Mastering the game of Connect 4 through self-play

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Abstract

Alpha Zero is an AI algorythem, that is capable of learning to play zero sum stated multiplayer games. These types of games include Go, Chess, Phi Sho and so forth. This is done by training a neural network and from data generated by a Monte Carlo Tree Serch. This document also explains how neural networks work and a short explenation of the infrastructure around the AI to allow for playing on remote devices. [4][5]

Contents

Alpha Zero is an algorithm published in 2018 by Google Deepmind as the generalization of AlphaGo Zero, an algorithm that learned to play the game of Go using only the rules of the game. In the generalized version, the same principles were applied to Chess and Shogi. Unlike previous algorithms such as StockFish or Elmo that use hand-crafted evaluation functions along with alpha-beta searches over a large search space, Alpha Zero uses no human knowledge. Rather, it generates all information through self-play. It has been shown to achieve superhuman performance in Chess, Shogi and Go. In this project the AI will be trained to play connect4. The entire algorithm is implemented in C++. Furthermore all agents have been evaluated against each other using the Elo evaluation system [2]. Additionally, I have added a short introduction on how neural networks work and how they are trained in section 1.4 on page 14.

1 Methods

The Alpha Zero algorithm is a reinforcement learning algorithm using two major parts: a) a *Monte Carlo tree search* (MCTS) that is guided by b) the *neural network* to improve performance. The agent (computer player) runs a certain amount of simulation games using its MCTS and neural network. At each step, the MCTS evaluates the most promising next states as given by the neural network's estimation. The MCTS, by simulating games starting from the current state, will improve the neural network's prediction for that state. At the end of each game, the winner is determined and used to update the neural network's estimation of who would win a game starting from a certain state. Training an AI by teaching it to prefer advantagious actions is called reinforcement learning.

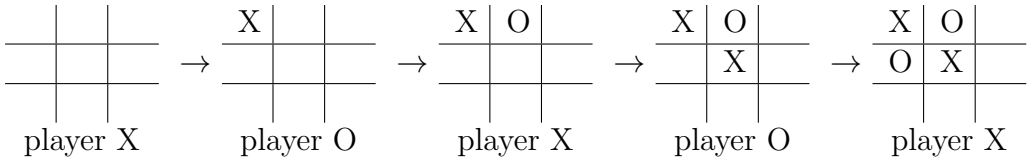
1.1 Reinforcement Learning

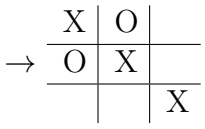
When training neural networks, there are three major possible situations: Supervised learning, unsupervised learning, and reinforcement learning. The first uses predetermined data with known in- and outputs the network is trained to predict. An example of supervised learning is the recognition of handwriting as the data is defined by humans. This method consists of creating a large database of examples, and the neural network is then trained to predict a given output for all examples.

Unsupervised learning or self-organization is used when there is no previous available data and the neural network has to create those classifications itself. An example of unsupervised learning is Vector quantization. The algorythems sorts points in n-dimensional space into a predetermined amount of groups. Every group is defined by its centroid point. Training happens by selecting a sample point at random, and moving the closest centroid point towards the sample point by a fraction of the distance betwean them. The sample point is selected from the input data [6]. An example of both supervised and unsupervised learning can be seen in the demo[1].

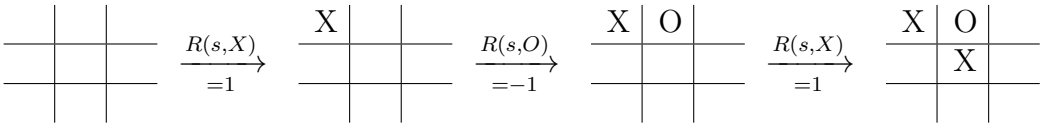
These two methods represent the extreme ends of the spectrum. Reinforcement leaning on the other hand can be thought of as an intermediate form. It uses a predetermined environment which gives positive, neutral and negative feedback. The neural network is then discouraged from taking actions leading to negative feedback and encouraged to take actions leading to positive feedback. The feedback is determined by the environment the agent learns to interact with. In this case, losing a game would be bad and result in negative feedback whereas winning a game leads to positive feedback. Ties lead to neutral feedback. The agents learning is set up in such a way, that it is encouraged to take actions leading to positive feedback and discouraged from taking actions that lead to negative feedback. However actions, can lead to a loss that only occurs many game steps in the future. A common approach to solve this problem is to have the feedback propagate backwards to previous actions. In Alpha Zero, this is handled by the memory (see section 1.5.2 on page 25). When the game reaches an end state and a winner is determined, the feedback is propagated backwards up threw all states used to get to the end state. If the player won, the feedback is positive. If he lost, it is negative. More specifically, if a player takes an action a_s at a state s, that leads to a win for that player, the reward for that state is defined as $R(s, a_s) = 1$. On the other hand, if the action leads to a loss, the reward will be $R(s, a_s) = -1$. If the game ends in a tie, the reward is $R(s, a_s) = 0$. Every agent p will try to maximize $\sum_{s \in g \cap p} R(s, a_s)$. $g \cap p$ is the set of all states in which the player p takes an action. Let's look at a tic tac toe example of the following game:

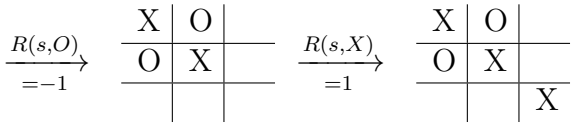
[1] demo is at https://github.com/JulianWww/Matura-AlphaZero-demos





Since player X won the game, the reward for every state $s \in g \cap X$ is $R(s, a_s) = 1$ and the reward for every state $s \in g \cap O$ is $R(s, a_s) = -1$. The reward for the entire game is:





> The important thing to keep in mind is that reinforcement learning algorithms encourage actions that lead to a positive feedback and discourage actions that lead to a negative feedback.

1.2 Game

In order to train a reinforcement learning AI, it must interact with an environment. In Alpha Zero the game is the the environment. The game consists of a series of constant unchanging game states. Every game state consists of a game board and a player. An end game state is a state at which the game is done, every game ends in an end game state. At an end game state one

player won or the game ended in a tie. Togather the states form a graph. Any possible path thought this graph starting from a root state (the inital state of the board) and ending in any end game state, is a possible game. From an end game state, there is no where left to go. For connect4 an end game state has either four stones in a line or a full game board. Let $\mathbb{G}$ be the set of all legal game states. Let $\mathbb{G}_{done} \subset \mathbb{G}$ be the set of all game states for which the game is done. At every gamestate one player is at turn. This means that that player will take an action next. Let $\phi(s) : \mathbb{G} \to \{1, -1\}$ be the function mapping states to players. In the tick-tack-toe example from earlyer we could say that:

$$\phi(s) = \begin{cases} 1 & s \in g \cap X \\ -1 & s \in g \cap O \end{cases} \tag{1}$$

More generally $\phi(s) = 1$ if the first player (the player that starts the game) is at turn and $\phi(s) = -1$ if the other player is a turn.

1.2.1 Game Board

Board games consist of placing stones of different types on a board with a certain amount of fields. Many games, like Go, Chess and Connect4, arrange their fields in a rectangular pattern. These games have two distinct stones. We can represent these game boards as stack of binary layers. Every layer is associated with one kind of stone. Each layer contains a one, where the board has a stone of the appropriate type and zeros everywhere else. For instance, the following tic tac toe game board can be represented by the following binary plane stack.

$$\begin{array}{|c|c|c|} \hline & \text{X} & \text{O} \\ \hline \text{O} & \text{X} & \\ \hline \text{O} & & \text{X} \\ \hline \end{array} \rightarrow \left[\begin{bmatrix} 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix} \right]$$

Internally, the game board is represented by a flat vector. The conversion from a game state $s \in \mathbb{G}$ to vector is defined as $vec(T_s(s))$. Where $T_s(s) : \mathbb{G} \to \mathbb{R}^{\cdots}$ is the board's 3-dimensional board tensor. The *vec* function is

defined in section 3.5.1 on page 32.

$$vec\left(\left[\begin{bmatrix} a_{111} & \cdots & a_{11o} \\ \vdots & \ddots & \vdots \\ a_{1n1} & \cdots & a_{1no} \end{bmatrix} \cdots \begin{bmatrix} a_{m11} & \cdots & a_{m1o} \\ \vdots & \ddots & \vdots \\ a_{mn1} & \cdots & a_{mno} \end{bmatrix}\right]\right) = \begin{pmatrix} a_{111} \\ \vdots \\ a_{11o} \\ \vdots \\ a_{1n1} \\ \vdots \\ a_{1no} \\ \vdots \\ a_{m11} \\ \vdots \\ a_{m1o} \\ \vdots \\ a_{mn1} \\ \vdots \\ a_{mno} \end{pmatrix} \tag{2}$$

This operation for the tic tac toe board from before would look like this:

$$vec\left(T_s\left(\begin{array}{c|c|c} & \text{X} & \text{O} \\ \hline \text{O} & \text{X} & \\ \hline \text{O} & & \text{X} \end{array}\right)\right) = [0\,1\,0\,0\,1\,0\,0\,0\,1\,0\,0\,1\,1\,0\,0\,1\,0\,0]^T \tag{3}$$

1.2.2 Actions

Actions are numbers used to identify changes to the game. Every game has a set of all possible actions $\mathbb{A}_{possible} \subset \mathbb{N}_0$. In connect4, the set of all possible actions for the current player is $\mathbb{A}_{possible} = [0, 41]$. There is no need to have actions for the player, that is not at turn as these will never be taken. Every number is associated with a position on the game board. The mapping a to game fields is the following:

0	1	2	3	4	5	6
7	8	9	10	11	12	13
14	15	16	17	18	19	20
21	22	23	24	25	26	27
28	29	30	31	32	33	34
35	36	37	38	39	40	41

Let $\mathbb{A}(s)$ be the set of all legal actions for a given state $s \in \mathbb{G}$. For all states $s_{done} \in \mathbb{G}_{done}$ the set of all legal actions $\mathbb{A}(s_{done})$ is the empty set. The function $\mathcal{A} : \mathbb{G} \times \mathbb{A} \to \mathbb{G}$ is used to get from one game state to another by taking an action. Where $\mathbb{A}$ is the set of all legal actions the chosen game state. If we were to map action to position for tick tack toe as follows and that the game board is the following:

0	1	2
3	4	5
6	7	8

X	O	

State s

In this example player X is allowed to place a stone in any empy field $\mathbb{A}(s) = \{2, 3, 4, 5, 6, 7, 8\}$. Therefor $\mathcal{A}(a, s)$ is valid if $a \in \mathbb{A}(s)$ and otherwise invalid.

1.3 MCTS

A Monte Carlo tree search (MCTS) is a tree search algorithm that can be used to find sequences of actions leading to a desirable outcome. This is done by procedurally generating a directed graph of possible successor states to the current state or root state. In Alpha Zero it is used to improve the neural networks prediction. Because a MCTS changes during simulation, idices are used to specify which simulation step the tree is in. A MCTS simulation consists of three phases Leaf Selection, Node Evaluation and Expansion and Backfill.

The MCTS graph consists of nodes and edges. The edges represent connections betwean nodes while the nodes represent game states. Let $\mathbb{M}_{possible} = \{\mathcal{N}(s) \mid s \in \mathbb{G}\}$ be the set of all possible nodes , where $\mathcal{N} : \mathbb{G} \to \mathbb{M}_{possible}$ is a bijective function that maps a game state to a node. $\mathcal{S} : \mathbb{M}_{possible} \to \mathbb{G} = \mathcal{N}^{-1}$ is the inverse of $\mathcal{N}$. For notational simplicity, the set of all allowed actions for any node $n \in \mathbb{M}_{possible}$ is $\mathbb{A}(n) = \mathbb{A}(\mathcal{S}(n))$. The

ammount of nodes and structure of the MCTS is changed by the algorythem itself during simulation. Therefor Let l be the index of the current simulation step. Let $\mathbb{L} = [0, S]$ be the set of all l, where S is a constant defined in the algorythems configuration file (section **??** on page **??**). During the first simulation, the Tree contains only the root node n_0. The root node is the starting point of the simulation. Let $\mathbb{M}_l \subseteq \mathbb{M}_{possible}$ be the set of all nodes in the tree at step $l \in \mathbb{L}$.

Every node $n_l \in \mathbb{M}_l$ has a set of edges $\mathbb{E}_l(n_l)$ at step l that point from it to another nodes. Let $\mathbb{E}_l$ be the set of all edges in the current graph. $\mathcal{E}_l : \mathbb{M}_l \times \mathbb{A}_{possible} \to \mathbb{E}_l$ is a bijective function used to map nodes and actions to edges. Furthermore for $\mathcal{E}_l(n_l, a)$ to be valid a must be an element of $\mathbb{A}(n_l)$. The function $\mathcal{N}_{to_l} : \mathbb{E}_l \to \mathbb{M}_l$ maps an edge to the node it is pointing to while $\mathcal{N}_{from_l} : \mathbb{E}_l \to \mathbb{M}_l$ is used to find the node an edge is pointing from. Furthermore it is usefull to distingush expanded nodes from leaf nodes. Leaf nodes are nodes that don't have edges leading out of them. Let $\mathbb{M}_{leaf_l} \subseteq \mathbb{M}_l$ be the set of leafnodes. For every node $n_l \in \mathbb{M}_{leaf_l}$, the following is true by definition $\mathbb{E}_l(n_l) = \emptyset$. Expanded nodes are have edges leading out of them. Let $\mathbb{M}_{expanded_l} \subseteq \mathbb{M}_l$ be the set of expanded nodes. For every node $n_l \in \mathbb{M}_{leaf_l}$, the following is true by definition $\mathbb{E}_l(n_l) \neq \emptyset$.

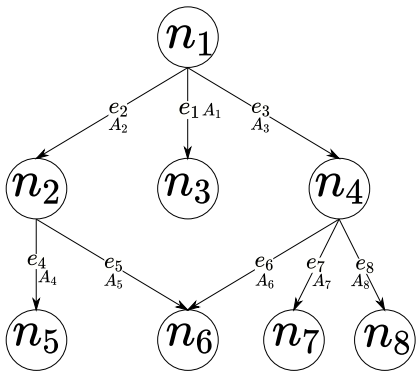


Figure 1: In the following small MCTS tree represents a possible graph at step l, where $n_?$ are nodes, $e_?$ are edges connecting the nodes and $A_?$ are actions associated with the edge they are next to. The questionmark represents the indices. The set of all nodes $\mathbb{M}_l = \{n_1, n_2, \ldots, n_8\}$ and $\mathbb{E}_l = \{e_1, e_2, \ldots, e_5\}$. We can also see that $\mathbb{E}_l(n_1) = \{e_1, e_2, e_3\}$, $\mathbb{E}_l(n_2) = \{e_4, e_5\}$, $\mathbb{E}_l(n_3) = \emptyset$ and so forth. Because e_1 represents action A_1 taken at node n_1, $\mathcal{E}_l(n_1, A_1) = e_1$. By the same logic $\mathcal{E}_l(n_2, A_2) = e_2$ and so forth. Becuase edge e_1 connects node n_1 to n_3, $\mathcal{N}_{from_l}(e_1) = n_1$ and $\mathcal{N}_{to_l}(e_1) = n_3$. The same logic applies to all other nodes. The set of all expanded nodes $\mathbb{M}_{expanded_l} = \{n_1, n_2, n_4\}$ because they have at least one edge leading away from them. On the other hand, the set of all leaf nodes $\mathbb{M}_{leaf_l} = \{n_3, n_5, n_6, n_7, n_8\}$. Finally $\mathbb{M} = \mathbb{M}_{expanded} \cup \mathbb{M}_{leaf}$ (see section 4.1 on page 35 for all data)

1.3.1 Evaluation Basis

The MCTS's goal is to find a good estimations of the reward for a certain action at a certain state. This reward estimation is $Q_l : \mathbb{E}_l \to \mathbb{R}$. To define Q_l, the functions $W_l : \mathbb{E}_l \to \mathbb{R}$ and $N_l : \mathbb{E}_l \to \mathbb{N}_0$ are required. $N_l(e_l)$ is the amount of times an edge $e_l \in \mathbb{E}_l$ has been traversed. This means how many times σ (equation 6 on page 12) has chosen to follow the edge e_l to a new node. $W_l(e_l)$ is the sum of the reward computations from all $N(e_l)$ times the edge has been evaluated. With these two functions Q_l is defined as:

$$Q_l(e_l) = \begin{cases} 0 & N_l(e_l) = 0 \\ \frac{W(e_l)}{N(e_l)} \end{cases} \tag{4}$$

The fourth and last of these functions is $P_l : \mathbb{E}_l \to \mathbb{R}$. P_l is the policy function, it's the neural network's preliminary estimation of how valuable the action is. To see what $P_l(e_l)$ is trained to aproximate see equation 47 on page 24. This function is used to guide the search to more promising edges.

1.3.2 Leaf Selection

MCTS's evaluation starts by simulating future moves within the tree. This is done by selecting an edge and then following that edge to a new node. From there, the next edge and node are selected. This is repeated until a leaf node is reached. To select an edge and thus a node from the current node $n \in \mathbb{M}_l$ the function σ_l is used. To define σ_l we must first define the edge evaluation function $v_l : \mathbb{E}_l \to \mathbb{R}$. v_l is defined as follows:

$$v_l(e) = Q_l(e) + c_{puct} P_l(e) \cdot \frac{\sqrt{\Sigma_{b \in \mathbb{E}(\mathcal{N}_{from_l}(e))} N_l(b)}}{1 + N_l(e)} \tag{5}$$

Where $c_{puct} \in \mathbb{R}^+$ is the exploration constant used to define how important exploration is. The smaller c_{puct} is, more important Q and less important exploration and P. σ_l, for a given node $n \in \mathbb{M}_l$, is then defined as:

$$\sigma_l(n) = \mathcal{N}_{to_l}(\text{argmax}_l(\mathbb{E}_l(n))) \tag{6}$$

argmax_l returns the edge $e \in \mathbb{E}_l$ with the largest $v_l(e)$.
In order to find a leaf node n_{L_l} starting from the root node n_0 and be able to update the tree later on, the following algorithm is run L times, until a leaf node is found. First let $i \in [0, L[$ be the index of the iteration of this algorithm. Let $\mathbb{M}_{back,l,i} \subseteq \mathbb{M}$ be the set of nodes traversed by the algorithm at set i during simulation l. By definition $\mathbb{M}_{back,l,0} := \{n_0\}$. Than:

$$n_{L_i+1} = \sigma(n_{L_i}) \tag{7}$$

$$\mathbb{M}_{back,l,i+1} = \mathbb{M}_{back,l,i} \cup \{n_{L_i+1}\} \tag{8}$$

Once a leaf-node $n_{L_l} \in \mathbb{M}_{leaf_l}$ is found that node is evaluated. $\mathbb{M}_{back,l,L}$ will be important in section 1.3.4 on page 14.

1.3.3 Node Evaluation and Expansion

When a leaf node n_{L_l} is reached, there are two possible cases. Ether $\mathcal{S}(n_{L_l})$ is an end game state or not.

1.3.3.1 end game state $\mathcal{S}(n_{L_l}) \in \mathbb{G}_{done}$

In this case the tree is not changed but backfill is still performed. If the player at turn at the end game state is $\phi(\mathcal{S}(n_{L_l}))$. The value $v_l \in \mathbb{R}_{-1,1}$ (69) of n_{L_l} is defined as:

$$v_l = \begin{cases} -\phi(\mathcal{S}(n_{L_l})) & \phi(\mathcal{S}(n_{L_l})) \text{ lost} \\ 0 & \phi(\mathcal{S}(n_{L_l})) \text{ tied} \\ \phi(\mathcal{S}(n_{L_l})) & \phi(\mathcal{S}(n_{L_l})) \text{ won} \end{cases} \tag{9}$$

1.3.3.2 not end game state $\mathcal{S}(n_{L_l}) \notin \mathbb{G}_{done}$

In this case the nodes state is passed to the neural network (section 1.4 on page 14). The neural networks prediction function outputs a policy vector $\pi_l \in \mathbb{R}_{0,1}^{|\mathbb{A}|}$ (69) and a scalar $v_l \in \mathbb{R}_{-1,1}$ (69). The scalar v_l is the neural networks estimation of the expected reward at n_{L_l}. π_l is the estimation of the advantageousness of every action in $\mathbb{A}$. After evaluation, the leaf node is expanded. Let $\mathbb{E}_{new}$ be the next set of all edges pointing away from n_{L_l}. This set contains one edge for every action in $\mathbb{A}(n_{L_l})$. Let $\mathbb{M}_{new}$ be the set of nodes, that the nodes in $\mathbb{E}_{new}$ are pointing to. The various Tree sets and functions are then updated as follows for step $l+1$.

$$\mathbb{M}_{l+1} = \mathbb{M}_l \cup \mathbb{M}_{new} \tag{10}$$

$$\mathbb{E}_{l_+1} = \mathbb{E}_l \cup \mathbb{E}_{new} \tag{11}$$

$$\mathbb{E}_{l+1}(n) = \begin{cases} \mathbb{E}_{new} & n = N_{L_l} \\ \mathbb{E}_l(n) \end{cases} \tag{12}$$

$$\mathcal{E}_{l+1}(n,a) = \begin{cases} \mathcal{E}_l(n,a) & n \neq n_{L_l} \\ e \end{cases} \tag{13}$$

Where $e \in \mathbb{E}_{new}$ is the edge associated with action a at node n_{L_l}.

$$\mathcal{N}_{to_{l+1}}(e) = \begin{cases} \mathcal{N}_{to_l}(e) & e \in \mathbb{E}_l \\ n \end{cases} \tag{14}$$

Where $n \in \mathbb{M}_{new}$ is the node, that edge e is pointing to.

$$\mathcal{N}_{from_{l+1}}(e) = \begin{cases} \mathcal{N}_{from_l}(e) & e \in \mathbb{E}_l \\ n_{L_l} \end{cases} \tag{15}$$

$$\mathbb{M}_{expanded_{l+1}} = \{n \in \mathbb{M}_{l+1} \ : \ \mathbb{E}_{l+1}(n) \neq \emptyset\} \tag{16}$$

$$\mathbb{M}_{leaf_{l+1}} = \{n \in \mathbb{M}_{l+1} \ : \ \mathbb{E}_{l+1}(n) = \emptyset\} \tag{17}$$

$$P_{l+1}(\mathcal{E}_{l+1}(n,a)) = \begin{cases} P_l(\mathcal{E}_{l+1}(n,a)) & e \in \mathbb{E}_l \\ \pi_{l_a} \end{cases} \tag{18}$$

1.3.4 Backfill

The value v_l is used to update the P, W and Q function as follows for every edge $e \in \mathbb{E}_{l+1}$:

$$N_{l+1}(e) = \begin{cases} 0 & e \notin \mathbb{E}_l \\ N_l(e) + 1 & \mathcal{N}_{to_{l+1}}(e) \in \mathbb{M}_{back,l,L} \wedge \mathcal{N}_{from_{l+1}}(e) \in \mathbb{M}_{back,l,L} \\ N_l(e) \end{cases} \tag{19}$$

$$W_{l+1}(e) = \begin{cases} 0 & e \notin \mathbb{E}_l \\ W_l(e) + v_l & \mathcal{N}_{to_{l+1}}(e) \in \mathbb{M}_{back,l,L} \wedge \mathcal{N}_{from_{l+1}}(e) \in \mathbb{M}_{back,l,L} \\ W_l(e) \end{cases} \tag{20}$$

Q_{l+1} is already defined according to (4). $\mathcal{N}_{to_{l+1}}(e) \in \mathbb{M}_{back,l,L} \wedge \mathcal{N}_{from_{l+1}}(e) \in \mathbb{M}_{back,l,L}$ checks if the edge e has been traversed during leaf selection. [1] In constrast to [4], this implementation stores the MCTS simulation values in the edges to allow for the fact that actions from two differant nodes leading to the same node are not identical and therefore should not be treated as such. But nodes of the same game state are identical and should be treated as such.

1.4 Neural Network

Search algorithms like MCTS are able to find advantageous action sequences. In game engines, the search algorithm is improved by using evaluation functions. These functions are generally created using human master knowledge. In the Alpha Zero algorithm, this evaluation function is a biheaded deep convolutional neural network trained by information gathered from the MCTS. In order to understand the training process, one must first understand how the neural network functions.

1.4.1 Introduction to Neural Networks

An artificial neural network or just neural network is a mathematical function inspired by biological brains. Although there are many types of neural networks, the only relevant one to this work is the feed forward network. These models consist of multiple linear computational layers separated by non-linear activation functions. Every layer takes the outputs of the previous layer, and applies a linear transformation to it [8]. There are many different feed-forward neural network layers and activation functions to chose from when designing a neural network. To focus this explanation, only the relevant ones will be discussed along with the back-propagation algorithm.

1.4.1.1 Fully Connected Layer

A fully connected layer is the most basic layer. It applies a simple matrix multiplication. The layer takes a $1 \times n$ dimentional matrix $x \in \mathbb{R}^{1\times n}$ as an input and multiplies it by a weight matrix $w \in \mathbb{R}^{n\times m}$. This operation outputs a $1 \times m$ dimensional matrix to which a bias $b \in \mathbb{R}^{1\times m}$ is added to form the output matrix $v \in \mathbb{R}^{1\times m}$ containing the output values of the layer. v is then fed to the next layer. The addition of the bias vector b is optional. In some situations it is worth dropping the bias in favour of computational speed. The fully connected layer forward propagation function shall be defined as $\delta_{wb} : \mathbb{R}^n \to \mathbb{R}^m$

$$\delta_{wb}(x) = w \cdot x + b \tag{21}$$

1.4.1.2 Convolutional Layer

Convolutional layers are commonly used for image processing. They perform the same operations over the entire image searching for certain patterns. In order to achieve this, a set of kernels $\mathbb{K}$, of size $m \times n$, are defined for the layer. Kernels are similar to fully connected layers. They consist of a weight tensor $w \in \mathbb{R}^{m\times n\times l}$ and an optional bias scalar $b \in \mathbb{R}$. For every kernel $k \in \mathbb{K}$, the kernel's forward operation $\xi_k : \mathbb{R}^{m\times n\times l} \to \mathbb{R}$ is defined as:

$$\xi_k(i) = \langle w_k, i \rangle_I + b \tag{22}$$

where $<>_I$ is the Tensor inner product defined in equation 63 on page 31. The convolutional operation $\Lambda : \mathbb{R}^{i\times j\times l} \to \mathbb{R}^{i-m+1\times j-n+1\times|\mathbb{K}|}$ is an element

wise opperation. Given that $I \in \mathbb{R}^{i \times j \times l}$ is the layer input, every element of $\Lambda(I)_{abc}$ with $a \in [1, i-m+1]$, $b \in [1, j-n+1]$ and $c \in [1, |\mathbb{K}|]$ is defined as:

$$\Lambda(I)_{abc} = \xi_{k_c}(\langle I \rangle_{S_{m \times n,\, ab}}) \tag{23}$$

The submatrix indexing operation $\langle\rangle_s$ is defined in section 3.4 on page 31. For example given the following input tensor $I \in \mathbb{R}^{4 \times 4 \times 1}$:

$$I = \begin{bmatrix} [3] & [0] & [1] & [5] \\ [2] & [6] & [2] & [4] \\ [2] & [4] & [1] & [0] \\ [3] & [0] & [1] & [5] \end{bmatrix}$$

and the following kernel weight matrix $w_k \in \mathbb{R}^{3 \times 3 \times 1}$ along with the scalar $b \in \mathbb{R}$,

$$w_k = \begin{bmatrix} [-1] & [0] & [1] \\ [-2] & [0] & [2] \\ [-1] & [0] & [1] \end{bmatrix}$$
$$b = 7$$

there are four possible locations in which w_k can be placed within I. As there is only one kernel, the length of the set of all kernels $|\mathbb{K}| = 1$. This also means that $\Lambda(I) \in R^{2 \times 2 \times 1}$. To calculate $\Lambda(I)_{111}$, we compute the kernel operation $\xi_k(I[[1,3],[1,3],\{1\}])$

$$\Lambda_{111}\left(\begin{bmatrix} [3] & [0] & [1] & [5] \\ [2] & [6] & [2] & [4] \\ [2] & [4] & [1] & [0] \\ [3] & [0] & [1] & [5] \end{bmatrix}\right) = \begin{bmatrix} [3] & [0] & [1] \\ [2] & [6] & [2] \\ [2] & [4] & [1] \end{bmatrix} \circ \begin{bmatrix} [-1] & [0] & [1] \\ [-2] & [0] & [2] \\ [-1] & [0] & [1] \end{bmatrix} + 7 \tag{24}$$

$$= -1 \cdot 3 + 0 \cdot 0 + 1 \cdot 1 - 2 \cdot 2 + 0 \cdot 6 + 2 \cdot 2 - 1 \cdot 2 + 0 \cdot 4 + 1 \cdot 1 + 7$$
$$= 4$$

The same is done for $\Lambda(I)_{121}$, $\Lambda(I)_{211}$ and $\Lambda(I)_{221}$. This leads to a $\Lambda(I)$ of:

$$\Lambda(I) = \begin{bmatrix} [4] & [3] \\ [4] & [2] \end{bmatrix}$$

1.4.1.3 Activation Function

All neural network layers are linear functions. Thus, given two layer evaluation functions $f_1(x) = ax + b$ and $f_2(x) = cx + d$, the chained function $f(x) = f_1(f_2(x))$ is also linear. In order to represent non linear functions, a non linear activation function f_a is added between two neural network layers. Thus, the chained function becomes $c(x) = f_1(f_a(f_2(x)))$. In this neural network, three different activation functions are used: $tanh$, $softmax$, and $LeakyReLU$. These functions are defined as follows:

tanh:

$\mathbb{R} \to \mathbb{R}$

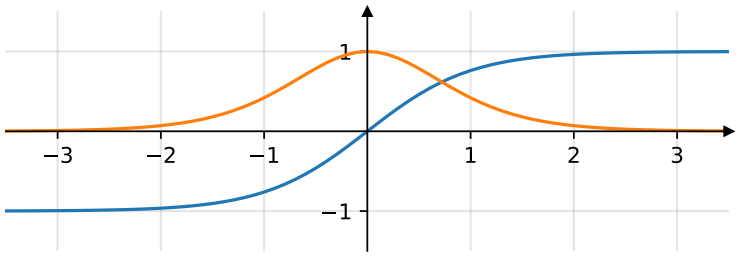


Figure 2: tanh function in blue and the tanh's derivative is in orange

$$tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}} \tag{25}$$

$$\frac{d}{dx} tanh(x) = sech(x)^2 \tag{26}$$

see section 5.1 on page 36 for proof.
Therefor for a given n dimensional vector $v \in \mathbb{R}^n$, $tanh(v)$ is deffined as:

$$tanh(v) = \langle tanh, x \rangle_E \tag{27}$$

Where $\langle \rangle_E$ is defined in equation 68 on page 33. For simplicity later on the derivative of $tanh(v)$, $tanh'(v) \in \mathbb{R}^{n \times n}$ is a $n \times n$ dimensional matrix. It is defined as

$$tanh'(v)_{ij} = \begin{cases} tanh'(v_{ij}) & i = j \\ 0 \end{cases} \tag{28}$$

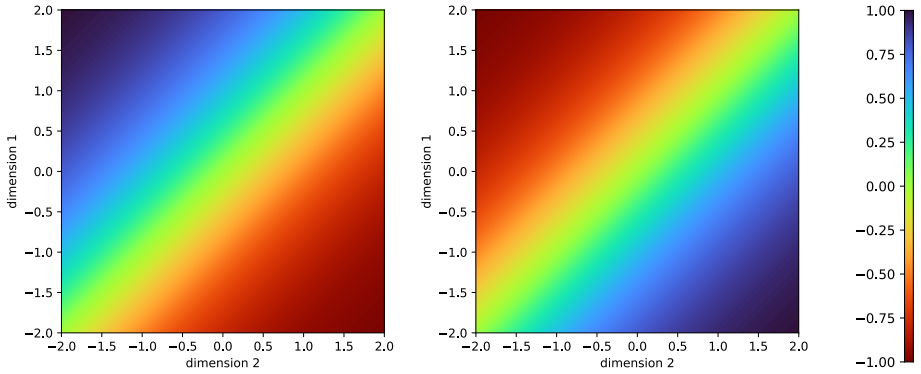
for every element i, j in the derivative matrix.

softmax:

$\mathbb{R}^n \to \mathbb{R}^n$

For a given input vector $v \in \mathbb{R}^n$. The output vector $o \in \mathbb{R}^n$ at every position $i \in [1, n]$ is:

$$o_i = softmax(v)_i = \frac{e^{v_i}}{\sum_{j \in v} e^j} \tag{29}$$



(a) $i = 1$ (b) $i = 2$ scale

Figure 3: Graph of the softmax function from $\mathbb{R}^2 \to \mathbb{R}^2$. i is the index of the output dimension. Therefore, $i = 1$ referes to the output's first dimension and $i = 2$ referes to it's second dimension.

Because the function's in- and outputs are n dimensional vectors, the derivative is an $n \times n$ dimensional matrix. When taking its derivative, $\frac{d}{dv_j} softmax(v)_i$, there are two possible cases.

case $j = i$:

$$\frac{d}{dv_j}\left[\frac{e^{v_i}}{\sum_{b \in v} e^b}\right] = softmax(v)_i \cdot (1 - softmax(v)_j) \tag{30}$$

case $j \neq i$:

$$\frac{d}{dv_j}\left[\frac{e^{v_i}}{\sum_{b \in v} e^b}\right] = -softmax(v)_i \cdot softmax(v)_j \tag{31}$$

Therefore, the derivative of the softmax function is:

$$softmax'(v)_{ij} = \begin{cases} softmax(v)_i \cdot (1 - softmax(v)_j) & i = j \\ -softmax(v)_i \cdot softmax(v)_j & i \neq j \end{cases} \tag{32}$$

LeakyReLU:

$\mathbb{R} \to \mathbb{R}$

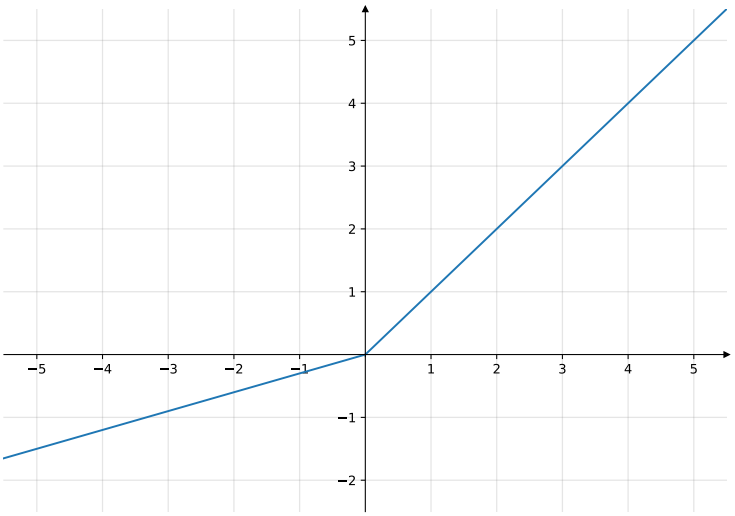


Figure 4: LeakyReLU with $c = 0.3$

$$\text{LeakyReLU}(x) = \begin{cases} x & x \geq 0 \\ x \cdot c & x < 0 \end{cases} \tag{33}$$

$$\frac{d}{dx}\text{LeakyReLU}(x) = \begin{cases} \frac{d}{dx}x & x \geq 0 \\ \frac{d}{dx}c \cdot x & x < 0 \end{cases}$$

$$\text{LeakyReLU}'(x) = \begin{cases} 1 & x > 0 \\ c & x < 0 \end{cases} \tag{34}$$

where c is a constant describing the slope of the function for negative input values. The derivative of the LeakyReLU function is undefined for $x = 0$. However as we will be performing gradient descent on these functions the derivative must befined for all $x \in \mathbb{R}$. A possible definition that accomplisches the objective is:

$$g(x) = \begin{cases} 1 & x \geq 0 \\ c & x < 0 \end{cases} \tag{35}$$

Therefor for a given n dimensional vector $v \in \mathbb{R}^n$, LeakyReLU(v) is deffined as:

$$\text{LeakyReLU}(v) = \langle \text{LeakyReLU}, x \rangle_E \tag{36}$$

Where $\langle \rangle_E$ is defined in equation 68 on page 33. For simplicity later on the derivative of LeakyReLU(v), LeakyReLU$'(v) \in \mathbb{R}^{n \times n}$ is a $n \times n$ dimensional matrix. It is defined as

$$\text{LeakyReLU}'(v)_{ij} = \begin{cases} g(v_{ij}) & i = j \\ 0 \end{cases} \tag{37}$$

for every element i, j in the derivative matrix.

1.4.1.4 Training

To make this explanation easier, I will use a fully connected neural network. Neural network training or backpropagation can be mathematically expressed as minimizing a loss function $\ell(Y_{pred}, Y_{true})$ describing how inaccurate the network is. In our case, ℓ takes the neural network's predicted value vector Y_{pred} and the correct value vector Y_{true}. Y_{true} must be known before the computation begins. In AlphaZero, Y_{true} is generated by the MCTS. As with the activation, function there are many different possible loss functions. In this implementation, the mean-square-error(mse) loss function is used. $mse : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ is defined as:

$$\ell(Y_{pred}, Y_{true}) = \frac{|Y_{pred} - Y_{true}|^2}{n} \tag{38}$$

The network then performs gradient descent to find parameters that minimize ℓ. Let $\ell' : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}^n$ be the derivative of ℓ'.

$$\ell'(Y_{pred}, Y_{true}) = \frac{1}{n}(Y_{pred} - Y_{true}) \tag{39}$$

Given a neural netowrk consisting of n layers, training will start at the last layer and probagate thought the network from back to front. Hence the name backpropagation. To change the values of the parameters of every layer in the network of the network, the algorythem must fist determine the in which direction and by how much, the variables should be moved. Let $j \in \mathbb{N}_{0,n-1}$ be the index of the layer. The indeces start at the first layer (0)

and count upwards. The layer at any particualer index j is f_j. For the last layer $j = n - 1$, the change to its output ΔY_j is described by (39) as follows:

$$\Delta Y_j = \langle l, \ell'(Y_{pred}, Y_{true}) \rangle_E \tag{40}$$

$$l(x) = \frac{2}{x} \tag{41}$$

Where $\langle \rangle_E$ is the elementwise vector opperator defined in equation 68 on page 33. In Generall f_j is always followed by an activation function f_{a_j}. Let A_j be the precomputed inputs to f_{a_j}. Let ΔA_j be the wisched for change to A.

$$\Delta A = f'_a(A) \Delta Y_j \tag{42}$$

Next comes the update to the weight matrix w. Let Δw describe the change to w and let X be the input vector of the layer. Δw is than defined as:

$$\Delta w = \Delta A \cdot X^T \tag{43}$$

The layer's bias vector is updated in the direction of ΔA:

$$\Delta b = \Delta A \tag{44}$$

Lastly, the change to the output of the previous layer ΔY_{j-1} is computed.

$$\Delta Y_{j-1} = \Delta A \cdot w^T \tag{45}$$

This process is repeated until the foremost layer of the neural network is reached. This layer has the index $j = 0$.

1.4.2 Network used by AlphaZero

The neural network in Alpha Zero is used to estimate the value v and policy p for any game state or node n. v is the neural network's estimation of the state's expected reward. The policy $p \in \mathbb{R}^{|\mathbb{A}|}$ of a game state n represents the advantageousness of every action $a \in \mathbb{A}$, as estimated by the neural network.

1.4.2.1 Neural Network input

The neural network input is a game state or node n represented by two 7 x 6 binary images stacked on top of each other. One image X represents the stones belonging to the current player. While the second image Y represents

the stones belonging to the other player. In both images, the pixel values are one where a stone belonging to the player they represent is located and zero if the field is empty or a stone belonging to the other player is located there. X and Y are then stacked on top of each other in the third dimension to form the input tensor $i_n = [X, Y] \in \mathbb{R}^{7\times6\times2}$. Consider the following Connect4 board (fig 5 on page 22).

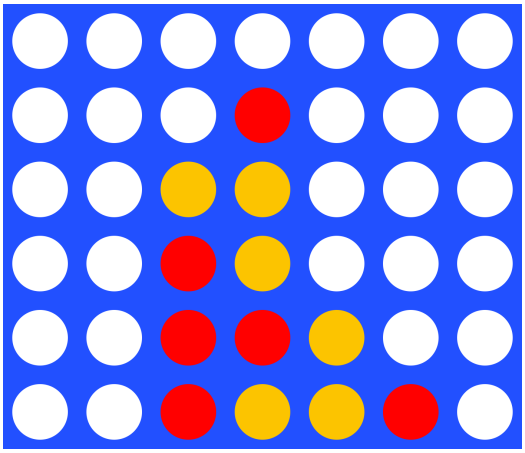


Figure 5

If red is the current player then:

$$X = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 \end{bmatrix}$$

$$Y = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 & 0 \end{bmatrix}$$

For clarification, the numbers are coloured in the same colour as the stones

at that position. After stacking X and Y, i_n is:

$$i_n = \begin{bmatrix} [0,0] & [0,0] & [0,0] & [0,0] & [0,0] & [0,0] & [0,0] \\ [0,0] & [0,0] & [0,0] & [1,0] & [0,0] & [0,0] & [0,0] \\ [0,0] & [0,0] & [0,1] & [0,1] & [0,0] & [0,0] & [0,0] \\ [0,0] & [0,0] & [1,0] & [0,1] & [0,0] & [0,0] & [0,0] \\ [0,0] & [0,0] & [1,0] & [1,0] & [0,1] & [0,0] & [0,0] \\ [0,0] & [0,0] & [1,0] & [0,1] & [0,1] & [1,0] & [0,0] \end{bmatrix}$$

1.4.2.2 Neural Network Architecture

The neural network used by Alpha Zero consists of three main sub-modules, namely the residual tower, the value head and the policy head. The residual tower's purpose is to preprocess the data for the two heads. The value head determines the value v from the output of the residual tower. While the policy head computes the policy p. The residual tower consists of a convolutional block followed by six residual blocks.
The convolutional block consists of the following:

1. A convolutional layer consisting of 75 filters with a kernel size of 3 x 3
2. Batch normalization [3]
3. A non-linear rectifier (LeakyReLU).

Every residual block consists of the following modules:

1. A convolutional layer consisting of 75 filters with a kernel size of 3 x 3
2. Batch normalization [3]
3. A non-linear rectifier (LeakyReLU)
4. A convolutional layer consisting of 75 filters with a kernel size of 3 x 3
5. Batch normalization [3]
6. Batch normalization outputs are added to the block's input.
7. A non-linear rectifier (LeakyReLU)

Outputs are then passed to the value and policy head of the network for further evaluation. The value head consists of the following modules:

1. A convolutional layer consisting of 10 filters with a kernel size of 1 x 1
2. A fully connected layer of size 210
3. A non-linear rectifier (LeakyReLU)
4. A fully connected layer of size 1
5. *tanh* activation function

The policy head consists of the following modules:

1. A convolutional layer consisting of 2 filters with a kernel size of 1 x 1
2. A fully connected layer of size 1

The output of the policy head p_{pre} is then masked with the allowed actions to form p_{masked} in such a way that p_{masked} is -1000 for all non-allowed actions. Finally, p_{masked} is passed throught the softmax function to form π:

$$\pi = \text{softmax}(p_{masked}) \tag{46}$$

1.4.2.3 Training

Training is performed in batches of 256 states. The value head is updated using mean square error. The policy head is updated using mean square error as well. However all non-legal actions are ignored. This avoids unnecessary updating of the neural network. The value, the neural network is trained to predict for a certain MCTS node n, is equivalent to 1 if the player who took an action at node n did win, -1 if that player did lose and 0 if the game ended in a tie. The policy p_{a_l} to train for, for a given legal action $a_l \in \mathbb{A}(n)$ is:

$$p_{a_l} = \frac{N(n, a_l)}{\sum_{a \in \mathbb{A}(n)} N(n, a)} \tag{47}$$

For non legal actions $a_n \in (\mathbb{A}_{possible} - \mathbb{A}(n))$, p_{a_n} is defined as:

$$p_{a_n} = p_{pre_{a_n}} \tag{48}$$

1.5 Data generation

The data used to train the neural network is generated by letting the best agent play several games against itself, until enough data has been generated to allow for training. In every game, at every game state, the MCTS performs 50 simulations. Once the simulations are done the action is chosen.

1.5.1 Action selection

There are two methods for action selection for a given node n_t: deterministic and probabilistic. The first will always return the action $a = argmax(N(\mathcal{E}(n_t, a \in \mathbb{A}(n_t))))$ of the most traversed edge, while the second will return a random action where the probability of selecting an action $a_i \in \mathbb{A}(n_t)$ is:

$$P(X = a_i, n_t) = \frac{N(\mathcal{E}(n_t, a_i))}{\sum_{j \in \mathbb{A}(n_t)} N(\mathcal{E}(n_t, j))} \tag{49}$$

($\mathbb{A}(s)$ are the allowed actions for state s.) Action selection during the training phase shall initially be probabilistic, and deterministic later on. The handover point shall be defined as the configurational constant 'probabilistic_moves' $\in \mathbb{N}^+$. During games outside the training loop, actions are always selected deterministically.

1.5.2 Memory

The memory stores a certain amount of memory elements. A memory element consists of a gamestate $g \in \mathbb{G}$, its action values $v \in \mathbb{R}^{|\mathbb{A}|}$ and the true reward $r \in \{1, -1, 0\} = R(g, a)$ where a is the action taken during play at that game state. The memory stores memory elements in a long list. After an action has been selected, but before any updates to the game simulation are made, the current game state is passed to temporary memory along with its action values v. Together they create a new memory element. This element's r is currently undefined. v is defined as:

$$v_a = \begin{cases} P(X = a, \mathcal{N}(g)) & a \in \mathbb{A}(g) \\ p_{pre_a} \end{cases} \tag{50}$$

$\mathbb{A}(g)$ is the set of all legal actions. p_{pre} is defined in section **??** on page **??**, and is used for all non legal actions. P is defined in equation 49 on page 25.

1.5.2.1 Memory update

Once the game is over, the winning player is determined and the value r of every memory element in the temporary memory is updated. r is 1 if the player taking an action at that state won, -1 if he lost and 0 if the game ended in a draw. The updated states are then passed to memory.

1.5.2.2 Model Training

Once the memory size exceeds 30'000 states, the self-playing stops and the neural network is trained as described in section: 1.4.2.3.

1.6 Model evaluation

In order to train the neural network, the "best player" generates data used to train the current network. After every time the current neural network has been updated, it plays 20 games against the best player. If it wins more than 1.3 times as often as the current best player, it is considered better. If this is the case, the neural network of the "current player" is saved to file and the old "best player" is replaced with the "current player" to become the new "best player". It is advantageous to force the network to win 1.3 times as often as that reduces the chance of the network just getting lucky.

2 Evaluation

To give us an idea of how good a player is, it would be useful to express performance using a single number. This number should not only give us a ranking but also allow for predictions of the winner of a game between two players and thus give us a measure of the relative strength of the players. One such rating method is the so called elo-rating method. [2]

2.1 Elo-rating

The elo-rating system assigns every player p a number $r_p \in \mathbb{R}$. In general, the larger r_p the better the player. More specifically, given two players a and b with elo-ratings r_a and r_b, the expected chance E of a winning against b is

[4]:

$$E = \frac{1}{1 + e^{(r_b - r_a)/400}} \tag{51}$$

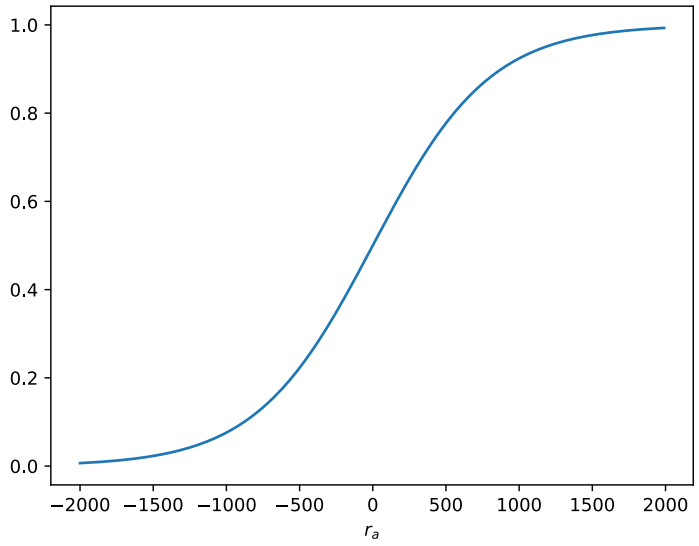


Figure 6: elo-rating win probability for $r_b = 0$

This function describes a sigmoid curve. This makes sense, because if the players have major strength discrepancies E converges to 1 or 0. When a and b play a game against each other, their elo,ratings are updated as follows[2]:

$$r_{n+1} = r_n + K(W - E) \tag{52}$$

with:

r_{n+1} the new rating for the player.

r_n the current rating of the player.

$W = s_a$ which is defined by equation 53 where a is the player to be updated.

E the expected chance of winning, see equation 51.

K is a constant controlling the sensitivity of the update function.

However, to avoid slow convergence of elo-ratings, a more direct formula is used to approximate the rating of an agent a. This is done by playing a predetermined amount of games against player b whose elo-rating r_b is known and unchanged throughout this process. First, a and b play a predetermined amount of games m and the score s_a of a is computed as [2]:

$$s_a = \frac{1}{m} \sum \begin{cases} 1 & a \text{ wins} \\ \frac{1}{2} & \text{tie} \\ 0 & a \text{ looses} \end{cases} \tag{53}$$

Assuming that this is the probability of a winning against b, a's elo-rating can be computed by solving equation 51 to r_a (fig 7 on page 28):

$$r_a = r_b - ln\left(\frac{1 - s_a}{s_a}\right) \cdot 400 \tag{54}$$

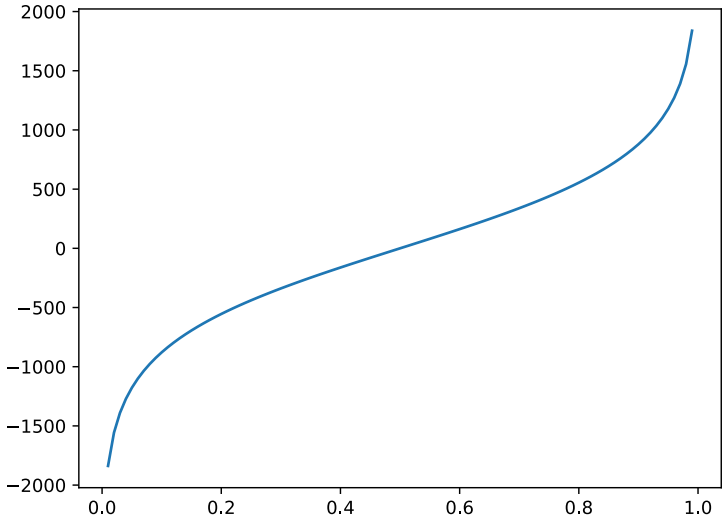


Figure 7: elo inverse function

Since a ranking of all the agents already exists (see section 1.6 on page 26), an agent's elo-rating can be computed by playing against an older version and then using equation 54 to determine its elo-rating.

2.1.1 Relativity of the Elo-rating

The only problem is that elo is a relative rating. The rating of any other agent depends on its performance against other agents and their elo-ratings. Therefore, one must give the system a base rating for at least one predefined agent. In this case, there are no previously known elo-rated agents , so I defined the untrained agent's elo-rating as 100. All other elo-ratings are relative to that.

2.2 Elo results

The rating r_i of any agent version i must in general be greater than the rating of the last version $r_i > r_{i-1}$. Furthermore, the expected minimal increase in rating $\Delta r_{min} = r_i - r_{i-1}$ is:

$$\Delta r_{min} = -ln\left(\frac{1-s_i}{s_i}\right) \cdot 400 \tag{55}$$

As a certain scoring threshold $\theta = 1.3$ was used during training to minimize the effect of noise in the evaluation, a prediction of s_i can be made. Given that s_a and s_b are the scores of two players that play aginst each other, then by definition:

$$s_a + s_b = 1 \tag{56}$$

Due to the imposed scoring threshold θ and the assumption that there are no ties:

$$s_a \geqslant s_b \cdot \theta \tag{57}$$

(if s_a has a higher version number than s_b)

For $\theta = 1.3$ this means that the expected average change in rating Δr:

$$\Delta r \geqslant -ln\left(\frac{1}{\theta}\right) \cdot 400 = \Delta r_{min} \cong 105 \tag{58}$$

Collected data shows this to be true (fig 8 on page 30). The same data shows that the average Δr is in fact roughly 408, which would equate to a θ of

$$\theta = \frac{1}{e^{\frac{-\Delta E}{400}}} \cong 2.8 \tag{59}$$

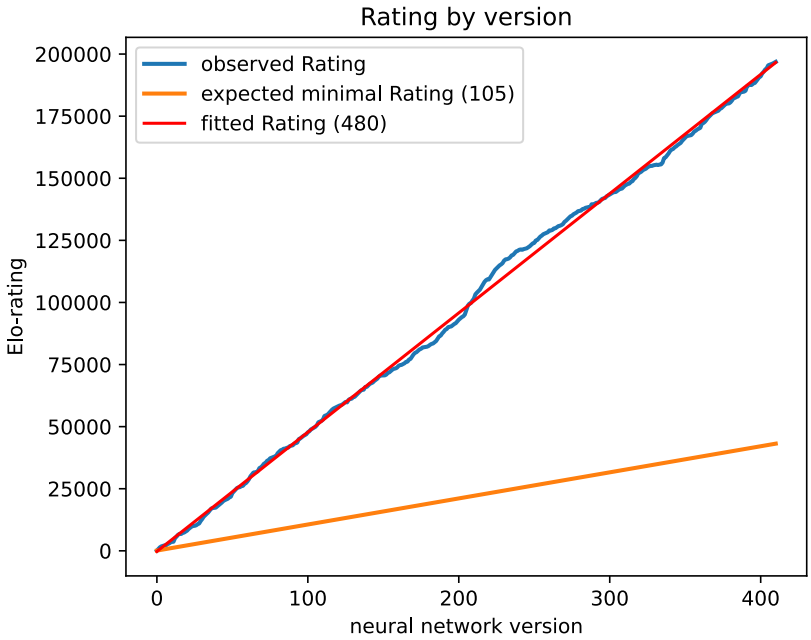


Figure 8: Elo-rating of agents based on their version along with the expected minimal rating Δr_{min} and the best fitted rating Δr.

3 Further definitions

3.1 Set Exclusion

Let $\mathbb{A} - \mathbb{B}$ be the set exclusion of $\mathbb{A}$ and $\mathbb{B}$.

$$\mathbb{A} - \mathbb{B} = \mathbb{A} \setminus \mathbb{B} = \{x : x \in \mathbb{A} \text{ and } x \notin \mathbb{B}\} \tag{60}$$

3.2 Hadamard product

Let A and B be 2 $m \times n$ matrices. For all $i \in [1, m]$ and $j \in [1, n]$ the hadamard product $A \circ B$ is defined as:

$$(A \circ B)_{ij} = A_{ij} \cdot B_{ij} \tag{61}$$

For example consider the following 2×3 matrices:

$$\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \\ a_{31} & b_{32} \end{bmatrix} \circ \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \\ b_{31} & b_{32} \end{bmatrix} = \begin{bmatrix} a_{11}b_{11} & a_{12}b_{12} \\ a_{21}b_{21} & a_{22}b_{22} \\ a_{31}b_{31} & a_{32}b_{32} \end{bmatrix}$$

3.3 Inner Product

3.3.1 Matrices

Let $A \in \mathbb{R}^{m \times n}$ and $B \in \mathbb{R}^{m \times n}$ be two $n \times m$ matrices.
Let their Inner Product $\langle A, B \rangle_I : \mathbb{R}^{m \times n}, \mathbb{R}^{m \times n} \to \mathbb{R}$ be defined as:

$$\langle A, B \rangle_I = \sum_{i=1}^{m} \sum_{j=1}^{n} A_{ij} B_{ij} = \sum_{i=1}^{m} \sum_{j=1}^{n} (A \circ B)_{ij} \tag{62}$$

For example consider the following 2×3 matrices:

$$\left\langle \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \\ a_{31} & b_{32} \end{bmatrix}, \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \\ b_{31} & b_{32} \end{bmatrix} \right\rangle_I = \begin{array}{l} a_{11}b_{11} + a_{12}b_{12} + a_{21}b_{21} \\ + a_{22}b_{22} + a_{31}b_{31} + a_{32}b_{32} \end{array}$$

3.3.2 n-dimensional Tensors

Let $A \in \mathbb{R}^{m \times \dots}$ and $B \in \mathbb{R}^{m \times \dots}$ be two n dimensional $m \times \dots$ tensors with $n > 2$
Let the Inner product $\langle A, B \rangle_I : \mathbb{R}^{m \times \dots}, \mathbb{R}^{m \times \dots} \to \mathbb{R}$ be defined as:

$$\langle A, B \rangle_I = \sum_{i=0}^{m} \langle A_i, B_i \rangle_I \tag{63}$$

3.4 Submatrix

Let $m = m_{ijk}$ be an $m \times n \times o$ dimensional tensor.
Let $<>_{S\, x \times y,\, ab}$ be the matrix slicing opperator. $x \times y$ is the size of the submatrix the operation should output. ab is the top left position of the submatrix within the outer matrix. For the operation to be defined, the

following must be true: $x \in [0, m[$, $y \in [0, n[$, $a \in [1, m-x]$ and $b \in [1, n-y]$. The submatrix $< m >_{S\, x \times y,\, ab}$ is defined as:

$$< m >_{S\, x \times y,\, ab} = \begin{bmatrix} [m_{ab1}, \ldots, m_{abo}] & \ldots & [m_{(a+x)b1}, \ldots, m_{(a+x)bo}] \\ \vdots & \ddots & \vdots \\ [m_{a(b+y)1}, \ldots, m_{abo}] & \ldots & [m_{(a+x)b1}, \ldots, m_{(a+x)(b+y)o}] \end{bmatrix} \tag{64}$$

3.5 Vectorization

The vectorization of an $m \times n$ matrix A, denoted $\text{vec}(A)$, is the $mn \times 1$ column vector obtained by stacking the columns of the matrix A on top of one another:

$$\text{vec}(A) = [A_{11} \ \ldots \ A_{1m}\, A_{21} \ \ldots \ A2m \ \ldots \ A_{n1} \ \ldots \ Anm]^T \tag{65}$$

Taken verbatim from:[7]

For example, the 3×2 matrix $A = \begin{bmatrix} a & b & c \\ d & e & f \end{bmatrix}$ vectorizes to

$$\text{vec}(A) = \begin{pmatrix} a \\ b \\ c \\ d \\ e \\ f \end{pmatrix}$$

3.5.1 Tensors

Let $T \in \mathbb{R}^{n \times \cdots}$ be a n-dimensional Tensor. Let $vec(T)$ be defined as:

$$vec(T) = T_0 \frown T_1 \frown \cdots \frown T_n \tag{66}$$

Where $\frown$ is defined defined in section 3.6 on page 32. For those who are familiar with python's numpy library, vec is equivilent to numpy.flatten.

3.6 Vector Concatination

Vector Concatination of two vectors v and u of dimensions n_v and n_u, denoted $v \frown u$, is the $n_v + n_u$ dimensional vector obtained by placing both vectors

one on top of the other.

$$v \frown u = \begin{pmatrix} v_1 \\ \vdots \\ v_{n_v} \\ u_1 \\ \vdots \\ u_{n_u} \end{pmatrix} \tag{67}$$

3.7 Elementwise vector operations

Let $v \in \mathbb{R}^n$ be a n dimensional vector. The Elementwise vector opperator $\langle s, v \rangle_{E_s}$ of some statement s is defined as:

$$\langle s, v \rangle_D = \begin{pmatrix} s(v_1) \\ s(v_2) \\ \vdots \\ s(v_n) \end{pmatrix} \tag{68}$$

For example let $v = [1, 4, 2]^T$, than $\langle v \rangle_T = [1, 0.25, 0.5]^T$.

3.8 Sets

Let

$$\mathbb{R}_{a,b} = \{x \in \mathbb{R} \ : \ a \leq x \leq b\} \tag{69}$$
$$\mathbb{N}_{a,b} = \{x \in \mathbb{N} \ : \ a \leq x \leq b\} \tag{70}$$

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4 Examples

4.1 Mcts

The full set of data as seen by the computer in the mcts example (fig 1 on page 11). The node sets are as follows defined by the amount of edged leaving each node.

$$\mathbb{M} = \{n_1, n_2, n_3, n_4, n_5, n_6, n_7, n_8\} \tag{71}$$
$$\mathbb{M}_{leaf} = \{n_3, n_5, n_6, n_7, n_8\} \tag{72}$$
$$\mathbb{M}_{expanded} = \{n_1, n_2, n_4\} \tag{73}$$

The edge sets for every node are as follows.

$$\mathbb{E}(n_1) = \{e_1, e_2, e_3\} \tag{74}$$
$$\mathbb{E}(n_2) = \{e_4, e_5\} \tag{75}$$
$$\mathbb{E}(n_3) = \emptyset \tag{76}$$
$$\mathbb{E}(n_4) = \{e_6, e_7, e_8\} \tag{77}$$
$$\mathbb{E}(n_5) = \emptyset \tag{78}$$
$$\mathbb{E}(n_6) = \emptyset \tag{79}$$
$$\mathbb{E}(n_7) = \emptyset \tag{80}$$
$$\mathbb{E}(n_8) = \emptyset \tag{81}$$

The edge by action and node function $\mathcal{E}$ looks af follows:

$$\mathcal{E}(n_1, A_1) = e_1 \tag{82}$$
$$\mathcal{E}(n_1, A_2) = e_2 \tag{83}$$
$$\mathcal{E}(n_1, A_3) = e_3 \tag{84}$$
$$\mathcal{E}(n_2, A_4) = e_4 \tag{85}$$
$$\mathcal{E}(n_2, A_5) = e_5 \tag{86}$$
$$\mathcal{E}(n_4, A_6) = e_6 \tag{87}$$
$$\mathcal{E}(n_4, A_7) = e_7 \tag{88}$$
$$\mathcal{E}(n_4, A_8) = e_8 \tag{89}$$

The node an edge points from function $\mathcal{N}_{from}$ looks af follows:

$$\mathcal{N}_{from}(e_1) = n_1 \tag{90}$$
$$\mathcal{N}_{from}(e_2) = n_1 \tag{91}$$
$$\mathcal{N}_{from}(e_3) = n_1 \tag{92}$$
$$\mathcal{N}_{from}(e_4) = n_2 \tag{93}$$
$$\mathcal{N}_{from}(e_5) = n_2 \tag{94}$$
$$\mathcal{N}_{from}(e_6) = n_4 \tag{95}$$
$$\mathcal{N}_{from}(e_7) = n_4 \tag{96}$$
$$\mathcal{N}_{from}(e_8) = n_4 \tag{97}$$

The node an edge points to function $\mathcal{N}_{to}$ looks af follows:

$$\mathcal{N}_{to}(e_1) = n_3 \tag{98}$$
$$\mathcal{N}_{to}(e_2) = n_2 \tag{99}$$
$$\mathcal{N}_{to}(e_3) = n_4 \tag{100}$$
$$\mathcal{N}_{to}(e_4) = n_5 \tag{101}$$
$$\mathcal{N}_{to}(e_5) = n_6 \tag{102}$$
$$\mathcal{N}_{to}(e_6) = n_6 \tag{103}$$
$$\mathcal{N}_{to}(e_7) = n_7 \tag{104}$$
$$\mathcal{N}_{to}(e_8) = n_8 \tag{105}$$

5 Proofs

5.1 tanh derivative

$tanh : \mathbb{R} \to \mathbb{R}$ is defined as:

$$tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}} \tag{106}$$

$$\begin{aligned}\frac{d}{dx}\left[\frac{e^x - e^{-x}}{e^x + e^{-x}}\right] &= \frac{(e^x + e^{-x})\frac{d}{dx}\left[e^x - e^{-x}\right] - (e^x - e^{-x})\frac{d}{dx}\left[e^x + e^{-x}\right]}{(e^x + e^{-x})^2} \\ &= \frac{(e^x + e^{-x})^2 - (e^x - e^{-x})^2}{(e^x + e^{-x})^2} \\ &= \frac{e^{2x} + 2e^x e^{-x} + e^{-2x} - e^{2x} + 2e^x e^{-x} - e^{-x}}{(e^x + e^{-2x})^2} \\ &= \frac{4}{(e^x + e^{-x})^2}\end{aligned} \tag{107}$$

because

$$sech(x) := \frac{2}{e^x + e^{-x}} \tag{108}$$

using (107) and (108) we can see, that

$$\frac{d}{dx}\left[tanh(x)\right] = sech(x)^2 \tag{109}$$

5.2 Softmax Derivative

The Softmax $s : \mathbb{R}^n \to \mathbb{R}^n$, $n \in \mathbb{N}$, is defined as

$$s(v)_i := \frac{e^{v_i}}{\sum_{j \in v} e^j} \tag{110}$$

for all $i \in [1, n]$. Due to the multidimensional natur of this function we are taking the derivative $\frac{d}{dv_j} s(v)_i$, with $i \in [1, n]$ and $j \in [1, n]$.

case $i \neq j$

$$\begin{aligned}\frac{d}{dv_j}\left[\frac{e^{v_i}}{\sum_{a \in v} e^a}\right] &= -\frac{\frac{d}{dx}\left[\sum_{a \in v} e^a\right] e^{v_i}}{(\sum_{a \in v} e^a)^2} \\ &= -\frac{e^{v_j} e^{v_i}}{(\sum_{a \in v} e^a)^2} \\ &= -s(v)_j s(v)_i\end{aligned} \tag{111}$$

case $i = j$

$$\begin{aligned}
\frac{d}{dv_j}\left[\frac{e^{v_i}}{\sum_{a\in v} e^a}\right] &= \frac{\frac{d}{dx}\left[e^{v_i}\right]\sum_{a\in v} e^a - e^{v_i}\frac{d}{dx}\left[\sum_{a\in v} e^a\right]}{(\sum_{a\in v} e^a)^2} \\
&= \frac{e^{v_i}\sum_{a\in v} e^a - e^{v_i}e^{v_j}}{(\sum_{a\in v} e^a)^2} \\
&= s(v)_i - s(v)_i s(v)_j \\
&= s(v)_i(1 - s(v)_j)
\end{aligned} \tag{112}$$

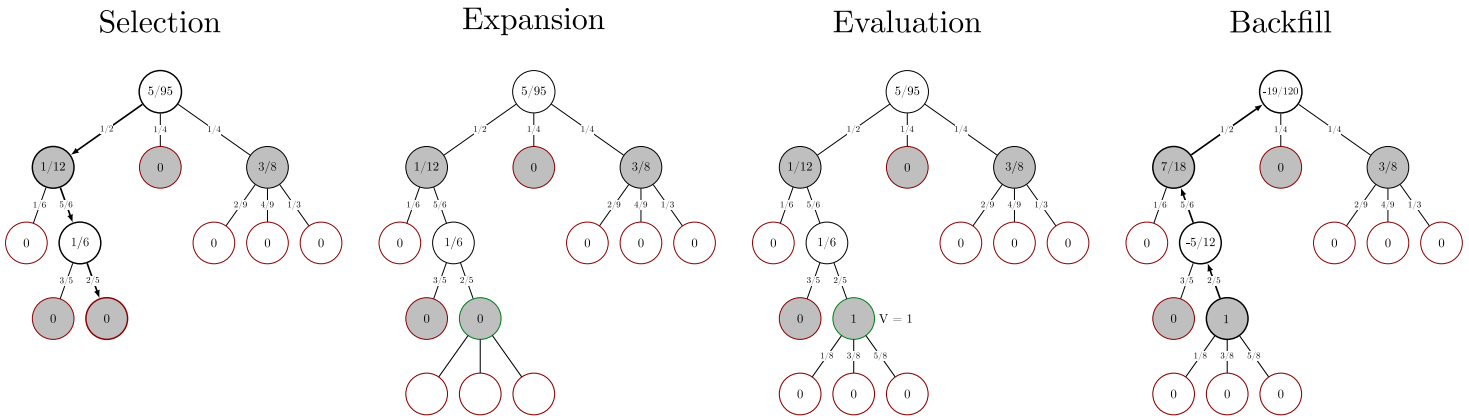

Figure 9: MCTS simulation steps. In this diagram, the numbers in the node represent Q and the number on the arrow is P. The red nodes are leaf nodes and the green one is the leaf node n_L. During the **selection** phase, σ is used to find successive nodes until the node n_L is reached. This is shown with the arrows. During the **expansion** phase, new nodes and edges are added for all possible legal actions at the node n_L. The **evaluation** phase gives the new nodes the following values $Q = 0$ and $P = \pi_a$. The value of the leaf v is then used during the **backfill** phase to update the Q's of all nodes traversed during selection.

Source: modified from https://en.wikipedia.org/wiki/File:MCTS-steps.svg
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