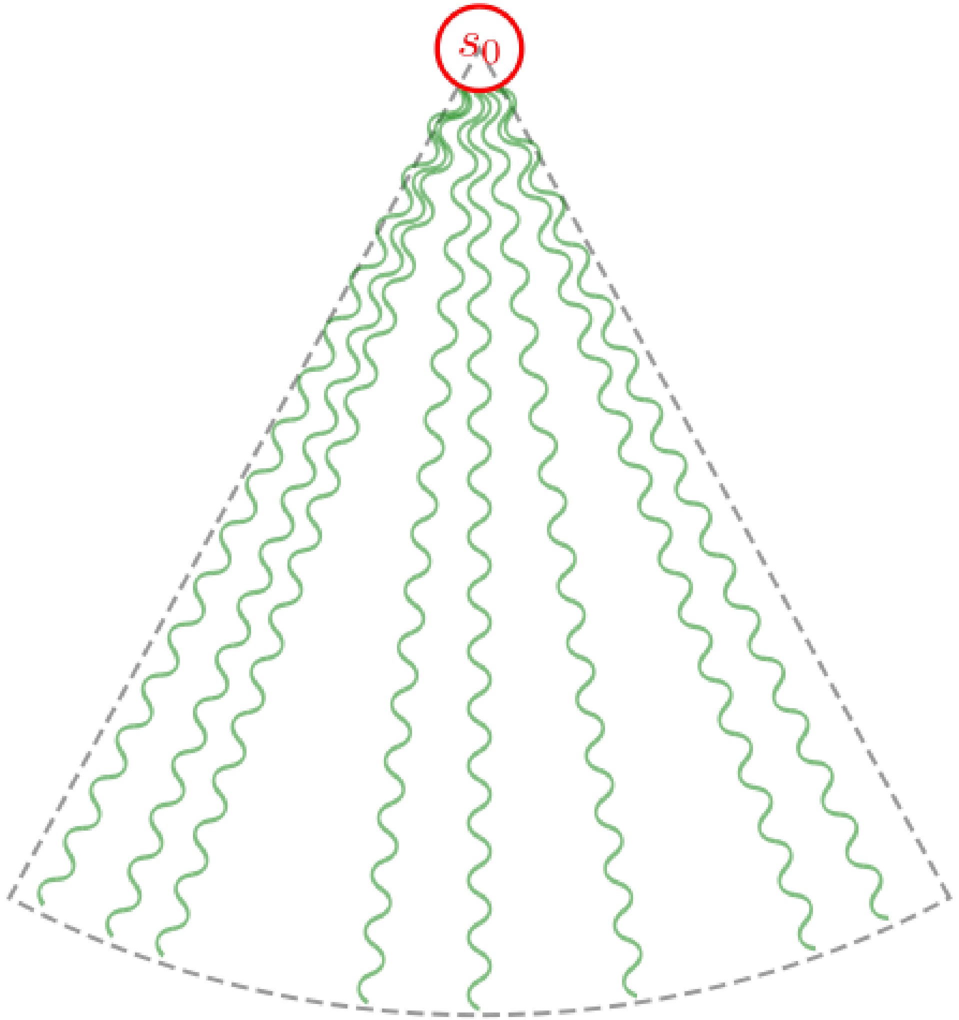
number of playouts with first action a

reward of i^{th} playout with first action a

4) $a^* := \text{argmax}_a \hat{Q}(s,a)$ is 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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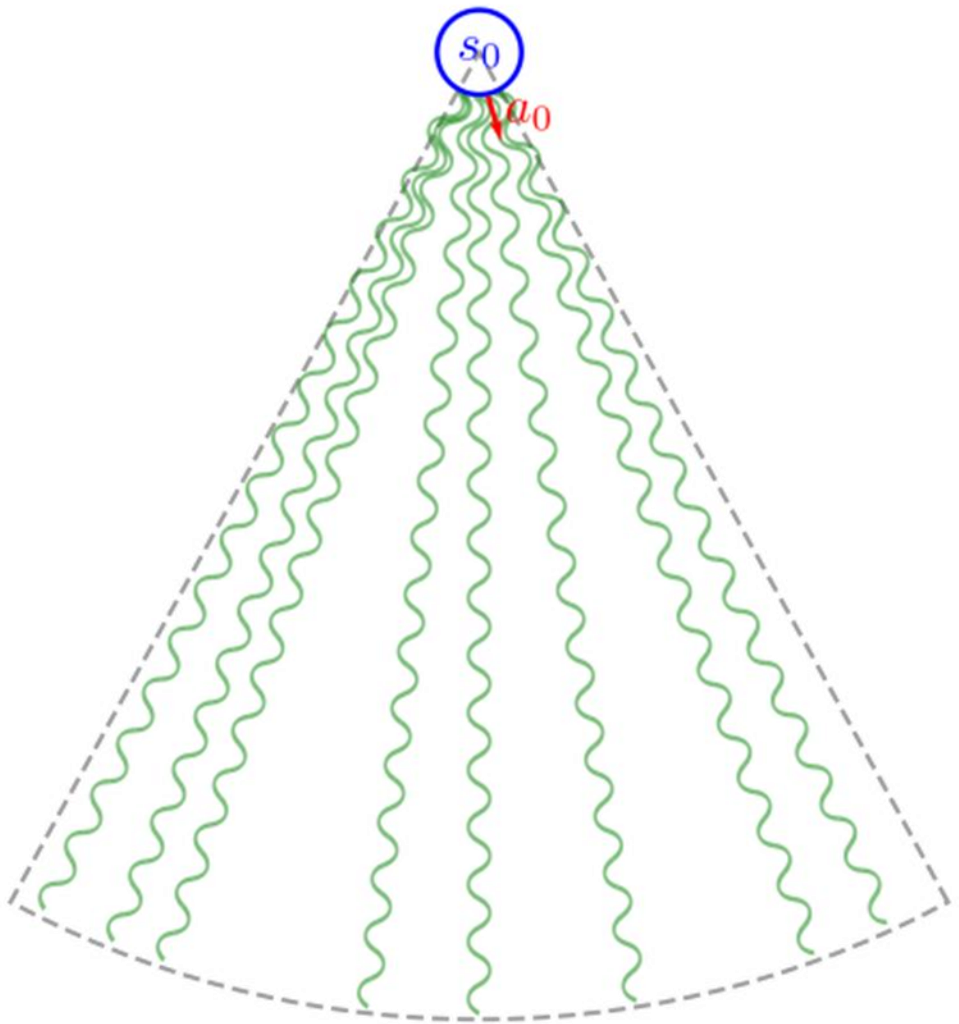

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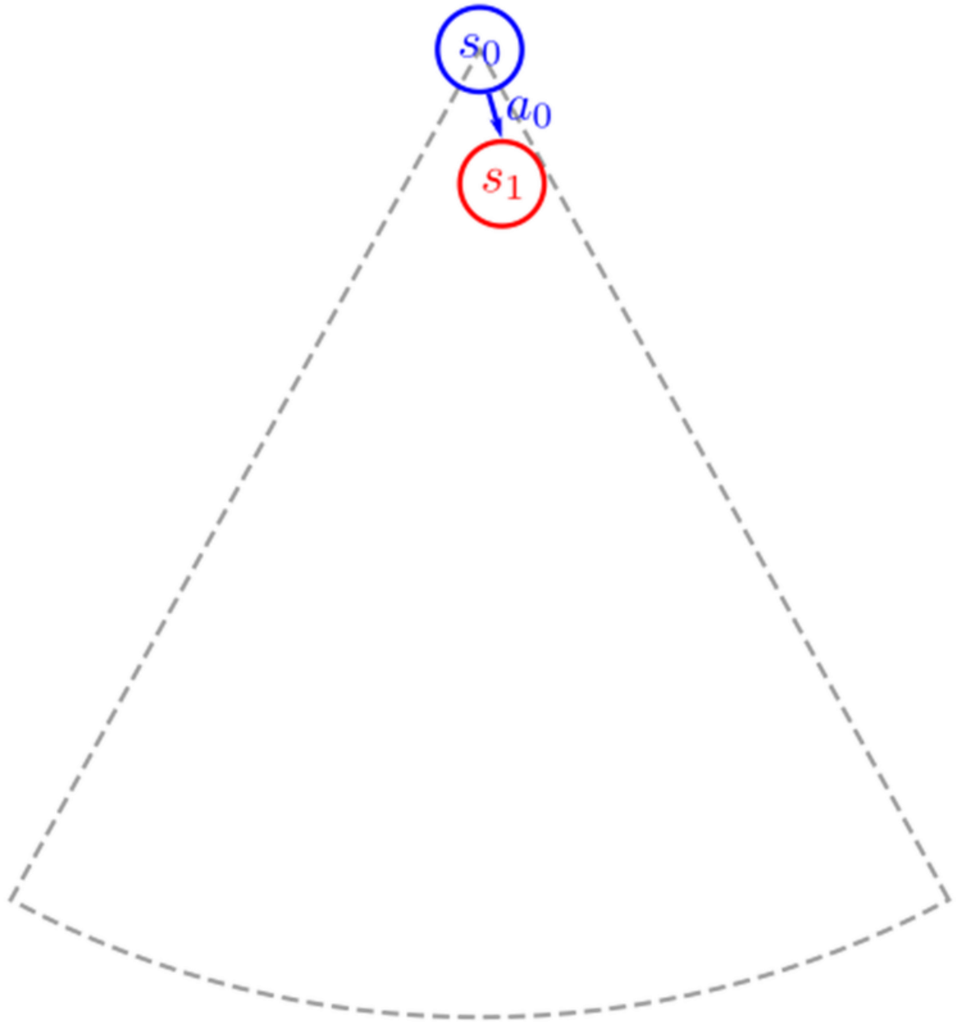

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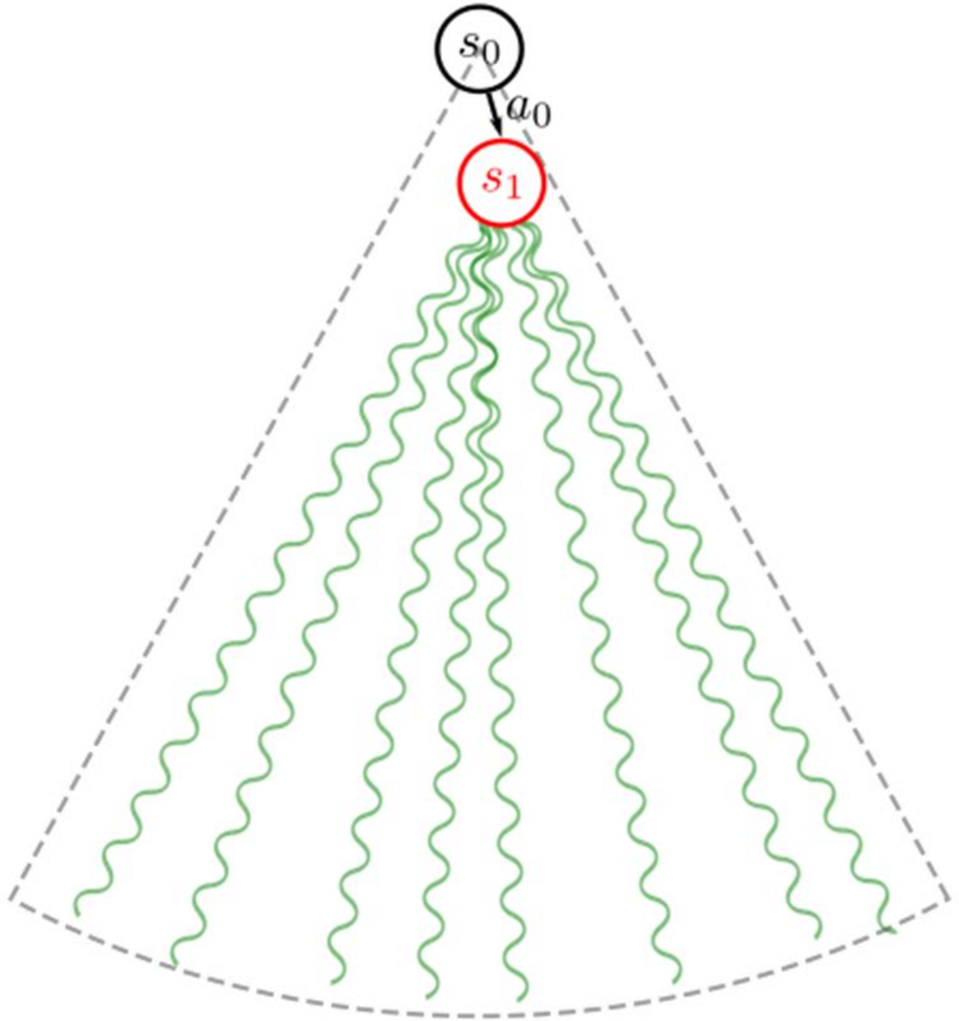

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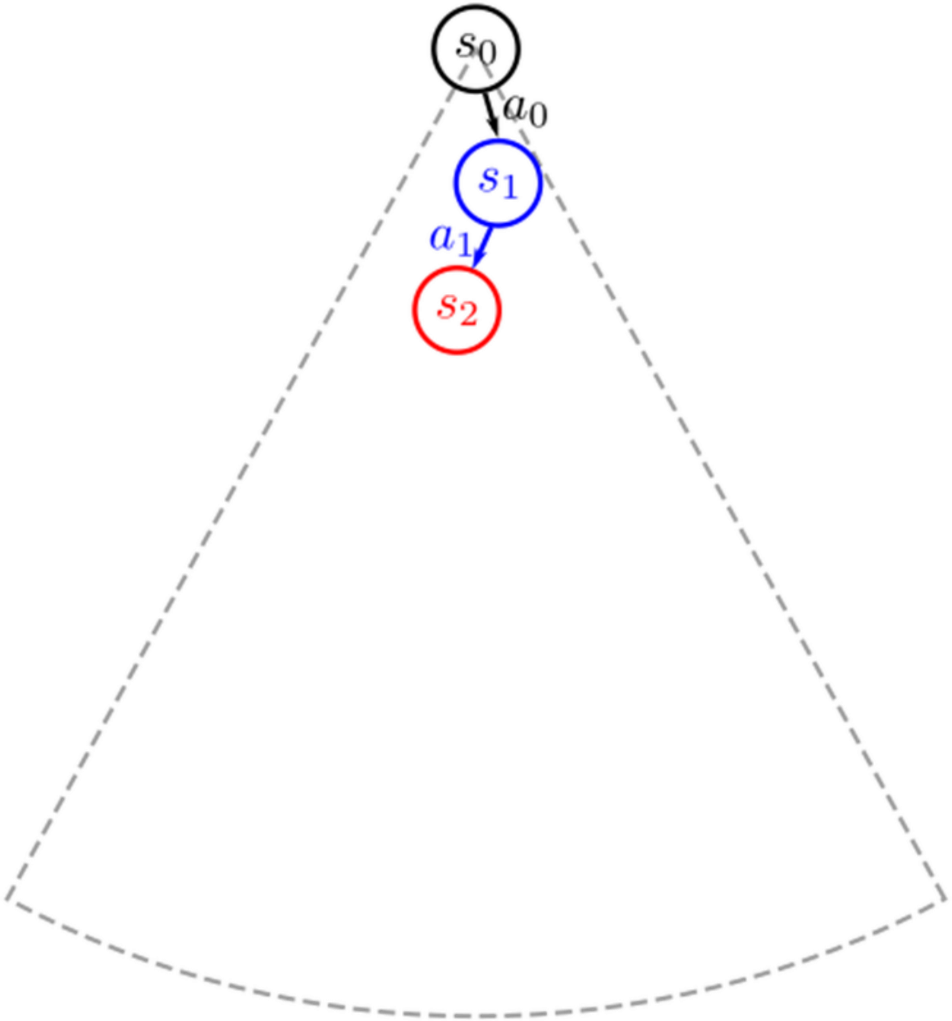

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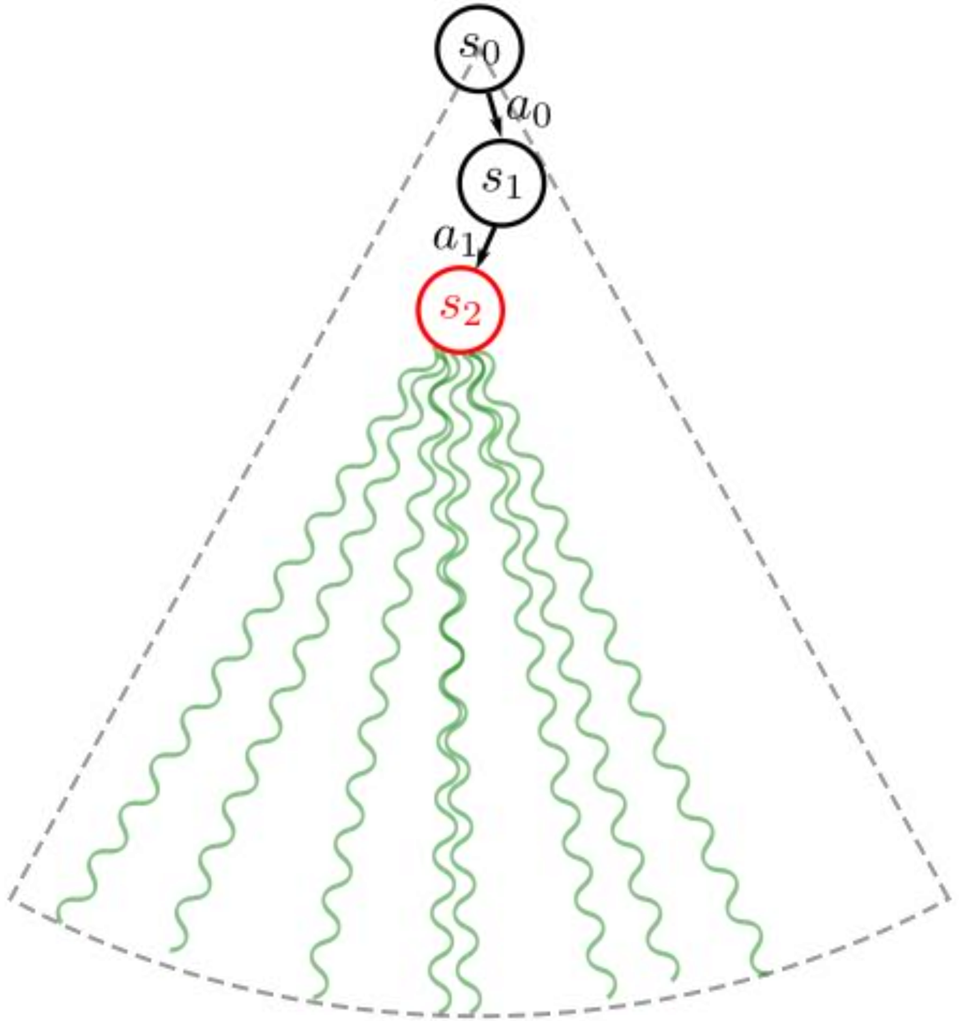
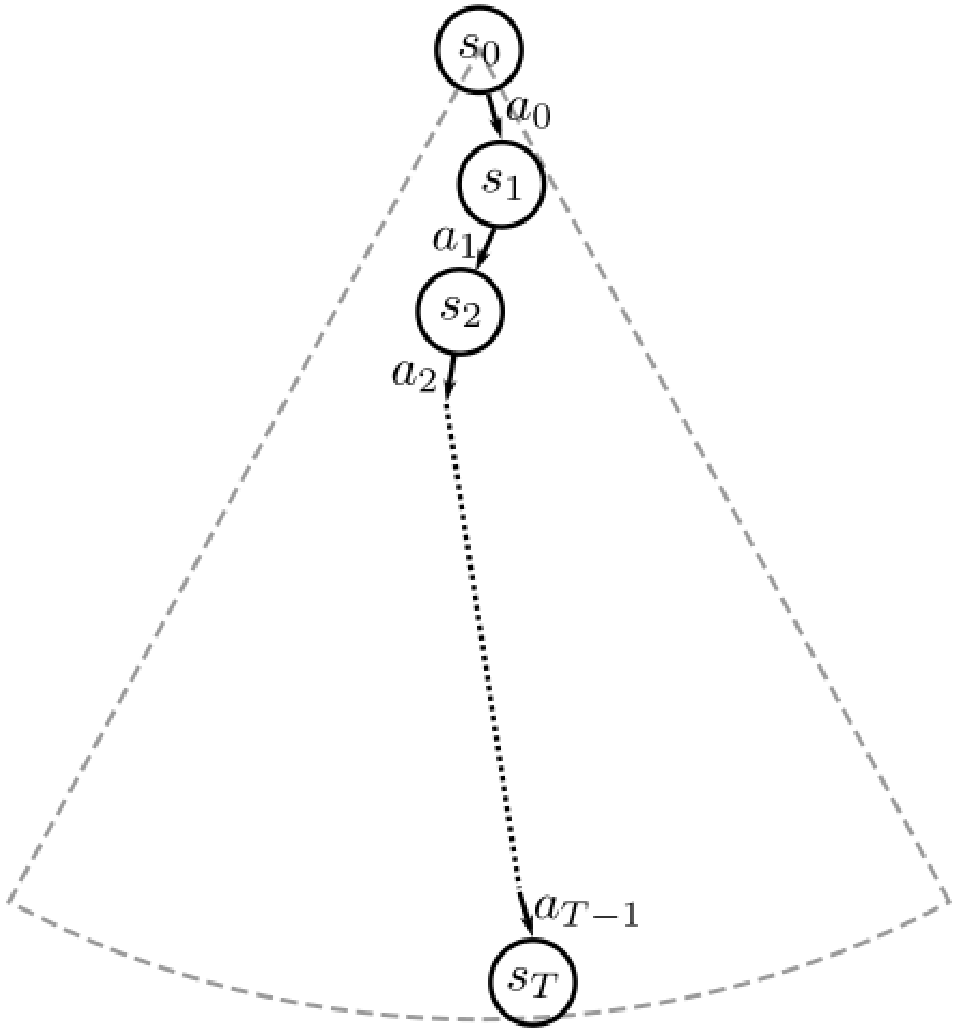


Monte Carlo method

- ***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 construction* of game subtree
  - optimal policy only *partially* defined
    (on actually computed states)
  - *intrinsically stochastic* policy optimization
    (the same initial state
    can give rise to different optimizations)
  - *no knowledge transfer*
    between *MC episodes*

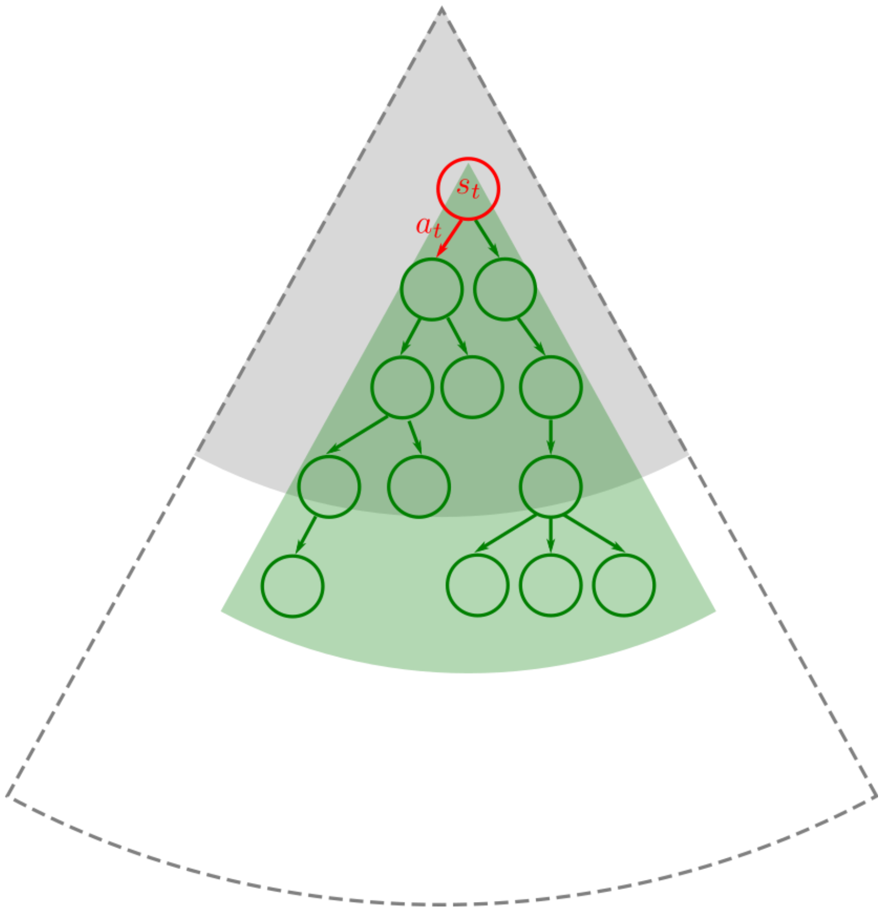


Monte Carlo Tree Search (MCTS):

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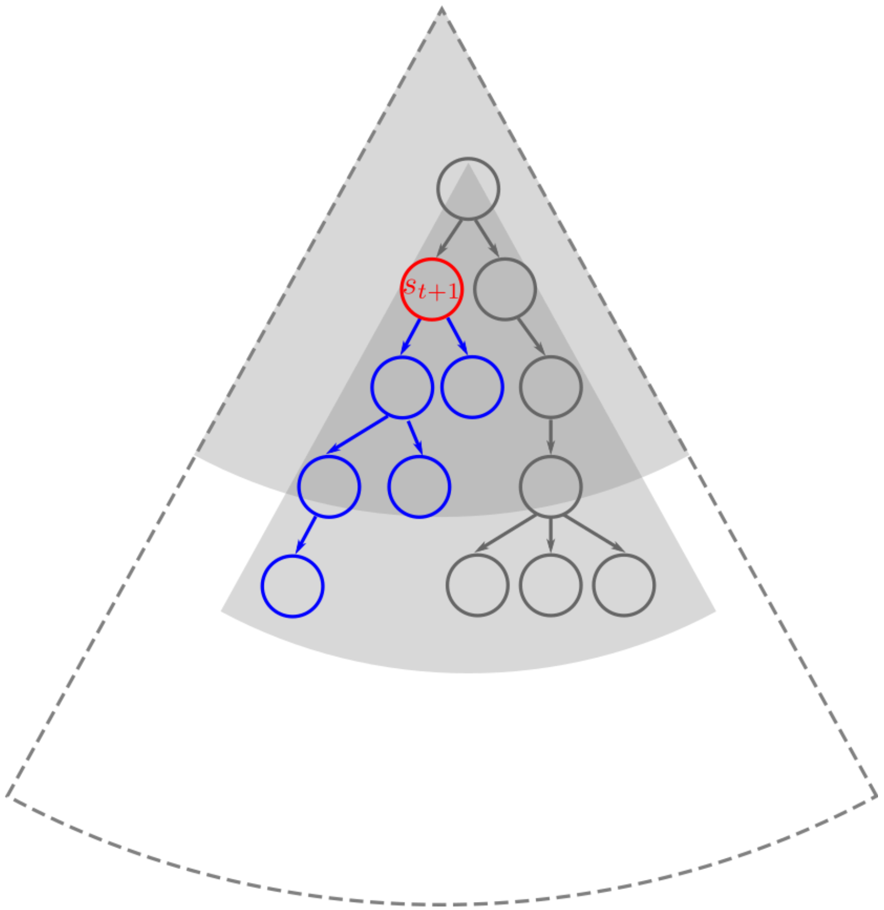
- *In the next step (with current state s_{t+1}):*
  - the subgraph of G_t with root s_{t+1} is ***expanded*** to create G_{t+1}
  - the statistics are ***updated*** and saved
  - best action a_{t+1} is decided
  - next state $s_{t+1} := \tau(s_t, a_t)$ is computed



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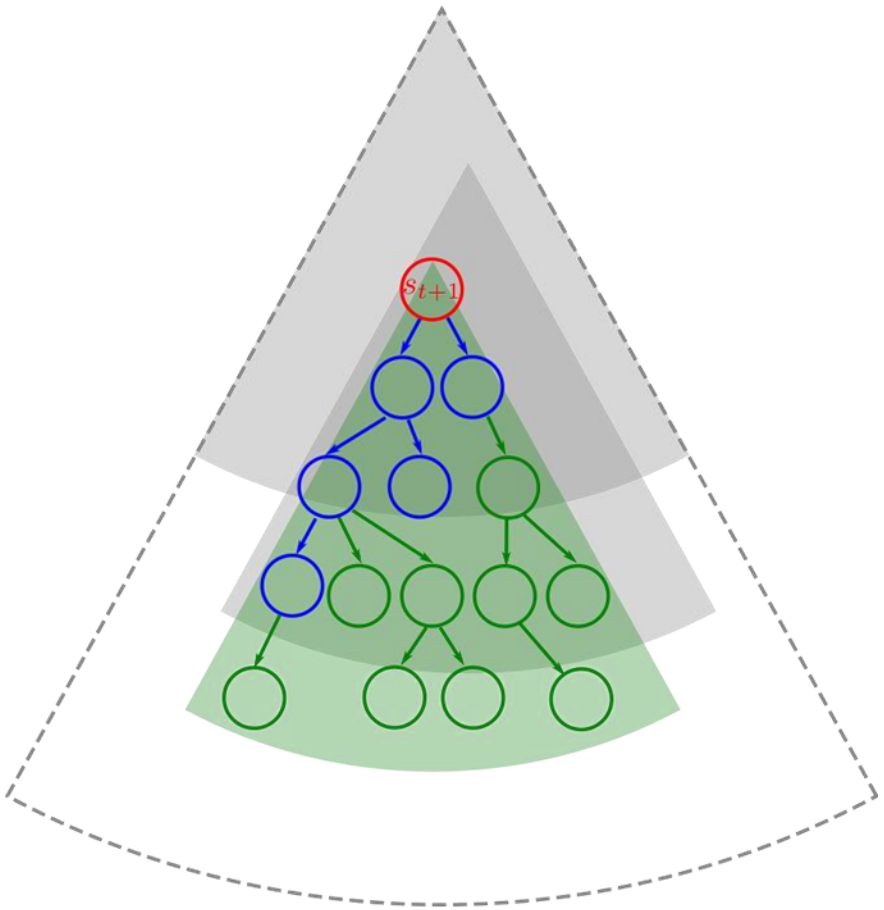
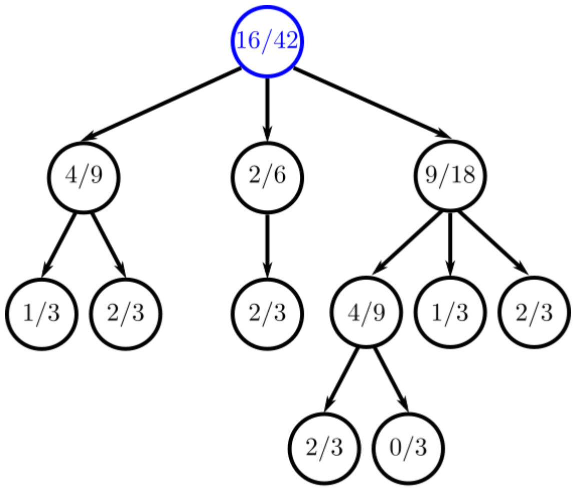


Monte Carlo Tree Search (MCTS) step

- ***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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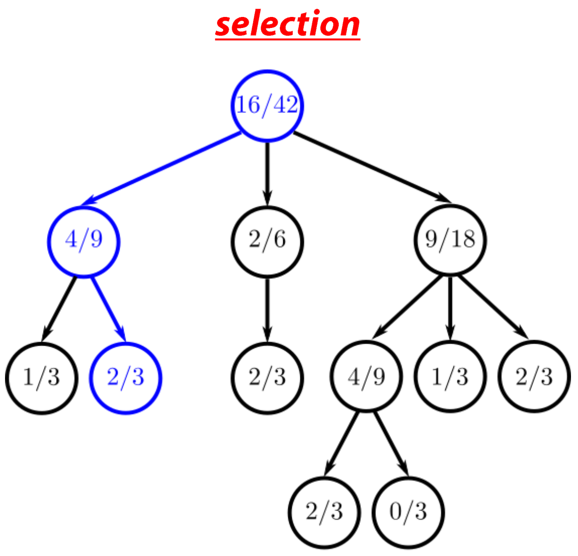
  1) start from current state s *(and the –possibly empty– stored tree with root s)*
  2) traverse the tree by following the ***selection policy***

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

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



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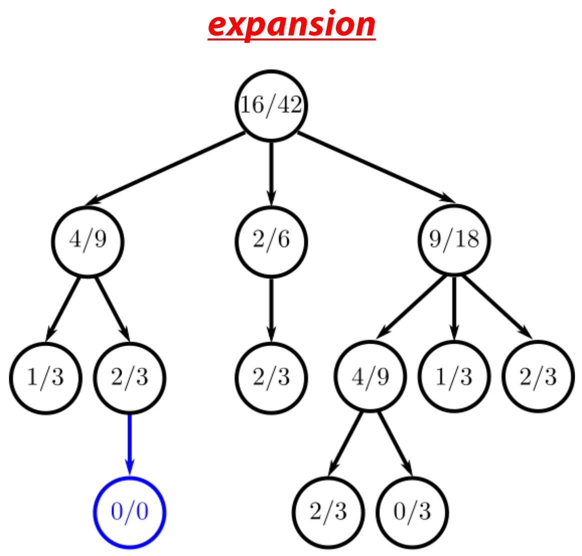
3) *expand* the tree by adding s_L



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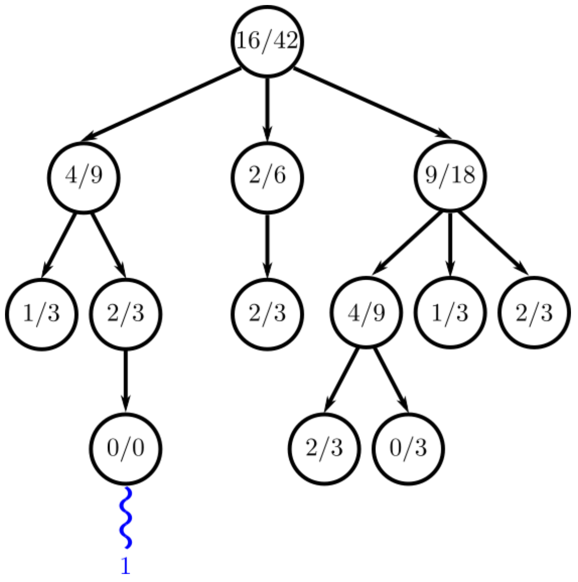
3) *expand* the tree by adding s_L
4) play one random playout from state s_L by following the *simulation policy*

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

and obtain the reward r

simulation



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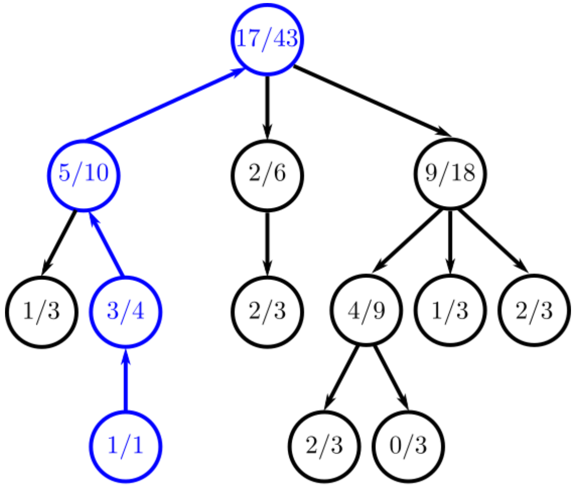
  and obtain the reward r

  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:

1) start from current state s *(and the –possibly empty– stored tree with root s)*
2) traverse the tree by following the ***selection policy***

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

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:

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Monte Carlo Tree Search (MCTS) step

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

repeat m times

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

- <u>Greedy</u> policy:

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

- <u>Selection</u> policy: ***Upper Confidence Bound applied to Trees (UCT)***

parameter
(default=1)

$$\pi^{\text{sel}}(s) := \pi^{\text{UCT}}(s) := \underset{N(s,a)>0}{\operatorname{argmax}} \left\{ \hat{Q}(s,a) + c\sqrt{\frac{2\log N(s)}{N(s,a)}} \right\}$$

<u>exploitation</u>
of actions
that look currently the best

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

<u>Convergence</u> [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:

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

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

$$\pi^{\text{sel}}(s) := \pi^{\text{UCT}}(s) := \underset{N(s,a)>0}{\text{argmax}} \left\{ \hat{Q}(s,a) + c\sqrt{\frac{2\log N(s)}{N(s,a)}} \right\}$$

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

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

set of admissible actions in state s

Monte Carlo Tree Search (MCTS) step

Algorithm 2 UCT

procedure UCTSEARCH(s_0)
  while time remaining **do**
    $\{s_0, ..., s_T\}, R = $ SIMULATE(s_0)
    BACKUP($\{s_0, ..., s_T\}, R$)
  end while
  return $\underset{a \in \mathcal{A}}{\text{argmax}}\, Q(s_0, a)$
end procedure

procedure SIMULATE(s_0)
  $t = 0$
  $R = 0$
  repeat
    if $s_t \in \mathcal{T}$ **then**
      $a = $ UCB1(s_t)
    else
      NEWNODE(s_t)
      $a_t = $ DEFAULTPOLICY(s_t)
    end if
    $s_{t+1} = $ SAMPLETRANSITION(s_t, a_t)
    $r_{t+1} = $ SAMPLEREWARD(s_t, a_t, s_{t+1})
    $R = R + r_{t+1}$
    $t \mathrel{+}= 1$
  until $Terminal(s_t)$
  return $\{s_0, ..., s_t\}, R$
end procedure

procedure UCB1(s)
  $a^* = \underset{a}{\text{argmax}}\, Q(s, a) + c\sqrt{\frac{2 \log N(s)}{N(s,a)}}$
  return a^*
end procedure

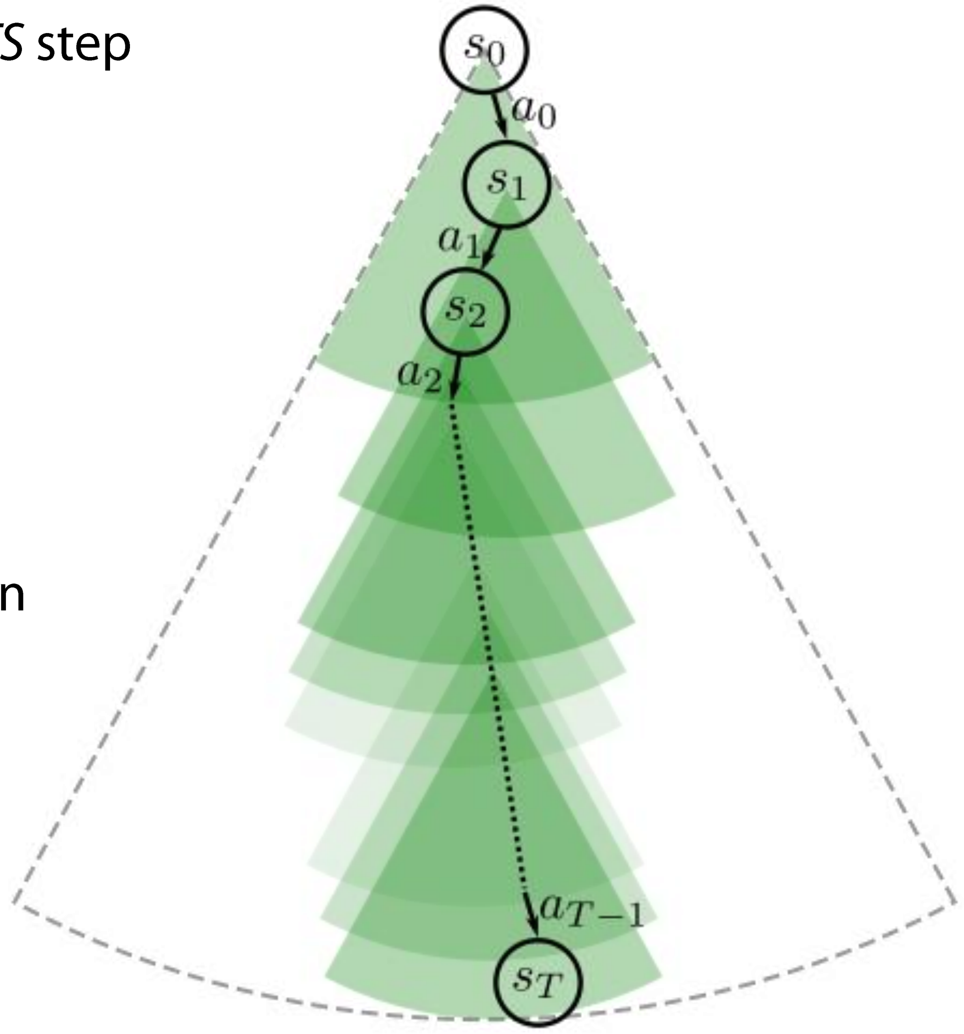
procedure BACKUP($\{s_0, ..., s_T\}, R$)
  for $t = 0$ **to** $T - 1$ **do**
    $N(s_t) \mathrel{+}= 1$
    $N(s_t, a_t) \mathrel{+}= 1$
    $Q(s_t, a_t) \mathrel{+}= \frac{R - Q(s_t, a_t)}{N(s_t, a_t)}$
  end for
end procedure

procedure NEWNODE(s)
  $N(s) = 0$
  for all $a \in \mathcal{A}$ **do**
    $N(s, a) = 0$
    $Q(s, a) = \infty$
  end for
  $\mathcal{T}.Insert(s)$
end procedure

From: D. Silver, Reinforcement Learning and Simulation-Based Search in Computer Go, PhD Thesis, 2009

Monte Carlo Tree Search (MCTS) method

- ***Monte Carlo Tree Search*** *method:*
  - <u>*memory*</u> of past playouts in a single *MCTS* step
    (collected in the tree statistics)
  - <u>*knowledge transfer*</u> between *MCTS* steps
    (by reusing subtrees already explored)
  - optimal policy only <u>*partially*</u> defined
    (on actually computed states)
  - <u>*intrinsically stochastic*</u> policy optimization
    (the same initial state
    can give rise to different optimizations)
  - What about <u>*knowledge transfer*</u>
    between *MCTS episodes*?
    transferring the entire MCTS tree
    would rapidly cause its explosive growth…



Dealing with Stochasticity and Uncertainty

Stochasticity and Uncertainty: general setting

- Stochastic reward:
  - *immediate reward* $r(s_t, a_t)$ is obtained when performing action a_t in state s_t
  - *delayed reward* is obtained only at the end of the game

$$r(s_t) := \begin{cases} 0 & \text{if } s_t \text{ is not a terminal state} \\ r & \text{otherwise} \end{cases}$$

possibly with $P(r \mid s_t, a_t)$ or $P(r \mid s_t)$ respectively

- Stochastic policy:

policy $\pi(s, a) := P(a \mid s)$ is a *probability distribution*

- Uncertainty of execution:

stochastic transition function $\tau : (s_t, a_t) \mapsto s_{t+1}$ as $P(s_{t+1} \mid s_t, a_t)$

Reinforcement Learning (RL)

- *Value function:*

$$V^\pi(s) := \mathbb{E}_\pi[R \mid s_0 = s]$$

mean over the trajectories following policy π

Optimal value: $V^*(s) := \max_\pi V^\pi(s)\ \forall s$

- *Action-value function:*

$$Q^\pi(s_t, a) := \mathbb{E}_\pi[R \mid s_0 = s, a_0 = a]$$

Optimal action-value: $Q^*(s,a) := \max_\pi Q^\pi(s,a)\ \forall s, a$

Optimal policy: $a^*(s) = \operatorname*{argmax}_a [Q^*(s,a)]$

Connection: $V^\pi(s) = \mathbb{E}_\pi[Q^\pi(s,a)]$ and $V^*(s) = \max_a [Q^*(s,a)]$