Computing Science (CMPUT) 455

Search, Knowledge, and Simulations

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Part III

Simulations and Monte Carlo Tree Search

455 Today - Lecture 12

- Start Part 3 - Simulations and Monte Carlo Tree Search
- Simulation methods in computing science
- Early examples simulating physics
- Examples in heuristic search
- Flat Monte Carlo
- Simulation-based TicTacToe player
- Simulation-based Go player, `Go3`

Coursework

- Assignment 2:
  - Feedback by end of today (via email)
  - Resubmission (with 20% penalty) due Wednesday at 11:55pm
- Reading: Rémi Coulom, *Computing Elo Ratings of Move Patterns in the Game of Go.*
- Lecture 12 activities
- Quiz 7: Simulations
  - due Monday (Oct 25)

CMPUT 497 Plug (Winter 2022)

CMPUT 497 — Artificial Intelligence Capstone, ★3

Students will experience the challenges, and rewards, of working in a team to address a real-world task, related to artificial intelligence or machine learning. This will involve first identifying the task itself, then iteratively addressing relevant issues (typically with feedback from a domain expert), leading to an implementation and culminating in evaluating that system. Students will also learn about best practices in organizing team projects, as well as important information about effective communication.

Instructor: Russ Greiner
Prerequisites: **ONE OF** CMPUT 267, 365, or 366.

- Note: best to take this capstone course after completing **all** of these.

Simulation Methods

Simulation Methods

- Wikipedia definition:

  Simulation is the imitation of the operation of a real-world process or system over time.

- Huge number and variety of applications
- Here, we focus on Monte Carlo (MC) simulation
- Main idea: learn information from **random sequences** of decision steps
- First simple examples:
  - No real sequence, just a single random step
  - That step is repeated many times for the same decision problem

Example 1: Estimate π with Monte Carlo

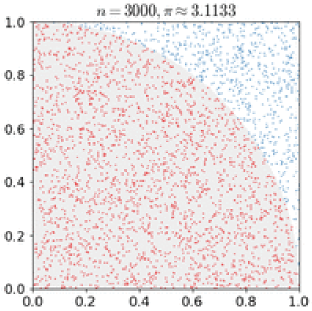


Image source: `https://upload.wikimedia.org/wikipedia`

- Generate random point (x, y) in $[0, 1) \times [0, 1)$ square
- Check if within circle: $x^2 + y^2 < 1$
- Repeat many times
- Fraction of points within circle is estimate for its area, $\pi/4$
- See code `estimate_pi.py` and do **Activity 12a**

Example 2: Numerical Integration with Monte Carlo Sampling

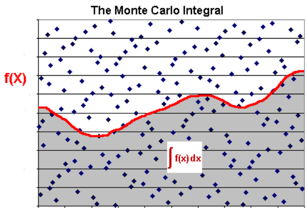


Image source:

`http://cedric-augonnet.com`

- Numerical Integration
- Similar idea as with π example
- Given arbitrary function *f*
- Count fraction of random points “under the curve”
- Need to find enclosing rectangle
- Deal with negative function values
- Demo of code `numerical_integration_MC.py`

Discussion - Monte Carlo Sampling for Numerical Integration

- Very general method
- No assumptions on type of function to integrate
- Can also use it in higher dimensions
  - Example in Activity 12a: volume of unit ball
  - Can estimate volume of irregularly shaped object
- All you need is:
  - Bounding box containing object
  - Random point generator
  - Reasonably fast method to check if point is inside or outside the object

Discussion continued - Limitations

Limitations

- Convergence of the basic method is slow
    - High variance (but no bias)
- Much faster methods exist if:
    - Functions have “nice” properties such as smoothness
- Decades of work on specialized MC methods
- Basic Monte Carlo (MC) is a fall-back
  for cases without “nice” structure

Origins of Monte Carlo Method - Manhattan Project

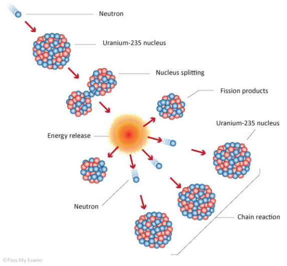


Image source: `http://www.nuclear-power.net`

- 1940's Manhattan Project: developed the first atomic bombs
- Extremely complex physics modeling required
- First computers were just becoming available
- One key problem: Neutron diffusion

Neutron Diffusion

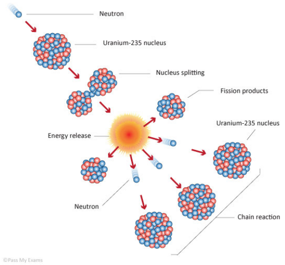
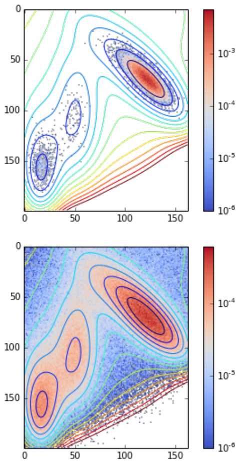


Image source: `http://www.nuclear-power.net`

- To obtain a nuclear chain reaction:
- Each neutron must create >1 neutron, before being absorbed
- Physicists could not solve this problem with "pure calculation"
- Ulam and von Neumann developed first *Markov Chain Monte Carlo* simulation methods
- Simulate many random neutrons flying through a substance
- Count how often new ones are generated in simulation

Markov Chain Monte Carlo



- Main idea:
  simulate *random walk* of particles
- Walk is biased by physics constraints
- Particle distribution approximates...
- ...true distribution of what should be measured
- Very popular in physics, engineering for modeling complex systems

Image source:

`bougui505.github.io/`

`python/2014/11/17/`

`simple-markov-chain-monte-carlo-mcmc-algorithm-in-python.`

`html`

Markov Chain Monte Carlo

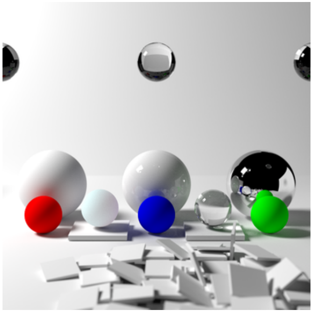


Image source:

`https://en.wikipedia.org/wiki/Path_tracing`

- Application:
  image rendering by path tracing
- Each light source emits many photons
- Many light rays sent out in random directions from source
- Model the physics of reflection, absorption etc. of those particles
- Number of particles hitting an area gives its illumination

Simulation Model

- To simulate something we need a model
- Neutron diffusion: physics - laws of motion, speed of neutrons, absorption by different materials, radioactive decay of different uranium isotopes,...
- Path tracing: light sources, laws of optics, shadows, reflection/light scattering, indirect light, ...
- Games:
  legal moves, outcome at the end
- Games with chance:
  simulated dice throws,
  possible distributions of unknown cards,...

Garbage In - Garbage Out Principle (GIGO)

- A simulation can only be as good as the underlying model
- If you feed great data to an invalid model, you typically get garbage
- Examples:
    - Missing relevant physics
    - Wrong initial conditions
    - Numerical instability, cascading errors
    - Bugs in computer code and/or hardware
    - Not implementing the rules of Go properly

Simulation in Heuristic Search

Simulation and Random Walks in Heuristic Search

- Early application: GSAT and WalkSAT for Boolean Satisfiability Problem (SAT)
- Given a boolean formula
- Example: $(x_0 \vee x_2) \wedge (\neg x_1 \vee \neg x_2)$
- Check if it is *satisfiable*: an assignment of true and false to the variables which makes the formula true
- Example: Set $x_0 = \mathit{True}, x_1 = \mathit{False}, x_2 = \mathit{False}$
- Whole formula becomes true
- Solving large SAT formulas is a difficult problem (NP-Hard!)
- Best solvers use heuristic search

Solving SAT by Systematic Search

- Given SAT formula with n variables, $x_0, ... x_{n-1}$
- Can solve by systematic search, trial and error
- Set $x_0 = \textit{True}$
    - Simplify formula
    - Solve SAT problem with $n - 1$ variables
- If fail: Set $x_0 = \textit{False}$
    - Simplify formula
    - Solve SAT problem with $n - 1$ variables
- Question: What is the worst-case cost of this procedure?

Solving SAT by Systematic Search

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- If fail: Set $x_0 = \textit{False}$
  - Simplify formula
  - Solve SAT problem with $n - 1$ variables
- Question: What is the worst-case cost of this procedure?
- Worst case cost: exponential in n
  - Need to try many of the 2^n variable assignments

GSAT and WalkSAT: Solving SAT by Biased Random Walk

- Local search methods developed in 1990's
- Start with random assignment of True or False to each variable
- If formula is true: stop, success
- If not, use heuristics to *flip* value of one variable
- Balance *exploitation* and *exploration*
  - Exploitation: flip a variable that makes the "largest possible improvement" of the formula
  - Exploration: flip a random variable
- Restart if no progress for a while

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GSAT and WalkSAT: Solving SAT by Biased Random Walk

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    - Exploitation: flip a variable that makes the "largest possible improvement" of the formula
        - Question: What could "improvement" mean?
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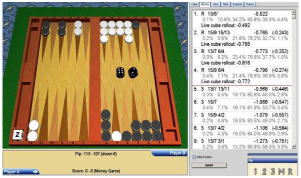
- Restart if no progress for a while
- How does local search compare to systematic search?
    - No clear winner, different strengths/weaknesses

Simulation in Game Tree Search - Backgammon



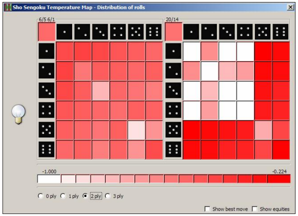
```
1. R  13/5*                -0.522
      0.1%  10.6% 34.2% 65.8% 39.3% 4.4%
   Live cube rollout: -0.492
2. R  15/9 15/13           -0.765  (-0.243)
      0.2%  5.6%  21.8% 78.2% 32.7% 1.1%
   Live cube rollout: -0.765
3. R  13/7 6/4             -0.773  (-0.252)
      0.0%  6.2%  23.4% 76.6% 37.7% 1.0%
   Live cube rollout: -0.816
4. R  15/9 6/4             -0.796  (-0.274)
      0.4%  7.1%  21.4% 78.6% 36.9% 0.6%
   Live cube rollout: -0.772
5. 3  13/7 13/11           -0.968  (-0.446)
      0.3%  5.5%  19.1% 80.9% 45.0% 2.8%
6. 3  15/7                 -1.068  (-0.547)
      0.4%  7.1%  18.1% 81.9% 53.7% 3.4%
7. 3  15/9 4/2             -1.079  (-0.557)
      0.2%  4.6%  16.5% 83.5% 49.0% 2.7%
8. 3  13/7 4/2             -1.106  (-0.584)
      0.2%  4.3%  16.0% 84.0% 49.9% 2.9%
9. 3  13/7 3/1             -1.273  (-0.751)
      0.2%  3.6%  13.2% 86.8% 58.3% 3.9%
```

Image sources:

`www.backgammoned.net`

- Early success of simulation methods in games: Backgammon
- “Rollout” games with many different sequences of dice throws
- Play move that is most successful in these rollouts
- Backgammon was also an early success story for neural networks
  We will discuss that story later

Simulation in Backgammon



0 ply 1 ply [✓ 2 ply] 3 ply

Image sources: `www.bkgm.com/gnu/AllAboutGNU.html`

- Picture: simulation result of all possible dice throws
- white = good winrate, red = bad
- Right side: risky move
  - Many throws lead to sure win
  - Many other throws lead to sure loss
- Left side: safe move
  - Outcomes more similar
  - Here, this move is better in expectation
- Knowing this distribution allows you to make better decisions

From Games With Chance Elements to Games With No Chance

- Games with chance element (dice, hidden cards)
  - Using random simulations is a natural idea
  - Tried even in the earliest programs

- Games without chance element (chess, checkers, Go,...)
  - Using random simulations is much less natural
  - It took a lot longer to develop those methods
  - Often, it also works very well
  - Our first example: TicTacToe
  - Second example: Go

Random Simulation in TicTacToe

- From given state, finish game
  with moves selected uniformly at random
- In TicTacToe, all empty squares are legal moves
- End simulation when game is over by rules:
  - Three in a row
  - Board full
- Implementation: method `simulate(self)`
  - In file `tic_tac_toe.py`

Method TicTacToe.simulate()

```
def simulate(self):
    allMoves = self.legalMoves()
    random.shuffle(allMoves)
    i = 0
    while not self.endOfGame():
        self.play(allMoves[i])
        i += 1
    return self.winner(), i
```

Method TicTacToe.simulate()

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```

Implementation note:

- For random play in TicTacToe, it's enough to shuffle the list of moves once, then play in that order
- Not true in Go (**why?**)

Use Simulations as Evaluation Function

Evaluate: how good is a game state?

- Exact answer:
    - Run solver
    - Compute minimax value
- Heuristic, first (old) answer:
    - Run depth-limited alphabeta search
    - At depth limit: call heuristic evaluation function
    - Compute minimax value
    - Problem: how to create evaluation function?
- **Heuristic, second (new) answer:**
    - Run simulations, score final result
        - Win = 1, loss = 0 (draw = 0.5)
    - Compute *winrate* over all simulations

Simulation-Based Player

- Uses 1-step (1-ply) lookahead to evaluate all moves
- For each legal move:
  - Run *n* simulations
  - Measure the winrate (winning percentage) for these simulations
- After all simulations:
  - Play move with highest winrate
- Implementation: `simulation_player.py`

Flat Monte Carlo

- The method based on 1-ply lookahead + simulations is sometimes called *Flat Monte Carlo*
- **Monte Carlo** method: uses random simulations
- **Flat:** does not build a deep tree,
  only 1 ply (1 move) lookahead
- Contrast: Monte Carlo Tree Search
  builds a (often very deep) tree

Simulation Player Implementation - simulate

`SimulationPlayer.simulate(self, state, move)`

- Play `move` from given `state` - changes state
- Evaluate state after the move:
- Run `self.numSimulations` from it
- After simulations: `undoMove` to restore previous state
- Evaluation of move:
  average outcome of these simulations

SimulationPlayer.simulate

```
def simulate(self, state, move):
    stats = [0] * 3
    state.play(move)
    moveNr = state.moveNumber()
    for _ in range(self.numSimulations):
        winner, _ = state.simulate()
        stats[winner] += 1
        state.resetToMoveNumber(moveNr)
    state.undoMove()
    eval = (stats[BLACK] + 0.5 * stats[EMPTY])
           / self.numSimulations
    if state.toPlay == WHITE:
        eval = 1 - eval # Negamax view
    return eval
```

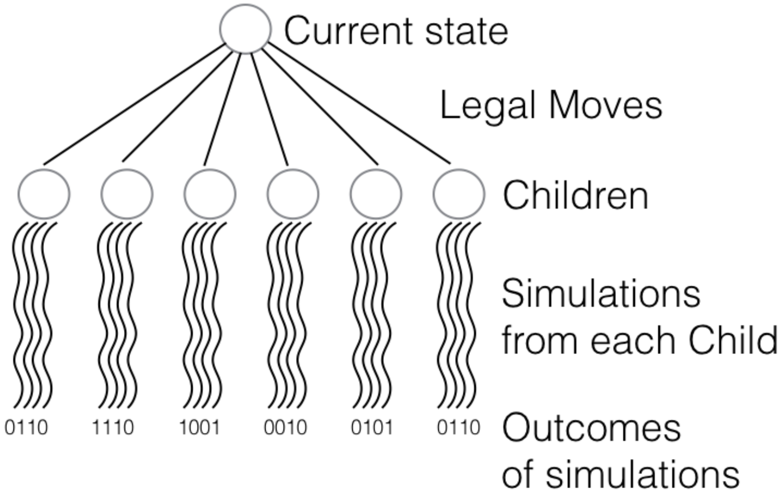
Simulation Player Implementation - genmove

- `SimulationPlayer.genmove(self, state)`
- For each move: Evaluate it by simulation
- Collect and compare winrates for all moves
- Pick the move with best winrate

SimulationPlayer.genmove

```
def genmove(self, state):
    moves = state.legalMoves()
    numMoves = len(moves)
    score = [0] * numMoves
    for i in range(numMoves):
        move = moves[i]
        score[i] = self.simulate(state, move)
    bestIndex = score.index(max(score))
    best = moves[bestIndex]
    return best
```

Simulation-Based Player



Match Simulation-Based Player vs Perfect and Random Players

- `simulation_player.py`
- `perfect_player.py`
  solves game at each step
- `random_player.py`
  selects move uniformly at random
- `play_match.py` run test games, print statistics
- How do these players compare?
- How does the strength of the Simulation Player change if we increase the number of simulations?

Match 1: 10 simulations/move, 100 games each color

- Results in table:
  - Black player (X, name on left side)
  - Result vs White player (O, name on top)
- Perfect player never loses with either color
- Going first is a big advantage (unless both are perfect)
- Note: numbers will change if re-run, but results will be similar with high probability

Table: Wins/Draws/Losses (W/D/L), 10 simulations/move, 100 games each color.

Black	Sim(10)	Perfect	Random
Sim(10)	**62W**/21D/17L	0W/**76D**/24L	**97W**/3D/0L
Perfect	**77W**/23D/0L	0W/**100D**/0L	**100W**/0D/0L
Random	9W/5D/**86L**	0W/20D/**80L**	**64W**/7D/29L

Scaling of Simulation Player vs Perfect

- Vary number of simulations 1, 10, 100, 1000
- Separate stats as Black, as White
- Results for Random and Perfect added for comparison
- Increasing simulations clearly helps
- 1000 simulations/move seem to play almost perfectly?
- Activity 12b: re-try this experiment, run more games
- TicTacToe is simple. In Go, Sim(1000) still plays poorly

Player	As Black	%	As White	%
Random	0W/20D/**80L**	10%	0W/0D/**100L**	0%
Sim(1)	0W/19D/**81L**	9.5%	0W/7D/**93L**	3.5%
Sim(10)	0W/**80D**/20L	40%	0W/24D/**76L**	12%
Sim(100)	0W/**100D**/0L	50%	0W/**77D**/23L	38.5%
Sim(1000)	0W/**100D**/0L	50%	0W/**100D**/0L	50%
Perfect	0W/**100D**/0L	50%	0W/**100D**/0L	50%

Scaling Simulation Player vs Random

- Vary number of simulations 1, 10, 100, 1000
- Separate stats as Black, as White
- Results for Random and Perfect added for comparison
- Increasing simulations clearly helps
- Sim(1000) as white better than perfect???

Player	As Black	%	As White	%
Random	64W/7D/29L	67.5%	29W/7D/64L	32.5%
Sim(1)	82W/9D/9L	86.5%	63W/15D/22L	70.5%
Sim(10)	97W/1D/2L	97.5%	78W/8D/14L	82%
Sim(100)	99W/1D/0L	99.5%	88W/9D/3L	92.5%
Sim(1000)	97W/3D/0L	98.5%	**91W/5D/4L**	93.5%
Perfect	100W/0D/0L	100%	**80W/20D/0L**	90%

Comments on Experiments

- 100 games is not enough to get precise numbers
  - Still large statistical error
  - Enough to get a rough first idea
- Benefit of more simulations is clear
- Does it play perfectly?
  - In TicTacToe, maybe close to perfect
  - In harder games like Go, not at all

Comments on Experiments (2)

- Sim(1000) can exploit Random better than the perfect player
- Confirmed with 1000 games - see below
- Probable reason:
- Tie-breaking towards moves that are more successful in random simulations
- Optional activity: write a perfect player with simulation-based tiebreaking

Player	As Black	%
Sim(1000)	988W/12D/0L	99.4%
Perfect	991W/9D/0L	99.55%

Player	As White	%
Sim(1000)	908W/59D/33L	**93.75%**
Perfect	799W/201D/0L	**89.95%**

Go3 - Simulation-Based Go Players

- `Go3` implements several variations of simulation-based players
- All choose their best move based on success in simulations
- `Go3` implements two different **simulation** policies
- `Go3` implements two different **move selection** algorithms at the root
- `Go4` will have even more simulation policies

Simulations in `Go3`

- As in TicTacToe, simulations used as state evaluation
- Use simulations to finish game many times from current position
- Keep winrate statistics to evaluate state
- How to do simulation in Go?
- Two simulation methods implemented in `Go3`
  - Almost-random
  - Rule-based (discussed later)

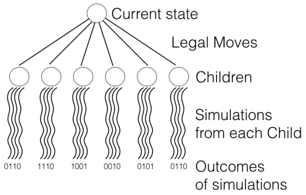
Almost-Random Simulations in `Go3`

- Remember `Go1` and `Go2`, random Go players
- Selected moves uniformly at random
    - *Except:* do not fill one-point eyes
- Almost-random simulation in `Go3` works the same way
- It will choose almost-random moves in its simulations
- Filter eye-filling moves only
- Pick all other moves with equal probability
- Pass in simulation only if all board moves are eye-filling

Move Selection in `Go3`

- Two algorithms: simple and UCB
- Simple is the same as in `simulation_player.py`
  - For each move, try *n* simulations starting with this move
- Second algorithm is UCB (later)
  - Smarter choice of which moves to simulate more often

Simple Move Selection Details



- For each legal move m_i
  - Play m_i
  - Run n random simulations
  - Undo move m_i
  - Count number of wins w_i
  - Compute winrate w_i/n
- Play the move with maximum winrate
- move $= \arg\max_i w_i/n$
- Difference to TicTacToe:
  - Legal moves include pass

Pass in Simulation vs Pass in Game

Simulations

- Regarding passing, behave like `Go1` and `Go2`
- No pass except at very end to avoid filling eyes

Move selection for player

- `Go3` player move selection is different from simulations, `Go1` and `Go2`
- In Go, pass is always legal
- `Go3` player can pass earlier if it has the best winrate
- Examples:
  - All moves on board are bad tactically
  - All moves on board are in own or opponent territory

Simulation Speed in Go vs TicTacToe

- Speed in Go is quite slow
- Simulations take much longer than in TicTacToe
- Max. 9 moves in TicTacToe
- Roughly $n \times n$ on board size n in the opening
- Example: 7×7 Go
- Simulation can be longer than 50 moves
- Reason:
  - Capture large blocks
  - Play back onto those newly empty points

Summary

- Simulation methods:
  - Approximate a quantity that is difficult to compute otherwise
  - Example: physics
  - Example: evaluation of game states
- Monte Carlo simulation - random sequences of actions
- First example - TicTacToe
  - Approaches (almost?) perfect play with enough simulations
- Second example - Go
  - Much better than random, but far from a good player