

Deep Reinforcement Learning and Control

# Monte Carlo Tree Search with Prior Knowledge

Spring 2021, CMU 10-403

Katerina Fragkiadaki



# Definitions

**Learning:** the acquisition of knowledge or skills through experience, study, or by being taught.

**Planning:** any computational process that uses a model to create or improve a policy



# Simplest Monte-Carlo Search

Given a deterministic transition function  $T$ , a root state  $s$  and a simulation policy  $\pi$  (potentially random)

Simulate  $K$  episodes from current (real) state:

$$\{s, a, R_1^k, S_1^k, A_1^k, R_2^k, S_2^k, A_2^k, \dots, S_T^k\}_{k=1}^K \sim T, \pi$$

Evaluate action value function of the root by mean return:

$$Q(s, a) = \frac{1}{K} \sum_{k=1}^K G_k \rightarrow q_\pi(s, a)$$

Select root action:  $a = \operatorname{argmax}_{a \in \mathcal{A}} Q(s, a)$

# Can we do better?

- Could we be improving our simulation policy the more simulations we obtain?
- Yes we can! We can have two policies:
  - Internal to the tree: keep track of action values  $Q$  not only for the root but also for nodes internal to a tree we are expanding, and use to improve the simulation policy over time
  - External to the tree: we do not have  $Q$  estimates and thus we use a random policy

**In MCTS, the simulation policy improves**

- Can we think anything better than  $\epsilon$  – greedy?

# Monte-Carlo Tree Search

## 1. Selection

- Used for nodes we have seen before
- Pick according to UCB

## 2. Expansion

- Used when we reach the frontier
- Add one node per playout

## 3. Simulation

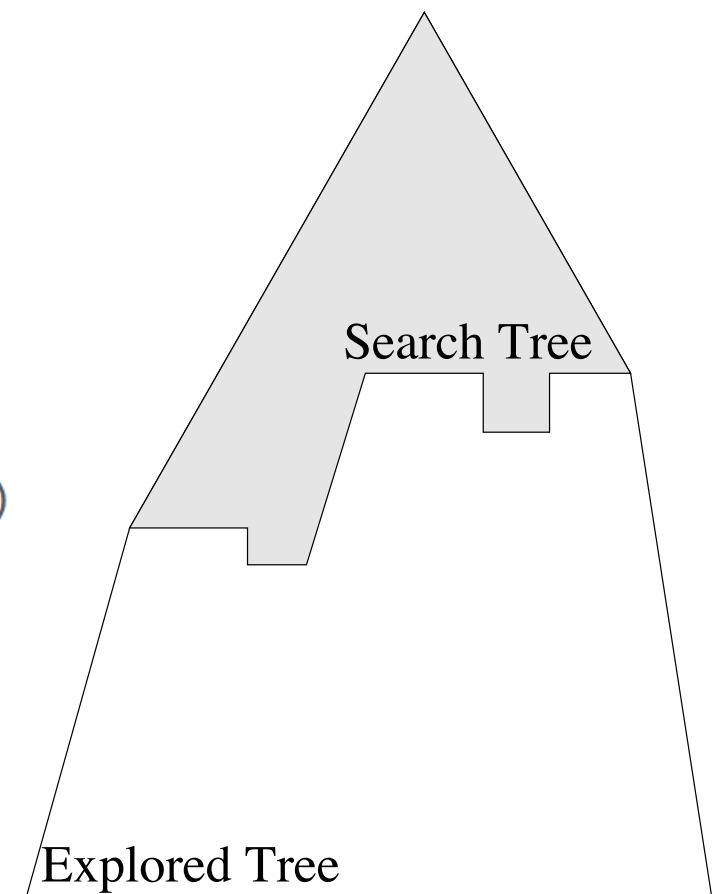
- Used beyond the search frontier
- Don't bother with UCB, just play randomly

## 4. Back-propagation

- After reaching a terminal node
- Update value and visits for states expanded in selection and expansion

# Basic MCTS pseudocode

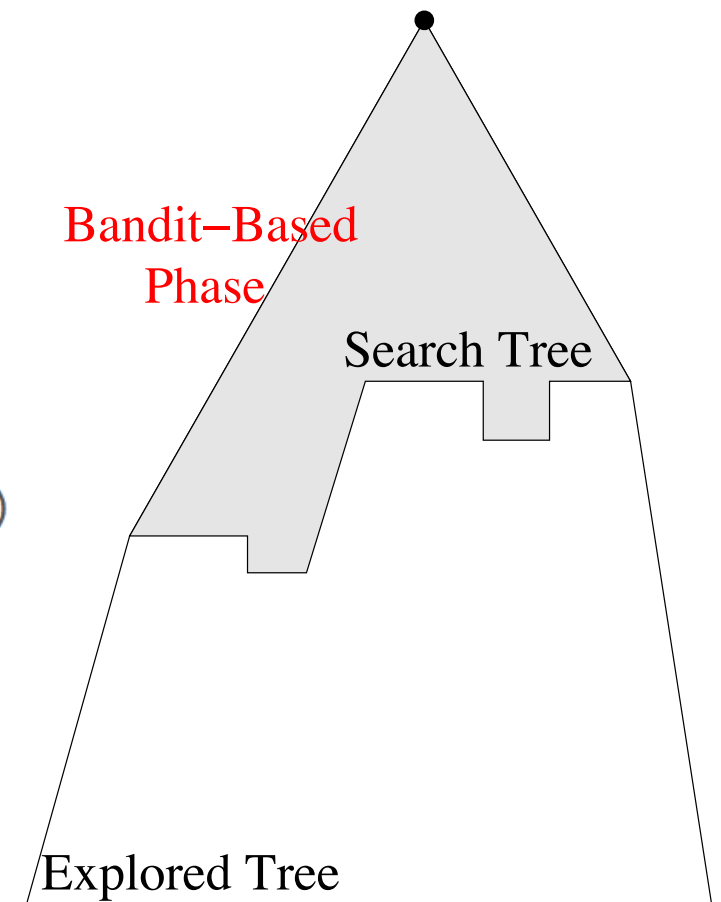
```
function MCTS_sample(state)
  state.visits++
  if all children of state expanded:
    next_state = UCB_sample(state)
    winner = MCTS_sample(next_state)
  else:
    if some children of state expanded:
      next_state = expand(random unexpanded child)
    else:
      next_state = state
    winner = random_playout(next_state)
  update_value(state, winner)
```



Search tree contains states whose all children have been tried at least once

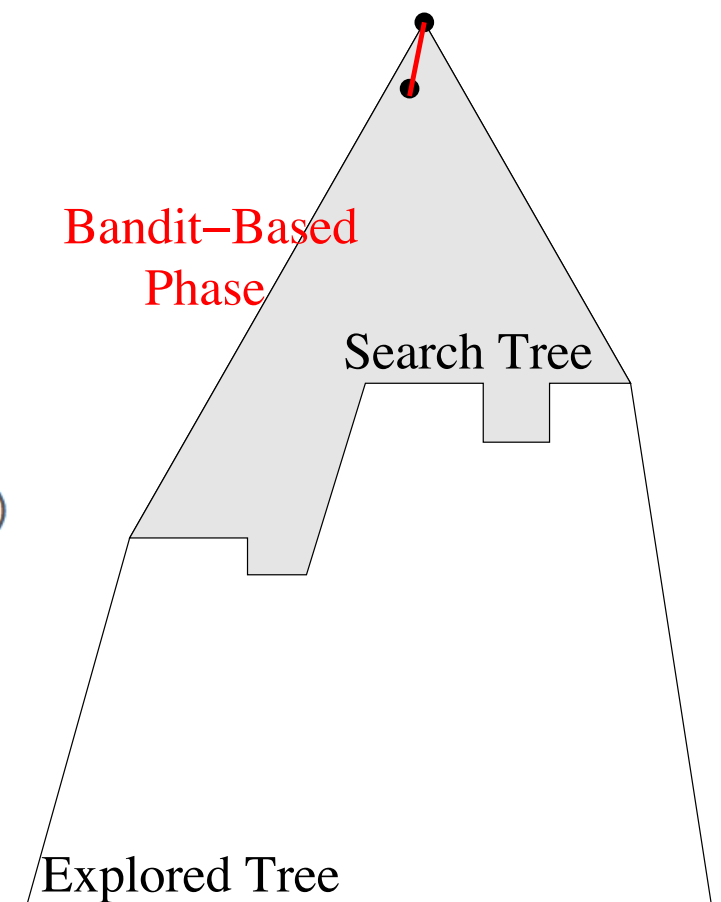
# Basic MCTS pseudocode

```
function MCTS_sample(state)
  state.visits++
  if all children of state expanded:
    next_state = UCB_sample(state)
    winner = MCTS_sample(next_state)
  else:
    if some children of state expanded:
      next_state = expand(random unexpanded child)
    else:
      next_state = state
    winner = random_payout(next_state)
  update_value(state, winner)
```



# Basic MCTS pseudocode

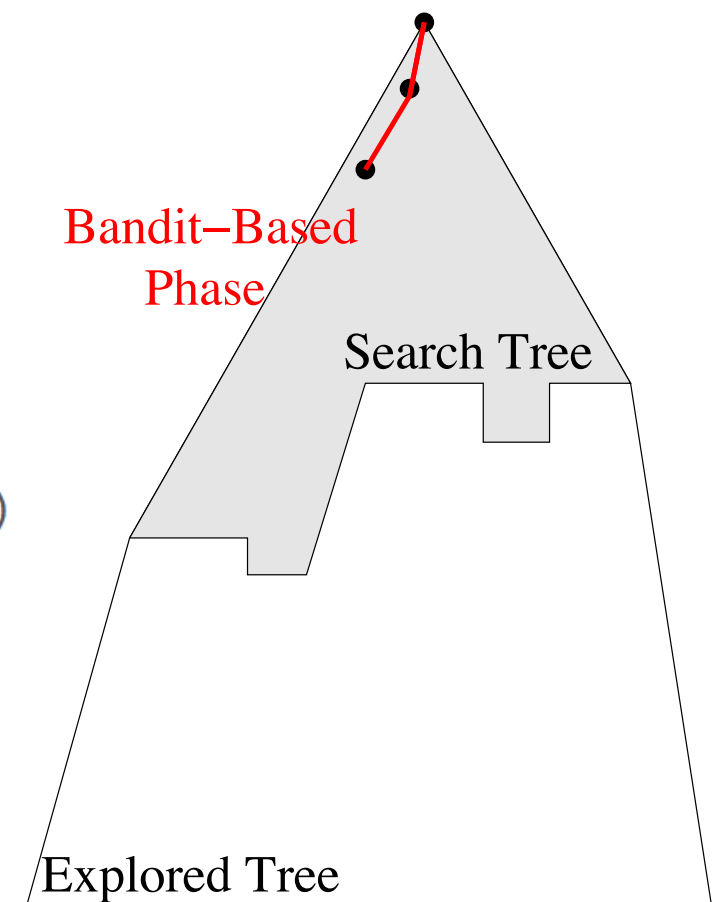
```
function MCTS_sample(state)
  state.visits++
  if all children of state expanded:
    next_state = UCB_sample(state)
    winner = MCTS_sample(next_state)
  else:
    if some children of state expanded:
      next_state = expand(random unexpanded child)
    else:
      next_state = state
    winner = random_payout(next_state)
  update_value(state, winner)
```





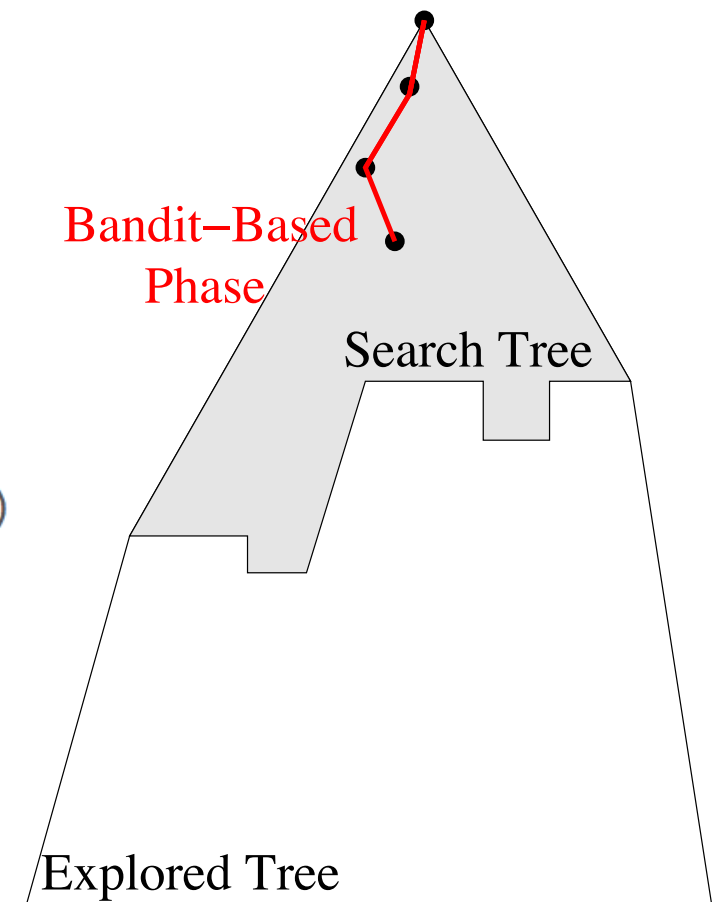
# Basic MCTS pseudocode

```
function MCTS_sample(state)
  state.visits++
  if all children of state expanded:
    next_state = UCB_sample(state)
    winner = MCTS_sample(next_state)
  else:
    if some children of state expanded:
      next_state = expand(random unexpanded child)
    else:
      next_state = state
    winner = random_playout(next_state)
  update_value(state, winner)
```



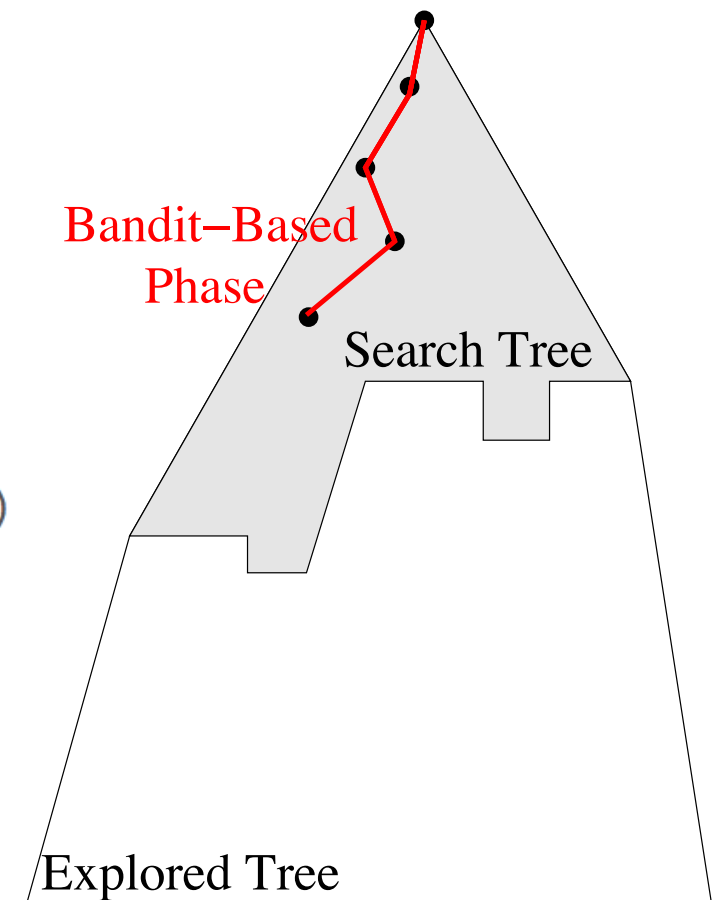
# Basic MCTS pseudocode

```
function MCTS_sample(state)
  state.visits++
  if all children of state expanded:
    next_state = UCB_sample(state)
    winner = MCTS_sample(next_state)
  else:
    if some children of state expanded:
      next_state = expand(random unexpanded child)
    else:
      next_state = state
    winner = random_playout(next_state)
  update_value(state, winner)
```



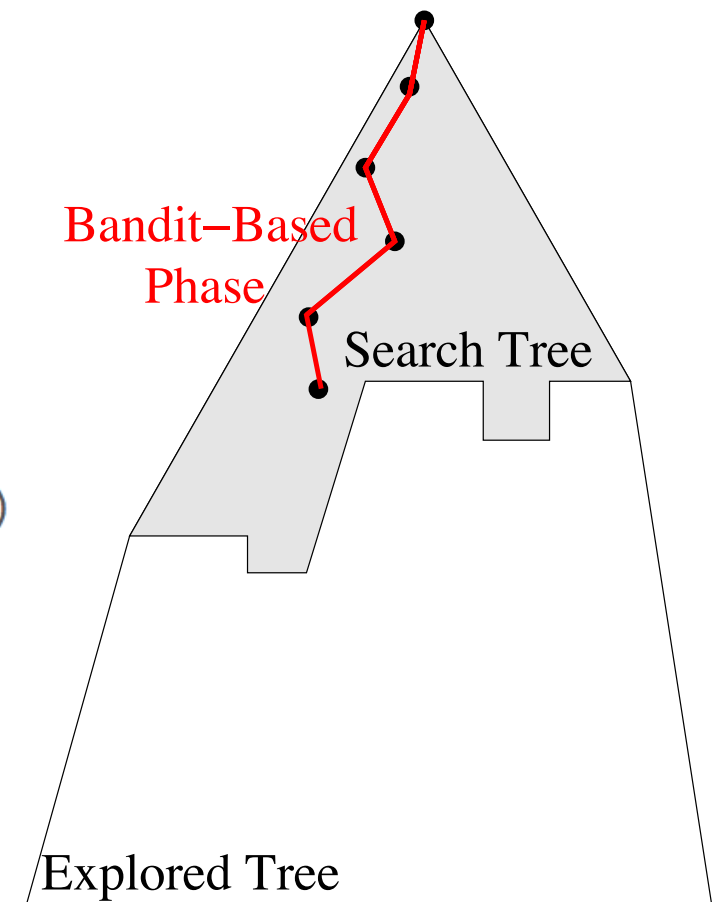
# Basic MCTS pseudocode

```
function MCTS_sample(state)
  state.visits++
  if all children of state expanded:
    next_state = UCB_sample(state)
    winner = MCTS_sample(next_state)
  else:
    if some children of state expanded:
      next_state = expand(random unexpanded child)
    else:
      next_state = state
    winner = random_playout(next_state)
  update_value(state, winner)
```



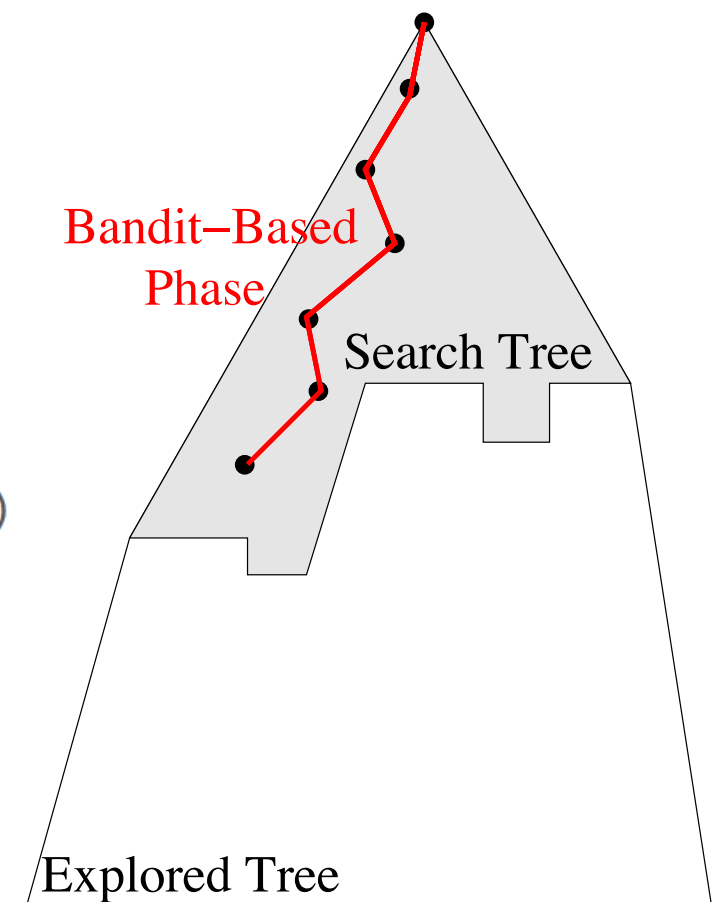
# Basic MCTS pseudocode

```
function MCTS_sample(state)
  state.visits++
  if all children of state expanded:
    next_state = UCB_sample(state)
    winner = MCTS_sample(next_state)
  else:
    if some children of state expanded:
      next_state = expand(random unexpanded child)
    else:
      next_state = state
    winner = random_playout(next_state)
  update_value(state, winner)
```



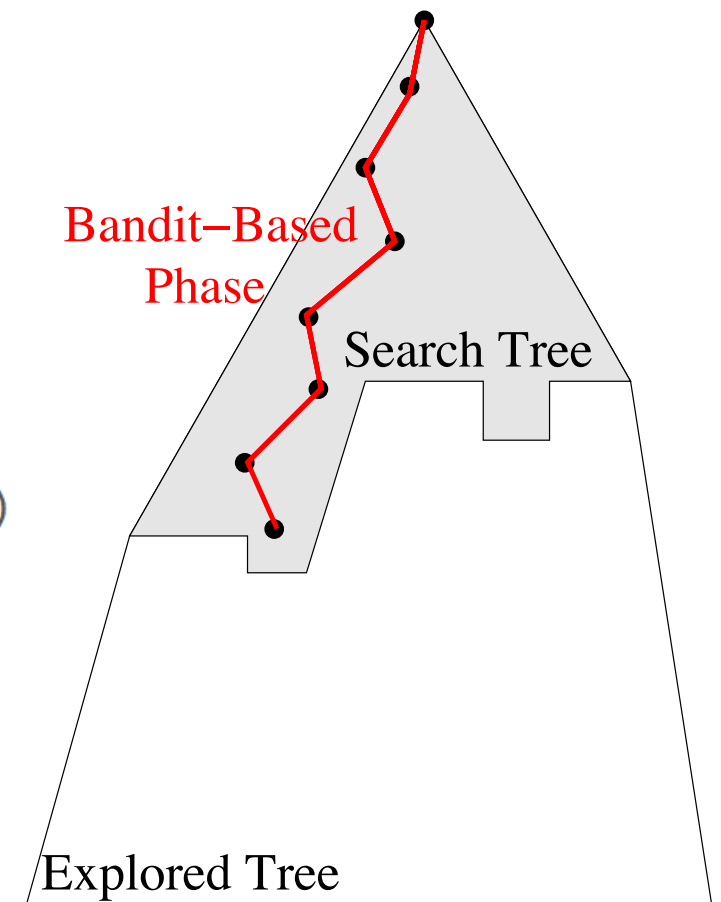
# Basic MCTS pseudocode

```
function MCTS_sample(state)
  state.visits++
  if all children of state expanded:
    next_state = UCB_sample(state)
    winner = MCTS_sample(next_state)
  else:
    if some children of state expanded:
      next_state = expand(random unexpanded child)
    else:
      next_state = state
    winner = random_playout(next_state)
  update_value(state, winner)
```



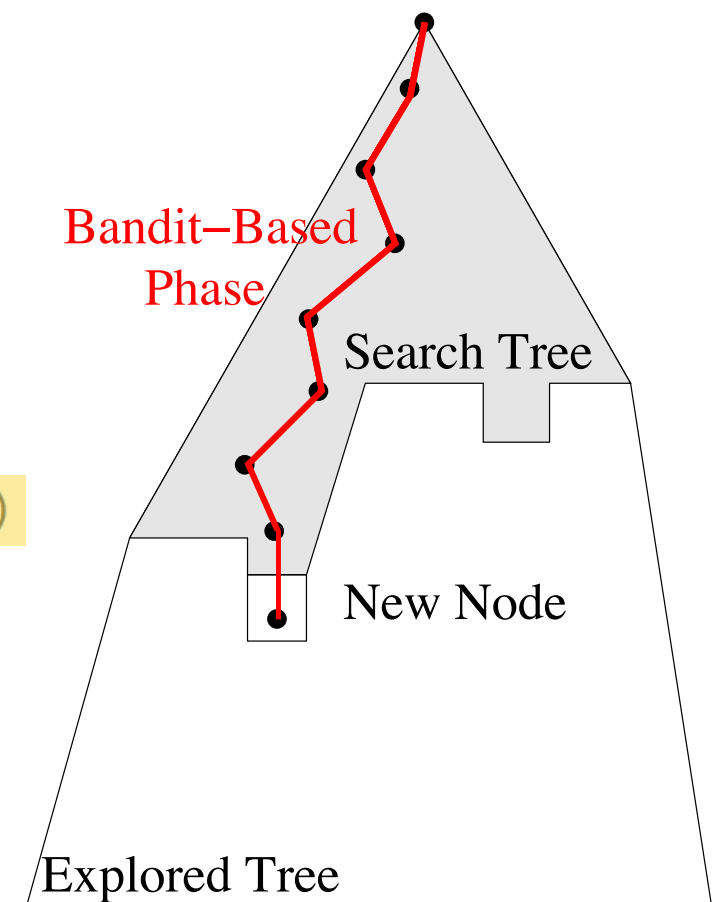
# Basic MCTS pseudocode

```
function MCTS_sample(state)
  state.visits++
  if all children of state expanded:
    next_state = UCB_sample(state)
    winner = MCTS_sample(next_state)
  else:
    if some children of state expanded:
      next_state = expand(random unexpanded child)
    else:
      next_state = state
    winner = random_payout(next_state)
  update_value(state, winner)
```



# Basic MCTS pseudocode

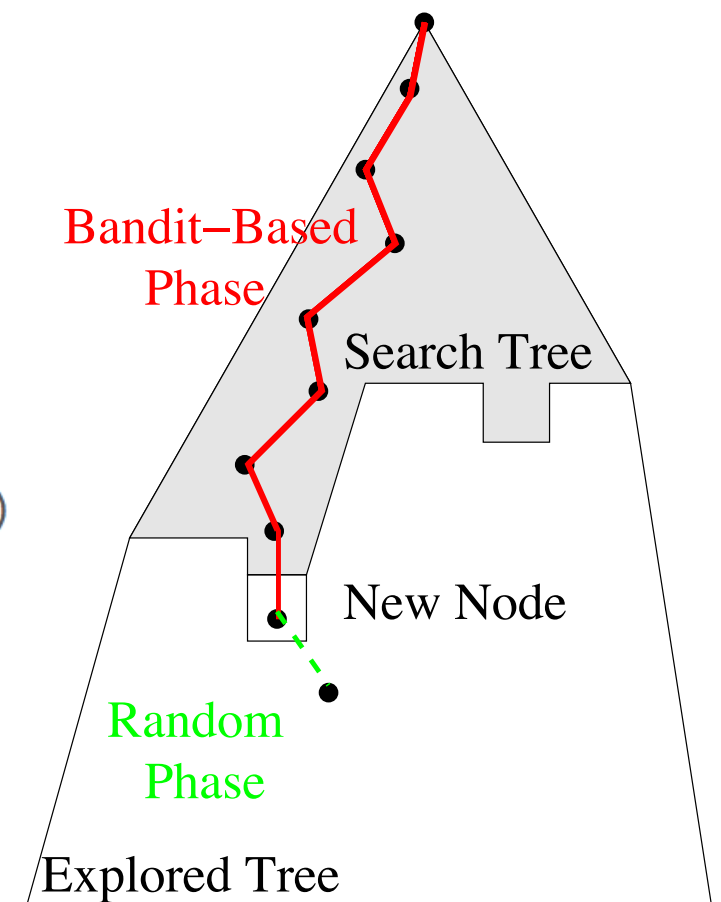
```
function MCTS_sample(state)
  state.visits++
  if all children of state expanded:
    next_state = UCB_sample(state)
    winner = MCTS_sample(next_state)
  else:
    if some children of state expanded:
      next_state = expand(random unexpanded child)
    else:
      next_state = state
    winner = random_payout(next_state)
  update_value(state, winner)
```



# Basic MCTS pseudocode

```
function MCTS_sample(state)
    state.visits++
    if all children of state expanded:
        next_state = UCB_sample(state)
        winner = MCTS_sample(next_state)
    else:
        if some children of state expanded:
            next_state = expand(random unexpanded child)
        else:
            next_state = state
        winner = random_playout(next_state)
    update_value(state, winner)
```

```
function random_playout(state):
    if is_terminal(state):
        return winner
    else: return random_playout(random_move(state))
```

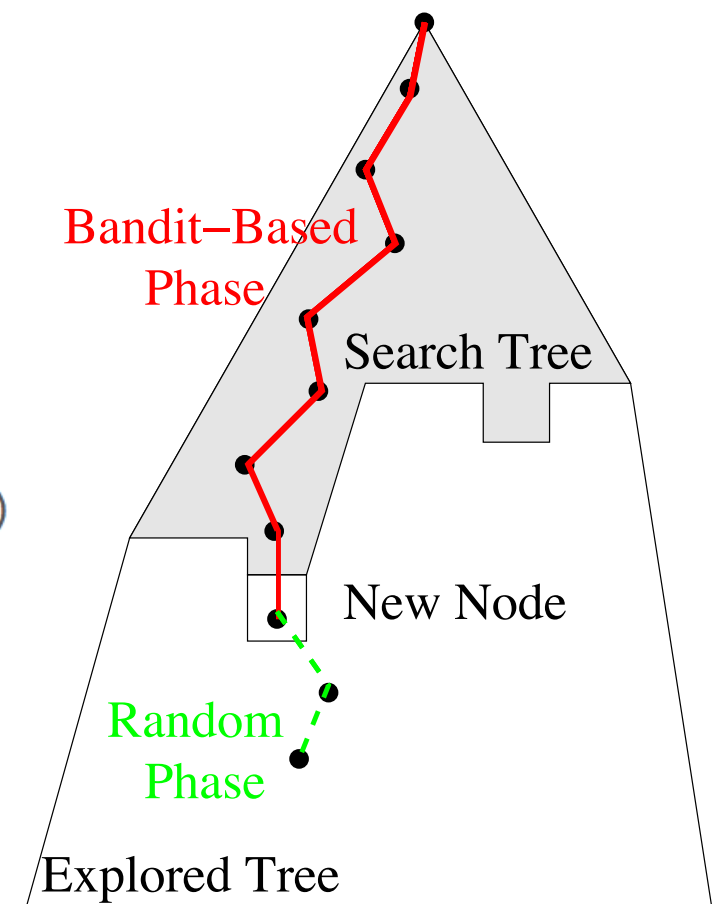




# Basic MCTS pseudocode

```
function MCTS_sample(state)
    state.visits++
    if all children of state expanded:
        next_state = UCB_sample(state)
        winner = MCTS_sample(next_state)
    else:
        if some children of state expanded:
            next_state = expand(random unexpanded child)
        else:
            next_state = state
        winner = random_playout(next_state)
    update_value(state, winner)
```

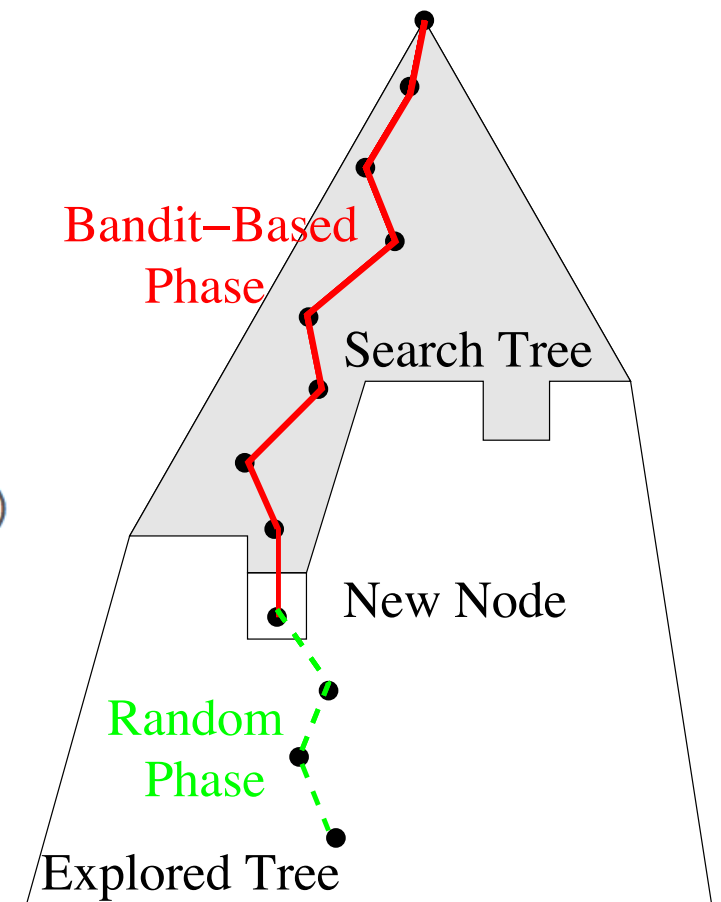
```
function random_playout(state):
    if is_terminal(state):
        return winner
    else: return random_playout(random_move(state))
```



# Basic MCTS pseudocode

```
function MCTS_sample(state)
    state.visits++
    if all children of state expanded:
        next_state = UCB_sample(state)
        winner = MCTS_sample(next_state)
    else:
        if some children of state expanded:
            next_state = expand(random unexpanded child)
        else:
            next_state = state
        winner = random_playout(next_state)
    update_value(state, winner)
```

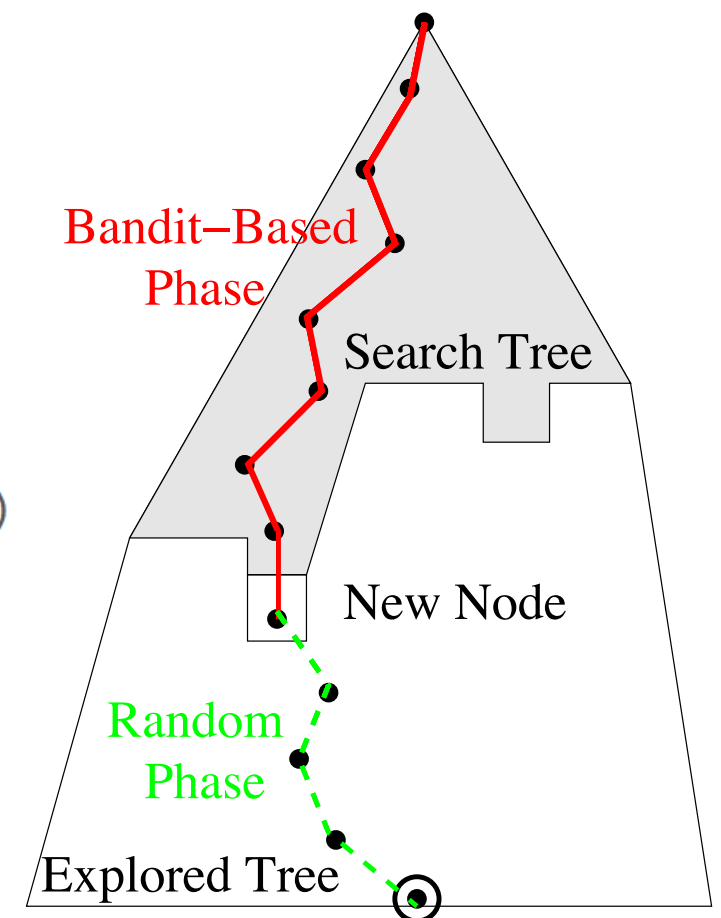
```
function random_playout(state):
    if is_terminal(state):
        return winner
    else: return random_playout(random_move(state))
```



# Basic MCTS pseudocode

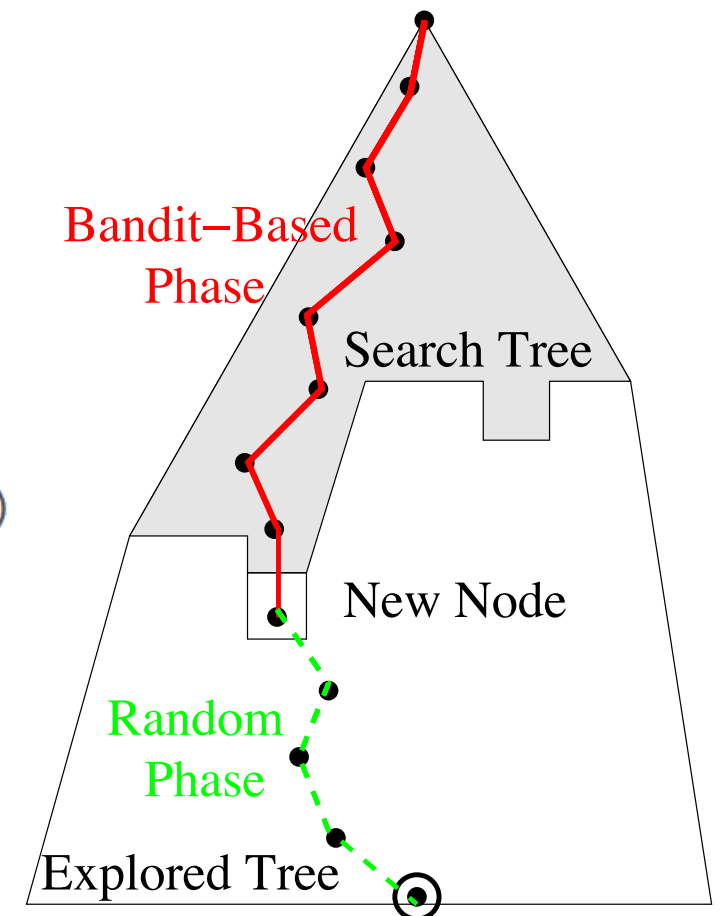
```
function MCTS_sample(state)
    state.visits++
    if all children of state expanded:
        next_state = UCB_sample(state)
        winner = MCTS_sample(next_state)
    else:
        if some children of state expanded:
            next_state = expand(random unexpanded child)
        else:
            next_state = state
        winner = random_playout(next_state)
    update_value(state, winner)
```

```
function random_playout(state):
    if is_terminal(state):
        return winner
    else: return random_playout(random_move(state))
```

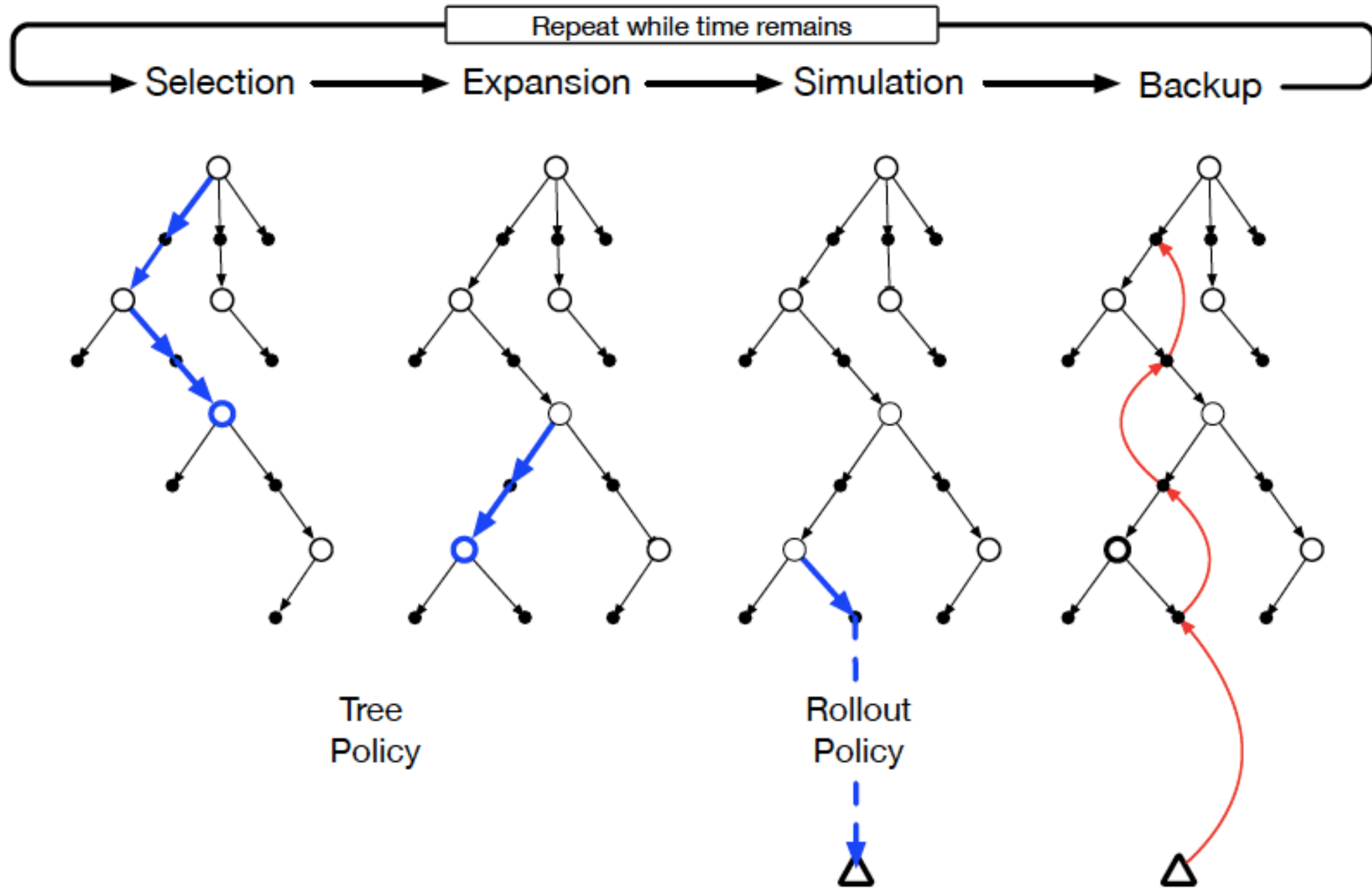


# Basic MCTS pseudocode

```
function MCTS_sample(state)
  state.visits++
  if all children of state expanded:
    next_state = UCB_sample(state)
    winner = MCTS_sample(next_state)
  else:
    if some children of state expanded:
      next_state = expand(random unexpanded child)
    else:
      next_state = state
    winner = random_playout(next_state)
  update_value(state, winner)
```



# Monte-Carlo Tree Search



# Monte-Carlo Tree Search

Use cases:

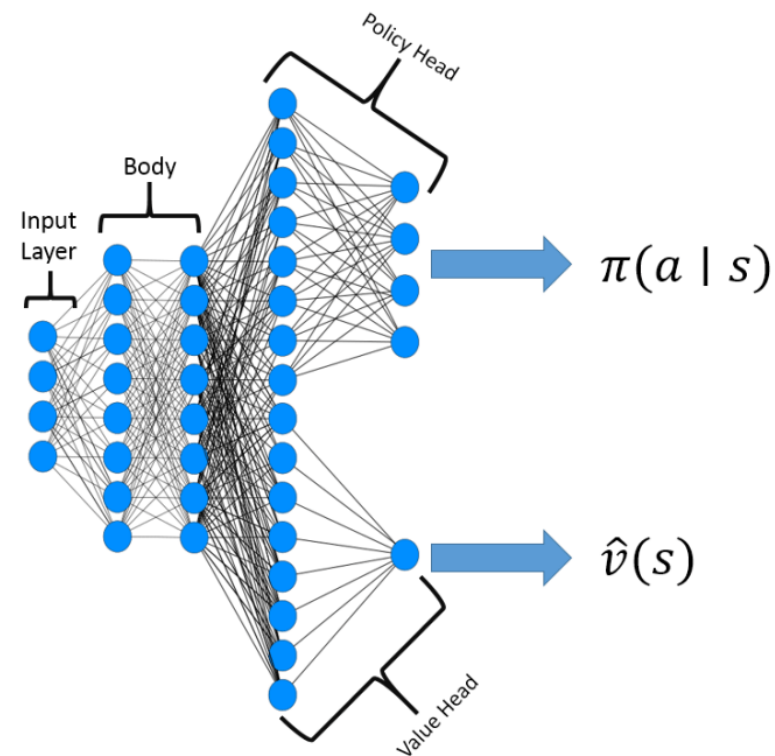
- As online planner for selecting the next move
- For state-action value estimation at training time. At test time just use the reactive policy network, without any lookahead planning.
- In combination with policy and value networks at test time (AlphaGo)
- In combination with policy and value networks at both train and test time (AlphaGoZero)

# Can we do better?

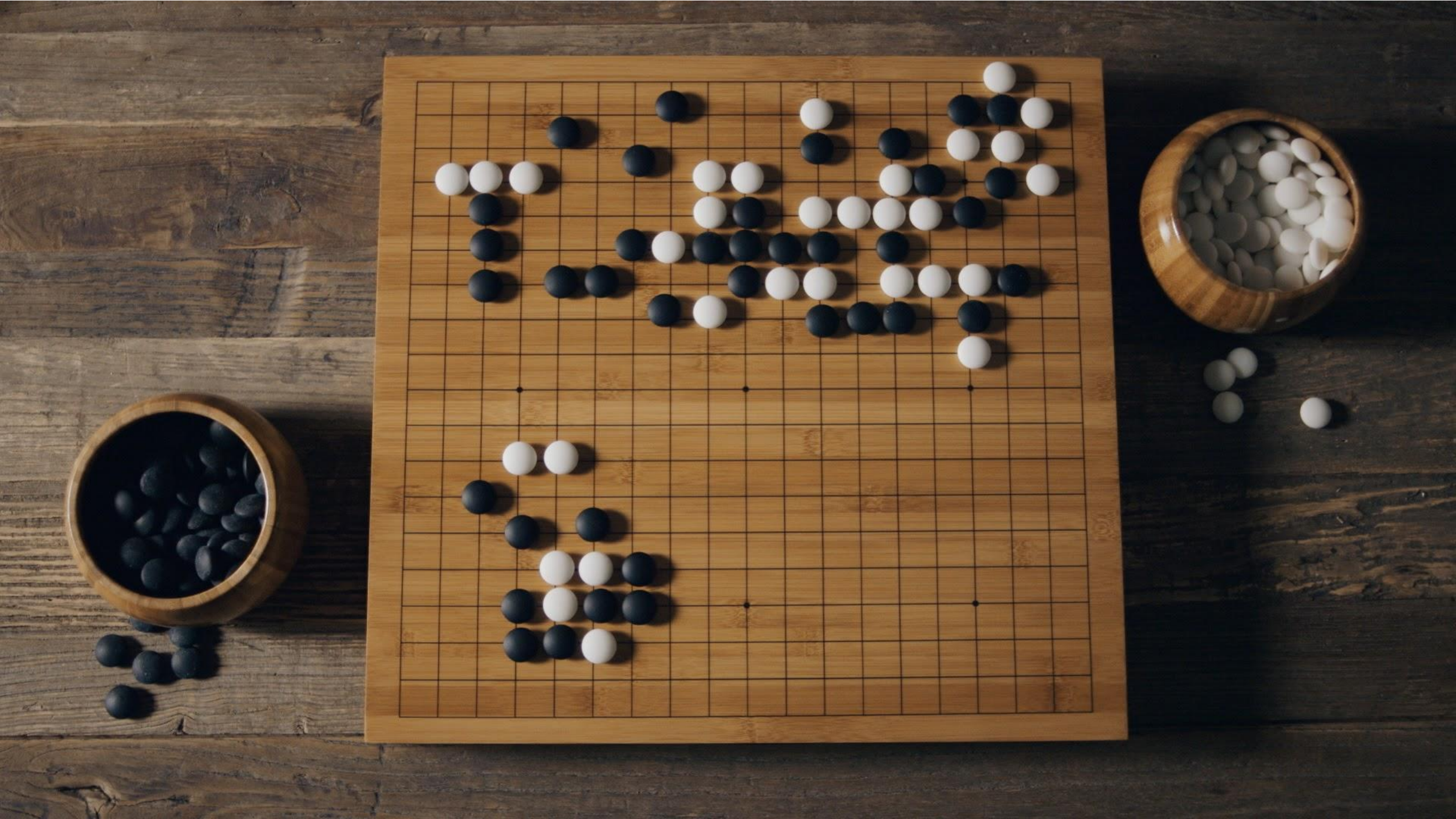
Can we inject prior knowledge into state and action values instead of initializing them uniformly?

# MCTS + Policy/ Value networks

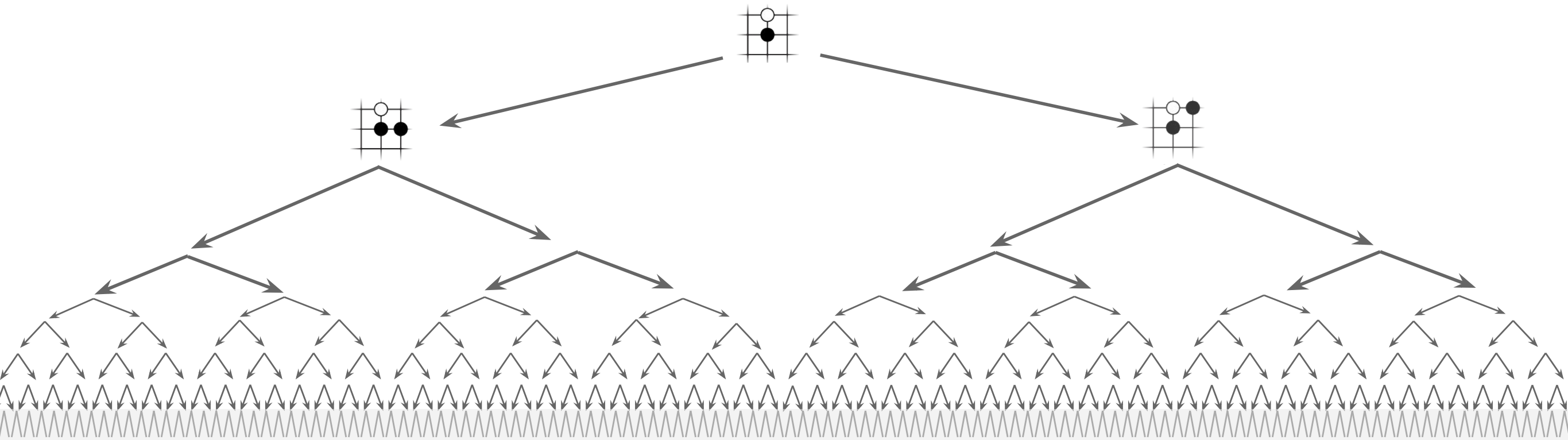
- Value neural net to evaluate board positions to help prune the tree depth.
- Policy neural net to select moves to help prune the tree breadth.







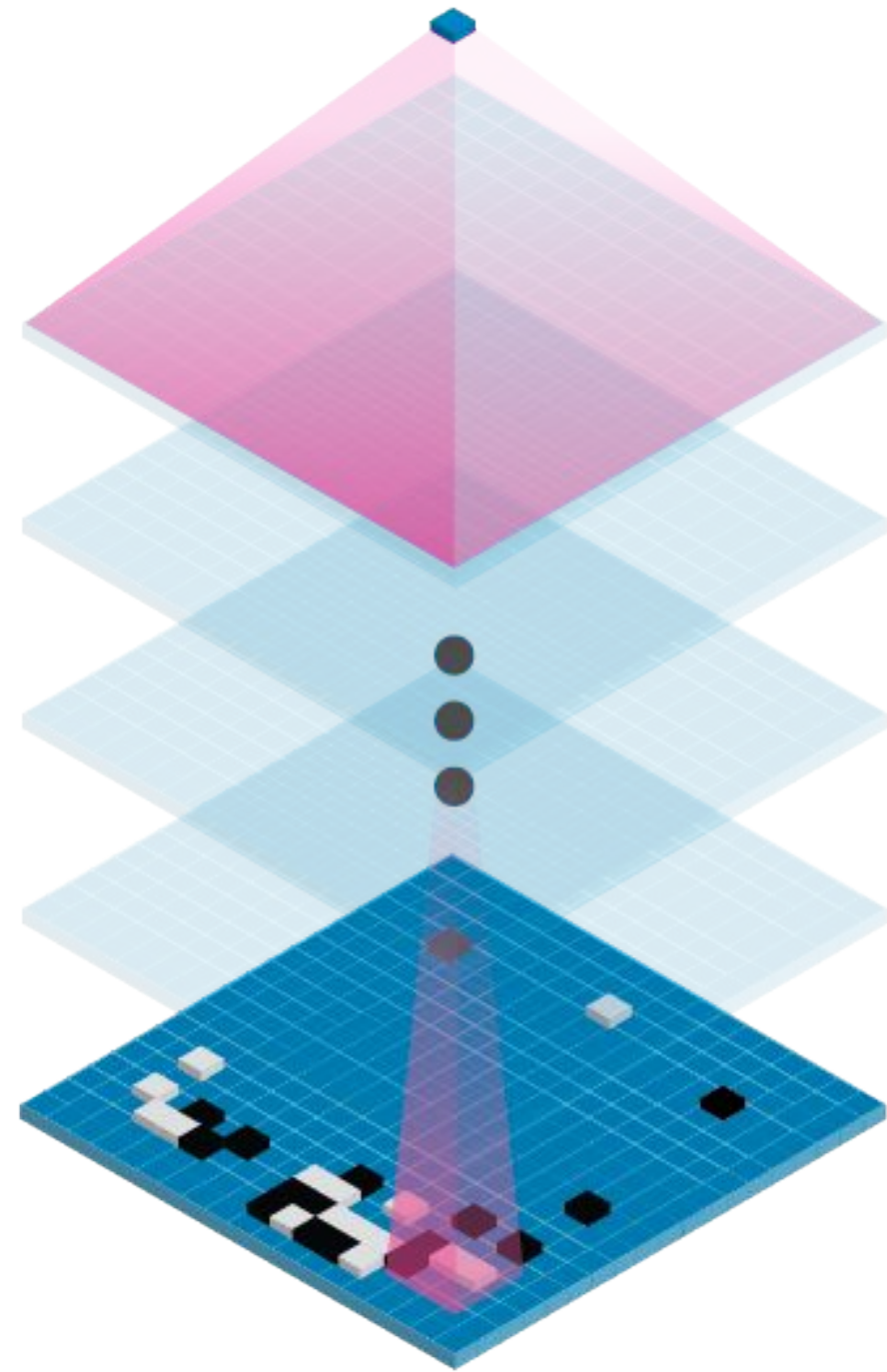
# Exhaustive Search



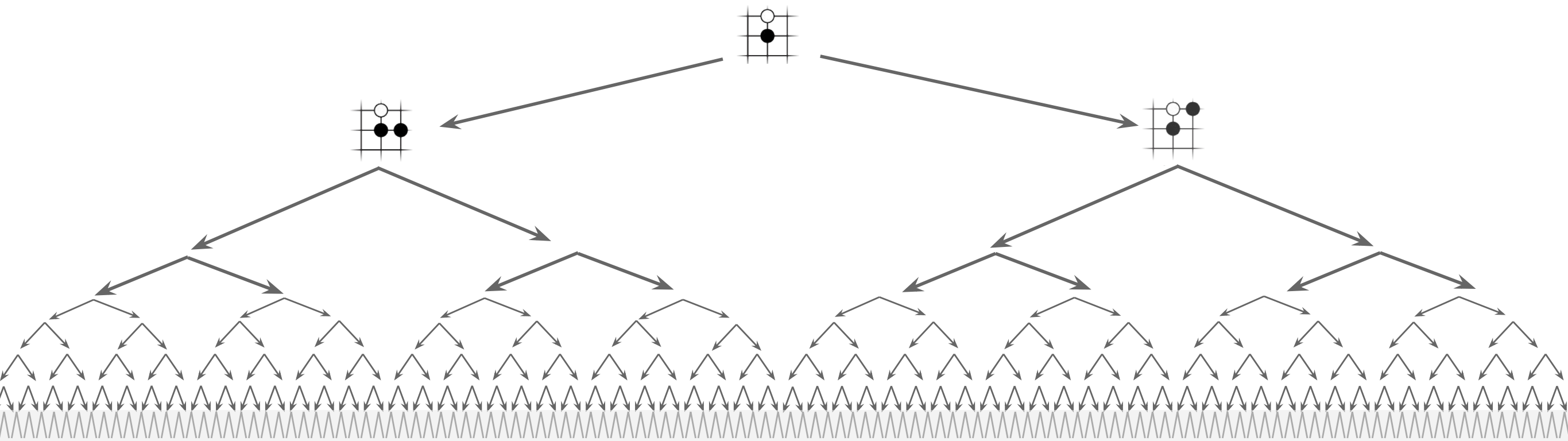


# Value Network

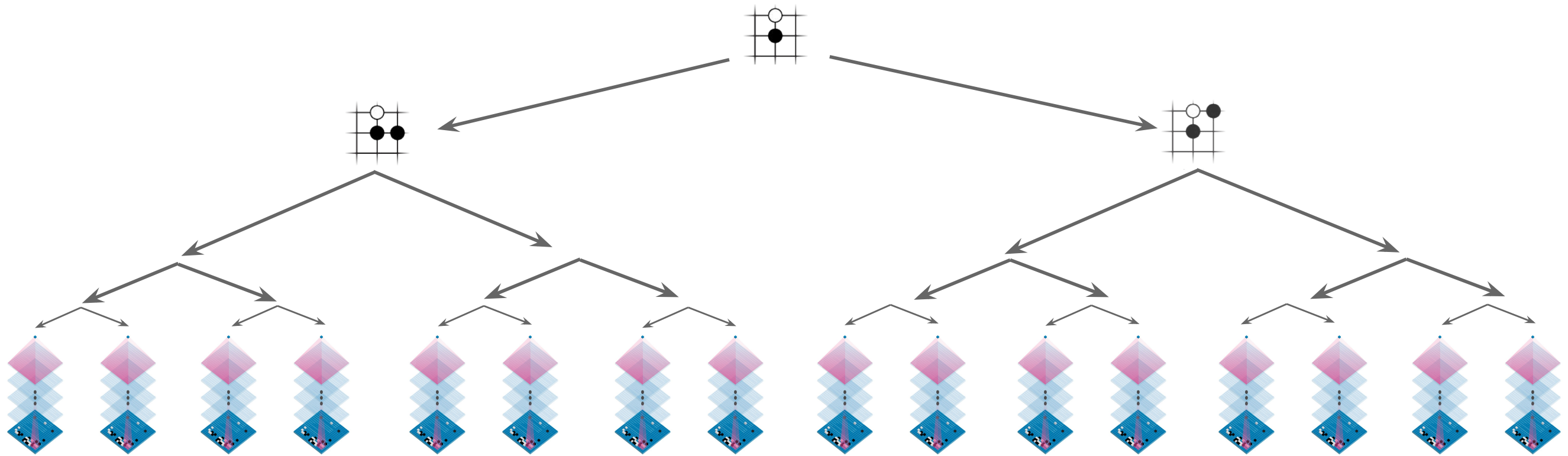
How well am I doing?



# Reduce Depth with Value Network

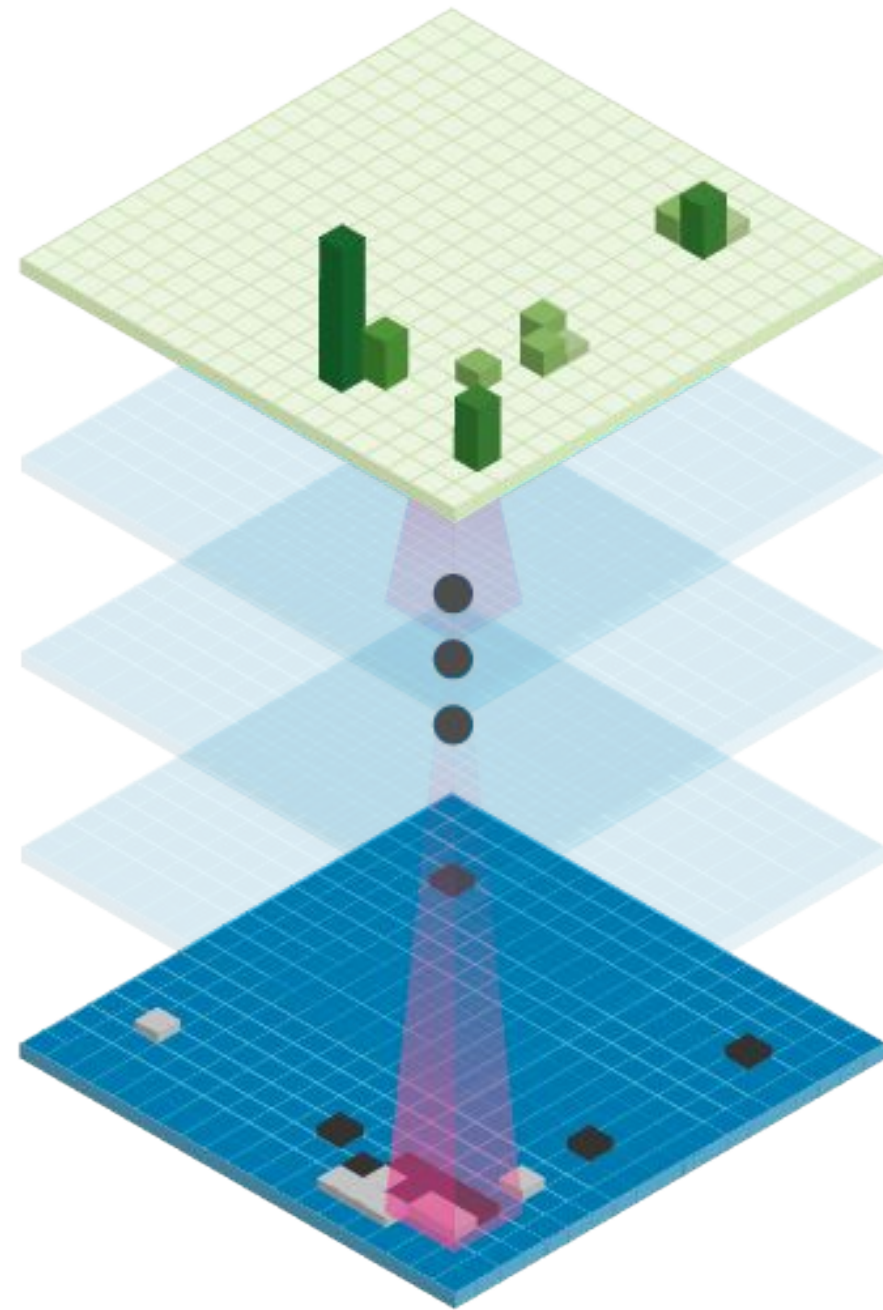


# Reduce Depth with Value Network

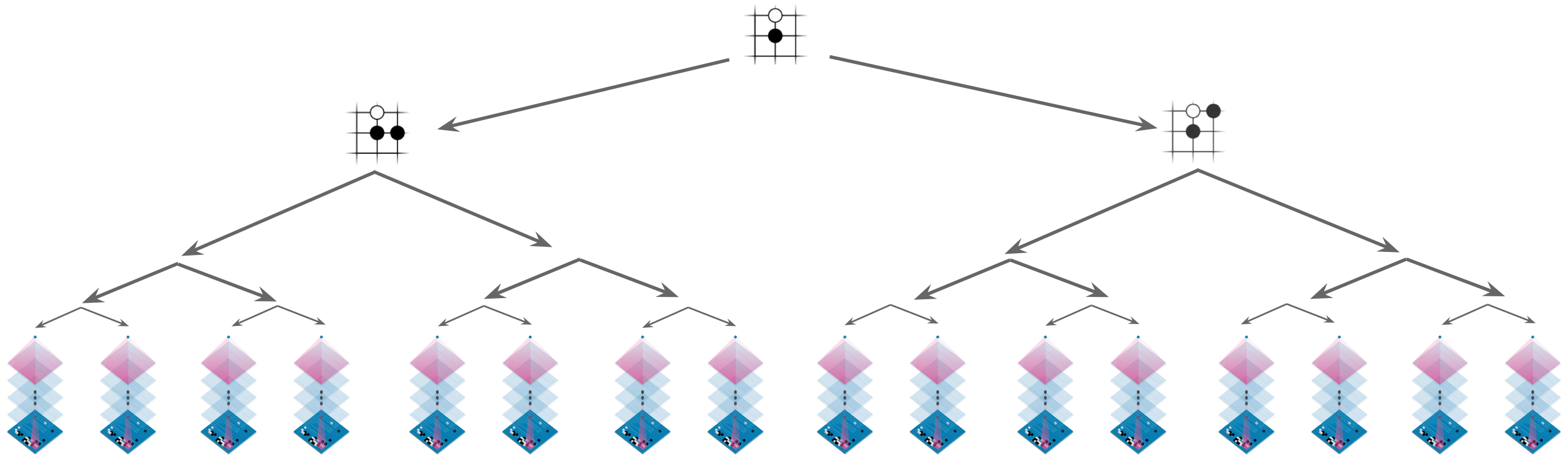


# Prior Network

What are the most likely actions?



# Reduce Breadth with Policy Network

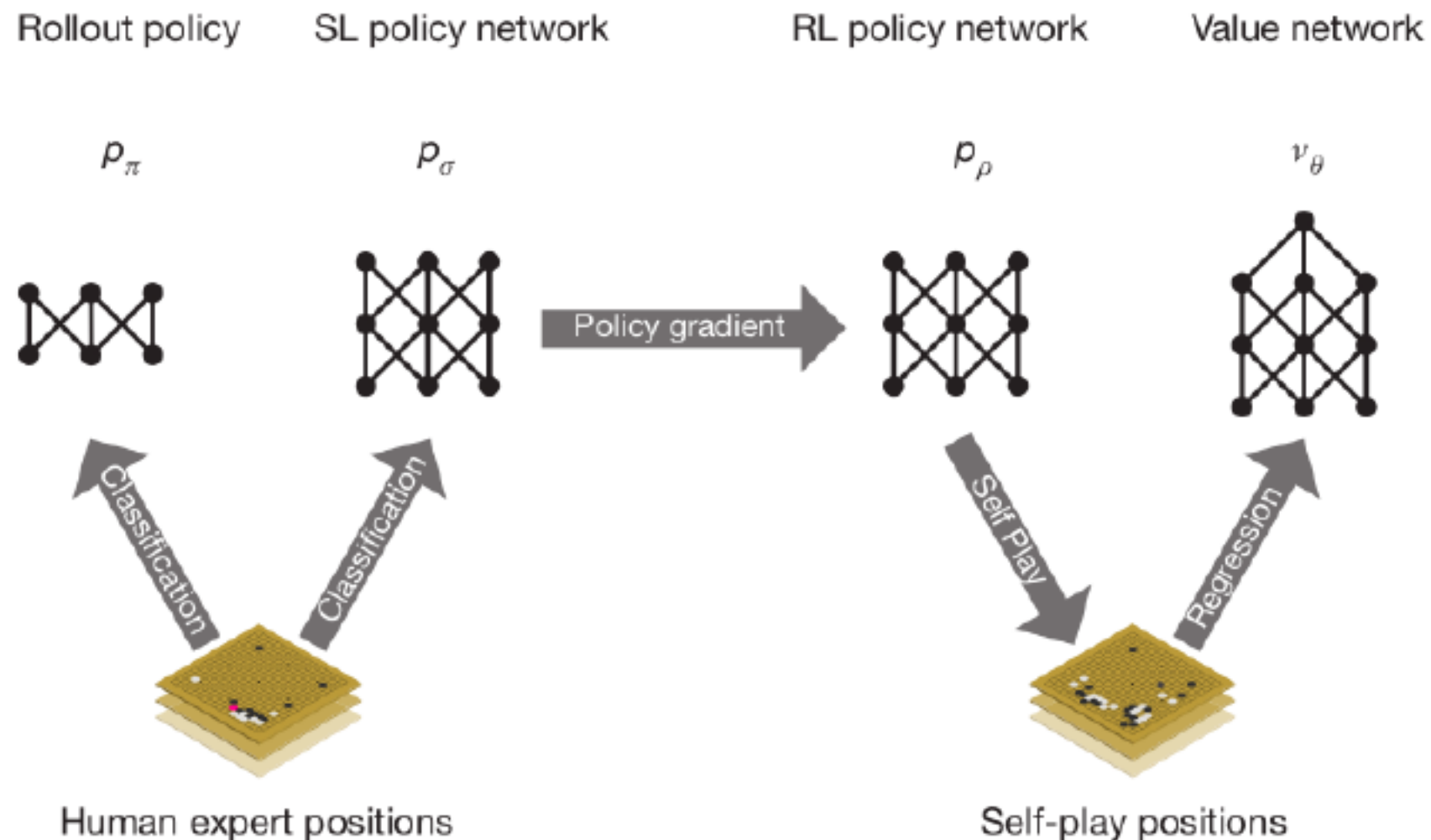






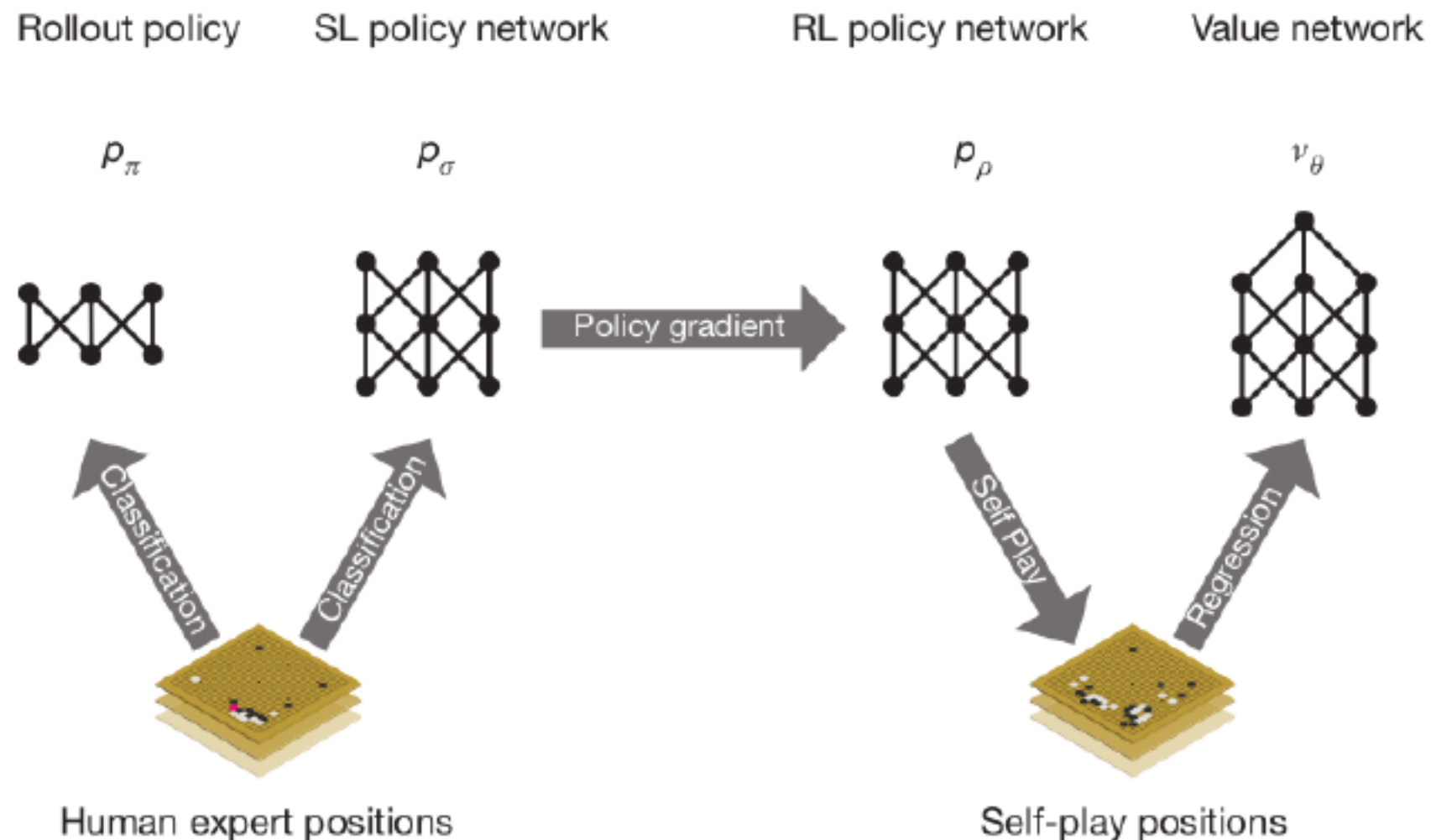
# AlphaGo

1. Train two policies, one cheap policy  $p_\pi$  and one expensive  $p_\sigma$  by mimicking expert moves.
2. Train a new policy  $p_\rho$  with RL and self-play  $p_\rho$  initialized from the  $p_\sigma$  policy.
3. Train a value network that predicts the winner of games played by  $p_\rho$  against itself.
4. Combine the policy and value networks with MCTS at test time.



# AlphaGo

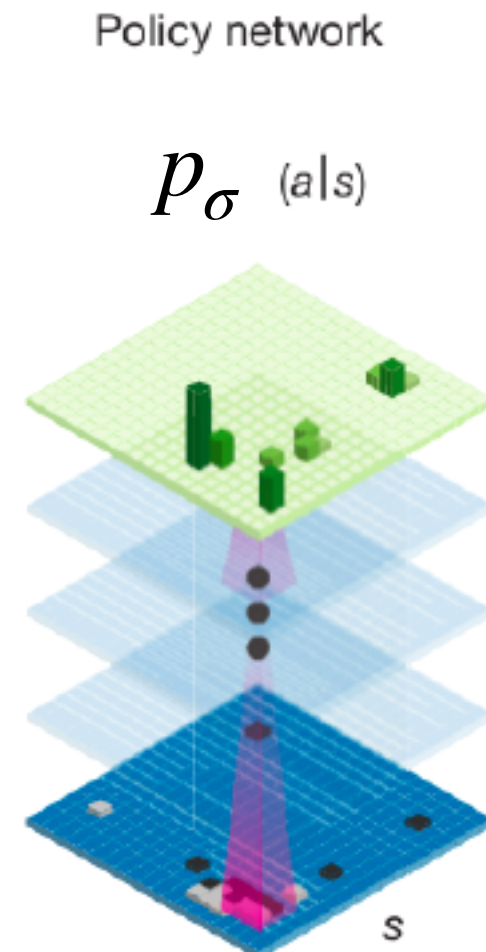
1. Train two policies, one cheap policy  $p_\pi$  and one expensive  $p_\sigma$  by mimicking expert moves.
2. Train a new policy  $p_\rho$  with RL and self-play  $p_\rho$  initialized from the  $p_\sigma$  policy.
3. Train a value network that predicts the winner of games played by  $p_\rho$  against itself.
4. Combine the policy and value networks with MCTS at test time.



# Supervised learning of policy networks

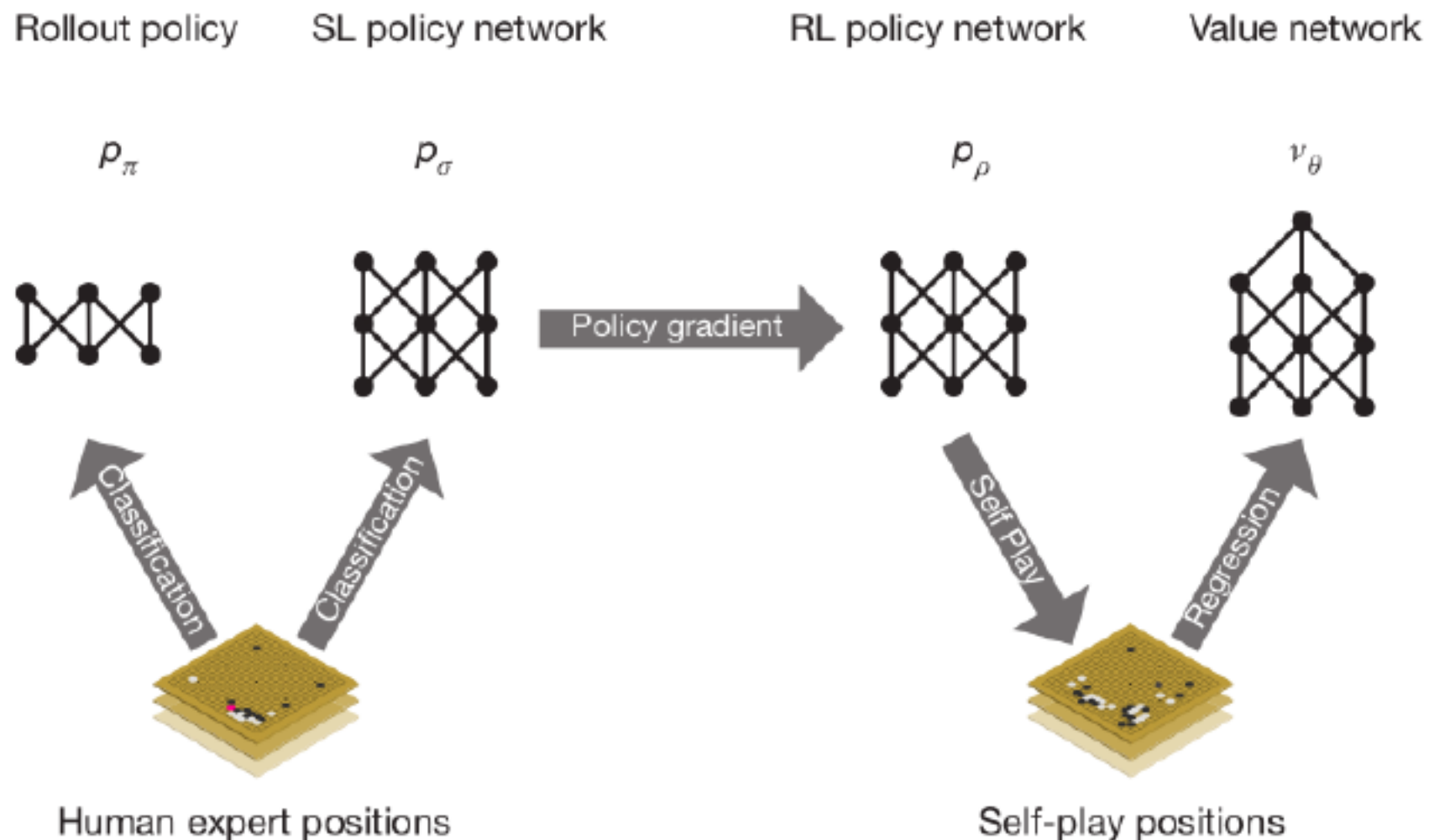
- Objective: predicting expert moves
- Input: randomly sampled state-action pairs  $(s, a)$  from expert games
- Output: a probability distribution over all legal moves  $a$ .

SL policy network: 13-layer policy network trained from 30 million positions. The network predicted expert moves on a held out test set with an accuracy of 57.0% using all input features, and 55.7% using only raw board position and move history as inputs, compared to the state-of-the-art from other research groups of 44.4%.



# AlphaGo

1. Train two policies, one cheap policy  $p_\pi$  and one expensive  $p_\sigma$  by mimicking expert moves.
2. Train a new policy  $p_\rho$  with RL and self-play  $p_\rho$  initialized from the  $p_\sigma$  policy.
3. Train a value network that predicts the winner of games played by  $p_\rho$  against itself.
4. Combine the policy and value networks with MCTS at test time.



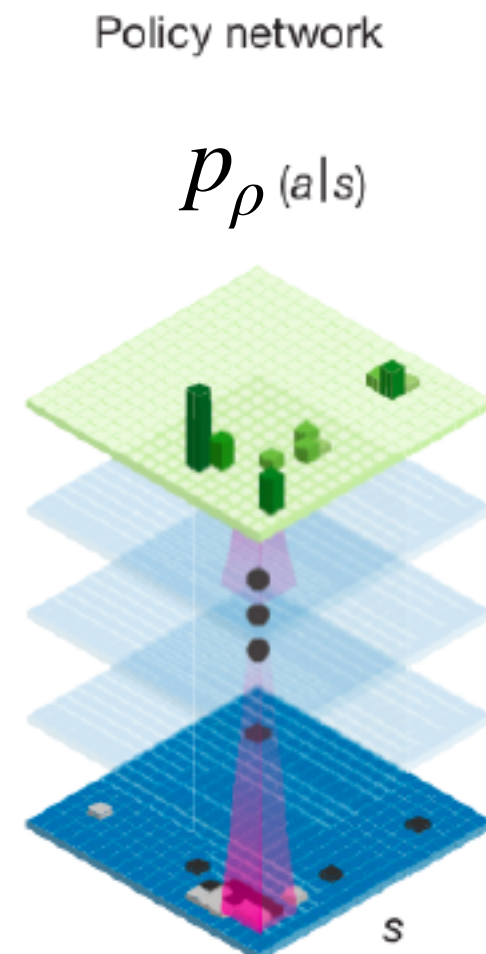
# Reinforcement learning of policy networks

- Objective: improve over SL policy
- Weight initialization from SL network
- Input: Sampled states during self-play
- Output: a probability distribution over all legal moves  $a$ .

Rewards are provided only at the end of the game, +1 for winning, -1 for loosing

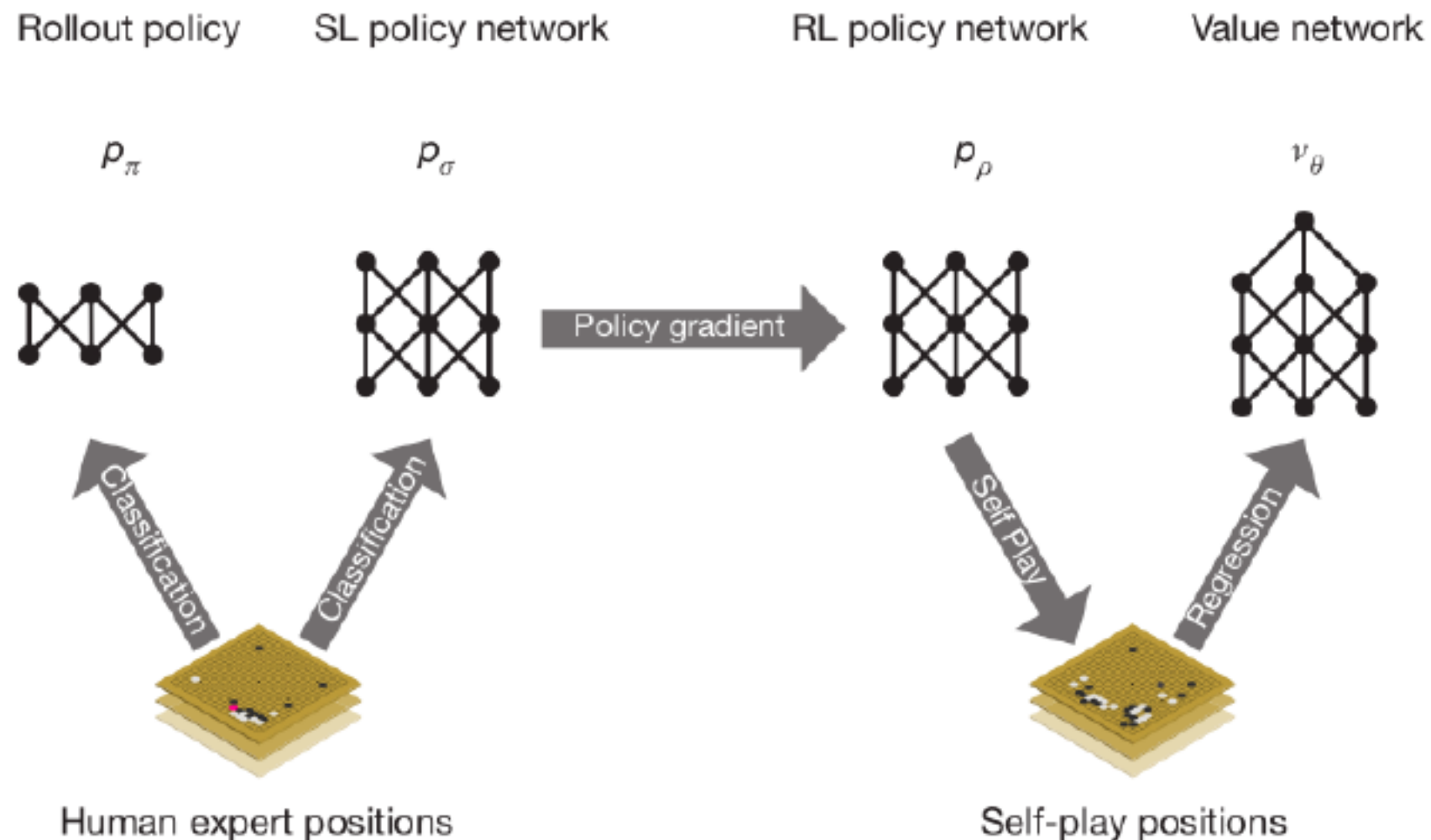
$$\Delta\rho \propto \frac{\partial \log p_\rho(a_t | s_t)}{\partial \rho} z_t$$

The RL policy network won more than 80% of games against the SL policy network.



# AlphaGo

1. Train two policies, one cheap policy  $p_\pi$  and one expensive  $p_\sigma$  by mimicking expert moves.
2. Train a new policy  $p_\rho$  with RL and self-play  $p_\rho$  initialized from the  $p_\sigma$  policy.
3. Train a value network that predicts the winner of games played by  $p_\rho$  against itself.
4. Combine the policy and value networks with MCTS at test time.





# Reinforcement learning of value networks

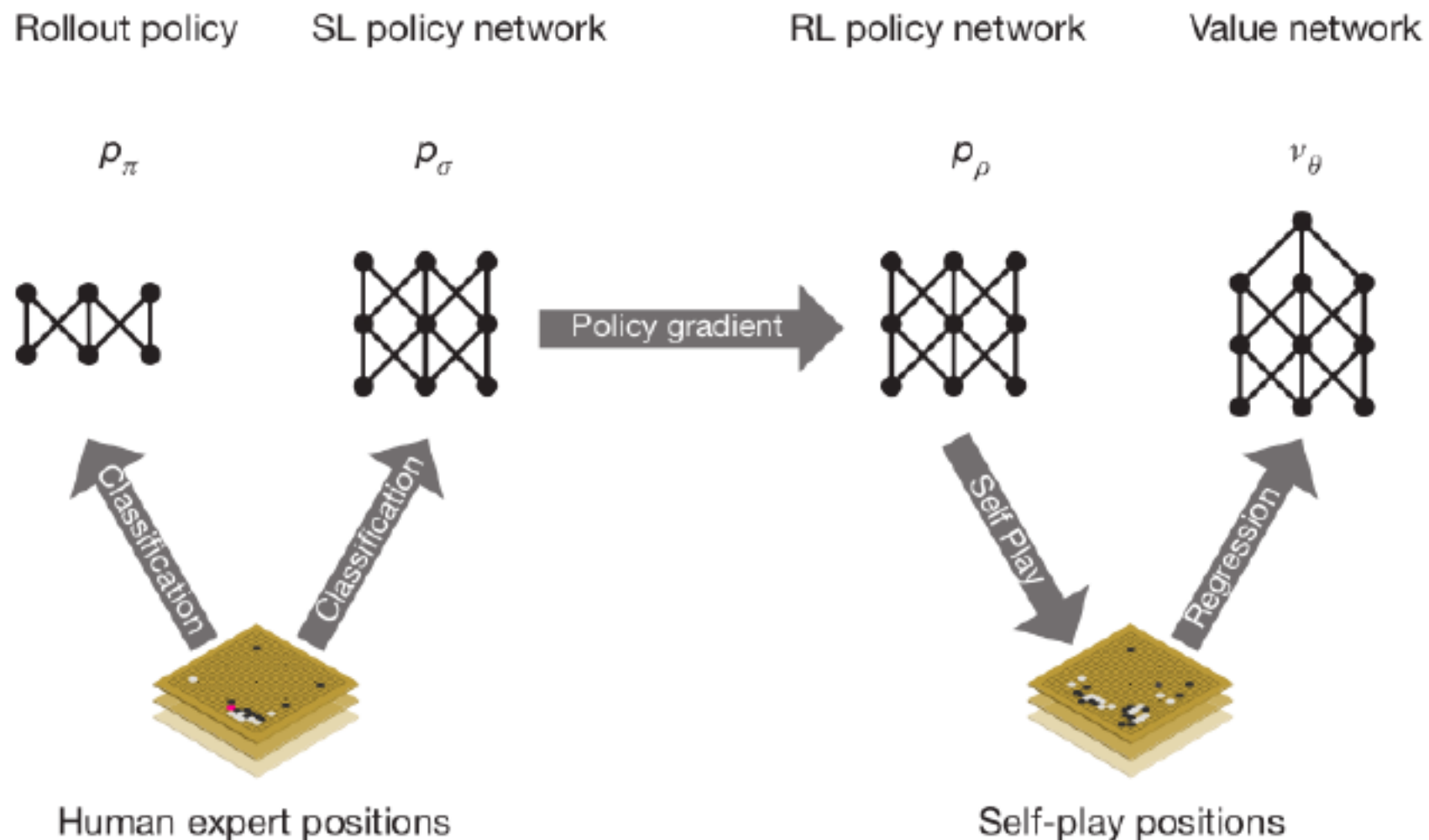
- Objective: Estimating a value function  $v_p(s)$  that predicts the outcome from position  $s$  of games played by using RL policy  $p$  for both players.
- Input: Sampled states during self-play, 30 million distinct positions, each sampled from a separate game.
- Output: a scalar value

Trained by regression on state-outcome pairs  $(s, z)$  to minimize the mean squared error between the predicted value  $v(s)$ , and the corresponding outcome  $z$ .



# AlphaGo

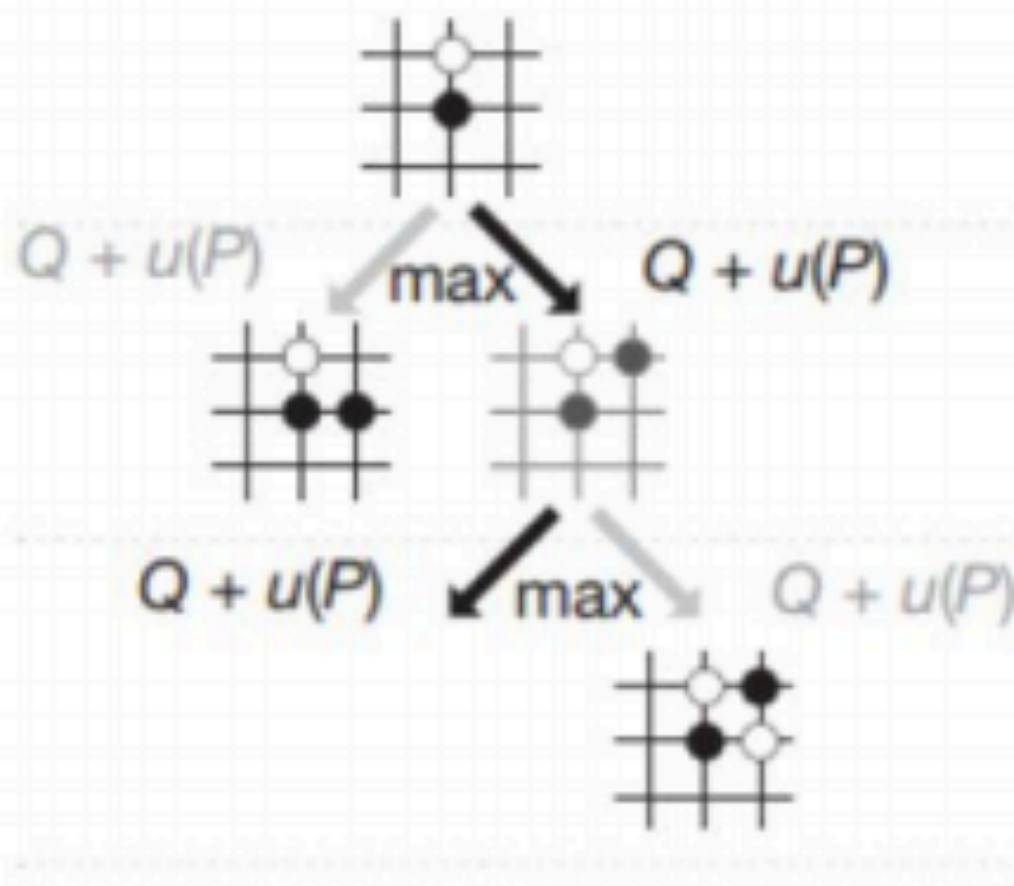
1. Train two policies, one cheap policy  $p_\pi$  and one expensive  $p_\sigma$  by mimicking expert moves.
2. Train a new policy  $p_\rho$  with RL and self-play  $p_\rho$  initialized from the  $p_\sigma$  policy.
3. Train a value network that predicts the winner of games played by  $p_\rho$  against itself.
4. Combine the policy and value networks with MCTS at test time.





# MCTS + Policy/ Value networks

**Selection:** selecting actions within the expanded tree



## Tree policy

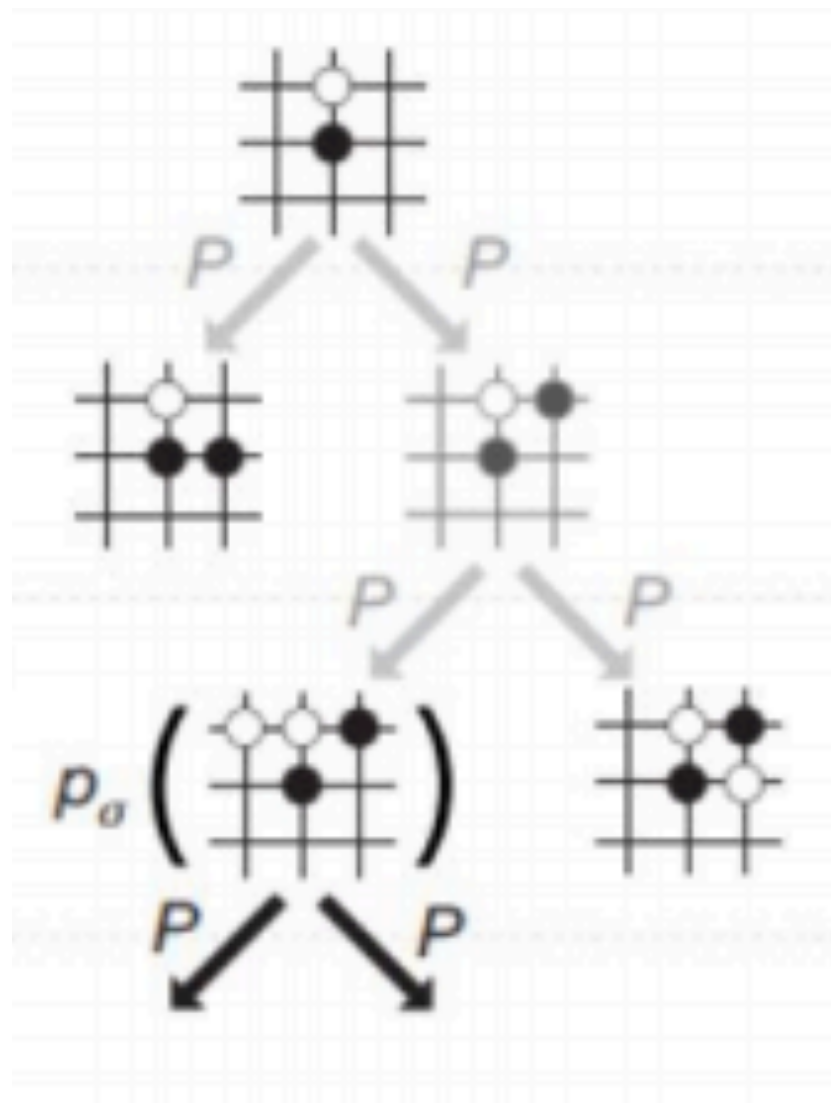
$$a_t = \operatorname{argmax}_a (Q(s_t, a) + u(s_t, a))$$

$$u(s, a) \propto \frac{P(s, a)}{1 + N(s, a)}$$

- $a_t$  - action selected at time step  $t$  from state  $s_t$
- $Q(s_t, a)$  - average reward collected so far from MC simulations
- $P(s, a)$  - prior expert probability provided by the SL policy  $p_\sigma$
- $N(s, a)$  - number of times we have taken action  $a$  from state  $s$  from MC simulations
- $u$  acts as a bonus value

# MCTS + Policy/ Value networks

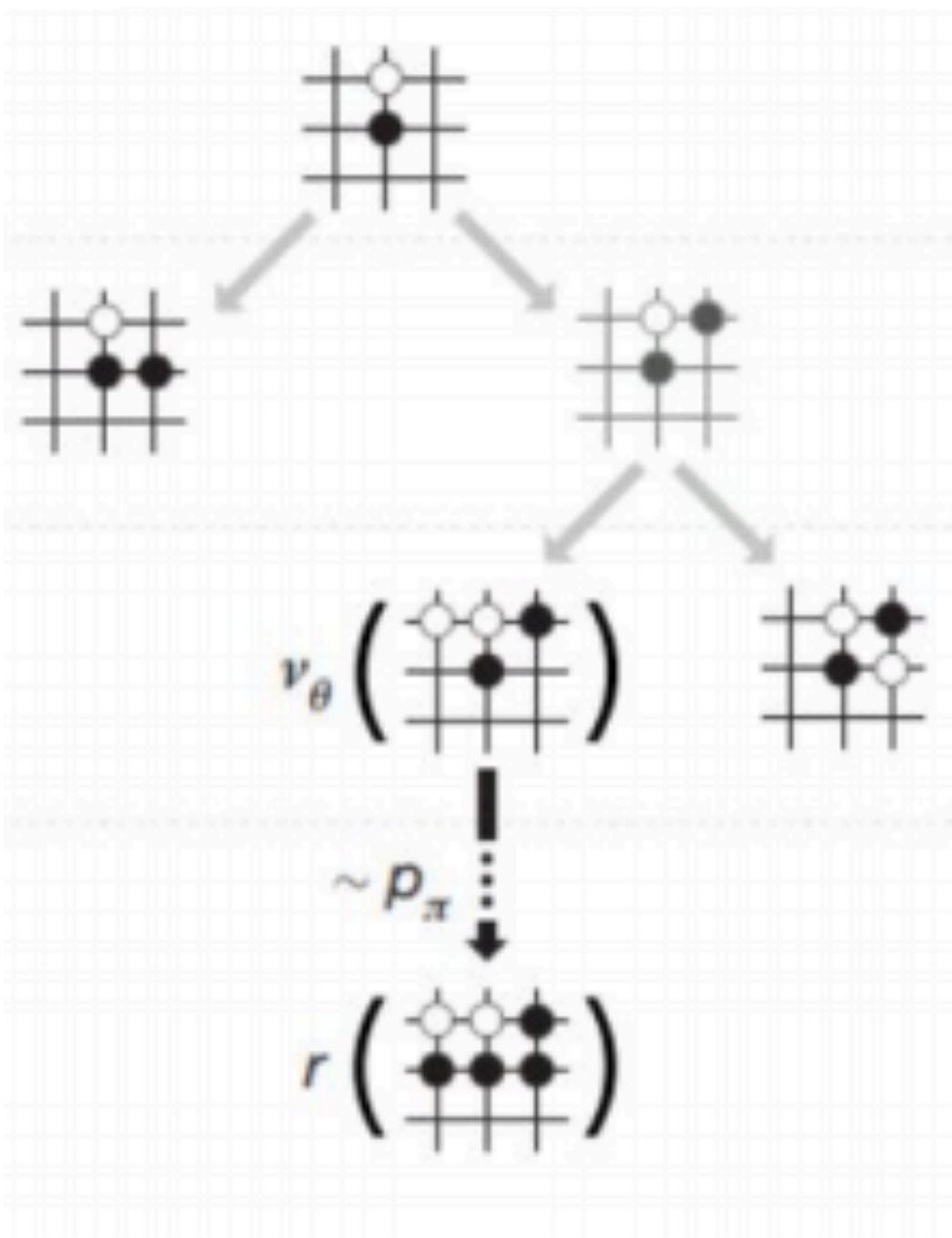
**Expansion:** when reaching a leaf, play the action with highest score from  $p_\sigma$



- When leaf node is reached, it has a chance to be expanded
- Processed once by **SL policy network** ( $p_\sigma$ ) and stored as prior probs  $P(s, a)$
- Pick child node with highest prior prob

# MCTS + Policy/ Value networks

**Simulation/Evaluation:** use the rollout policy to reach to the end of the game



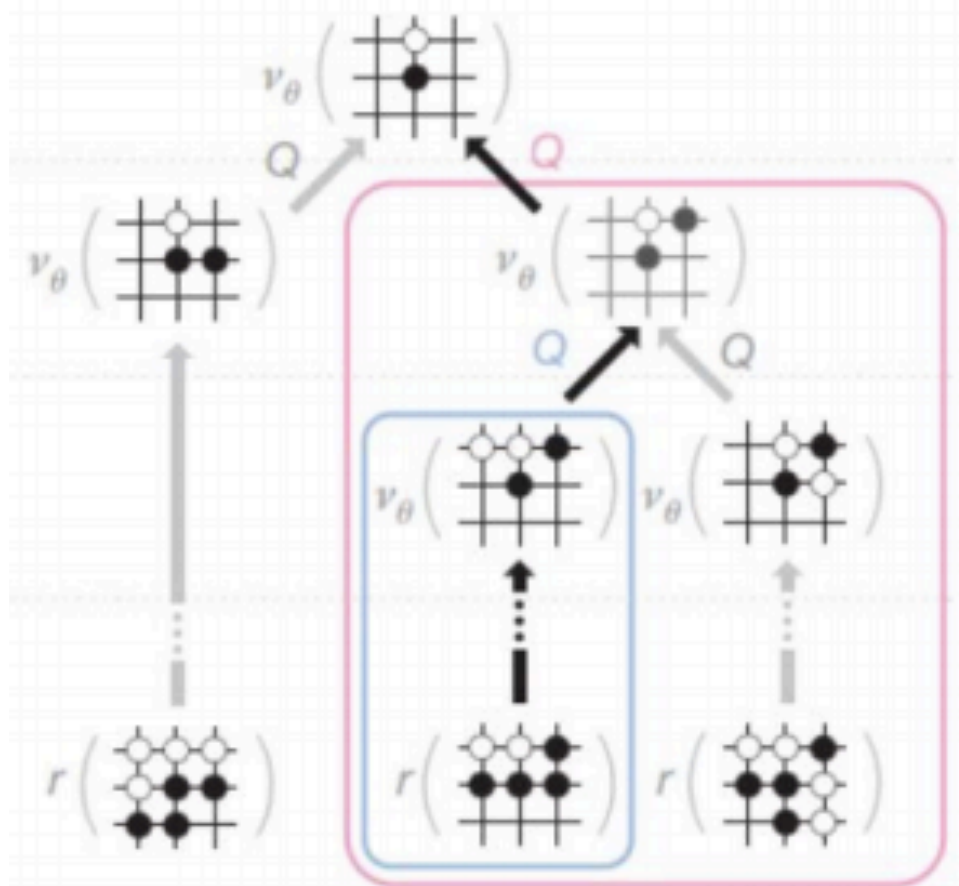
- From the selected leaf node, run multiple simulations in parallel using the rollout policy
- Evaluate the leaf node as:

$$V(s_L) = (1 - \lambda)v_\rho(s_L) + \lambda z_L$$

- $v_\rho$  : value from the trained value function for board position  $s_L$
- $z_L$  : Reward from fast rollout  $p_x$ 
  - Played until terminal step
- $\lambda$  - mixing parameter

# MCTS + Policy/ Value networks

- **Backup:** update visitation counts and recorded rewards for the chosen path inside the tree



$$N(s, a) = \sum_{i=1}^n \mathbf{1}_{(s,a) \in \tau_i}$$
$$Q(s, a) = \frac{1}{N(s, a)} \sum_{i=1}^n \mathbf{1}_{(s,a) \in \tau_i} V(s_L^i)$$

- Extra index is to denote the  $i$  simulation,  $n$  total simulations
- Update visit count and mean reward of simulations passing through node
- Once MCTS completes, the algorithm chooses the most visited move from the root position.

# AlphaGoZero: Lookahead search during training!

- So far, look-ahead search was used for online planning at test time!
- We saw in the last lecture that MCTS is also useful at training time: it in fact reaches superior Q values than vanilla model-free RL.
- AlphaGoZero uses MCTS during training instead.
- AlphaGoZero gets rid of human supervision.

# AlphaGoZero: Lookahead search during training!

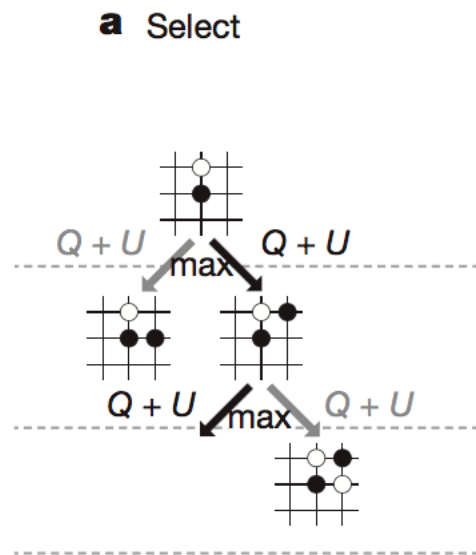
- So far, look-ahead search was used for online planning at test time!
- We have seen that MCTS is useful at training time: it in fact reaches superior Q values than vanilla model-free RL.
- AlphaGoZero uses MCTS during training instead.
- AlphaGoZero does not use any human supervision and outperforms human players while trained only by self-play.

# AlphaGoZero: Lookahead search during training!

- Given any policy, a MCTS guided by this policy for action selection (as described earlier), will produce an improved policy for the root node (policy improvement operator)
- Train to mimic such improved policy

# MCTS + Policy/ Value networks

## Tree policy



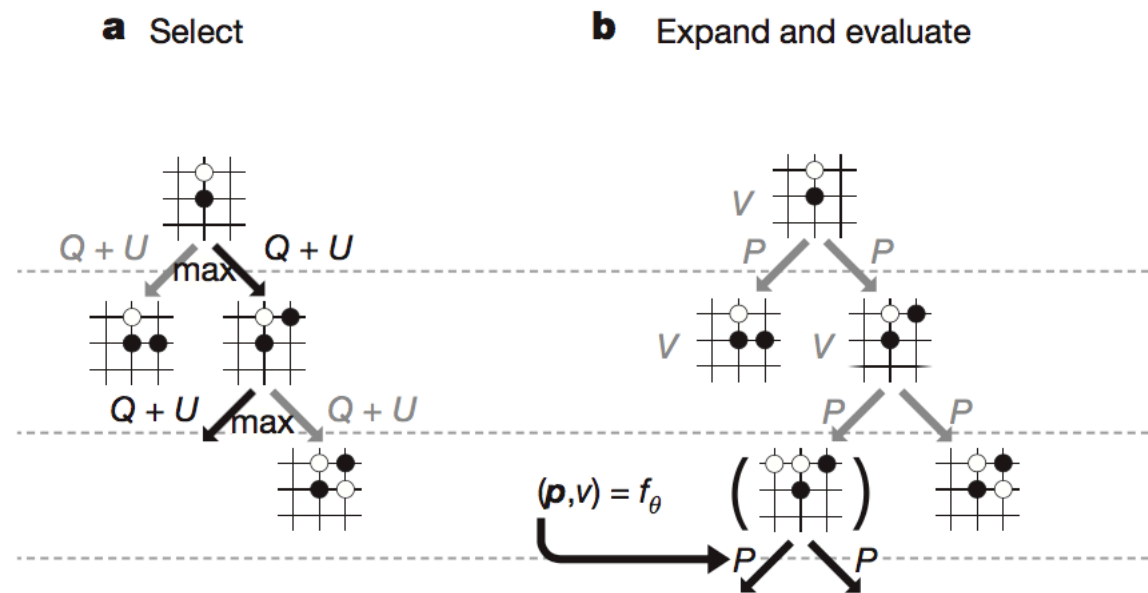
$$a_t = \operatorname{argmax}_a \left( Q(s_t, a) + U(s_t, a) \right)$$

$$U(s, a) \propto \frac{P(s, a)}{1 + N(s, a)}$$

- $a_t$  - action selected at time step  $t$  from state  $s_t$
- $Q(s_r, a)$  - average reward collected so far from MC simulations
- $P(s, a)$  - prior expert probability provided by the policy  $\pi_\theta$
- $N(s, a)$  - number of times we have taken action  $a$  from state  $s$  from MC simulations
- $U$  acts as a bonus value



# MCTS + Policy/ Value networks

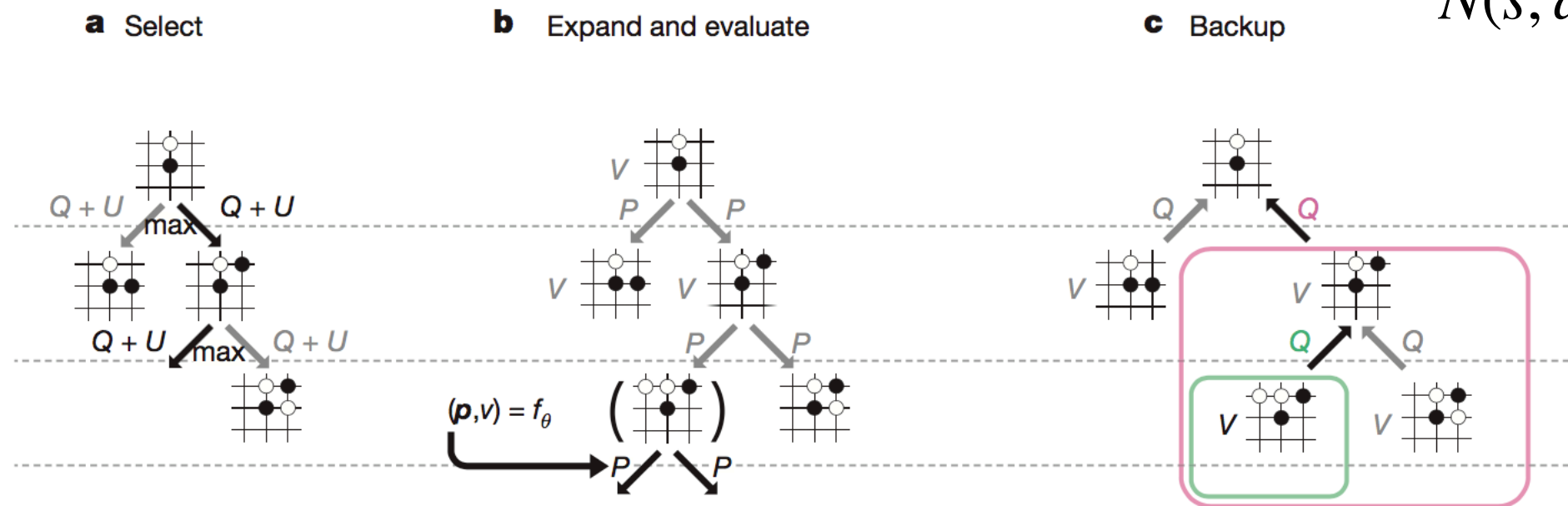


- When leaf node is reached, its value is computed  $v_\theta(s)$  and the prior probs  $P(s, a)$  for all its legal action-children are computed and stored.

# MCTS + Policy/ Value networks

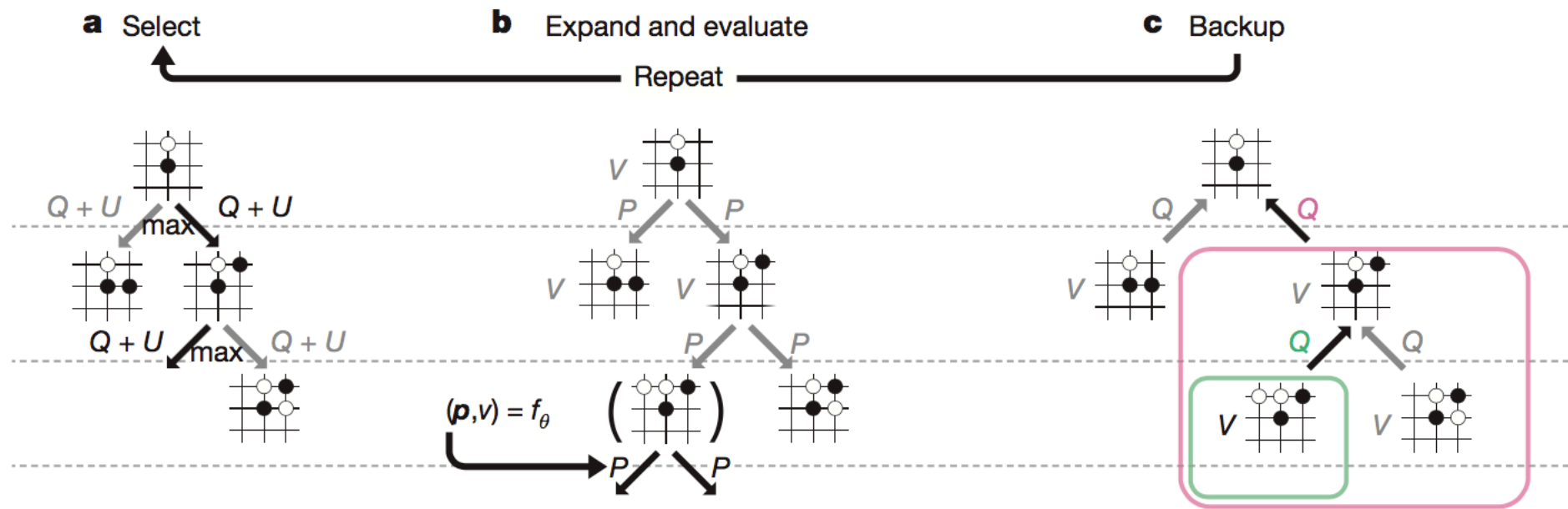
$$N(s, a) = \sum_{i=1}^n \mathbf{1}_{(s,a) \in \tau_i}$$

$$Q(s, a) = \frac{1}{N(s, a)} \sum_{i=1}^n \mathbf{1}_{(s,a) \in \tau_i} V(s_L^i)$$



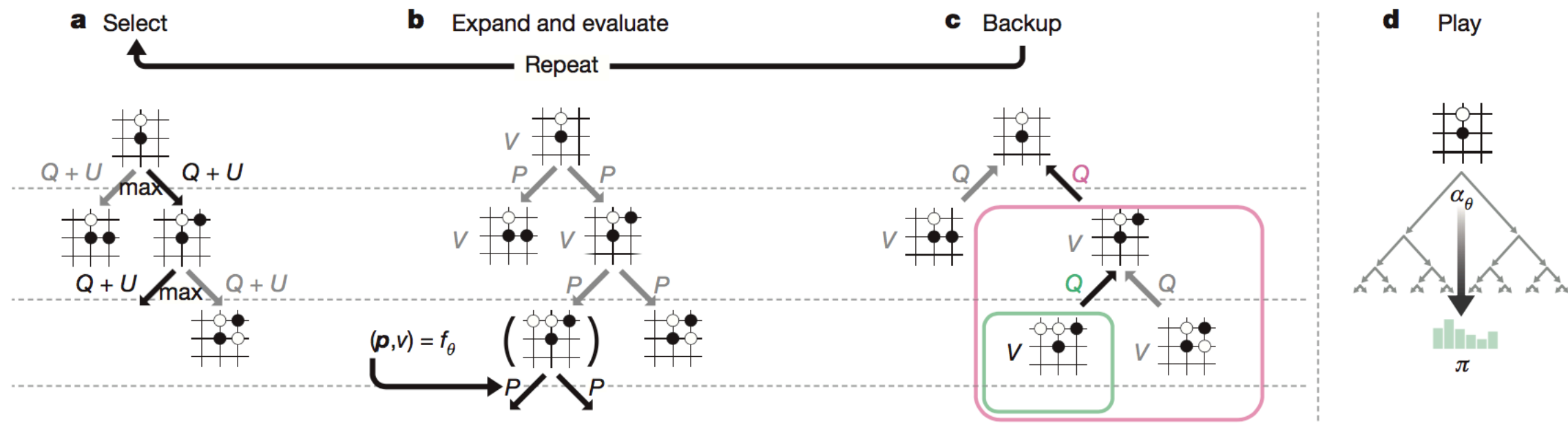
- No full rollouts till game termination!
- Update visit counts, total reward and mean reward for the actions used in the current rollout.
- $n$ : the # of MC simulations so far

# MCTS + Policy/ Value networks



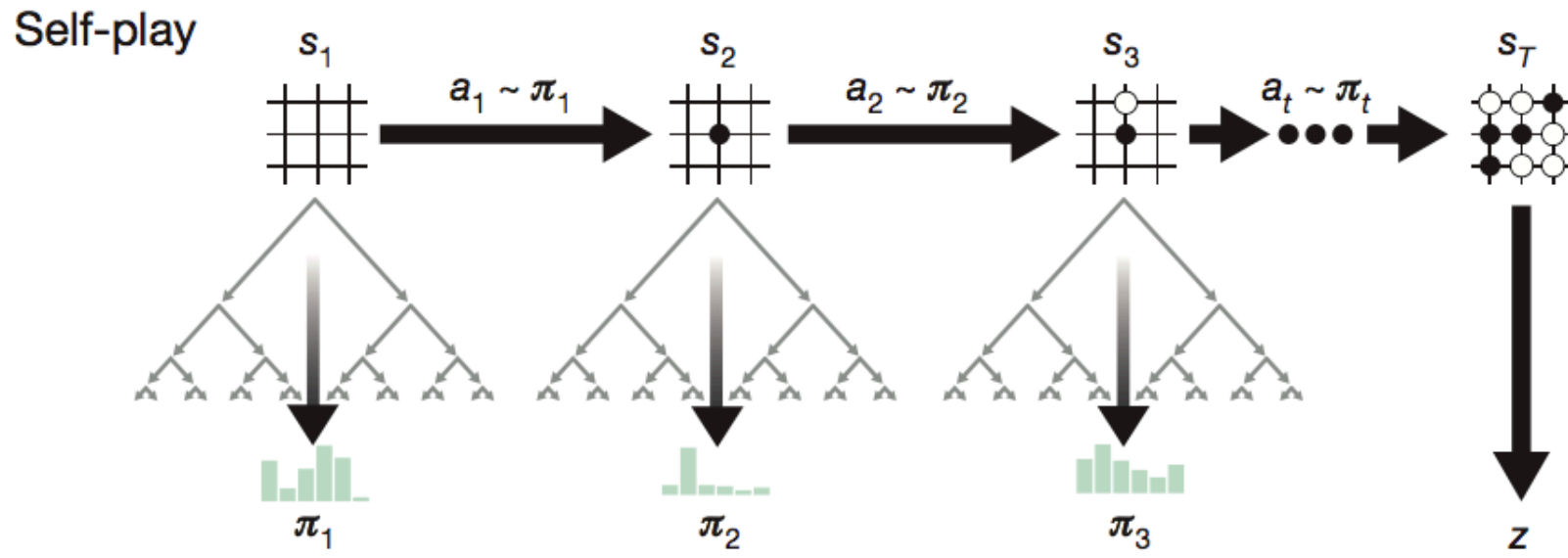
1600 MC rollouts were used to select each root action.

# MCTS + Policy/ Value networks



Once MCTS completes, the algorithm chooses the most visited move from the root position.

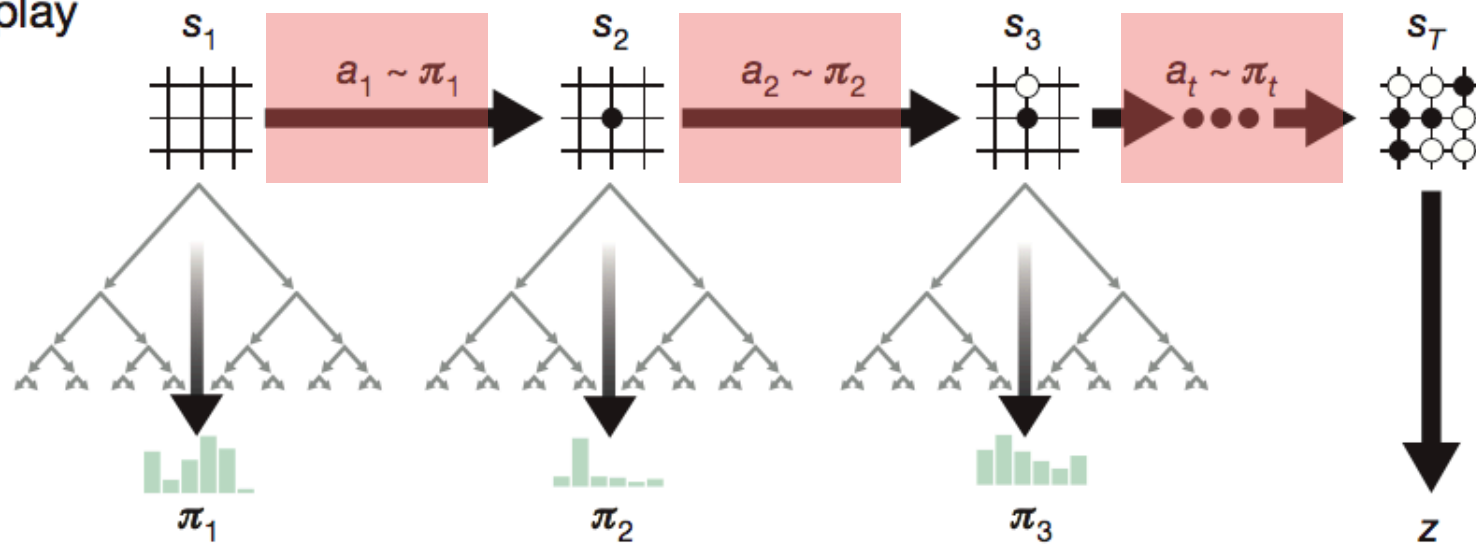
# Self-play



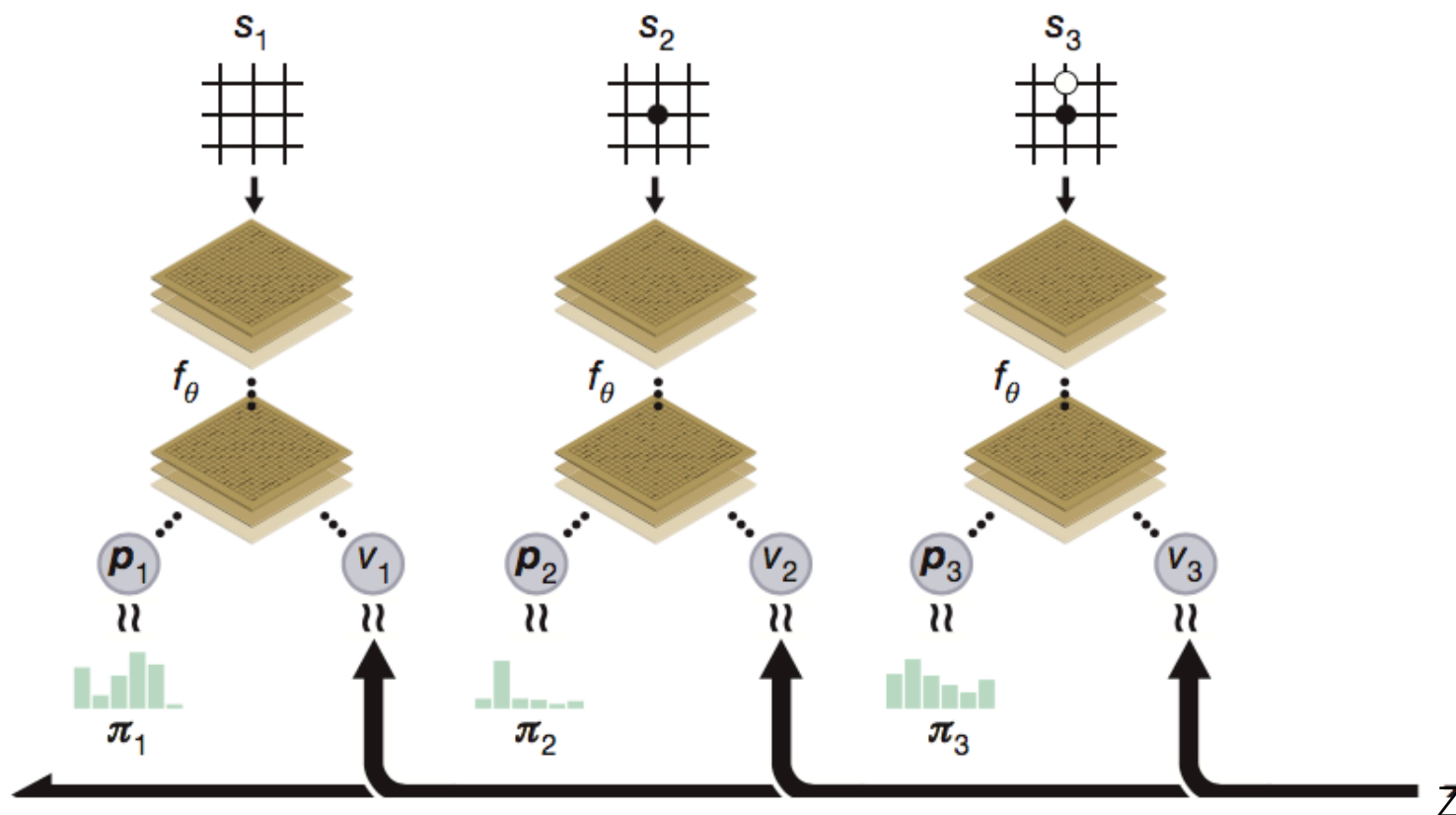
# MCTS as policy improvement operator

Each of those requires 1600 MC rollouts, i.e., about 0.4 secs thinking time per move.

Self-play

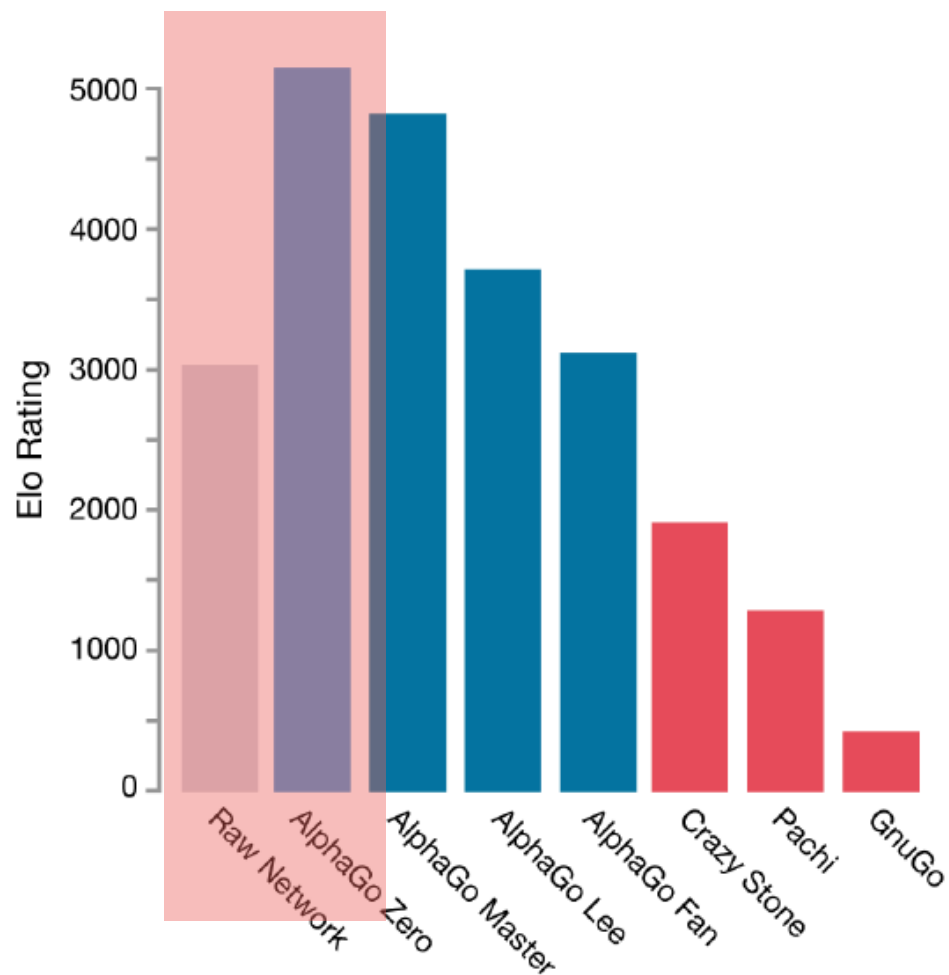
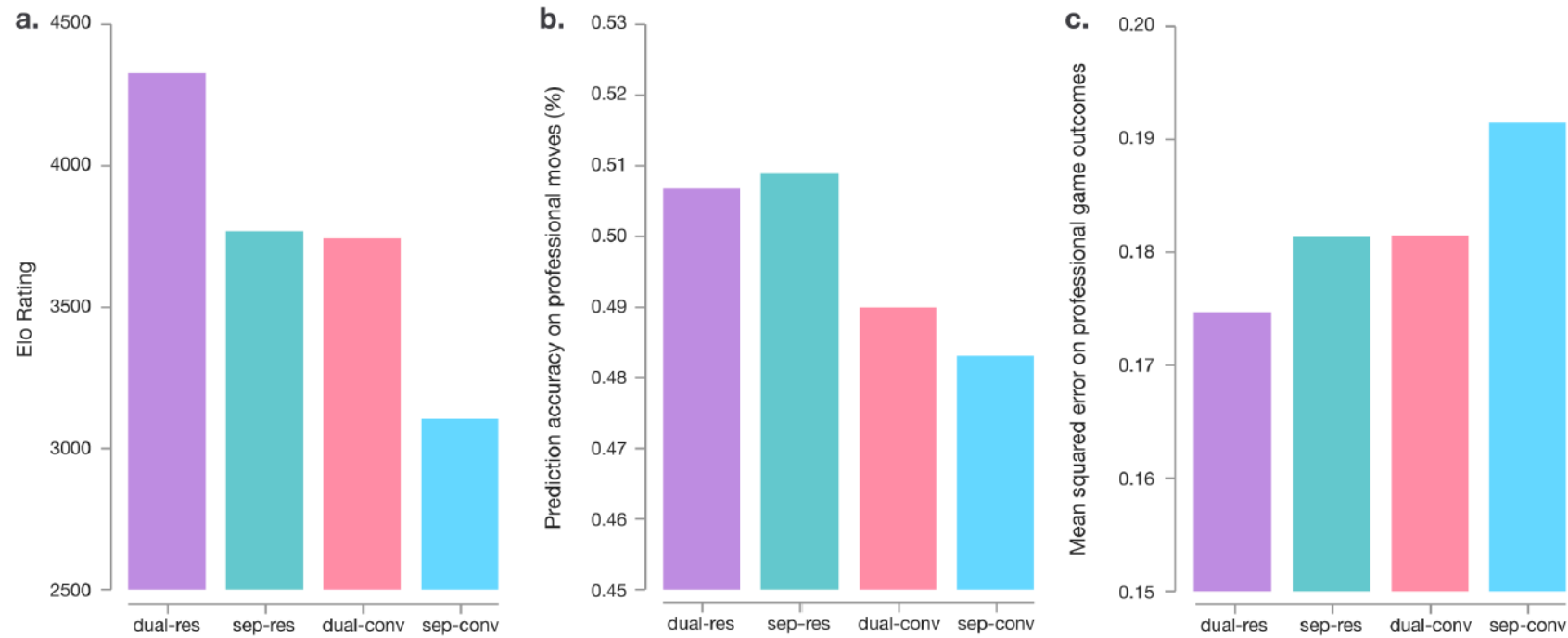


Neural network training



- Given a policy  $\pi_\theta$ , MC rollouts can provide for the root state an action distribution that is better than the initial policy  $\pi_\theta$ .
- Train so that the policy network mimics this improved policy
- Train so that the position evaluation network (value function approximator) output matches the outcome

# Architectures



- Resnets help
- Jointly training the policy and value function using the same main feature extractor helps
- Lookahead tremendously improves the basic policy