Investigation of self-play deep reinforcement learning for Tic-Tac-Toe

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Abstract

With the recent announcement by Google that they've developed the world's strongest chess AI, AlphaZero, with a self-play deep reinforcement learning algorithm, the idea of pairing a neural network with a Monte Carlo Tree Search algorithm (MCTS) for complex two player board games has become very popular. In this paper I attempt to understand how both neural networks and MCTS work and how Googled paired them together by attempting to train my own AlphaZero for a simpler game and compare how the algorithm compares with an AI that uses MCTS alone. I chose to train my version of AlphaZero, uninterestingly named BetaZero, on tic-tac-toe. My work shows that MCTS alone can play tic-tac-toe and unfortunately, because of a combination of issues, BetaZero didn't perform at all as expected. I reflect on my challenges when trying to train BetaZero.

Introduction

Designing powerful AI's for complex two player games like chess and Go have captured the attention of people for many years. Some of the best chess engines in the world like Stockfish continue to improve year on year. Recently Google's AlphaZero managed to create a world class AI from a form of self-play reinforcement learning called Tabula-Rasa. AlphaZero is differnet from how other strong chess engines because AlphaZero only knew the rules of the game and was only allowed to play against itself. AlphaZero works by combining Monte Carlo tree search (from now on denoted MCTS) and a neural network. The Alphazero paper by David Silver et al. describes at a high level how they modified MCTS to utilize the insights of the neural network, how they architected and trained their network, and how they evaluated a board position. [Silver et al.2017]

In this work I try to create an AI for tic-tac-toe similar to AlphaZero. Let the tic-tac-toe AlphaZero agent be called BetaZero from now on. The reason why such a simple game was chosen was because there are readily available AIs which play perfectly to test the BetaZero against. In fact, because of how simple tic-tac-toe is, a simple MCTS without deep learning plays the game perfectly when the MCTS agent is given enough time or simulation iterations to think. Another reason why tic-tac-toe was the game of choice was because of the hardware limitations faced. AlphaZero was trained on Google's infrastructure whereas I am limited to working with my laptop.

I investigate how augmenting a MCTS algorithm for tic-tac-toe with deep learning improves MCTS when it is limited to only a small number of simulation iterations. I also investigate how many fewer simulation iterations BetaZero needs to play perfectly when compared with a vanilla MCTS agent.

Monte Carlo Tree Search

Monte Carlo Tree Search (MCTS) is a search algorithm used for finding optimal decisions in game trees. MCTS determines the best move in a given game state by progressively, and asymetrically, exploring the game tree. Upon each iteration the algorithm chooses a new node to explore and then randomly plays out the game from the new state to get a game outcome. [Browne et al.2012] The total score and visits are stored at each explored state in the tree and the best action is the one leads into the state that has the best average score. The high level pseudocode for MCTS is

Algorithm 1 Generic MCTS

```
function MctsSearch(s_0)
    create root node n_0 with state s_0
    while within computation budget do
        v_l ←Tree Policy(v_0)
        △ ← Default Policy(s(v_l))
        Backup(v_l, △)
    end while
    return a(BestChild(v_0))
end function
```

where

- s_0 is the initial state
- v_l is a game state that is reachable from s_0
- $\triangle$ is the score of the played out game from state v_l
- a(BestChild(v_0)) is the action from s_0 to the next state that has the best expected outcome.

There are many variations of MCTS and in this case I chose the version of MCTS that generates one unvisited node each iteration. At each new unvisited node the default policy was to return the score of the game by playing out the game randomly. The result of the game, z, took on values $\{1, 0, -1\}$ where 1 meant that the player playing in state v_l won, 0 encoded a draw and -1 encoded a loss for the player acting in state v_l. The Backup function updates the nodes in the game tree that were visited in the current iteration. At each node the outcome of the game was added to the node's score and the node's number of visits is incremented by one.

In order for MCTS to be effective the tree policy must balance exploration and exploitation. Intuitively, the policy must minimize the amount of regret when it chooses the action for s_0. The UCB1 policy is known to produce an expected logarithmic growth in regret without any prior knowledge of the game outcomes for each action.

$$UCB1(v_l) = \overline{X} + c\sqrt{\frac{2\ln n}{n_j}}$$

$\overline{X} = \frac{\texttt{score at } v_l}{\texttt{visits to } v_l}$ indicates the expected score of the node v_l in the game tree. n_j represents the number of visits child j has received and n represents the number of visits v_l as received. c is a constant. If a node hasn't been visited its $UCB1$ score is set to infinity. The $UCB1$ score balances exploitation and exploration because a node with a low visit count will have a higher $UCB1$ score compared to another node with a higher visit cound (assuming their $\overline{X}$ scores are the same). Therefore the tree policy used for MCTS was to choose the child node with the highest $UCB1$ score.

AlphaZero Neural Network

The neural network that AlphaZero used, denoted as $f_\theta(s)$, took in as input a game representation and outputted a tuple $(\vec{p}, v)$ where θ are the parameters of the network, s is the game state, $\vec{p}$ is the policy that the network thinks is optimal at state s, and $v \in [-1, 1]$ is the expected outcome of the game.

Since AlphaZero was built to play complex board games like Chess, Go, and Shogi, they represented these games as a large $N \times N \times (MT + L)$ stack of images where the image stack is composed of T time steps of M planes of size $N \times N$ where each plane represents a board position along with M binary feature planes that denoting piece presence. [Silver et al.2018] This game representation seemed too complicated for a simple game of tic-tac-toe and as a result I represented a game position as a flattened 3×3 array. A value of 1 represented the player's piece, a value of -1 represented the opponent's piece and 0 represented an empty square on the board.

Similarly, a much simpler network architecture was chosen compared to the one used for AlphaZero however, the chosen architecture had the same high level structure as AlphaZero's network. AlphaZero's architecture consisted of three parts. For the first part, the body, AlphaZero had 20 rectified, batch-normalized covolutional layers. Afterwords the body split to the policy and value head. The policy head was composed of an additional convolutional layer where the number of filters represented the probabilities of $\vec{p}$. The value head added an addition convolution layer to the body, a rectified linear layer, and a $tanh$ layer of size 1. For BetaZero (the tic-tac-toe agent), I chose a much simpler network architecture because of hardware limitations and because tic-tac-toe is much simpler than chess.

The input to the network is $(X, 9)$ where X is the number of training examples. Next the body is composed of two hidden rectified, batch-normalized linear layers. This means that the activation function used is

$$relu(x) = \begin{cases} x & x \geq 0 \\ 0 & x < 0 \end{cases}$$

Each hidden layer in the body had 81 hidden units. The policy head added an

the output of the policy head to be a distribution the softmax function was applied to the last hidden layer.

$$softmax(\vec{p_j}) = \frac{e^{p_j}}{\sum_{k \in p} e^{p_k}}$$

The value head also adds an addition rectified batch-normalized hidden layer with 18 units to the body. Then a 1 unit layer is and the value is the $tanh$ of the output. Visually, the network for BetaZero looks like

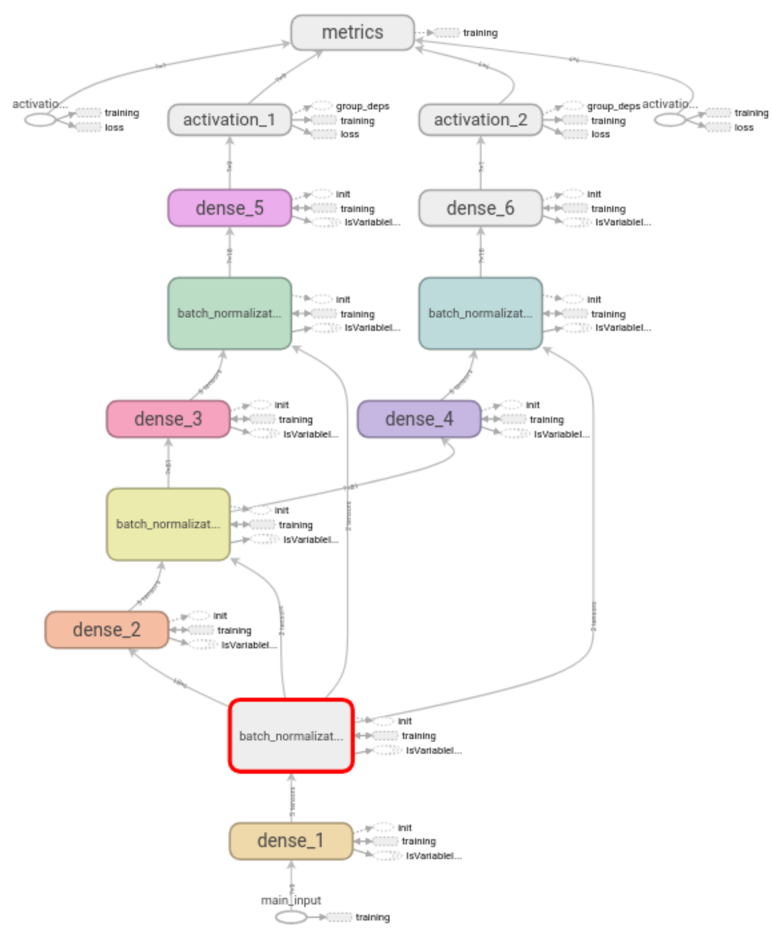


Figure 1: Network Architecture for BetaZero

AlphaZero MCTS

Since AlphaZero evaluates a given game state by using both an MCTS and the neural network described in the previous section. The following changes to MCTS are made that differ from what was described in the MCTS section. Even though I haven't described how the network is trained, assume for now that the network accurately predicts the correct policy vector and game outcome. The AlphaZero version of MCTS is

Algorithm 2 How AlphaZero finds the best move in a position

function ALPHAZEROSEARCH(s_0)
    create root node n_0 with state s_0
    while within computation budget **do**
        $v_l \leftarrow$TREE POLICY(v_0)
        $\triangle \leftarrow$ DEFAULT POLICY($s(v_l)$)
        BACKUP(v_l, $\triangle$)
    end while
    return COMPUTEPOLICY$\pi(n_0)$
end function

function TREEPOLICY(v_0)
    return argmax_{v_j}COMPUTEUCB1(v_j)
end function

function COMPUTEUCB1(v_0)
    $Q \leftarrow \overline{X}$
    $c \leftarrow \log\left(\frac{1+parent.visits+cbase}{cbase}\right) + cinit$
    $U \leftarrow c(prior)\left(\sqrt{\frac{parent.visits}{1+n}}\right)$
    return $Q + U$
end function

function DEFAULTPOLICY(v_0)
    $\vec{p}, v \leftarrow f(s_0)$
    return v
end function

AlphaZero differs from MCTS in the following ways:

- The default policy for AlphaZero just queries the neural network for the value of the game instead of randomly playing out the game.
- AlphaZero returns a policy vector π instead of the best action. For the case in BetaZero, the policy π is computed by

$$p_a = \frac{\overline{X_a} - X_{min}}{\sum_{a \in \text{actions}} \overline{X_a}} \qquad \forall a \in \text{ valid actions in } s$$

- AlphaZero augmented the UCB1 score of a node by introducing a $prior$ parameter. The $prior$ parameter for game state v_j is the probability of choosing the action that goes from the parent of state v_j to state v_j where the probability is given from the neural network, f_θ.

Another smaller addition that Alphazero implemented is that they add some noise into the $prior$ probability for each state. More specifically, they sample from a gamma distribution and update each probability as follows

$$prior = \frac{3}{4}prior + \frac{1}{4}noise$$

The intuition for adding the noise was to make sure that MCTS was properly exploring enough in the case that the neural network was tunneled into one certain move.

AlphaZero Training

The last component of AlphaZero that needs to be described is how it trains. Since Alphazero is only allowed to play against itself, training follows the following regime (See algorithm 3): During self-play each position is saved along with the policy π. At the end of the game the outcome of the game, along with the policies π generated during the game are used to train the neural network. The loss function for the network is, for a given board state,

Algorithm 3 AlphaZero learning process

function TRAIN()
    create a game with initial state $s \leftarrow s_0$
    while the game isn't over **do**
        $\pi \leftarrow$ALPHAZEROSEARCH(s)
        boards, policies $\leftarrow$ GETTRAININGDATA
        $s \leftarrow$ CHOOSEMOSTLIKELYMOVE(π)
    end while
    TRAINNEURALNETWORK(boards, policies)
end function

$$\ell = (z - v)^2 - \pi^T \log \vec{p} + c||\theta||^2$$

z is the outcome of the game of self play. v is the predicted outcome of the game for the given board state. π is the policy vector returned by the AlphaZero MCTS and $\vec{p}$ is the neural network's policy for the given board state the last term in the loss function just adds some ℓ_2 regularization. This means that the network will try to minimize the mean squared loss between the predicted and actual game outcome and it will try to minimize the log loss between the predicted and generated policies.

Intuitively, this loss function makes it such that the neural network will better predict the outcome of the game from a given board position and better predict the best policy from a board position. What is interesting is how AlphaZero's MCTS algorithm relies heavily on the neural network, f_θ and so even though neither the network nor MCTS can play chess very well the hope is that during each game of self play, the AlphaZero augmented MCTS will find a policy that is better than the network's predicted policy and that the network's current policy is better than randomly sampling the next set of actions. This would allow AlphaZero to slowly and iteratively learn how to play the game even though it knew nothing except the rules to begin with.

Differences between Beta and AlphaZero

Given that Chess and tic-tac-toe are very different I now list the differences I chose to make when building BetaZero. Some of the big design differences are already mentioned in the previous section.

- The network BetaZero uses is a much simpler multi output Feed forward network compared to AlphaZero's multi output CNN. (See the AlphaZero Neural Network section for more info)

- I removed the ℓ_2 regularization from the loss function because I thought it added unnecessary complexity.
- In the game tree, the score at each node is always with respect to the player that is going to move at the root of the tree. This means that when a label is generated, by either random play or from BetaZero's value prediction, every node's score will be w.r.t to the root player. Therefore when running $UCB1$ in nodes with the opposing player, we instead return $-Q + U$ instead of $Q + U$. (See psuedocode for reference). This differs from AlphaZero where for nodes with the opposing player playing they instead add (1-v) to that node's score instead of adding just v.
- Since the tic-tac-toe board has 8 axis' of symmetry, for each board position I also added the symmetric boards to the training set with the corresponding symmetric policy vectors. Alphazero also used this trick when learning how to play Go but didn't do so for chess because there are much fewer symmetries on the chess board since queen side castling is different from king side castling.
- I used a learning rate of 0.02 whereas in AlphaZero they first trained with a learning rate of 0.2 and decreased it by an order of magnitude every 100000 games.

Experiments

The first thing that I did was to determine how many iterations a regular MCTS AI needed to play perfect tic-tac-toe. Since tic-tac-toe is such an easy game, I tested whether the MCTS AI played perfectly by personally playing against it and then playing the MCTS against itself and making sure that it drew all its games. This was achieved for an MCTS that was allowed to search for 750 iterations. This is an intuitive answer because it means that the AI is allowed to approximately look 3 moves deep which is plenty for enough for tic-tac-toe.

From here I proceed to train BetaZero but limit its MCTS to fewer iterations and determine how many fewer (if any) iterations BetaZero needs to play perfectly. I trained a BetaZero agent for 20000 games but noticed that the training loss wasn't decreasing much after the first 200. The loss graph looked like The concerning thing was that the loss never bottomed out and that while the neural network had high accuracy when predicting the expected outcome of the game from a given position, it had very low accuracy when predicting the policy for a given position. Regardless of the concerning loss graph. I tested BetaZero against the perfect MCTS. I tested BetaZero 7 times. For each test I increased BetaZero's MCTS iteration depth. The Beta Zero's iteration depth started at 150 and increased to 750. Ideally BetaZero would perform optimally before it requires a 750 MCTS iteration depth. I track the draw percentage of BetaZero against the optimal MCTS AI. This is calculated simply as

$$\frac{\text{Number of draws}}{\text{Number of total games}}$$

Figure 2: The training loss of BetaZero during self play

At each iteration I play 100 games against the optimal MCTS AI.

Iterations	Draw percentage
150	0.0
250	0.0
350	0.0
450	0.0
550	0.0
650	0.0
750	0.0

Because the draw rate was 0.0 for every version of BetaZero, and since the MCTS AI plays perfectly, this meant that BetaZero lost all of its games to the regular MCTS AI.

Unfortunately this result means that something is obviously wrong with BetaZero. During troubleshooting I manually evaluated BetaZero against some positions and compared the predicted policies and predicted game outcomes with a regular MCTS AI. Here are the most interesting results

		O
	X	
X	O	

Here BetaZero correctly classifies the position with a expected game score of 0.943 and the predicted policy $\vec{p}$ is

0.176	$.153$	0.001
0.278	0.0088	0.2086
0.004	0.0023	0.167

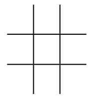
This shows that BetaZero has correctly identified that if a square is taken then the probability of taking that invalid action is very low. Also the best move BetaZero wants to make is indeed a winning move.

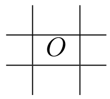
Here is another example of BetaZero classifying a given position

O	X	O
X	X	O
O	O	X

The position is clearly a draw but BetaZero estimates that the game score is 0.999.

Another alarming classification is for the following boards





BetaZero predicts that the expected outcome of the empty board is 0.92 which is way too high given that the expected the outcome, with perfect play is 0. It predicts the expected outcome for the second board is -0.98 which is too pessimistic.

From manually debugging BetaZero, it is clear that it correctly predicts the outcome and policy of some positions while for others it is wrong. This leads me to believe there is either an issue with the MCTS algorithm BetaZero is using or some board positions and their corresponding policies aren't being trained on. What is concerning about how AlphaZero evaluates positions is that instead of randomly playing out a game to get its label, it queries the neural network for the expected outcome. From the particular examples above, if the neural network is misclassifying the outcome of some states will misrepresent the score stored at each game state in the game tree which will cause BetaZero to recommend the incorrect move. Either way it is clear BetaZero still has a lot more to learn before it can compete with the perfect MCTS AI.

Conclusion

I attempted to mimic the success AlphaZero had with Chess, Go, and Shogi by creating a self-play reinforcement learning AI for tic-tac-toe. In doing so I learned how Monte Carlo Tree Search allows an AI to balance exploration and exploitation when playing games with large state spaces. The idea that finishing a game with random play during the $Default - Policy$ part of MCTS can, in aggregation, produce accurate assessments shows how powerful randomization is. I also learned about how Silver et al. at Google combined a neural network with MCTS. I tried my best to mimic the way their algorithm but during testing it seems like there are some bugs that still are preventing BetaZero from playing tic-tac-toe perfectly.

References

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