MCTS - Connect four

Markov Decision Processes and Reinforcement Learning

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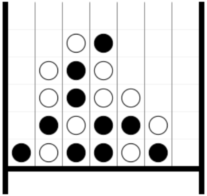
February 9, 2025

Overview

The objective of this project is to explore different reinforcement learning algorithm on the game **Connect Four**, starting from very simple mcts implementation to alphazero.

Algorithms:

- **Naive MCTS:** A basic Monte Carlo Tree Search approach without learning.
- **REINFORCE with Baseline:** A policy gradient method incorporating a baseline.
- **AlphaZero:** A self-play RL algorithm combining MCTS with deep learning.



Connect Four is a two-player game played on a vertical 7-column, 6-row grid where players take turns dropping colored discs into the slots, aiming to connect four discs of their color horizontally, vertically, or diagonally.

Properties

- **Deterministic:** Outcome fully determined by player actions. $S_{t+1}, R_t = p(S_t, a_t)$
- **Episodic:** Sequence of actions leading to a terminal state. Episode: $\{(S_1, a_1), \ldots, (S_T, a_T)\}$
- **Two-Player:** Players 1 and 2 alternate moves, strategies π_1 and π_2.
- **Zero-Sum:** Rewards sum to zero. $R_1 = -R_2$. Terminal rewards: Win (+1/-1), Draw (0/0)
- **Perfect Information:** Both players have complete knowledge of the current state.

- **Trajectory Length:** Max 42 moves (7 columns x 6 rows).
- **State Space:**
  - Naive: $3^{42} \approx 1.1 \times 10^{20}$
  - Improved: $\approx 4.5 \times 10^{12}$ states
  - Storage: 4.5×10^{12} states $\times$ 8 bytes/state $=$ 36 TB (64 bit state representation)
- **Tabular Methods:** Infeasible due to large state space.
- **Solvability:** Solved. Player 1 can always win with optimal play (Wikipedia). No readily available solvers for testing.

Framework: JAX provides a high-performance framework for computational efficiency and flexibility, allowing for scalable and efficient development of machine learning algorithm.

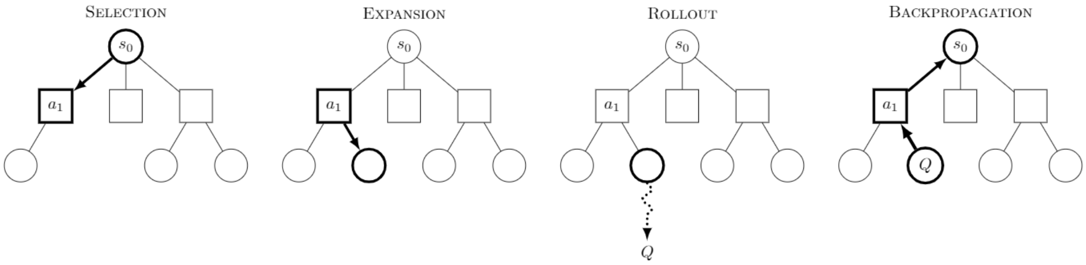
JAX Features:

- JIT Compilation
- GPU/TPU Acceleration
- Efficient Vectorization (vmap)
- Automatic Parallelization (pmap)
- Functional Programming (Pure Functions)

Libraries with links

- `mctx`: JAX-native MCTS implementations.
- `pgx`: Game environment simulation, diverse games, fast parallelization.
- `Haiku`: Neural network building and training in JAX.
- `optax`: Gradient processing and optimization.

Monte Carlo Tree Search is a decision-making algorithm that explores a decision space by constructing a search tree through repeated simulations. Given a computation budget it balances exploration and exploitation to refine the root node policy.



To perform a MCTS search using the MCTX library, two main functions must be provided:

RootFnOutput(state):

- Specifies the representation of the root state.
- Returns the prior logits and the estimated value of the root state.

recurrent_fn(state, action):

- Encapsulates the environment dynamics.
- Returns the reward, discount factor, and for the new state, the prior logits and value.

The search returns **action_weight**, representing the updated root node policy.

Negative Discount Factor

In alternating-turn games, a negative discount factor ($\gamma = -1$) is used to invert value estimates between players:

$$V(S_t) = r_t + \gamma \cdot V(S_{t+1}) = r_t + (-1) \cdot V(S_{t+1})$$

- S_t: Current state (Player 1's turn).
- S_{t+1}: Next state (Player 2's turn), where the value $V(S_{t+1})$ represents the opponent's optimal value.

This inversion maintains the zero-sum property by ensuring that a high value for one player corresponds to a low value for the opponent.

The neural network is a custom **ResNet**, a convolutional network with residual connections and batch normalization. It has two output heads:

$$l, v' = \mathrm{ResNet}_\theta(S_t)$$

1. **Policy Head:** Produces a probability distribution over possible actions:

$$\pi(a \mid S_t) \approx \hat{\pi}(a \mid S_t) = \mathrm{softmax}(l)$$

2. **Value Head:** Outputs a scalar value approximating the value function:

$$V(S_t) \approx \hat{V}(S_t) = v'$$

Description

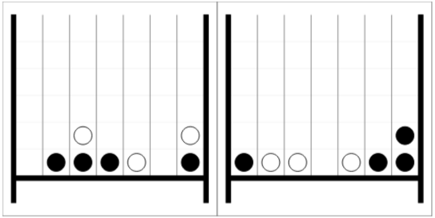
Naive implementation of Monte Carlo Tree Search:

- **no learning**
- MCTS
  - policy: uniform
  - value: single random rollout

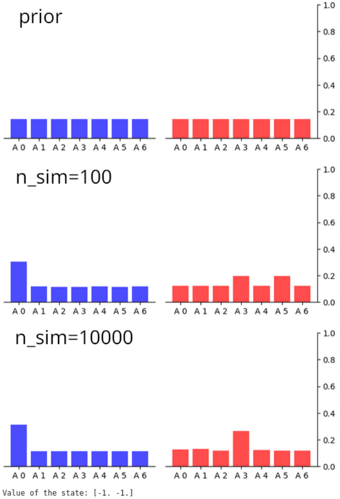
Pseudocode MCTS Inference


```
def RecurrentFn(s, a)
    s', reward <- env_step(s, a)
    V, pi <- random_rollout(s'), uniform_prior
    discount <- -1.0
    return s’, pi, V, reward, discount

def RunMCTS(s)
    root = (V, pi(a|s)) <- random_rollout(s), uniform_prior
    policy_output <- MCTS(root, RecurrentFn, num simulation)
    return arg max_a policy_output
```



Value = [-1, -1]


Policy output
prior
n_sim=100
n_sim=10000
A 0 A 1 A 2 A 3 A 4 A 5 A 6
1.0
0.8
0.6
0.4
0.2
0.0
Value of the state: [-1. -1.]

Description

Reinforce baseline algorithm:

- Policy based algorithm
- no MCTS
- on policy, batch
- neural network function approximation

```
Initialize: Neural Network, Optimizer, Replay Buffer

Main Loop:
    for iteration in 1..MaxIterations:
        # Self-play Phase
        Collect Games:
            for N games:
                def step_fn(s):
                    root = V_nn, pi_nn(a|s) <- nn_forward(s)
                    run MCTS(root, num_simulation):
                        s', reward <- env
                        V', pi <- nn_forward

                    a <- MCTS.policy_out.action

                    s', r <- env_step(s, a)

                    return (s, policy_out, s', r, discount=-1),
                        s'

                s_init <- env.reset()
                data <- jax.scan(step_fn, s_init)

                samples <- compute_loss_input(data) # cumulative rewards
                Save samples to Replay Buffer # (s_t, pi_t, G_t:value target)


        Shuffle samples and make minibatches (Replay Buffer)






        # Training Phase
        Train Network:
            batch ~ Replay Buffer # sample (s_t, a_t, G_t)
            compute_loss:
                V_nn, pi_nn(a|s_t) <- nn_forward(s_t)
                A(s_t, a_t) <- G_t - V_nn(s_t) # compute advantage
                policy_loss <- -mean[log(pi_nn(a_t|s_t) * A(s_t, a_t)]
                value_loss  <- MSE(V_nn(s_t), G_t)
                entropy_loss <- entropy(pi_nn)

                loss <- policy_loss + value_loss + 0.1 entropy_loss

            Compute gradient (loss)
            Update model parameters

        # Saving Phase (periodic)
        if iteration % saving_interval == 0:
            Save checkpoint
```

Total Loss:

$$L = \mathcal{L}_{\text{policy}} + \mathcal{L}_{\text{value}} + 0.1 \times \mathcal{L}_{\text{entropy}}$$

Where:

$$\mathcal{L}_{\text{policy}} = -\mathbb{E}\left[\log \hat{\pi}(a_t \mid S_t) \cdot A(S_t, a_t)\right]$$

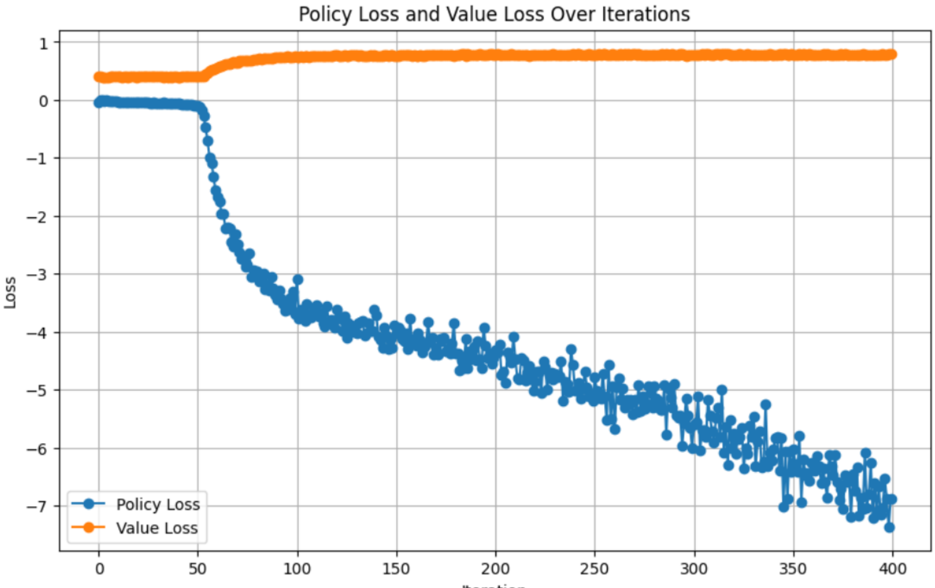
$$A(S_t, a_t) = G_t - \hat{V}(S_t)$$

$$\mathcal{L}_{\text{value}} = \mathbb{E}\left[\left(\hat{V}(S_t) - G_t\right)^2\right]$$

$$\mathcal{L}_{\text{entropy}} = -\mathbb{E}\left[\sum_a \pi(a \mid S_t) \log \pi(a \mid S_t)\right]$$

Gradient Clipping: ensures that the gradients do not exceed a specified threshold, preventing exploding gradients.

Loss plot


Policy Loss and Value Loss Over Iterations
1
0
−1
−2
−3
−4
−5
−6
−7
Loss
0
50
100
150
200
250
300
350
400
Policy Loss
Value Loss

Even with loss improvements, divergence still occurs.

The Deadly Triad:

Bootstrapping	$\times$
Function Approximation	$\checkmark$
Off-Policy (No Batch)	$\times$

Alphazero algorithm

- MCTS
  - policy: neural network policy head
  - value: neural network value head
- neural network function approximation

```
Initialize: Neural Network, Optimizer, Replay Buffer

Main Loop:
    for iteration in 1..MaxIterations:
        # Self-play Phase
        Collect Games:
            for N games:
                def step_fn(s):
                    root = V_nn, pi_nn(a|s) <- nn_forward(s)
                    run MCTS(root, num_simulation):
                        s', reward <- env
                        V', pi <- nn_forward

                    a <- MCTS.policy_out.action

                    s', r <- env_step(s, a)

                    return (s, policy_out, s', r, discount=-1),
                            s'

                s_init <- env.reset()
                data <- jax.scan(step_fn, s_init)

                samples <- compute_loss_input(data) # cumulative rewards
                Save samples to Replay Buffer # (s_t, pi_t, G_t:value target)


        Shuffle samples and make minibatches (Replay Buffer)





        # Training Phase
        Train Network:
            batch ~ Replay Buffer # sample (s_t, policy_out_t, G_t)
            compute_loss:
                V_nn, pi_nn(a|s_t) <- nn_forward(s_t)
                policy_loss <- cross_entropy(pi_nn(a|s_t), policy_out)
                value_loss  <- MSE(V_nn(s_t, G_t))

                loss <- policy_loss + value_loss + entropy_loss

            Compute gradient (loss)
            Update model parameters

        # Saving Phase (periodic)
        if iteration % saving_interval == 0:
            Save checkpoint
```

Total Loss:

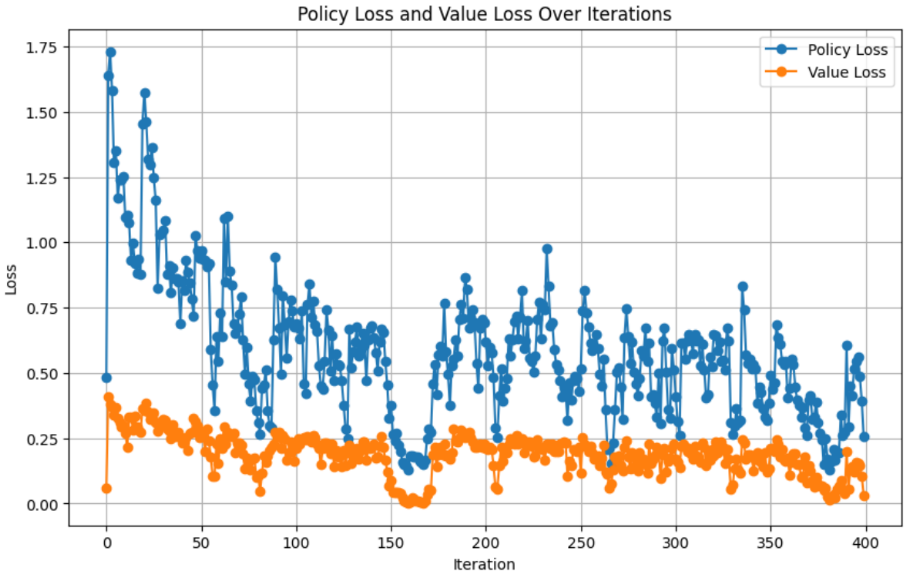
$$L = \mathcal{L}_{\text{policy}} + \mathcal{L}_{\text{value}}$$

Where:

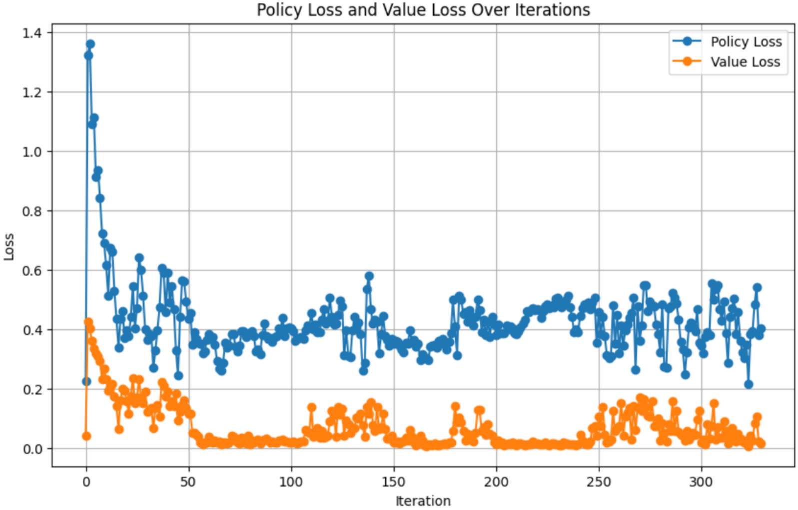
$$\mathcal{L}_{\text{policy}} = -\mathbb{E}_{a \sim policy\_out} [\log \hat{\pi}(a)]$$

$$\mathcal{L}_{\text{value}} = \mathbb{E}\left[\left(\hat{V}(S_t) - G_t\right)^2\right]$$

Loss plot


Policy Loss and Value Loss Over Iterations
Policy Loss
Value Loss
Loss
Iteration
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
0
50
100
150
200
250
300
350
400

With better training: increase num. MCTS simulation, batch size, neural network



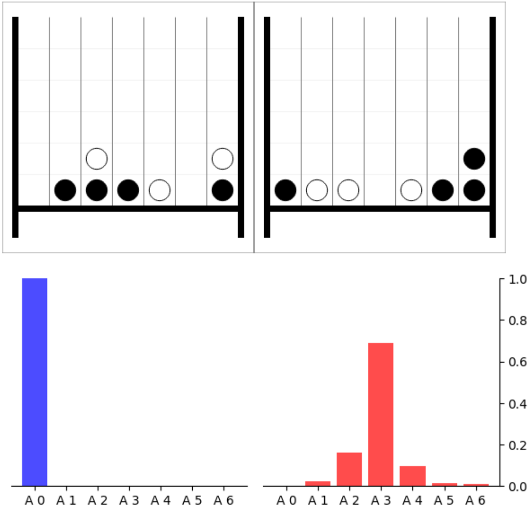
Inference MCTS vs One-shot

```
def RecurrentFn(s, a)
    s', reward <- env_step(s, a)
    V, pi <- nn_forward(s')
    discount <- -1.0
    return s', pi, V, reward, discount

def RunMCTS(s)
    root = (V, pi(a|s)) <- nn_forward(s)
    policy_output <- MCTS(root, RecurrentFn, num simulation)
    return arg max_a policy_output
```

```
def RunOneShot(s)
    pi_nn(a|s) <- nn_forward(s)
    return arg max_a pi_nn(a|s)
```

Example Network forward




```
Array([-0.93581444,  0.85516936], dtype=float32)
```

Notebook games and demo play

Future Experiments

- hyper-parameter tuning for better training
- longer training
- network architecture
  - increase capacity
  - transformer architecture
- MCTS: test different selection algorithm

References

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Mastering chess and shogi by self-play with a general reinforcement learning algorithm.

Silver, D., Schrittwieser, J., Simonyan, K., and et al. (2017b).
Mastering the game of go without human knowledge.
Nature, 550:354–359.

Thank you for your attention!