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# Monte-Carlo Game Tree Search: Basic Techniques

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# Abstract

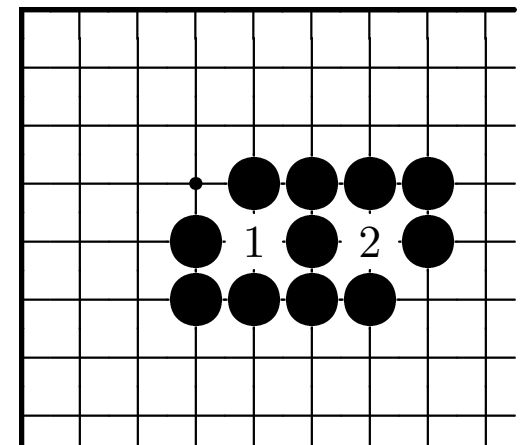
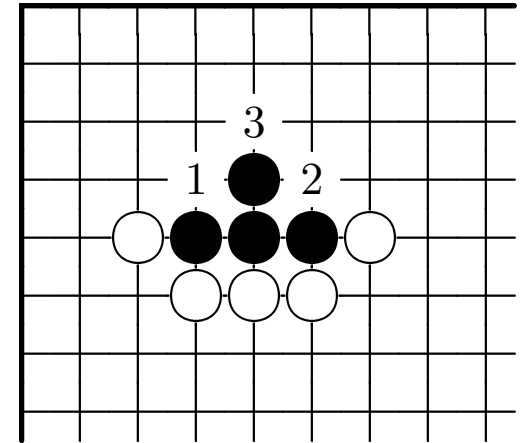
- **Introducing the original ideas of using Monte-Carlo simulation in computer Go.**
  - Pure Monte-Carlo simulation.
  - Using UCB scores.
  - In-cooperate with Mini-Max tree search.
  - Using UCT tree expansion.
    - ▷ *Best first tree growing.*
- **Introduce only sequential implementation here.**
  - Parallel implementation will be introduced later if time allows.
- **Conclusion:**
  - A new search technique that proves to be very useful in solving selective games including computer Go.

# Basics of Go (1/2)

- Black first, a player can pass anytime.
- The game ends when both players pass in consecutive turns.
- **intersection**: a cell where a stone can be placed or is placed.
- two intersections are **connected** if they are either adjacent vertically or horizontally, i.e., 4-neighbors.
- **string**: a connected, i.e., vertically or horizontally, set of stones of one color.
- **liberty**: the number of connected empty intersections.
  - Usually we calculate the amount of liberties for a string.
  - A string with no liberty is captured.
- **eye**:
  - Exact definition: very difficult to be understood and implemented.
  - Approximated definition:
    - ▷ *An empty intersection surrounded by outside borders or stones of one color with two liberties or more.*
    - ▷ *An empty intersection surrounded by outside borders or stones belonging to the same string.*

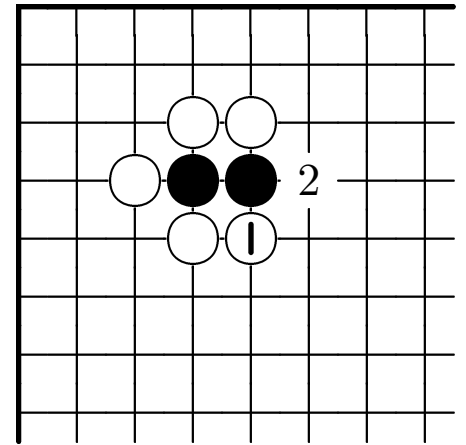
# Basics of Go (2/2)

- A black string with 3 liberties.
- A black string with 2 eyes.
  - A string with two eyes cannot be captured by the opponent unless you fill in one of the two eyes yourself first.



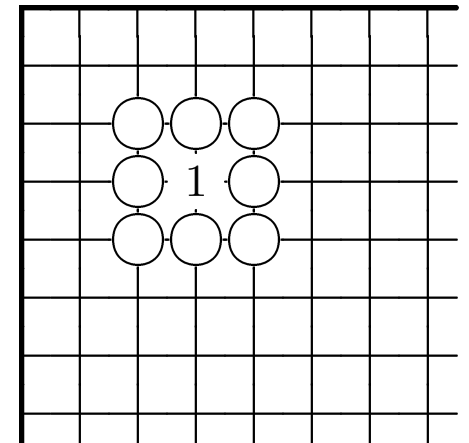
# Atari

- A string with liberty = 1 is in danger and is called **atari**.
  - Placing a white stone at the intersection 1 **threatens** the black string.
  - The black string is in danger.
  - The intersection at 2 is now critical.



# Legal ply

- Place your stone in an empty intersection, not causing **suicide** or **Ko**<sup>1</sup>.
  - Black cannot place a black stone at the intersection 1.
  - This is called a **suicide** ply<sup>2</sup>.



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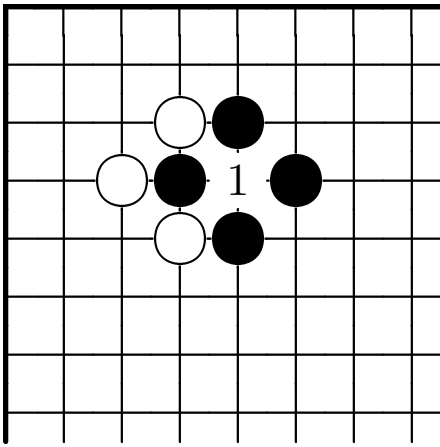
<sup>1</sup>Ko will be defined later.

<sup>2</sup>More discussion of suicide plys will be given later.

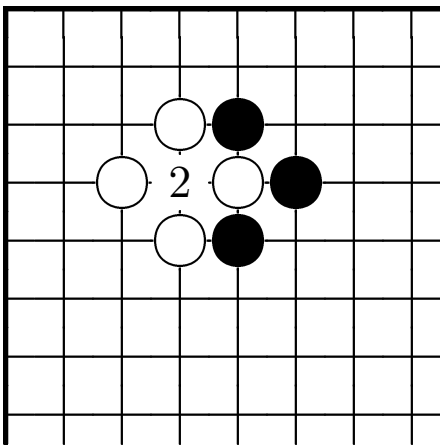
# The rule of Ko

- Use the rule of **Ko** to avoid endless repeated plys.

- Place a white stone at 1, a black stone is captured.



- Place a black stone at 2, a white stone is captured.



- This can go on forever and thus is forbidden (to the black).

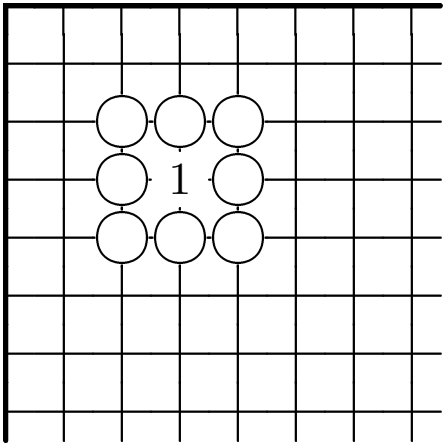
# General rules of Go

- Black plays first.
- A string without liberty is removed.
- You cannot place a stone and results in a position that is 2-plys ago after the removing of strings without liberty.
  - **You cannot create a loop.**
    - ▷ *Note: exact rules for avoiding loops are very complicated and have many different definitions.*
- You can **pass**, namely forfeit the right to play.
  - A **self-suicide** ply is one that causes the stone played, and this stone only, being removed immediately which is equivalent to a pass.
    - ▷ *In most rules, you cannot place a stone to cause more than one of your stones, including the one just played, being removed.*
    - ▷ *You can place a stone in an intersection without liberty if as a result you can capture opponent's stones.*
- When both players pass in consecutive plys, the game ends.
- The one with more stones and **eyes** wins at the end of the game after discounting **Komi**.
  - ▷ *Other scoring rules exists such as counting the number of stones captured as well.*

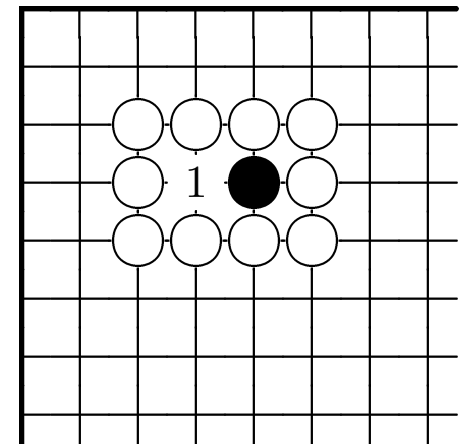


# More examples

- If black plays 1, then it is equivalent to a pass.



- Illegal move (suicide) at 1 for black for most rules unless it is Ing rules.



# Komi

- When calculating the final score, the black side, namely the first player, has a penalty of  $k$  stones, which is set by what is called **Komi**.
  - To offset the initiative.
  - When  $k$  is an integer, you may draw a game.
    - ▷ *It is possible to draw<sup>3</sup> a Go game by entering a loop whose length is more than 4 plys.*
- Go has different very subtle rules with different versions which set the value of Komi differently.
  - The value of Komi changes over the time.
  - For 9 by 9 Go, currently it is 7.
    - ▷ *It is possible to draw even no loop is involved!*
  - For 19 by 19 Go, it is either 6.5 or 7.5.
    - ▷ *No draw by score!*
    - ▷ *May be draw by entering a loop whose length is more than 4.*

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<sup>3</sup>Some rules disallow the creation of any loop.

# Ranking system

- **Dan-kyu system: from good to bad in the order of**
  - Professional level: dan.
    - ▷ 9, 8, ..., 2, 1
  - Amateur level: dan.
    - ▷ 9, 8, ..., 2, 1
    - ▷ *usually no more than 6*
  - Kyu:
    - ▷ 1, 2, 3, 4, ...
- **A higher ranked player has a better chance of winning, but not a sure win, against a lower ranked player.**

# Elo system

- **Elo: assign a numerical score to a player so that the larger the score, the better a player is.**
- **Usually between 100 to 3000+.**
- **Time dependent.**
- **More details in later lectures.**
- **Human: [www.goratings.org](http://www.goratings.org)**
  - **$\geq 2940$ : professional 9 dan**
  - **$\sim 2820$ : professional 5 dan**
  - **Human history high <sup>4</sup>**
    - ▷ *Nov. 2019: 3692.33 (Shin, Jinseo).*
    - ▷ *Nov. 2020: 3909.94 (!!) (Shin, Jinseo).*
    - ▷ *Nov. 2021: 3828 (Shin, Jinseo).*
    - ▷ *Nov. 2022: 3839 (Shin, Jinseo).*
    - ▷ *Oct. 2023: 3865 (Shin, Jinseo).*
  - **Alpha Go has an impact on human players. Whoever can make use of it for training can improve better than those who cannot.**

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<sup>4</sup><https://www.goratings.org/en/>

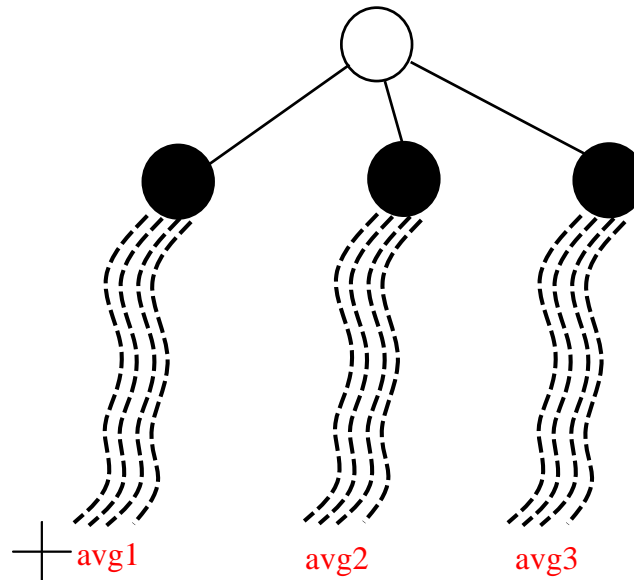
# Why Alpha-Beta cut won't work on Go?

- Alpha-beta based searching has been used since the dawn of CS.
  - Effective when a **good** evaluation function can be designed manually by human and computed **efficiently** by computers.
    - ▷ *Evaluation functions do not need to be designed purely by human anymore.*
    - ▷ *One can use machine learning techniques as well.*
    - ▷ *Example: the development of GNU Go before 2004 using manually designed heuristics, and the development of Alpha Go after year 2016 using deep learning.*
  - Good for games with a not-too-large branching factor, say within 40 and a relative small **effective** branching factor, say within 5.
    - ▷ *Effective plys mean those that are not obviously bad plys.*
- Go has a huge branching factor and a not too small effective branching factor. The evaluation function of Go is also difficult to be manually designed.
  - First Go program is probably written by Albert Zobrist around 1968.
  - Until 2004, due to a lack of major break through, the performance of computer Go programs is around 5 to 8 kyu for a very long time.

# Monte-Carlo search: original ideas

## ■ Algorithm $MCS_{pure}$ :

- For each child of the root
  - ▷ *Play a large number of **almost random games** from a position to the end, and score them.*
- Evaluate a child position by computing the average of the **scores** of the random games in which it had played.
- Play a move going to the child position with **the best score**.



# How scores are calculated

- **Score** of a game: the difference of the total numbers of stones and eyes for the two sides.
- Evaluation of the child positions from the possible next moves:
  - Child positions are considered independently.
  - Child positions were evaluated according to the **average scores** of the games in which they were played, not only at the beginning but at every stage of the games provided that it was the first time one player had played at the intersection.
- Can use winning rate or non-losing rate as the score.
  - **For ease of description, we use mostly winning rate in the rest of our slides here.**

# How almost random games are played

- No filling of the eyes when a random game is drawn.
  - The only **domain-dependent knowledge** used in the original version of GOBBLE in 1993.
- Moves are ordered according to their current scores.
- Ideas from “simulating annealing” were used to control the probability that a move could be played out of order.
  - The amount of randomness put in the games was controlled by the **temperature**.
    - ▷ *The temperature was set high in the beginning, and then gradually decreased.*
    - ▷ *For example, the amount of randomness can be a random value drawn from the interval  $[e^{v(i)/t(i)} - c, e^{v(i)/t(i)} + c]$  where  $v(i)$  is the value at the  $i$ th iteration,  $c$  is a positive constant and  $t(i)$  is the temperature at the  $i$ th iteration.*
    - ▷ *Note when  $t(i) \gg 1$ , then  $e^{v(i)/t(i)} \rightarrow 1$ .*
  - Simulating annealing is not required, but was used in the original 1993 version.



# Results

- **Original version: GOBBLE 1993 [Bruegmann'93].**
  - Performance is not good compared to other Go programs of the same era.
- **Enhanced versions used after year 2000.**
  - Adding the idea of using new scoring functions.
  - Using a mini-max tree search.
  - Using a best first tree growing.
  - Adding more domain knowledge.
  - Adding more techniques.
    - ▷ *Much more than what are discussed here.*
    - ▷ *In practice, works out well when the game is approaching the end or when the state-space complexity is not large.*
  - Building theoretical foundations from statistics, and on-line and off-line learning.
  - Using techniques from deep learning.

# Historical results (1/2)

## ■ MoGo (France):

- ▷ *Won Computer Olympiad champion of the 19 \* 19 version in 2007.*
- ▷ *Beat professional 8-dan player Myungwan Kim with a 9-stone handicap at August 2008 (US Go Congress).*
- ▷ *Judged to be in a “professional” level for 9 \* 9 Go in 2009.*
- ▷ *Very close to professional 1-dan for 19 \* 19 Go.*

## ■ Zen (Japan):

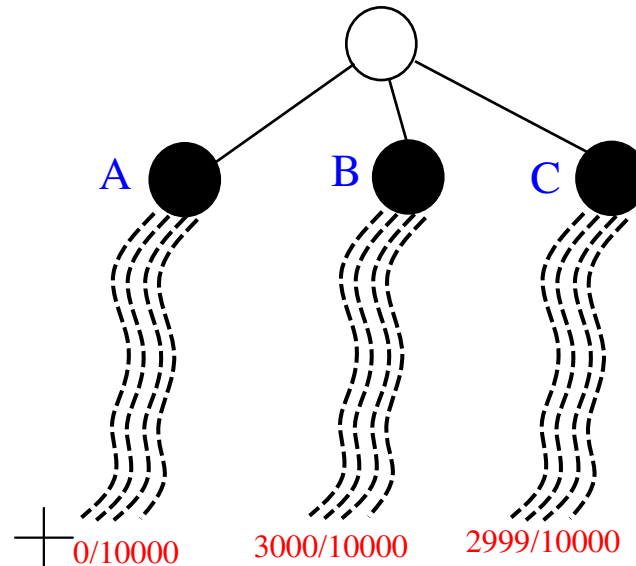
- ▷ *Close to amateur 3-dan in 2011.*
- ▷ *Beat a 9-dan professional master with handicaps at March 17, 2012.*  
*First game: Five stone handicap and won by 11 points.*  
*Second game: four stones handicap and won by 20 points.*
- ▷ *Add techniques from machine learning.*

# Historical results (2/2)

- **AlphaGo Lee: Beat a professional 9-dan at March 2016 with a record of 4 to 1 !**
  - ▷ *Using supervised deep learning.*
  - ▷ *Elo 3739 ~ 10-dan [Silver et al 2016] vs Sedol Lee (~ Elo 3580)*
- **AlphaGo Zero: An earlier version beat one of the very top professional players at May 2017 with a record of 3 to 0 !!!**
  - ▷ *Using unsupervised learning.*
  - ▷ *Elo 5185 !!! ~ (10 + x)-dan [Silver et al 2017] vs Ke, Jie (Elo 3761)*

# Problems of MCS<sub>pure</sub>

- May spend too much time on hopeless branches.
  - In the example below, after some trials on  $A$ , it can be concluded that this branch is hopeless.
  - From now on, time should be spent on  $B$  and  $C$  to tell their difference which is currently too close to call.



† **2999/10000** means winning 2,999 times out of 10,000 simulations.

# First major refinement

## ■ Observations:

- Some moves are obviously bad and do not need further exploring.
- Should spend some time to verify whether a move that is currently good will remain good or not.
- Need to have a mechanism for moves that are bad so far because of **extremely bad luck** to have a chance to be reconsidered later.

## ■ Efficient sampling:

- Original: equally distributed among all legal moves.
- Biased sampling
  - ▷ *Sample some moves more often than others.*
  - ▷ *Every move has some chance to be sampled from time to time.*

# Better playout allocation

## ■ $K$ -arm bandit problem:

- Assume you have  $K$  slot machines each with a different payoff, i.e., expected value of returns  $\mu_i$ , and an unknown distribution.
- Assume you can bet on the machines totally  $N$  times, what is the best strategy to get the largest returns?

## ■ Ideas:

- Try each machine a few, but enough, times and record their returns.
- For the machines that currently have the best returns, play more often later on.
- For the machines that currently return poorly, **give them a chance from time to time** just in case their distributions are bad for the runs you have tried so far.

# UCB

## ■ UCB: Upper Confidence Bound [Auer et al'02]

- For each child  $p_i$  of a parent node  $p$ , compute its

$$\text{UCB}_i = \frac{W_i}{N_i} + c\sqrt{\frac{\log N}{N_i}} \text{ where}$$

- ▷  $W_i$  is the number of win's for the position  $p_i$ ,
- ▷  $N_i$  is the total number of games played  $p_i$ ,
- ▷  $N = \sum_{\forall i} N_i$  is the total number of games played on  $p$ , and
- ▷  $c$  is a positive constant called **exploration** parameter which controls how often a slightly bad move be tried.

- Expand a new simulated game for the move with the highest UCB value.

## ■ Note:

- We only compare UCB scores among children of a node.
- It is meaningless to compare scores of nodes that are not siblings when later on tree search is in-cooperated.

# What is guaranteed by using UCB

- **Theorem 1:** a non-optimal machine is played only  $O(\ln N/\Delta^2)$  times for  $N$  operations where  $\Delta$  is the smallest amount of **regret** normalized to the range of  $[0,1]$  [Auer et al'02].
  - regret: the loss due to not picking the true best one.
  - the total amount of regrets is  $O(\ln N/\Delta)$ .
  - If there is no other information available, this is probably the best you can do theoretically.
- **How this helps in doing Monte Carlo simulation?**
  - Game search problem: finding the best ply among  $K$  possible moves.
    - ▷ *Each possible ply corresponds to a bandit.*
    - ▷ *A good ply leads to a position with a better win rate which is a bandit with a better payoff.*
  - Most of the time in the course of doing  $N$  simulations, except  $O(K \times \ln N/\Delta^2)$  of them, the simulation is done on plies with good win rates.
    - ▷ *The optimal machine is played exponentially more number of times than the non-optimal machines.*
  - Using the law of large number, you get a better in quality Monte Carlo simulation if more simulations are done.



# How UCB is derived (1/2)

- **Hoeffding inequality [Hoeffding 1963]:**
  - Assume  $X$  is a Bernoulli random variable in the range of  $[0, 1]$  with an expected value of  $E(X)$ .
  - Let  $X_i$  be the  $i$ th independent sampling of  $X$ .
  - Let  $\bar{X}_w = \frac{1}{w} \sum_{i=1}^w X_i$  be the average of the first  $w$  samplings.
  - $P(|E(X) - \bar{X}_w| \geq u) \leq e^{-2 \cdot w \cdot u^2}$  for  $u > 0$ .
    - ▷ *This means the real value  $E(X)$  has a chance of no more than  $e^{-2 \cdot w \cdot u^2}$  to be the observed value  $\bar{X}_w$  plus an upper bound of  $u$  if  $u > 0$ .*
- It gives an estimation on the difference between the real value and the observed average value at the time  $w$ .
  - Fixing  $u$ , when  $w$  increases, the chance of the difference to be  $\geq u$  decreases exponentially.
- **High level implications**
  - In a true random setting, it looks like something is “remembered” in the long run.
  - In observing a long sequence of random events, if the first half is bad, then the second half is likely to become better so that overall it is in the average case.

# How UCB is derived (2/2)

- Assume we want the chance of failure, i.e., different between the observed average value and the real value to be  $\geq u$ , to be exponentially decreasing when the number of total trials  $N$  increases, say in the rate of  $N^{-2 \cdot c^2}$  where  $c > 0$  is a constant.
  - Fix the chance of failure to be the small value of  $N^{-2 \cdot c^2}$  where  $c > 0$ .
  - This means the real value has a very small chance, namely  $N^{-2 \cdot c^2}$ , to be more than  $\bar{X}_w + u$  when  $N$  is large.

■ Then

$$e^{-2 \cdot w \cdot u^2} \leq N^{-2 \cdot c^2}$$
$$\implies u \leq c \sqrt{\frac{\log N}{w}}$$

- You may use error functions of forms other than  $N^{-2 \cdot c^2}$  with different approximation factor as stated in Theorem I.

# Exploitation or Exploration

$$\text{UCB}_i = \frac{W_i}{N_i} + c \sqrt{\frac{\log N}{N_i}}$$

- In the UCB formula,
  - $t$  is  $N_i$  and  $\bar{X}_t = \frac{W_i}{N_i}$  is the observed value.
  - $\frac{W_i}{N_i} + c \sqrt{\frac{\log N}{N_i}}$  is the upper bound of  $E(X)$  with a good confidence.
- Using  $c$  to keep a balance between
  - **Exploitation**: exploring the best move so far.
  - **Exploration**: exploring other moves to see if they can be proven to be better.
- No  $N_i$  should be zero.
  - Give each child at least some trials.
- The theoretical value for  $c$  in [Auer et al'02] is
  - $\sqrt{2 \cdot \frac{\log 2}{\log e}} \sim 1.18$  where  $e$  is the base of the natural logarithm which is about 2.718.

# Comments

- It is worthy to note that Hoeffding's inequality also states
  - $P(\bar{X}_t - E(X) \geq u) \leq e^{-2 \cdot t \cdot u^2}$  for  $u > 0$ .

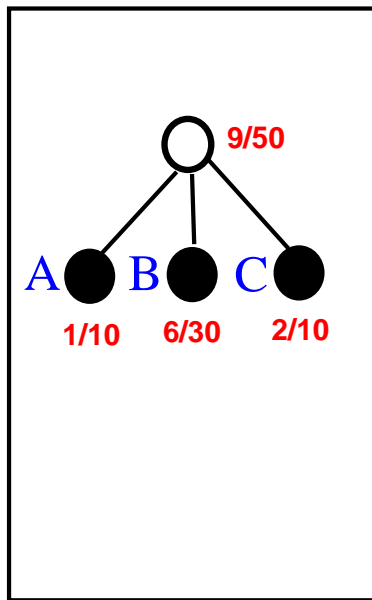
- This means the lower confidence bound (LCB)

$$\text{LCB}_i = \frac{W_i}{N_i} - c \sqrt{\frac{\log N}{N_i}}$$

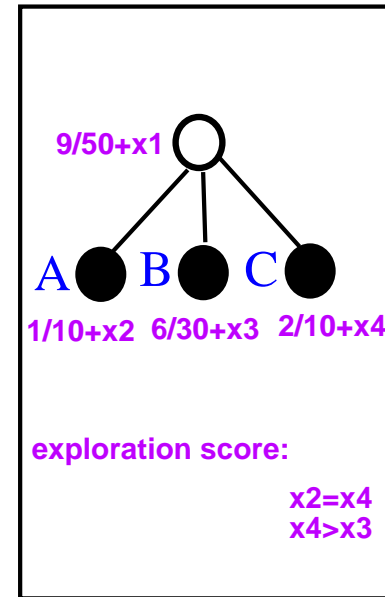
- Hence if your observation so far from the first  $N$  observations is  $\frac{W_i}{N_i}$ , then the real value is within  $\text{LCB}_i$  and  $\text{UCB}_i$  with a high probability.
- $\text{LCB}_i$  can be used when you are in great advantage.
- The value  $c$  can be varied during different phases of a game.
  - Q: What to set in the opening?
  - Q: What to set in the middle?
  - Q: What to set in the endgame?

# Illustration: using UCB scores

- Using winning rate,  $B$  and  $C$  are tied.
- Using UCB scores,  $C$  is better than  $B$  because  $C$  obtained the score using less trials.



+ score = winning rate



UCB score

# Other formulas for UCB (1/2)

- Other formulas are available from the statistic domain.
  - Ease of computing
  - Better statistical behaviors
    - ▷ *For example, consider the variance of scores in each branch.*

# Other formulas for UCB (2/2)

- **Example of UCB using variance:** consider the games having results drawn from Bernoulli random variable in the range of  $[0, 1]$ .
  - Then  $\mu_i$  is the expected result of the playouts simulated from this position.
  - Let  $\sigma_i^2$  be the variance of the results of the playouts simulated from this position.
  - Define  $V_i = \sigma_i^2 + c_1 \sqrt{\frac{\log N}{N_i}}$  where  $c_1$  is a constant to be decided by experiments.
  - A revised UCB formula [Auer et al'02] [Gelly et al '06] is

$$\mu_i + c \sqrt{\frac{\log N}{N_i} \min\{V_i, c_2\}},$$

where  $c$  and  $c_2$  are both constants to be decided by experiments and  $c_2$  is used to bound the influence of  $V_i$ .

- **Note:** in [Auer et al'02],  $c_1$  is  $\sqrt{2}$ ,  $c_2$  is  $\frac{1}{4}$  and  $c$  is 1. However  $c_2$  really depends on how large the range of your scores are.

# Comments

- The above revised bound in practice gives a better result, but no theoretical bound is proved.
- $\mu_i = 0$  and  $\sigma_i^2 = 0$  means a sure to draw situation.
- $\mu_i = 0$  and  $\sigma_i^2 \gg 0$  means a tie and not-so-quiet situation.
- If  $\sigma_i^2 \gg 0$ , then no conclusion should be made, or no final decision should be made.
- Since the numerical value of  $\sigma_i^2$  can be very large, you need to consider not over using it.

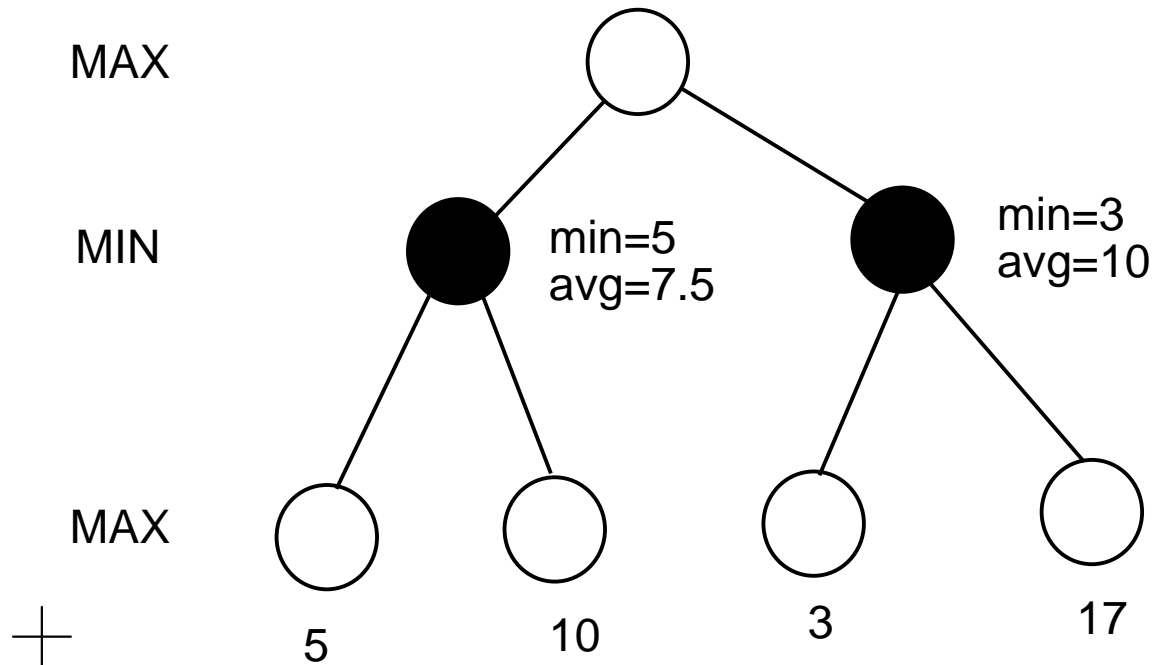


# Monte-Carlo search using UCB scores

- Doing Monte-Carlo search by first performing  $x$  trials on each child, and then  $y$  trials each time on the current best child.
- Algorithm  $\text{MCS}_{UCB}(\text{position } p, \text{int } x, \text{int } y)$ :
  - Generate all possible children  $p_1, p_2, \dots, p_b$  of the current position  $p$
  - for each child  $p_i$  do
    - ▷ Perform  $x$  almost random simulations for  $p_i$
    - ▷ Calculate the UCB score for  $p_i$
  - While there is still time do
    - ▷ Pick a child  $p^*$  with the largest UCB score
    - ▷ Perform  $y$  almost random simulations for  $p^*$
    - ▷ Update the UCB score of  $p^*$  as well as other nodes
  - Pick a child with **the largest winning rate** to play
- It is usually the case we pick a child with the largest winning rate, not with the largest UCB score to play.
  - After enough trials, one with the largest winning rate is usually, but not always, the one with the largest UCB score.

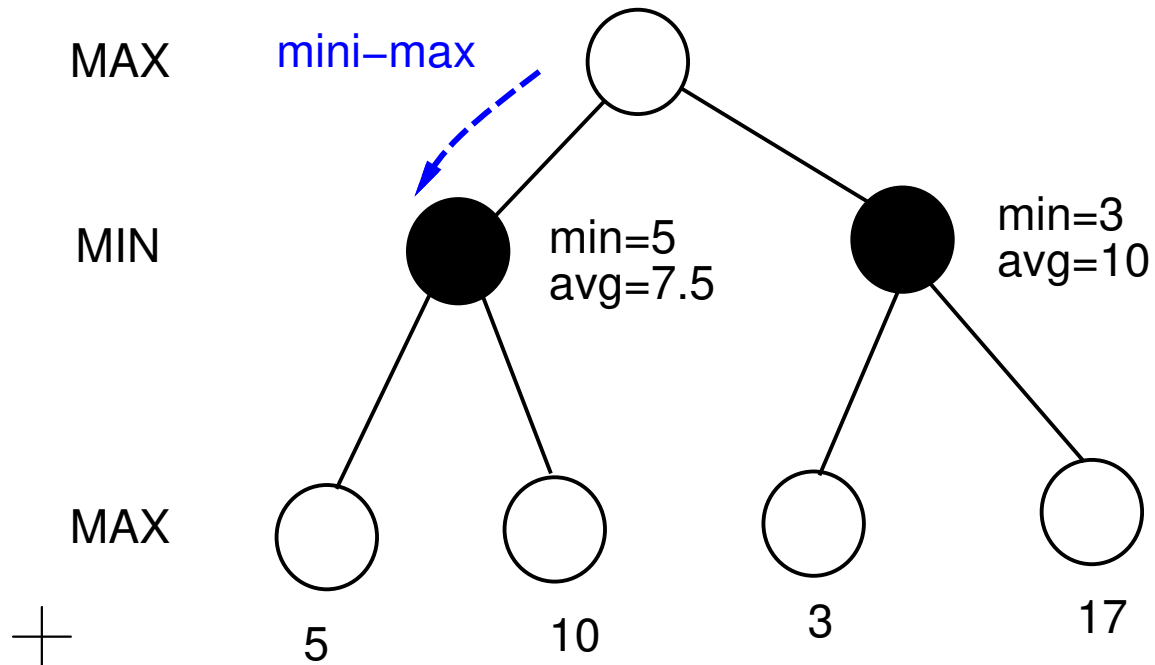
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- The average score of a branch sometimes does not capture the essential idea of a mini-max tree search.



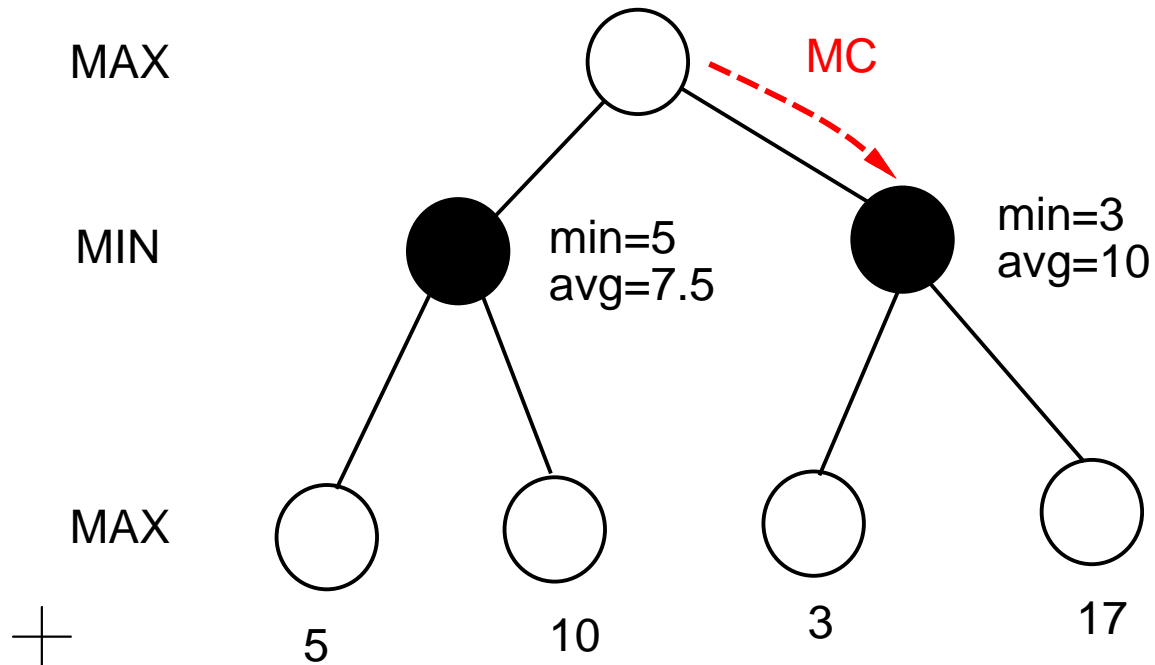
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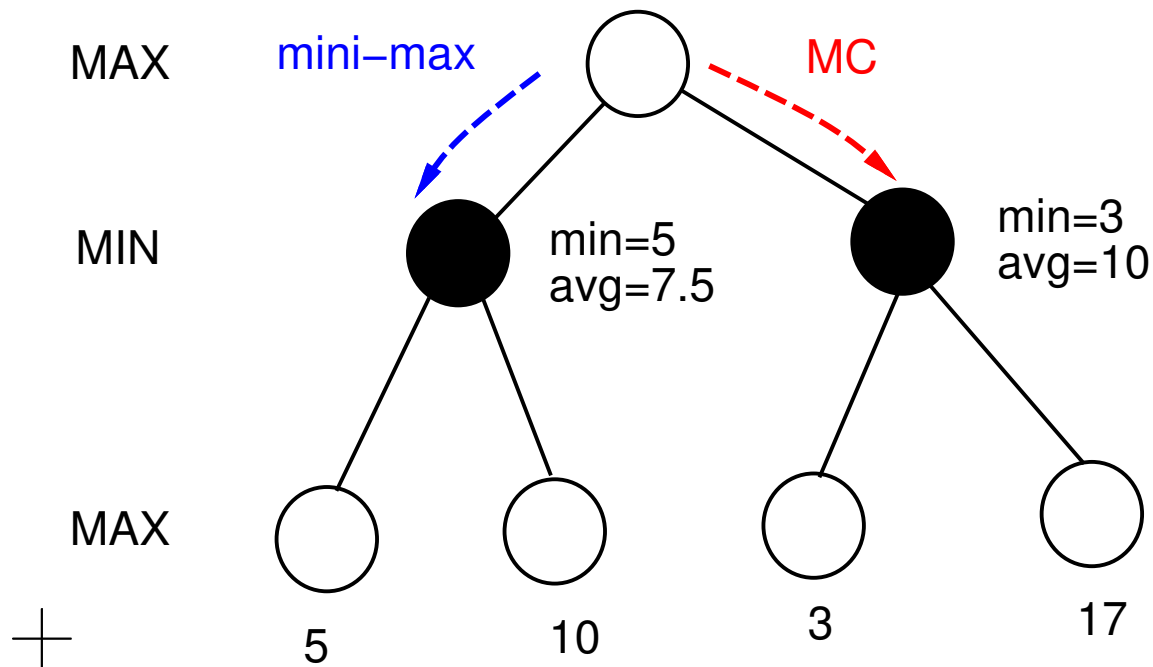
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# More problem of MCS<sub>pure</sub>

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- May spend too much time on the wrong branch.

# Second major refinement

## ■ Intuition:

- Initially, obtain some candidate choices that are needed to be further investigated.
- Perform some simulations on the leaf at a principle variation (PV) branch.
  - ▷ *A **PV path** is a path from the root so that each node in this path has the best score among all of its siblings.*
  - ▷ *Note: In a mini-max tree, “best” means differently for a min or a max node.*
- Update the scores of nodes in the current tree using a mini-max formula.
- Grow a best leaf at the PV one level.
- Repeat the above process until time runs out.

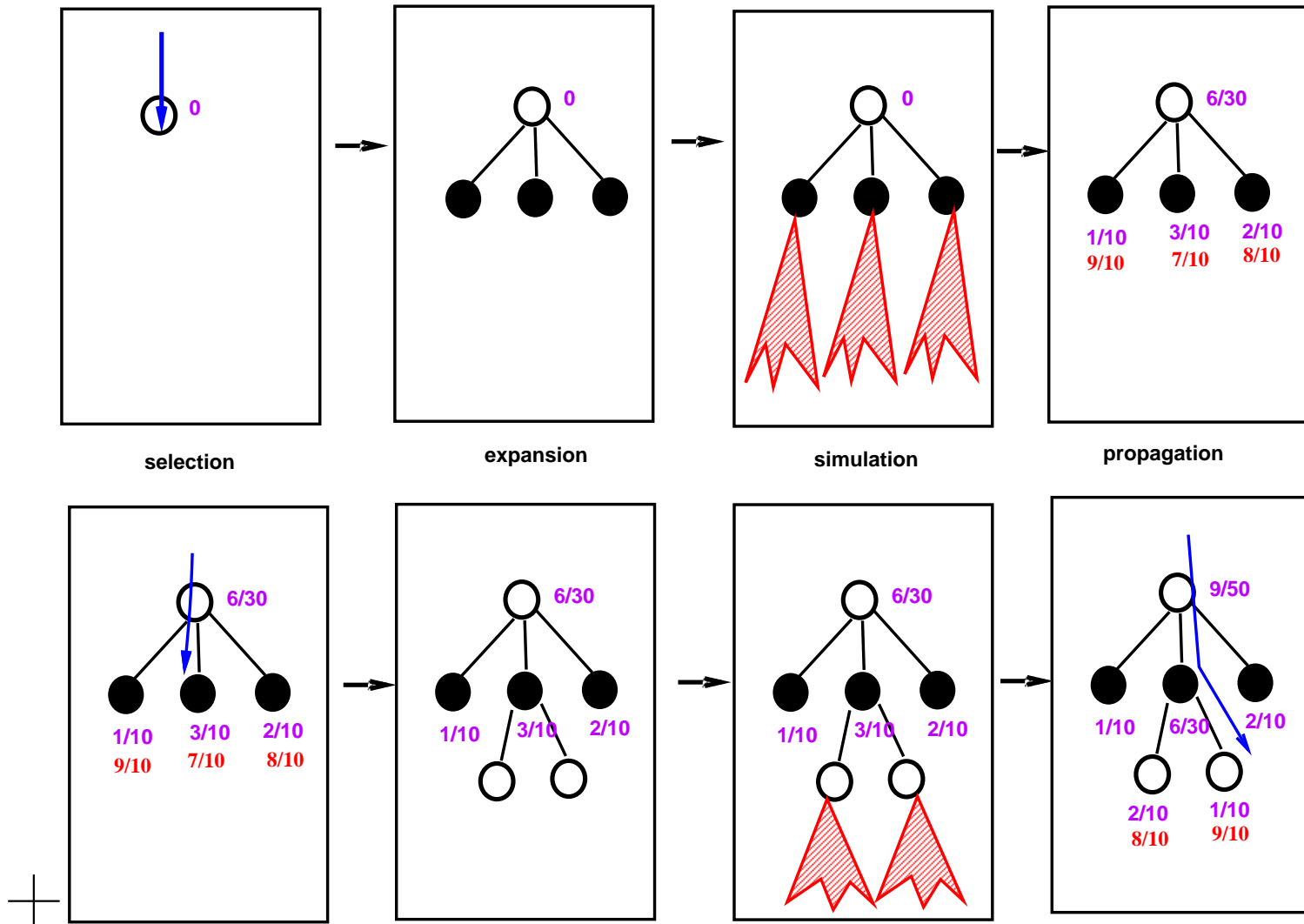
## ■ **Best-first tree growing** [Coulum'06].

- Keep a partial game tree and uses the mini-max formula within the partial game tree kept.
- Grow the game tree **on demand**.

# Monte-Carlo based tree search

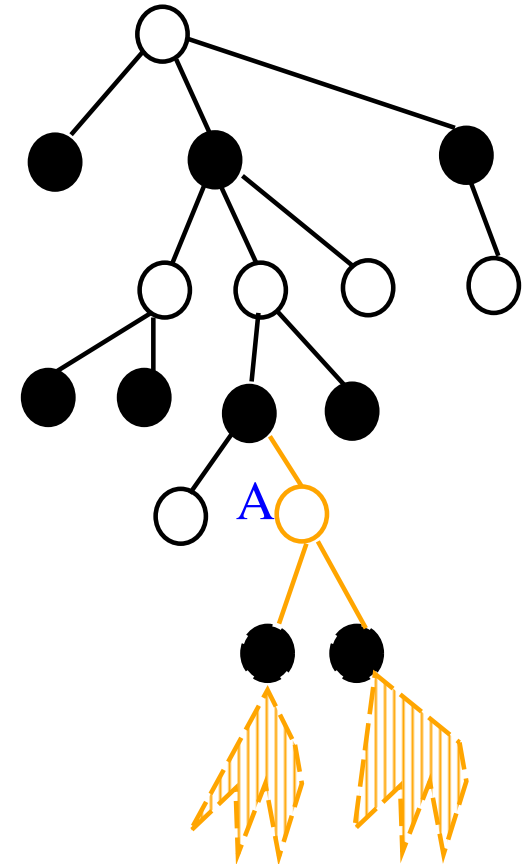
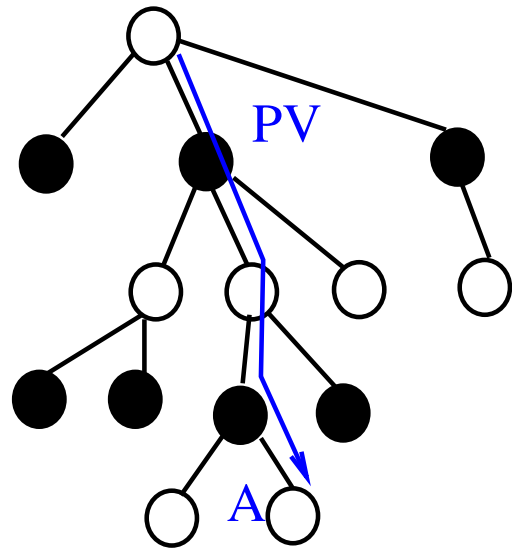
- Algorithm  $\text{MCTS}_{basic}(\text{int } x)$ : // Monte-Carlo mini-max tree search
- 1: Obtain an initial game tree
- 2: Repeat the following sequence  $N_{total}$  times
  - 2.1: Selection
    - ▷ From the root, pick one path to a leaf with the best “score” using a mini-max formula.
  - 2.2: Expansion
    - ▷ From the chosen leaf with the best “score”, expand it by one level using a good **node expansion** policy.
  - 2.3: Simulation
    - ▷ For each expanded leaf, perform  $x$  trials (playouts).
  - 2.4: Back propagation
    - ▷ Update the “scores” for nodes from the selected leaves to the root using a good **back propagation** policy.
- Pick a child of the root with the current best winning rate as your move.

# Illustration: Tree growing using win rate





# Illustration: Best first tree growing



Grow the best leaf

find the PV from top to bottom  
and then pick the best leaf to expand



# Comments (1/2)

- In finding the PV path in a Monte-Carlo tree:
  - We do this by a **top-down** fashion.
  - From the root, which is a max node, pick a child  $p_1$  with the largest possible score and then go one step down.
  - From  $p_1$ , which is a MIN node, pick a child with the smallest score  $p_2$  and then go one more step down.
  - We keep on doing this until a leaf is reached.
- In updating the scores of nodes in a Monte-Carlo tree when some more simulations are done in a leaf  $q$ :
  - We do this by a **bottom-up** fashion.
  - We first update the score of  $q$ .
  - Then we update the score of  $q$ 's parent  $q^*$  by merging the newly generated statistics of  $q$  with the existing statistics of  $q^*$ .
  - We keep on doing this until the root is reached.
  - **This is different from the updating operations done in a mini-max tree.**
  - The reasons to merge, not to replace, are
    - ▷ *the value is a winning chance from sampling, not really an actual value obtained from an evaluation function;*
    - ▷ *after merging you get a statistical value that is more trustful since the sample size is increased.*

# Comments (2/2)

- **When the number of simulations done on a node is not enough, the mini-max formula of the scores on the children may not be a good approximation of the true value of the node.**
  - For example on a MIN node, if not enough children are probed for enough number of times, then you may miss a very bad branch.
- **When the number of simulations done on a node is enough, the mini-max value is a good approximation of the true value of the node.**
- **Use a formula to take into the consideration of node counts so that it will initially act as returning the mean value and then shift to computing the normal mini-max value [Bouzy'04], [Coulom'06], [Chaslot et al'06].**

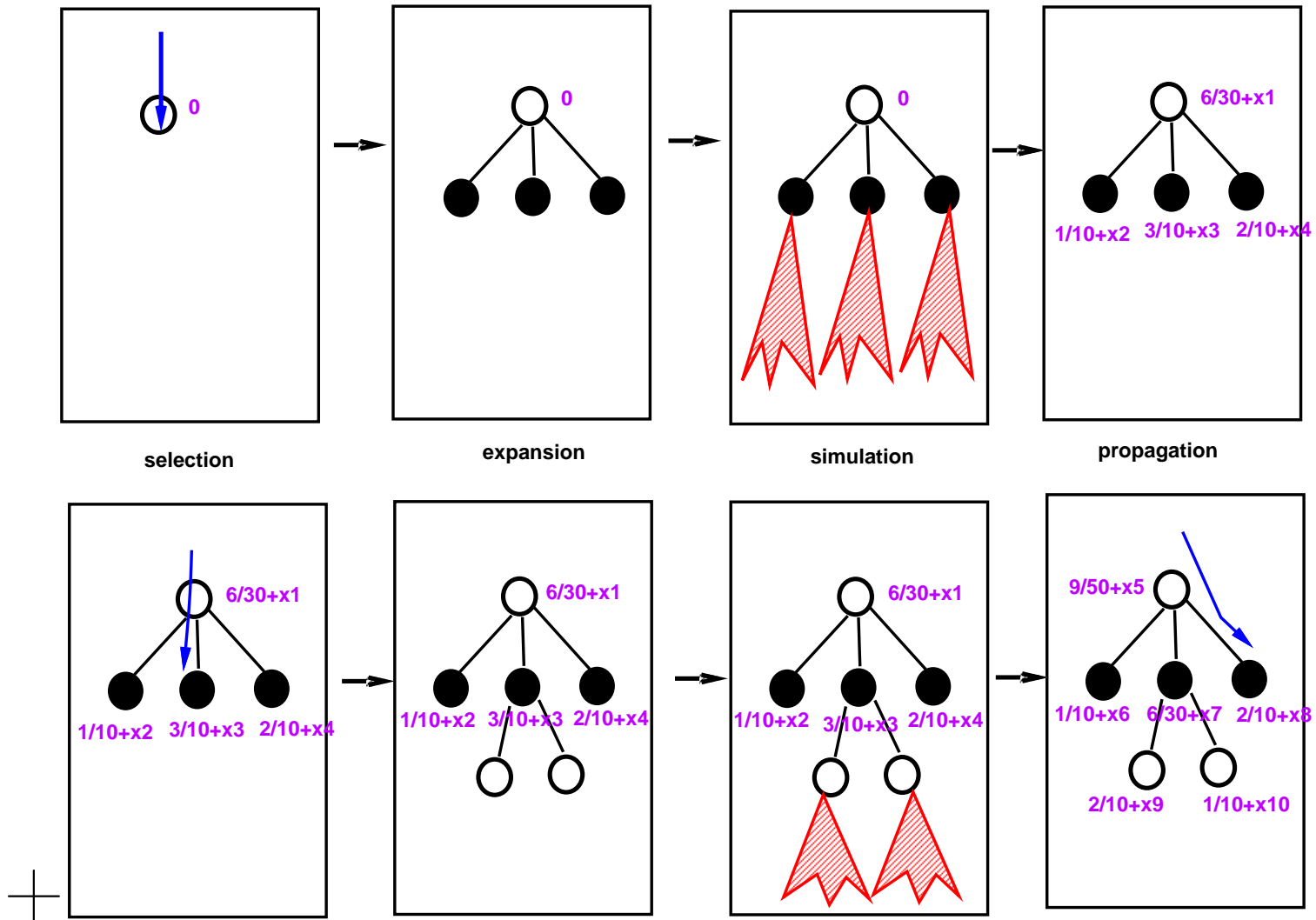
# UCT

- **UCT: Upper Confidence Bound for Tree [Chaslot et al '08]**
  - Maintain the UCB value for each node in the game tree that is visited so far.
  - Best first tree growing:
    - ▷ *From the root, pick a  $PV_{UCB}$  path such that each node in this path has a **largest UCB score** among all of its siblings.*
    - ▷ *Pick the leaf-node in the PV path and has been visited more than a certain amount of times to expand.*
- **UCT approximates mini-max tree search with cuts on proven worst portion of trees.**
- **Effective when the “density of goals” is sufficiently large.**
  - When there is only a unique goal, Monte-Carlo based simulation may not be efficient.
  - The “density” and distribution of the goals may be something to consider when picking the threshold for the number of playouts needed to reach a statistical conclusion.

# Monete Carol with UCB: MCTS

- Algorithm MCTS(int  $x$ ):
- 1: Obtain an initial game tree
- 2: Repeat the following sequence  $N_{total}$  times
  - 2.1: Selection
    - ▷ From the root, pick a  $PV_{UCB}$  path to a leaf such that each node has a best UCB score among its siblings.
    - ▷ May decide to “trust” the score of a node if it is visited more than a threshold number of times.
    - ▷ May decide to “prune” a node if its raw score is too bad to save time.
  - 2.2: Expansion
    - ▷ From a leaf with the best UCB score, expand it by one level.
    - ▷ Use some node expansion policy to expand.
  - 2.3: Simulation
    - ▷ For each expanded leaf, perform  $x$  trials (playouts).
    - ▷ May decide to add knowledge into the trials.
  - 2.4: Back propagation
    - ▷ Update the UCB scores for nodes using a good back propagation policy.
- Pick a child of the root with the best **winning rate** as your move.

# Tree growing using UCB scores



# Comments about the UCB value

- For node  $i$ , its  $UCB_i = \frac{W_i}{N_i} + c\sqrt{\frac{\log N}{N_i}}$ .
- What does “winning rate” mean?
  - For a MAX node,  $W_i$  is the number of win’s for the MAX player.
  - For a MIN node,  $W_i$  is the number of win’s for the MIN player.
- When  $N_i$  is approaching  $\log N$ , then  $UCB_i$  is nothing but the current winning rate plus a constant.
  - When  $N$  is very large, then the current winning rate is a good approximation of the real winning rate for this node.
  - If you walk down the tree from the root along the path with largest UCB values, namely  $PV_{UCB}$ , then it is like walking down the traditional mini-max PV.

# Important notes

- We only describe some specific implementations of Monte-Carlo techniques.
  - Other implementations exist for say UCB scores.
- It is important to know the underlying “theory”, not a particular implementation, that makes a technique work.
- Depending on the amount of resources you have, you can
  - decide the frequency to update the node information,
  - decide the frequency to re-pick PV,
- You also need to know the precision and cost of your floating-point number computation which is the core of calculating UCB scores.



# Implementation for Go

- **How to partition stones into strings?**
  - Visit the stones one by one.
  - For each unvisited stone
    - ▷ *Do a DFS to find all stones of the same color that are connected.*
  - Can use a good data structure to maintain this information when a stone is placed.
    - ▷ *Example: disjoint union-find.*
- **How to know an empty intersection is a **potential** eye?**
  - Check its 4 neighbors.
  - Each neighbor must be either
    - ▷ *out of board, or*
    - ▷ *it is in the same string with the other neighbors.*
- **How to find out the amount of liberties of a string?**
  - for each empty intersection, check its 4 neighbors:
    - ▷ *check it is a liberty of the string where its neighbors are in;*
    - ▷ *make sure an empty intersection contributes at most 1 in counting the amount of liberties of a string.*

# Generating random numbers

- The success of MCTS based algorithms depends heavily on good quality in the pseudo random numbers generated.
  - Using a good seed.
  - The period of random numbers generated.
  - Whether the sequence produced can pass some statistical tests.
- Using good third-party pseudo random number generators.
  - Some good ones include PCG at <https://www.pcg-random.org/index.html>.

# General implementation hints (1/4)

- Each node  $p_i$  maintains 3 counters  $W_i$ ,  $L_i$  and  $D_i$ , which are the number of games won, lost, and drawn, respectively, for playouts simulated starting from this position.
  - Note that  $N_i = W_i + L_i + D_i$ .
  - For ease of coding, the numbers are from the view point of the root, namely MAX, player.
- Assume  $p_{i,1}, p_{i,2}, \dots, p_{i,b}$  are the children of  $p_i$ .
  - $W_i = \sum_{j=1}^b W_{i,j}$
  - $L_i = \sum_{j=1}^b L_{i,j}$
  - $D_i = \sum_{j=1}^b D_{i,j}$
- “Winning rate”:
  - For a MAX node, it is  $W_i/N_i$ .
  - For a MIN node, it is  $L_i/N_i$ .

# General implementation hints (2/4)

- Only nodes in the current “partial” tree are maintaining the 3 counters.
- Assume  $p_{i,1}, p_{i,2}, \dots, p_{i,b}$  are the children of  $p_i$  that are currently in the “partial” tree.
  - It is better to maintain a “default” node representing the information of playouts simulated when  $p_i$  was a leaf.
- When any counter of a node  $v$  is updated, it is important to update the counters of all of its ancestors.
  - ▷ *For example: the winning rates of all  $v$ 's ancestors are also changed.*
- Need efficient data structures and algorithms to maintain the UCB value of each node.
  - When a simulated playout is completed, the UCB scores of all nodes are changed because the total number of playouts,  $N$ , is increased by 1.

# General implementation hints (3/4)

## ■ How to incrementally update mean and variance of a node?

- Assume the results of the simulation form the sequence

$x_1, x_2, x_3, \dots, x_i, x_{i+1}, x_{i+2}, \dots$

- Let  $var(n)$  be the variance of the first  $n$  elements. Hence

$var(n) = \frac{1}{n} \sum_{i=1}^n (x_i - \mu(n))^2$  where  $\mu(n) = \frac{1}{n} \sum_{i=1}^n x_i$ .

- In each node, we maintain the following data:

▷  $n$

▷  $sum2(n) = \sum_{i=1}^n x_i^2$

Hence  $sum2(n+1) = sum2(n) + x_{n+1}^2$

▷  $sum1(n) = \sum_{i=1}^n x_i$

Hence  $sum1(n+1) = sum1(n) + x_{n+1}$

- $\mu(n) = \frac{1}{n} \cdot sum1(n)$

●

$$\begin{aligned} var(n) &= 1/n \cdot (sum2(n) - 2 \cdot \mu(n) \cdot sum1(n) + n \cdot \mu(n)^2) \\ &= 1/n \cdot sum2(n) - 2 \cdot \mu(n) \cdot \mu(n) + \mu(n)^2 \\ &= 1/n \cdot sum2(n) - \mu(n)^2 \end{aligned}$$

# General implementation hints (4/4)

- In general, we do not perform a division operator unless it is really needed to do so.
- $sum1(n) = sum2(n)$  if
  - the value of a leaf can only be 0 or 1;
- If the value of a node can be something else, then  $sum1(n)$  and  $sum2(n)$  may be different.
  - The possible range of the value of a leaf defines how “rich” your variance can be.
  - If the range is too large, then the value of the variance can be very large.
  - Pick a suitable range so that you can better tradeoff the mean and the variance in computing UCB values using more involved formulas with the variance.

# Hints on updating UCB scores

- When  $x$  more simulations are done on a node  $p$ , then
  - the winning rates of  $p$  and  $p$ 's ancestors may change;
  - the exploration scores of  $p$  and  $p$ 's ancestors decrease;
    - ▷  $c\sqrt{\frac{\log N}{N_i}} \rightarrow c\sqrt{\frac{\log(N+x)}{(N_i+x)}}$
  - the winning rates of the siblings of  $p$  and  $p$ 's ancestors do not change;
  - the exploration scores of the siblings of  $p$  and  $p$ 's ancestors increases;
    - ▷  $c\sqrt{\frac{\log N}{N_i}} \rightarrow c\sqrt{\frac{\log(N+x)}{N_i}}$
- Calculating  $\log$  and division is time consuming, do not do it unless it is necessary.
  - Assume you have to find the max UCB value among children of a node with a total of  $N$  simulations.
    - ▷ *The value  $\log N$  needs to be calculated only once among all children.*
    - ▷ *Save  $\frac{W_i}{N_i}$  and reuse it if it is not changed.*

# Hints on UCT tree maintaining

- After a certain rounds of best-first tree growing as used in UCT tree growing, the shape of the tree is critical in getting a fast and correct convergence.
  - Shape of the tree can be roughly quantified by
    - ▷ *Total number of nodes:  $n$*
    - ▷ *Average depth of leaves:  $avgd$*
    - ▷ *Maximum depth:  $maxd$*
    - ▷ *Depth of PV:  $pvd$*
    - ▷ *Average branching factor:  $avgb$*
  - If  $avgd$  and  $maxd$  are about the same, then you do not have a good direction of searching.
  - If  $n$  is too small, then your code is not efficient.
  - If  $n$  is too large, then your code does not prune enough.
  - ...



# Slow code

```
long double maxV,Ntotal,N[maxChild],W[maxChild];
int b; // number of children
int i;
...
Ntotal = 0.0;
// compute total number of simulations
// done on children
for (i=0;i<b;i++)
    Ntotal += N[i];
maxV = -99999.9; // default for finding the max
// linearly scan and compute
for(i=0;i<b;i++)
    if(maxV < W[i]/N[i] + c * sqrt(log(Ntotal)/N[i]))
        maxV = W[i]/N[i] + c * sqrt(log(Ntotal)/N[i]);
```

# Slightly faster code

```
int Ntotal, // the total value is calculated when it is updated
    N[maxChild],W[maxChild];
int b; // number of children
int i;
long double maxV, temp,
    // precomputed terms used in UCB
    CsqrtlogN, // = c * sqrt(log(Ntotal))
    sqrtN[maxChild], // = sqrt((long double) N[i])
    WR[maxChild]; // winning rate = (long double) W[i]/ (double) N[i]
...
// initial value comes from the first element
maxV = WR[0] + CsqrtlogN/sqrtN[0];
for(i=1;i<b;i++){
    // save intermediate result
    temp = WR[i] + CsqrtlogN/sqrtN[i];
    if(maxV < temp)
        maxV = temp;
}
```

# Data structure for an UCB-tree

```
// using array instead of pointers to represent the MCTS search tree
struct NODE {
    int ply; // the ply from parent to here
    int p_id; // parent id, root's parent is the root
    int c_id[MaxChild]; // children id
    int depth; // depth, 0 for the root
    int Nchild; // number of children
    int Ntotal; // total # of simulations
    long double CsqrtlogN; // c*sqrt(log(Ntotal))
    long double sqrtN; // sqrt(Ntotal)
    int Wins; // number of wins
    long double WR; // win rate
} nodes[MaxNodes];

#define parent(ptr) (nodes[ptr].p_id) // id of ptr's parent
#define child(ptr,i) (nodes[ptr].c_id[i]) // the ith child of ptr
```

# Updating from leaf to root

```
...
// add deltaN simulations with deltaW wins to the node "id"
void update(int id, int deltaW, int deltaN)
{
    nodes[id].Ntotal += deltaN; // additional # of trials
    nodes[id].CsqrtlogN = C*sqrt(log((long double) nodes[id].Ntotal))
    nodes[id].sqrtN = sqrt((long double) nodes[id].Ntotal);
    nodes[id].Wins += deltaW; // additional # of wins in trials
    nodes[id].WR = (long double) nodes[id].Wins
                  / (long double) nodes[id].Ntotal;
}
...
do{
    update(ptr, deltaW, deltaN);
    ptr = parent(ptr);
}until(ptr == root);
update(root);
```

# Finding PV

```
// compute the UCB score of nodes[id]
long double UCB(int id)
{
    return (nodes[id].depth%2) ? (nodes[id].WR) : (1.0 - nodes[id].WR)
        + nodes[parent(id)].CsqrtlogN/nodes[id].sqrtN;
}

...
PV[0] = ptr = root;
while(nodes[ptr].Nchild > 0){ // while not reaching a leaf
    maxchild = child(ptr,0); // current index of child with max UCB
    maxV = UCB(maxchild); // current max UCB value
    for(i=1;i<nodes[ptr].Nchild;i++){
        ctemp = child(ptr,i);
        temp = UCB(ctemp);
        if(maxV < temp){ maxV = temp; maxchild = ctemp; }}
    PV[nodes[ptr].depth] = ptr = maxchild; // go deeper in tree
}
```

# Advanced data structure

```
// save computed intermediate values
struct NODE {
    int ply; // the ply from parent to here
    int p_id; // parent id, root's parent is the root
    int c_id[MaxChild]; // children id
    int depth; // depth, 0 for the root
    int Nchild; // number of children
    int Ntotal; // total # of simulations
    long double CsqrtlogN; //  $c * \sqrt{\log(Ntotal)}$ 
    long double sqrtN; //  $\sqrt{Ntotal}$ 
    int sum1; // sum1: sum of scores
    int sum2; // sum2: sum of square of each score
    long double Mean; // average score
    long double Variance; // variance of score
} nodes[MaxNodes];
```

# Advanced UCB routine

```
// compute the UCB score of nodes[id]
// for a range of scores [MinS .. MaxS]
long double UCB(int id)
{
    long double Range = MaxS - MinS; // can be stored as a constant
    // normalized the average score to be between 0 and 1
    long double SR = (nodes[id].Mean - MinS) / Range;
    return (nodes[id].depth%2) ? (SR) : (1.0-SR) +
        nodes[parent(id)].CsqrtlogN / nodes[id].sqrtN;
}
```

# Advanced updating routine

```
...
// add deltaN simulations with deltaS additional scores
// and sum of square of scores deltaS2
void update1(int id, int deltaS, int deltaS2, int deltaN)
{
    nodes[id].Ntotal += deltaN; // additional # of trials
    nodes[id].CsqrtlogN =
        c * sqrt(log((long double) nodes[id].Ntotal));
    nodes[id].sqrtN = sqrt((long double) nodes[id].Ntotal);
    nodes[id].sum1 += deltaS; // additional scores in trials
    nodes[id].sum2 += deltaS2;
    nodes[id].Mean = (long double) nodes[id].sum1
        / (long double) nodes[id].Ntotal;
    nodes[id].Variance = (long double) nodes[id].sum2
        / (long double) nodes[id].Ntotal -
        nodes[id].Mean * nodes[id].Mean;
}
```



# Comments (1/2)

- Using the idea of sampling to evaluate a position was used previously for other games such as 6x6 Othello [Abramson'90].
- Proven to be successful on a few games.
  - Very successful on computer Go.
- Not very successful on some games.
  - Not currently greatly outperform alpha-beta based programs on Chess or Chess-like games.
- Performance becomes better when the game is going to converge, namely the endgame phase.
- Need a good random playout strategy that can simulate the **average behavior** of the current position efficiently.
  - On a bad position, do not try to always get the best play.
  - On a good position, try to usually get the best play.
- **It is still an art to find out what coefficients to set.**
  - Need a theory to efficiently find out the values of the right coefficients.
  - It also depends on the speed of your simulation.
  - Deep learning based techniques may be helpful in speeding up the fine tuning the parameters.

# Comments (2/2)

- The “reliability” of a Monte-Carlo simulation depends on the number of trials it performs.
  - The rate of convergence is important.
  - Do enough number of trials, but not too much for the sake of saving computing time.
- Adding more knowledge can slow down each simulation trial.
  - There should be a tradeoff between the amount of knowledge added and the number of trials performed.
  - Similar situation in searching based approach:
    - ▷ *How much time should one spent on computing the evaluation function for the leaf nodes?*
    - ▷ *How much time should one spent on searching deeper?*
  - Another witness on how the art of **tradeoff** governs the design of a complex system.
- Knowledge, or patterns, about Go can be computed off-lined using statistical learning or deep learning.

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