

Strategic Evaluation of Deep Neural Networks in Board Games

by

Sigurður Helgason

Thesis of 60 ECTS credits submitted to the School of Computer Science at Reykjavík University in partial fulfillment of the requirements for the degree of Master of Science (M.Sc.) in Computer Science

January 2021

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Abstract

Deep neural networks have exceeded expectations in many areas where they can generate accurate predictions of the real world. This is going to be a powerful tool for the future, and we require a method of examining them to understand why and how they come to a specific prediction to alleviate trust issues. This paper examines which strategies a deep neural network that plays the game Breakthrough uses to reach its predictions. We explain the process of creating a neural network that can achieve success in playing board games only from playing against itself, without any human input. We outline the process of creating a model to examine the internal representation of the neural network of the game state to evaluate whether it both recognizes and uses strategies applied by humans that play the game. These strategies are compared against each other to infer which is best, and which the neural network uses the most. We show that the neural network emphasizes strategies that are considered the most successful handcrafted strategies for the game Breakthrough.

Herkænsku mat á djúptauganetum í leikjum

Sigurður Helgason

janúar 2021

Útdráttur

Djúptauganet hafa farið fram úr væntingum á mörgum sviðum, þau geta framkallað öflugar og nákvæmar spár um raunvöruleikann. Þetta mun verða öflugt tól í framtíðinni og við munum þurfa aðferðir til að geta rýnt í þessar spár til að styrkja traust okkar á þeim. Þessi ritgerð skoðar hvaða herkænsku aðferðir djúptauganet sem spilar leikinn Breakthrough nýtir sér til að taka ákvarðanir. Við útskýrum ferlið að smíða tauganet sem getur náð árangri í borðspilum með því einungis að spila gegn sjálfu sér, án inngrips frá mönnum. Við útskýrum ferlið að búa til líkan til að skoða innri framsetningu tauganets á leikstöðu til að meta hvort tauganetið þekki eða nýtir sér aðferðir sem menn hafa notað til að spila leikinn vel. Þessar aðferðir eru bornar saman til að álykta hver sé best og hver tauganetið notar mest. Við sýnum að tauganetið leggur áherslu á aðferðir sem eru taldar bestar fyrir leikinn Breakthrough. Að lokum skoðum við þjálfað tauganet með hóp af auðveldum sem og flóknum aðferðum til að rýna í hver herkænsku aðferð er mest notuð af tauganetinu.

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date		
Sigurður Helgason		
Master of Science		



I dedicate this thesis to my family, who while not understanding most of what I do, always support me and the friends that still want to talk to me even though my schedule has rendered me unmeetupwithable. Lastly, my girlfriend Hulda, who always helps me get through the tough times, and makes the good times even better.



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List of Abbreviations

MSc Masters of Science
ML Machine Learning
AI Artificial Intelligence
ANN Artificial Neural Network
DNN Deep Neural Network
MCTS Monte-Carlo Tree Search
CAV Concept Activation Vector

DL Deep Learning

MI Model Interpretability
ME Model Explainability



Chapter 1

Introduction

The world of deep learning (DL) is exciting. We have models that can examine images and reliably identify their content[1]. Deep learning models have outperformed ophthalmologists in identifying diabetic retinopathy[2] and identified cancer cells where others have not[3]. Deep learning models are used for the bleeding edge of protein folding, to gain further understanding of the underlying structure of organisms, such as viruses[4]. These models have done these things accurately, cheaply, and fast.

DL in conjunction with a randomized state-space search algorithm, Monte-Carlo Tree Search, was used to defeat the standing world champion Lee Sedol in the incredibly expansive game of Go, using a DL architecture called AlphaGo[5]. This was done using supervised learning on expert human knowledge, as well as a form of reinforement learning (RL) method called self-play where the agent learns from playing against itself. Later, this research was iterated on to create AlphaGo Zero[6], where no human knowledge was used to learn the game only self-play. AlphaGo Zero beat AlphaGo 100 to 0. Iterating on AlphaGo Zero, AlphaZero[7] was created, that approach is generalized to handle a diverse set of board games, namely: Chess, Shogi, and Go. AlphaZero will be the architecture we will use during this thesis. The results from these approaches imply that given enough time to learn a computer agent can gain a deep insight into how a game should be played.

The field of examining deep learning models to gain a richer understanding of how they work, and what makes them so much better than humans at various tasks, is still new. This is the field of Explainable Artificial Intelligence (XAI). If we wish to continue using artificial intelligence (AI) and machine learning (ML) to improve our lives, we must examine how they work. Not only to improve the models themselves but also to augment our ability, for example, if we have a superhuman chess agent but we understand exactly why and how that agent makes it decisions. We could use that superhuman agent to further our understanding of the game. Furthermore, these explanations are a legal requirement now in many areas[8], namely, legal and medical. Recently, XAI has been focused on Model Interpretability (MI), in particular, interpreting the model in such a way that we can predict what the model will do given a particular input [9]. Another class of XAI is Model Explainability (ME), where we attempt to explain how the internal mechanics of the model works. A simple example of ME would be when we explore a decision tree generated by an ML algorithm. The decision tree nodes and conditions explain exactly what the tree will do with a given input. This differs from MI where we would have to predict the results, without going into details as to why.

In this thesis, we outline a process of how we can examine an artificial neural network (ANN) to understand which higher-level concepts (HLC) it deems important for a given state within a game. Such a game can be simple like Tic-Tac-Toe or Breakthrough and complicated like Chess or Go.

The method of examining HLC's within games has generally been done by examining the current state of the game by evaluating them using some heuristic. A heuristic within games are evaluations of the expected end reward for a state, for example, the number and type of pieces left within a game of chess, we would call this material advantage. Intuitively, the material advantage is a higher-level concept we can use to evaluate a chess position. Of course there are many other relevant concepts to consider, for example whether the king is safe from attack, and the pawn structure. This thesis examines the evaluation of a neural network of a given state with respect to four different higher-level concepts namely, *Material Advantage*, *Aggressiveness*, *Unity*, and *Lorentz-Horey*. More precisely, we define the following research questions:

- 1. Given a NN that plays Breakthrough, can we determine if that NN has learned the HLCs that human players use.
- 2. Does a NN that trains itself using self-play learn some HLCs over time, and does it start to emphasize the HLCs that are generally considered better the more it trains, and conversely, does it start to demphasize HLCs that are considered worse.

Summary

In this thesis, we take an example game of Breakthrough, we train a neural network to play the game using only self-play. That is, the neural network is trained only by playing against itself with no external input other than the rules of the game itself. And we examine the neural networks against popular higher-level concepts (heuristics) that we use to play the game.

Chapter 2

Background

In this chapter, we discuss traditional artificial intelligence in the context of search, and explain the algorithms we used. Additionally, we discuss similar methods for searching state-spaces. We allocate a large portion of the section to Breakthrough as that will be our testbed. We discuss the different classes of machine learning as well as neural networks.

2.1 Environments

When researching artificial intelligence it is important to select an environment that is a suitable abstraction for the task at hand. Environments vary significantly and can be identified by their characteristics. The characteristics that are commonly used to describe environments can be seen in Table 2.1[10].

Table 2.1: Characteristics of environments

characteristic	Values	Description
Observable	Fully, Partially	How much of the environment can
		your agent percieve.
Agents	Single, Multi	Are there multiple agents playing
		in the environment.
Deterministic	Deterministic, Stochastic	Do the actions your agents ex-
		ecute deterministicly impact the
		environment.
Episodic	Sequential, Episodic	Can the actions be divided into
		atomic episodes or are future ac-
		tions sequentially affected by pre-
		vious actions.
Static	Static, Semi-Static, Dynamic	Does the environment change
		without agent input, or does it
		wait until agents take actions.
Discrete	Discrete, Continuous	Is your environment discrete w.r.t
		actions.

Categorizing environments using Table 2.1 gives one the power to find an environment in which a method works and know it can be applied to different environments

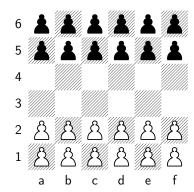


Figure 2.1: Initial 6×6 Breakthrough board

with the same characteristics. Additionally, it allows us to talk about agents in the context of environments as the entities that act within the environment.

2.2 Game Environment

Classical artificial intelligence game environments are commonly used to validate a method, e.g game environments can be games like Tic-Tac-Toe or Breakthrough, or simulation environments like driving simulators. Game environments are a suitable place to apply AI as they serve as an abstraction of the real world, for instance, a self-driving car agent who is verified to avoid driving into walls in a simulation is possibly safer than one who is not.

2.3 Breakthrough

The board game Breakthrough can be thought of as a simplified version of chess; the game is set up on a $M \times N$ board, M wide and N high, with squares similar to chess, and each player starts with two rows of pawns at opposite ends. The objective of the game is for a player to move one of their pawns to the opposite end of the board. A player wins if either they have reached the opposite end of the board or have captured all of their opponents' pawns. The pawns differ from chess pawns in such a way that they can not move two squares on the first move and they can both move and capture diagonally. This leads to the game being impossible to draw as pieces are always able to move or capture. An example of an initial board in Breakthrough can be seen in Figure 2.1.

Categorizing Breakthrough with the characteristics described in Section 2.1 we end up with the description shown in Table 2.2. These characteristics are identical to that of Tic-Tac-Toe, and chess. This categorization is the most common in board games where two players compete.

Some sizes of breakthrough boards have been solved, that is we know if both players play optimally we know who will be victorious. The solved boards are: 6×5 , 5×5 , and $3 \times 7[11]$. The size of board that is used in this thesis is 6×6 .

Characteristic	Value
Observable	Fully
Agents	Multi
Deterministic	Deterministic
Episodic	Sequential
Static	Static
Discrete	Discrete

Table 2.2: Categorization of Breakthrough

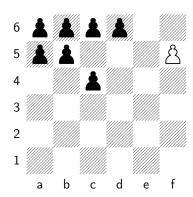


Figure 2.2: Breakthrough board where Material Advantage does not work well

2.3.1 Heuristics of Breakthrough

To evaluate the game of Breakthrough we may consider many heuristics (higher-level concepts), for instance a very simple heuristic would be a player's material advantage. *Material Advantage* is the amount of pieces the player has minus the amount of pieces the opponent has. This heuristics gives us some insight into how well the game is progressing, however, there are cases where this does not tell us much, for example when your opponent has a single piece left that is on the row immediately before the row needed for them to win. No matter how many pieces you have left, this state is bad for you if you're not able to capture that piece. An example of such a state can be seen in Figure 2.2.

A different heuristic would be the distance of your most advanced pawn minus your opponent's most advanced pawn; this could give you insight into how close you are to winning the game or how close your opponent is. As a higher-level concept, we can call this concept your aggressiveness, as it closely resembles how aggressive you are going for the win. Generally, in Breakthrough, it is favorable to move your whole team as a unit and play more defensively[12]. More advanced heuristics for Breakthrough will be discussed in detail later in a later chapter.

2.4 State-Space Search

Traditionally, methods for playing games search through the environment using a heuristic to guide the search. A simple way of doing a heuristic-based search would be to give all non-terminal states a 0 score and terminal states positive or negative scores based on whether it is a positive or negative result respectively. We say that such

a search algorithm is not guided, and the algorithm will probably have to evaluate a large portion of the state-space. This method of searching is generally extremely inefficient as the state-spaces of game environments are often extremely large, even infinite. For instance, an upper-bound estimate of the state-space for Breakthrough is $3^{(M-1)\times(N-1)}+2N$ where M is the height of the board N is the width of the board. The $3^{(M-1)\times(N-1)}$ represents each position of the board having either a white, or black piece, or being empty. And, the 2N component represents each square the final piece to move could have moved to. So for a small board, 5×4 the upper-bound estimation of the state-space is 531,449 states.

This is why a good heuristic is needed because we can identify paths in the game tree that will lead to a bad outcome early, allowing us to disregard a significant amount of states, reducing the time required to search.

The algorithms that are used in traditional state-space search are for instance Depth-first search (DFS), Breadth-first Search (BFS), Alpha-Beta Search (AB-Search)[13], and Monte-Carlo Tree Search (MCTS).

More modernly, these search methods have been augmented by Machine Learning, in such a way that we do not need to figure out a good heuristic for a given state, but rather, we apply a machine learning model to learn a function that takes in a state and returns an evaluation of that state[14]. This can lead to a significant time reduction as we do not need to simulate a whole game from a state to receive its evaluation but rather receive the evaluation from the model.

2.4.1 Monte-Carlo Tree Search

Monte-Carlo Tree Search (MCTS), described by R. Coulom[15], is a state space search algorith where we attempt to find the most advantageous action we can take that leads us towards a goal state we want, this goal state in Breakthrough would be be winning the game. While doing MCTS we construct a tree called a search tree. This search tree has nodes and edges, where the nodes represent a state s in the environment. Additionally, each node maintains two values Q and N, where Q is the average return from that state. In a game of Breakthrough this would be the expected end result from being in that state. The N value represents the amount of times this node has been visited during MCTS. The edges in the search tree represent the actions we can take from the the state s in the node. MCTS has four phases: Selection, Expansion, Rollout, and Backpropagation. These states happen sequentially and repeatedly. To apply MCTS we begin by initializing our search tree with a single node n_0 the starting state of our game.

We describe the MCTS algorithm's four phases: Selection, Expansion, Rollout, Backpropagation, in more detail below.

Selection

During the selection phase, an unexpanded node n within the tree is found, an unexpanded node is a node which has not been selected before. This process uses Upper Confidence Bound on Trees (UCT)[16] to find that node n, the formula is described in Equation 2.1. For a parent node n_{parent} (initially the root of the tree) we select a child node n_{child} with the highest UCT value repeatedly until an unexpanded node is found. In the formula c_{uct} is a constant to adjust the amount of exploration. The process of UCT is done to balance the amount of exploration vs exploitation of nodes

in the tree, where exploration referrs to the idea of exploring paths you are unsure of the true value for, and exploitation referrs to continuing exploring paths you already know are valuable.

$$UCT(n_{child}) = Q_{n_{child}} + c_{uct} \cdot \frac{\sqrt{log(N_{n_{parent}})}}{N_{n_{child}}}$$
 (2.1)

Expansion

During the expansion phase the node n which was selected during the selection phase is expanded. This generates all child nodes n' from n by applying the actions a available in the state s maintained by the node n.

Rollout

Next during rollout, we consider the state s of the node n and take a random action from there to get to state s'. This process is repeated until some terminal state is found. There the reward for that terminal state is recorded, in Breakthrough this would be 1 if white wins, or -1 if black wins. Environments need not be a binary outcome but for the purposes of this thesis we use only binary outcomes.

Backpropagation

The result from the terminal node found in rollout is then propagated up through the path that was taken during selection, updating the Q and N values along the path. As we do more and more repetitions of these four phases the Q values at the root node of the tree becomes more and more accurate towards the true value of the node. If MCTS is applied infinitely at a node the nodes Q value will represent the true value of the node, e.g. for Breakthrough, if we know that white is going to win from that node the true value of the node is 1. Secondly, the child node Q values will represent the best moves to take from the parent node, so they would represent an optimal policy vector.

2.4.2 Neural Network based UCT

When training a neural network the UCT formula is modified slightly to prefer selecting nodes that the neural network values highly by introducing a second scalar to the formula f(s) = (p, v), where f is the neural network, p is the policy vector returned by the neural network and v is the predicted value from the neural network. The resulting formula is described in Equation 2.2, and is a variant of PUCT[17]. Importantly, the p(a) factor is the probability of selecting the action a that leads to the node n_{child} in the policy vector p returned by the neural network. This approach was proven successful in [7]. Additionally, the rollout process is modified to instead of doing simulating the game by applying random actions to receive a reward, we rather use the predicted value v from the neural network and backpropagate that.

$$PUCT(n_{child}) = Q_{n_{child}} + c_{uct} \cdot p(a) \cdot \frac{\sqrt{\sum_{children=c} N_c}}{1 + N_{n_{parent}}}$$
(2.2)

2.5 Machine Learning

Machine Learning (ML) is a research field in which machines apply statistical functions on data to achieve a correct output, where by *correct* we mean the corresponding result that we expect. Generally, this a repetitive process where we look at examples of the data, and the algorithm progressively gets closer to the underlying function of the data it is fed. This process is therefore similar to trial and error for humans. ML is a sub-field of Artificial Intelligence.

We can categorize machine learning into three different sub-categories: Supervised Learning, Reinforcement Learning, and Unsupervised Learning.

2.5.1 Supervised Learning

In Supervised Learning, the ML algorithms attempt to build a model from a data set of labelled examples. The labelled examples are a set of input values and their corresponding output value. The ML algorithm then uses this data set to construct a model that is as accurate as possible at outputting the correct output value given the input value. In supervised learning many techniques are applied to maintain the generality of the model s.t. it does not just represent the data set it is given but also has high accuracy on a possible future data set it has not yet encountered.

Some examples of algorithms that are popular for Supervised learning would be, Decision Trees, Support Vector Machines, or Naive Bayes.

2.5.2 Reinforcement Learning

Reinforcement Learning focuses on the idea of trial and error for an ML algorithm, where the algorithm directly interacts with the environment it operates in, and from operating in the environment it is provided with either positive or negative feedback for its actions. Typically, the environment needs to be modeled as a Markov Decision Process. That is, the selection of actions in a state requires only the knowledge of being in that state, not the actions it took to get to that state.

Many algorithms are popular in reinforcement learning, for instance Q-learning[18], and TD-Lambda[19].

2.5.3 Unsupervised Learning

In Unsupervised Learning, the machine learning algorithms attempt to build a model from a data set of values that do not have a corresponding output value. These algorithms then generally attempt to find pattern within the data set, to which we could then later label upon examination of the patterns. Importantly, in Unsupervised Learning, all columns of values in the data set should be normalized to the same range, and should be standardized s.t. the mean of the values is 0 and it's standard deviation is 1. This is done in order for one value not to dominate the patterns in the data set.

Common algorithms in Unsupervised Learning are, K-Nearest Neighbours (KNN), K-Means[20], and DBScan[21].

2.5.4 Neural Networks

Neural networks (NN) are popular methods within a sub-field of ML known as Deep Learning (DL). Neural networks are generally used on a labelled dataset, and as such are a form of superwised learning. NN's are created to resemble how the human brain functions. In the brain, we have neurons which when they receive a signal they apply some function to them and if the resulting signal is high enough, they fire to the next neuron. This is how it is done in the neural network model as well. In NNs we have layers of neurons l_i , initial layer being l_0 and the last layer being l_n . These layers behave in such a way that when they get some input, generally a vector of numbers, each neuron in the layer takes a weighted sum of that vector by a learned weighing factor w_i , then applies an activation function to it. The result of doing this is then passed on to the next layer of neurons until a final layer is reached. At that point, we have reached a layer that corresponds to the prediction of the network. This value can be a binary classification, a regression value, or even the neural networks representation of the input, e.g where a neural network attempts to create an image from an example image [22]. It can then be said that a neural network is doing a function approximation of the input to some value. And, would be mathematically stated as $l_n(w_n \cdot l_{n-1}(w_{n-1} \cdot \dots \cdot l_0(w_0 \cdot \text{Input}))) = \text{Prediction}.$

The core of the learning in neural networks comes from optimizing the weighing factor. That weighting factor is gradually made to move in the direction of the actual correct output by algorithms, e.g the backpropagation algorithm [23].

2.6 Explainable Artificial Intelligence (XAI)

The field of XAI research is still far smaller than its counterpart of AI research [24]. Within XAI two fields are the largest: Model Interpretability and Model Explainability.

2.6.1 Model Interpretability

Model Interpretability is the more common approach of XAI, mainly because it is less constrained than model explainability. In order to achieve model interpretability, we must be able to answer the question of what prediction the model will return on a given input, with a high accuracy. Simple examples would be, given a neural network that has been trained to recognize if an image contains a dog, and a picture of a dog, if that model is highly interpretable, we can say with high certainty that the predicted value positive stating that the image does contain a dog.

2.6.2 Model Explainability

Model explainability within the context of neural networks is not possible today. Model explainability refers to firstly considering some input and output from a model. Then afterwards the model is examined to determine exactly what led to the predicted output. This concept is simple when we're working with Decision Trees. A decision tree is a tree whose nodes are representative of an input value and at every node a branch is selected based on the value of the input value. It is therefore easy to see how to examine the tree to explain the output. By following the branches in the tree we can exactly explain why the model predicted the output.

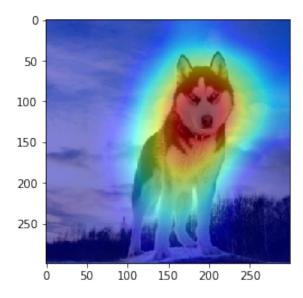


Figure 2.3: Example of a model's saliency map for an image of a dog

When we talk about neural networks this process is much more difficult; the underlying nodes are generally in the millions and the different layers of the neural network vary in the operations they apply to the input. During this process, the value is modified such that it becomes far removed from the initial input value. That being said, while the possibility of completely monitoring the training process and completely monitoring the evaluation process is possible it is not feasible.

2.6.3 Saliency Maps

Within XAI many methods have been developed to try to explain ANN's. In the field of image recognition there has been a lot of work examining which pixels of an image the model deems important. One such method is Saliency Maps[25]. There the pixel values the model deems important are colored s.t. a human can examine the image and get a sense of what portions of the image are important to the model. An example of a classification of a dog can be seen in Figure 2.3. This method is understandable to a human when the saliency map lines up to what we would focus on. However, this achieves no explanation on the prediction if the saliency map does not line up to human intuition or the prediction, for example, if in the same Figure 2.3 we had the same saliency map but the prediction would be dragon, or if the salience map was on the trees and the prediction was dog.

2.6.4 Shapley Values

Methods for explaining models that are not image recognition models include Shapley values, from Lundberg & Lee[26]. There the input is examined against its output, then iteratively input values are selected to be fixed. Then the other input values are varied and an average change in prediction is calculated. With this the Shapley value can be estimated for the fixed input value. This is done to examine which input values have the strongest link to the output value. Shapley values on a dataset can give insights on which input values the model deems most important.

2.7. SUMMARY

2.6.5 Concept Activation Vectors

A recent paper by Been Kim et al.[27], shows a method for examining a neural network giving a much more humanlike insight into a prediction. Using Concept Activation Vectors (CAV) a directional derivative for a given input can be examined with respect to some HLC's. For example, when a human looks at an image of an animal and is supposed to decide whether the image is of a horse or a zebra, an intuitive approach would be to check whether the animal has stripes, or the animal has both white and black colors. That method of determining if a horse is a zebra could then be called a higher-level concept, and if we're able to gather if a neural network uses this strategy for prediction we have a deeper understanding of its underlying structure, leading to an explanation of the result.

The construction of a CAV requires a method of labelling the values in your dataset with the corresponding concept in order to create a binary classifier on data. The binary classifier is constructed on the internal representation of the data points within the neural network. After training the neural network, and constructing the classifier, we run a new datapoint through the neural network and we examine the directional derivative of that datapoint. If the direction of that directional derivative is the same as the direction of the concept activation vector we say that the datapoint contains the concept.

2.7 Summary

This section discussed some of the important algorithms related to the research done in this thesis, as well as giving a foundation in the readers understanding of the test bed we will be using in future sections.

Chapter 3

Methods

In this chapter, we describe our implementation of the game Breakthrough and the methods for training a neural network to play the game. The training process uses MCTS, as described in Section 2.4.1, to guide its training. We outline the architecture we used for our neural network. We describe our process of constructing a concept activation vector for a higher-level concept in order to examine whether our neural network can recognize these higher-level concepts.

The training algorithm is a reinforcement learning self-play algorithm based on previous work by DeepMind[6].

3.1 Game Implementation

In this section, we will take a look at the implementation of the Breakthrough neural network, how we model its state representation and the pseudo-code for training.

3.1.1 Description of the input and output

For a neural network to be able to use input, that input needs to be numeric. We model a Breakthrough board numerically with a 3-dimensional matrix, $N \times M \times 3$, with two values $\{0,1\}$, where the first two indices on the z axis represent the players, and the last layer on the z axis represents which players turn it is. The first z index represents whites pawns, that is, each (x,y) position on the board where white has a pawn the corresponding (x,y,0) index in the 3-dimensional matrix has the value 1 otherwise it has 0, and similarly on the second layer for the black player. The last z layer, contains all 1's if it is the white players turn otherwise all 0's.

This representation of a Breakthrough board can now be passed through a neural network to receive a output. One of the outputs of the neural network is the policy vector. The policy vector is a 3-dimensional matrix where the lengths of the dimensions are $N \times M \times 6$ and each index of the matrix represents an action moving from cell x,y moving to the direction z. The directions are as follows: 0 represents moving upwards and to the left diagonally on the board, 1 upwards, 2 upwards and to the right diagonally, 3 downwards and to the left diagonally, 4 downwards, and lastly 5 downwards and to the right diagonally. The cell values indicate the probability distribution of the search selecting that move. Importantly, before we select a move from the neural networks prediction we zero out the illegal moves, and renormalize the array such that it sums to 1. We do this to not learn on illegal moves, and focus solely

on moves that we can actually make. The second output of the neural network is the value, which represents the predicted end value of the game from the given input state.

The policy head portion of the neural network is ultimately a neural network that handles a function approximation of the policy vector that is returned from Monte-Carlo tree search, and the value head of the neural network a function approximation of the final Q value of the root node in the search tree of a Monte-Carlo tree search. We will describe the data we use to effectively function approximate this MCTS function to train the neural network in Section 3.3.1.

3.2 Neural Network Architecture

The neural network architecture we opted to use was a single convolutional layer with a ReLU[28] activation function, followed by 5 residual layers each containing two layers of convolution, batch normalization, and a ReLU activation. Lastly, a split policy/value head, where the output of the last residual layer is split into two different outputs. The policy head are two layers: first a convolutional layer, and then a fully connected layer with a log softmax layer. The value head consists of three layers: first a convolutional layer, then a fully connected layer, and lastly a fully connected layer with a tanh activation function. Figure 3.1 depicts the architecture. Using this architecture we end up with 1,737,986 trainable parameters.

3.2.1 Convolutional Layers

It is important to understand why we use convolutional layers when dealing with board games as convolution is more typically associated with an image. This is because a convolutional layer is focused on merging multiple input parameters to a single neuron, making it an input parameter for the next layer representing the locality around the center point of the original input. Playing the game of Breakthrough, a piece is only able to capture pieces in its immediate vicinity. This lead to the selection of a 3-d convolutional kernel with a size of 3x3 and a stride of 1.

We require a global view of the board. This is why we use multiple residual layers with convolution. These residual layers stack convolutions on each other making the final convolution represent the locality of all the other localities, allowing the neural network to have a representation of the whole game state in its parameters. The selection of parameters was done for these reasons as well as to most closely resemble the architecture described in AlphaZero[7]. The decision to follow the architecture described in AlphaZero was taken as it has been tested in other board games that are similar to Breakthrough and proved successful.

3.2.2 Residual Layers

The residual layers add the output of the previous layer and the results of the residual layer. On a higher level, this leads to the internal representation of the neural network to maintain the whole game boards in its representation, s.t. two areas that are far away from each other maintain the same level of locality as two that are close.

The reason for why we use a residual layer for applying a convolution layer multiple times is to gain locality of the whole game board. A residual layer applies a function

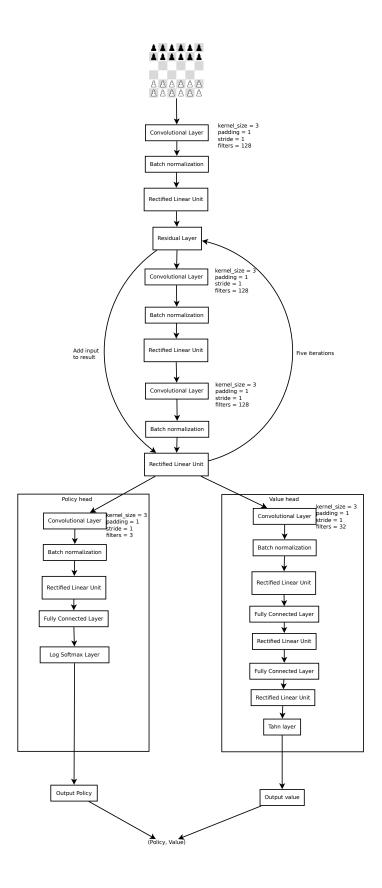


Figure 3.1: Neural Network Architecture

Algorithm 1 Neural network self-play pseudo-code

```
1: neural network nn1 = randomizedInitialNN()
2: neural network nn2 = randomizedInitialNN()
3: while true do
     dataset = generate dataset(nn1)
4:
     nn1.train on examples(dataset)
5:
     win rate = compete(nn1,nn2)
6:
     if win rate > 0.5 then
7:
       nn2 = nn1.copy()
8:
9:
     else
       nn1 = nn2.copy()
10:
     save(nn1)
11:
```

like this res(x) = x + l(x) where x is the input and l(x) is the function of the layer, commonly a convolutional layer.

3.3 Implementation

This subsection focuses on the implementation of the various functions required to train the neural network to play Breakthrough. The description is mainly through pseudo-code, and the code is available on GitHub for examination[29].

3.3.1 Self-play

To train the neural network to play Breakthrough we initialize two neural networks nn1 and nn2 with random weights. In line 4 we let nn1 play against itself using MCTS with PUCT to select moves. We collect data from this self-play to train on. The data collected is (s, π, τ, p, v) , where s is the state, π is the action policy vector provided by MCTS with PUCT, τ the end reward for the episode, 1 if white wins, -1 if black wins. p is the policy vector predicted by the neural network, and v is the predicted reward of the game by the neural network. Once the nn1 has finished training on the dataset we let nn1 and nn2 compete against each other 100 times see line 6. If nn1 is victorious in at least 51 of the 100 games, we say that nn1 did learn to play the game better, we then overwrite nn2 with nn1. Otherwise, the training did not achieve greater play and we overwrite nn1 with nn2. After each iteration we save nn1 to disk. After each iteration a new generation of our neural network is produced, everytime either getting better or not changing. This process is repeated indefinitely or until we are satisfied with our agent. Considering the training data returned by this process we see that the policy head learns on the difference between the policy vector it returned and the policy vector our MCTS with PUCT process returned, and our value head learns on the difference between what the value the neural network returned and the actual end reward of the game was. The pseudo-code is shown in Algorithm 1.

3.3.2 Compete

Algorithm 2 Neural network compete pseudo-code

```
1: Input: neural network nn1, neural network nn2
2: Output: win rate for white player
3: white_wins = 0
4: game = initial_breakthrough()
5: for 1 to 100 do
6: while not game.is_terminal() do
7: nn1.make_move()
8: nn2.make_move()
9: if game.white_wins() then
10: white_wins++
11: return white_wins/100
```

The compete function differs from the self-play function in such a way that we select the moves by a single pass through the neural network thereby only evaluating the neural networks ability to predict best actions. The pseudo-code shown in Algorithm 2.

3.3.3 Loss Function

The data collected is backpropagated through the NN moving the weights to the direction of this loss function $l = (p * \pi) + (\tau - v)^2$ for each state the NN encountered during self-play. Importantly the variable p has masked illegal actions to 0 to direct the NN to not learn on illegal moves.

3.4 Explainable State Representations

In this section we describe the process of training a Concept Activation Vector in order to linearly separate each state into points in a space with the concept and ones without the concept.

3.4.1 Testing with Concept Activation Vectors

Once the neural network has learned to play the game of Breakthrough, we examine its internal state with respect to higher level concepts that we understand. The first examined HLC is material advantage, that is, the number of pieces that a player has over their opponent. The higher-level idea to human players would be that they are in a better position since they have more pieces.

To examine the higher-level component we take a look at the internal state of the neural network itself. To do this, we take a state where we know whether or not that state contains or does not contain the concept in question, and run it through the neural network, and while the state is propagating through the network we select a layer to split the network, we call that layer l_{split} . This l_{split} layer is one that you can select arbitrarily, however some layers will be more representative of the concept you are currently viewing and as such this layer is one that should be selected through testing. As the state has been propagated up to l_{split} the state is a mutated vector $l_{split}(l_{split-1}(...l_0(state)))$ of the initial input state. We save that vector as a point in the N-dimensional space that it represents and label it with either having or not having

Algorithm 3 CAV creation pseudo-code

```
1: Input: neural network nn, column name, breakpoint, data set, sample size
2: Output: A concept activation vector for the column with column name
3: positive set = select positive samples(data set,
                                                          column name,
   ple size)
4: negative_set = select negative samples(data_set, column_name,
   ple size)
5: labelled set = positive set + negative set
6: unlabelled set = dataset - unlabelled set
7: model = StochasticGradientDescentClassifier()
8: for state in labelled set do
     //Modify labelled dataset to contain internal representations
10:
     state = nn.get internal representation(state)
11: train set, test set = train test split(labelled dataset)
12: model.train(train set)
13: prediction score, roc auc score = model.predict(test set)
14: return model
```

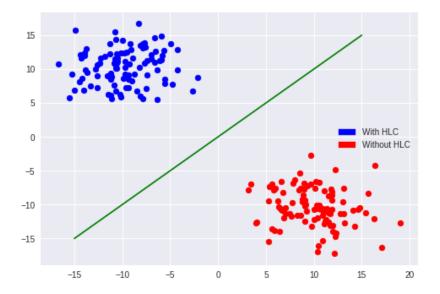


Figure 3.2: Trained linear classifier on a 2-dimensional space

the concept. Once we've gathered enough points in that N-dimensional space we train a linear classifier that attempts to split the N-dimensional space with a hyper-plane, where on one side we have states with the concept and on the other ones that do not have the concept. We use a Stochastic Gradient Descent classifier, from the SKLearn library[30]. We show pseudo-code of this process in Algorithm 3.

An example of how this would look where our N-dimensional space is two dimensional is shown in Figure 3.2. Once we have successfully trained this linear classifier, we create the concept activation vector which is simply a vector that is orthogonal to the decision boundary of the linear classifier. We can now examine new states with this concept activation vector, we do so by running another state s through the neural network and receive a (p, v) prediction. We then apply the backpropagation algorithm to receive the gradient at l_{split} with respect to the action with the highest value in the policy vector p. If that gradients direction is the same as the direction of the concept

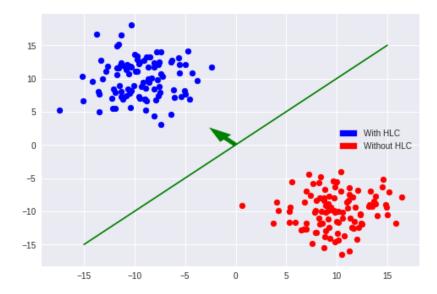


Figure 3.3: Trained linear classifier on a 2-dimensional space with arrow representing concept activation vector

Algorithm 4 Evaluate a neural network w.r.t concepts pseudo-code

```
1: Input: neural network nn, concept activation vector cav
2: Output: Portion of encountered states that contain the concept of the concept
   activation vector
3: state count = 0
 4: has tcav = 0
5: for 1 to 100 do
     current state = Breakthrough.initial state
7:
     while not current_state.terminal() do
       current internal_representation =
 8:
       nn.get internal representation(current_state)
       output = nn.finish propagating(current internal representation)
9:
       gradient direction =
10:
       nn.get gradient(current internal representation, output)
11:
       tcav score = cav \cdot gradient direction
       if same direction(tcav score, cav) then
12:
         has tcav++
13:
14:
       state count++
15:
       current state = nn.get next state(current state)
16: return has tcav / state count
```

activation vector (orthogonal of the decision boundary in the direction of our concepts) we say that the state includes the concept, and that it does not if the gradient moves in the other direction.

We show an example in Figure 3.3, where the arrow in the image represents the concept activation vector. If the gradient from running s through our neural network moves in that same direction we say the state s includes the concept otherwise it does not. Using this method we evaluate the internal representation of the state within the neural network and can see whether it recognizes the HLC.

In Algorithm 4 we show pseudo-code depicting how we evaluate if a neural network recognizes a given concept. The resulting value from running the algorithm is, the proportion of states where during the backpropagation algorithm of the neural network the network made its prediction using the knowledge of the higher level concept we are examining.

A clear limitation of this method is that we need the concepts we construct the concept activation vectors from to be a binary concept. That is, a state either is materially advantageous or it is not. This limitation comes from us applying the methods described in [27]. A second limitation is that we do not distinguish between a state where the gradient's magnitude at l_{split} is large or small, rather, we only identify whether it moves in the same direction as the concept activation vector.

3.5 Summary

In this chapter we described the architecture of the neural network, including how we model Breakthrough to be able to learn to play the game, we described the processes we use to learn from self play, and how we apply concept activation vectors to recognize if a neural network recognizes a given concept. In the following chapter we will evaluate the neural network.

Chapter 4

Results

In this chapter, we first evaluate the neural network against various agents to validate that it has learned how to play the game. Secondly, we describe each concept we intend to examine the neural network against. Thirdly, we take a look at the changes in the emphasis of the neural network during training. The main point of interest there being whether the neural network notices simple HLCs early then stops considering them as the network improves.

4.1 Evolution of the Neural Networks Win Rate

Examining the neural network is only interesting if the neural network can effectively play the game. We first examine the history of the neural network playing against an agent that takes moves completely at random. The win rate over every 10 generations can be seen in Figure 4.1. It is clear that very early on in the training process, almost immediately after generation 10, our agent performs nearly perfectly against the random agent. This implies that the agent does indeed learn some strategy in the game. The next agent we tried the neural network against was an agent that does regular Monte-Carlo tree search on the game space with 100 iterations of Monte-Carlo tree search for each move. The MCTS agent has a c_{uct} value of 0.9. A graph showing the win rate over generations is depicted in Figure 4.2. Again, our agent quickly

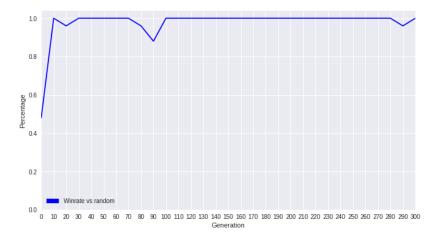


Figure 4.1: Winrate vs. random agent

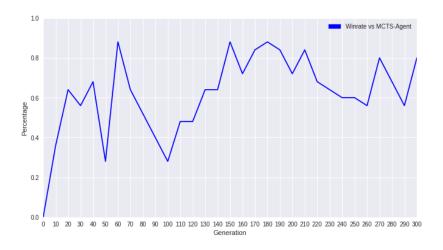


Figure 4.2: Winrate vs. MCTS agent

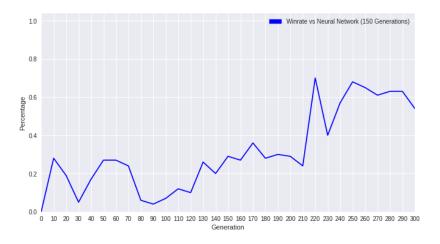


Figure 4.3: Winrate vs. neural network trained for 150 generations

learns some strategy and can win often, although not achieving a perfect win rate even after 300 generations. The last agent we tested against was the neural network itself, although only trained to 150 generations. The graph in Figure 4.3 shows win rate. As one would expect, the agent that has trained for less time performs poorly until it has trained for more than 150 generations where the win rate starts to increase.

These results imply that our agent certainly understands how to play the game of Breakthrough to a certain level. However, an intermediate level human player would most often be able to beat the agent, based on the author's experience playing against it. Note that the main focus of this was not to create an expert level agent. Rather, to gauge into the concepts the agent learns as described in the next section.

4.2 Selecting Concept Thresholds to Binarize the Concepts

As stated earlier, our method requires the concepts to be a binary classification of whether a state contains a concept or if it does not. It is difficult to argue for whether or not a state where you have one pawn up on your opponent or three constitues you being in a materially advantageous position. To identify a threshold where the concept is present we let a neural network that had been trained for 300 generations play against it self to generate 20,000 unique states. With this dataset of states we examine the distribution of each concept we created and evaluated samples from various thresholds, coming to a decision. This process of selecting a threshold can seem quite arbitrary and there could be a method of selecting this threshold in a more principled way, regardless, we took this approach of expert evaluations.

We test four concepts Material Advantage, Aggressiveness, Unity, and Lorentz-Horey score.

4.2.1 Description of Concepts

The first concept we examine is Material Advantage which conveys the idea of having more pawns than the opponent. Our dataset of 20,000 unique states show a distribution, see Figure 4.4. From examining this distribution and examining different thresholds we decided on the breakpoint of ≥ 2 , meaning that if you have 2 or more pieces than your opponent you are in a state that has this concept. From the 20,000 states only 5.5% of states have this concept.

The next concept is Aggressiveness, which describes how much closer your furthest piece is to the opponent's edge than your opponent's furthest piece to your edge. This is the minimum amount of how many moves it will take you to possibly win the game. A distribution of these values can be seen in Figure 4.5. We examined the distribution, and sampled states from various breaking points and decided on the value of ≥ 1 . That is, if the value of a state's furthest piece difference is greater than or equal to 1 that state has the concept of Aggressiveness. From the dataset 18.3% of states have this concept.

Our third concept is Unity. This concept represents the absolute average distance of your pawns from the center row of your pawns, and is calculated as follows: the row of your furthest pawn from the starting row r_{far} , the row of your nearest pawn from the starting row r_{near} . Finding the middle row is then $\frac{r_{far}+r_{near}}{2}$, we then take the absolute of the average distance from all of the players pawns to that row. The distribution of

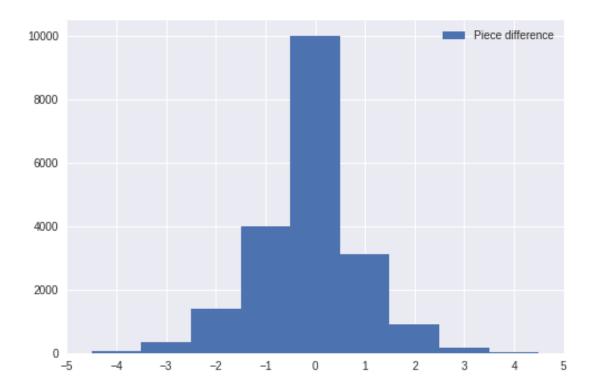


Figure 4.4: Distribution of piece amount difference

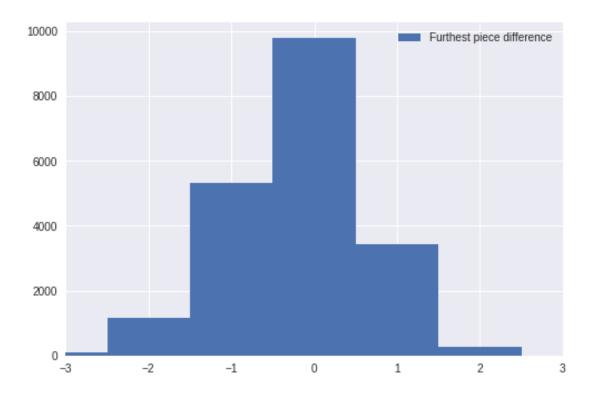


Figure 4.5: Distribution of difference of furthest pawns

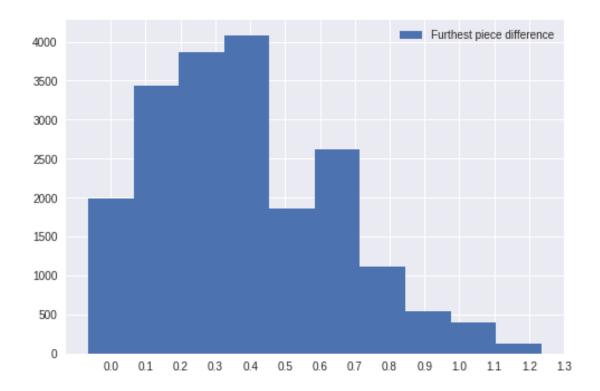


Figure 4.6: Difference of distance from center

Table 4.1: Lorentz-Horey cell values, from white players point of view, white player starting at the bottom of the board

21	21	21	21	21	21
11	15	15	15	15	11
7	10	10	10	10	7
4	6	6	6	6	4
2	3	3	3	3	2
5	15	5	5	15	5

the average distance values is shown in Figure 4.6. From sampling states from several points we decided on a breakpoint of ≤ 0.25 for identifying states as states where the Unity concept is precent. The value of 0.25 generally allows your states to have two rows that have the majority of the pawns and one or two pawns one row away from the group. From the dataset of 20,000 states 20% of states have this concept.

The last concept we examined was the Lorentz-Horey score. This concept is a popular heuristic in Breakthrough defined in the paper by Lorentz & Horey[12]. For this heuristic, we give each cell on the board a point value. For a given player the heuristic is then the sum of the cell values where they have pawns. The cell values are shown in Table 4.1. The matrix shown is flipped from the black player's point of view. The values are selected in such a way that as your pawns approach the opponent's side their value increases, having pieces on the edge is not optimal, as such a pawn will only be able to capture in one direction and can not escape capture as easily. To select the breakpoint for Lorentz-Horey heuristic, we generate a distribution of the difference in Lorentz-Horey Score over our dataset. The resulting distribution is shown in Figure 4.7. Our examination lead us to select the value of 5, as a breakpoint

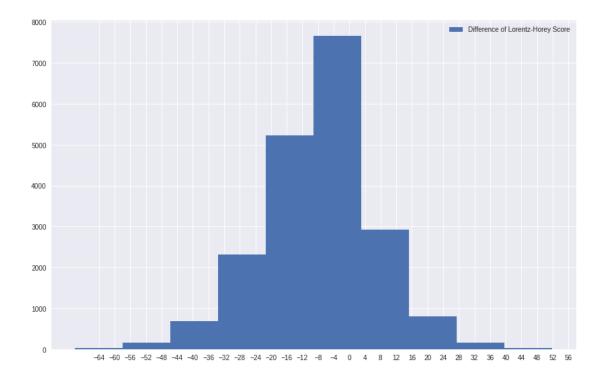


Figure 4.7: Difference of Lorentz-Horey Score

indicating that a state has the concept of Lorentz-Horey. Out of our dataset of 20,000 states 29.4% of states have this concept.

4.3 Evaluating Usage of Concepts Over Generations

To examine the neural networks usage we consider our neural network during training, going from generation 0 to generation 300. We examine the results at every 10 generations. The method of evaluating how much the neural network focuses on a given concept is shown in Section 3.4.1. In the following graphs, the red line represents the Area Under the Receiver Operating Characteristic Curve of the linear classifier used to construct the concept activation vector.

4.3.1 Material Advantage

The Figure 4.8. shows that throughout training the Material Advantage HLC is only ever a slight factor in the selection of states and we can say that the neural network does not consider number advantage in its selection process.

4.3.2 Agressiveness

From Figure 4.9, we can see that the aggressiveness HLC is a growing factor over as the neural network is trained. As a piece can always move forward, if your opponent does not capture that piece, this concept relates to how many moves it will take for you to win. Generally, when your opponent is not playing well this concept does well, and quickly becomes a bad heuristic in classical search algorithms.

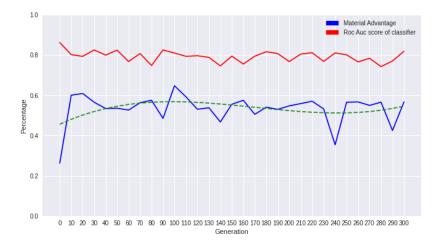


Figure 4.8: Percentage of selected states containing the HLC Material Advantage



Figure 4.9: Percentage of selected states containing the HLC aggressiveness

4.3.3 Unity

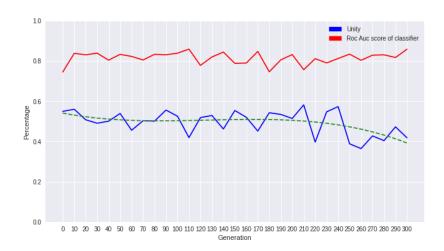


Figure 4.10: Percentage of selected states containing the HLC unity

Examining Figure 4.10, we see that the Unity HLC is steady, but then it drops as the network is trained. As this is considered a decent strategy in Breakthrough this is unexpected. However, this concept become increasingly unreliable as you lose pieces because it is the average of your remaining pieces distance to their center.

4.3.4 Lorentz-Horey Score

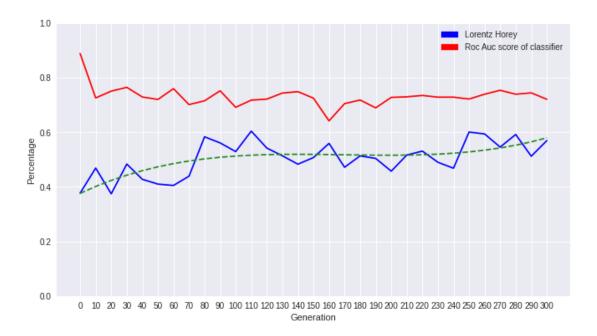


Figure 4.11: Percentage of selected states containing the HLC Lorentz-Horey

Examining Figure 4.11, we can see a trend where as the neural network is trained its use of this HLC increases over time. As this heuristic is the one most often cited as a successful strategy in Breakthrough, it is interesting to see that our Breakthrough agent is gradually learning a similar concept.

4.4 Summary

In this section we discussed some concepts that we believed would be representative of concepts that a nerual network would learn over time playing Breakthrough. An important note is that there are an infinite amount of concepts, and there could exist some that the neural network uses extensively that we overlooked. We examined the neural network against these concepts. In the following chapter we will discuss the next steps for this research.

Chapter 5

Discussion

This chapter discusses the results and the future work that could span from this research. Additionally, we conclude the work.

5.1 Summary

As seen in Chapter 4, our trained agent does indeed quickly start to recognize the higher-level concepts, thus answering our research question 1. The results are promising, as we see a popular concepts like Lorentz-Horey score rise in emphasis for the neural network, and a simple but effective concept like Material Advantage rise slowly but not exessively. We find the Unity concept to be disappointing as stated earlier in this paper; maintaining closeness of your pawns tends to be preferential. And lastly, for a the concept Aggressiveness, the fact that it falls off early is what we expected. It would have been the preferred result if we saw a greater variability in the concepts, but this could be a result from not enough training iterations, or not a complex enough model. Considering that the most emphasised HLC is the Lorentz-Horey score, and that the least is Unity, we can answer our research question 2. As we know from the literature, Lorentz-Horey is considered the leading heuristic for Breakthrough, and that HLC is highly emphasised by the neural network. Secondly, the Unity heuristic is not a validated heuristic, moreso, an attempt at creating a simple heuristic that closely resembles how tight-packed your pawns are. However, the fact that the resulting graphs are relatively steady the results are not as strong as we would have hoped.

Importantly, these concepts are only a few possibilities of an infinite set of concepts, and the neural network could be learning a completely different concept then those that we tested. However, that was not the focus of this research, it was to examine if a neural network does move towards HLC's that we humans use in games.

5.2 Limitations

There are clear limitations that this method of interpreting a trained neural network imposes. We only consider linear classifiers when constructing our concept activation vector, while there could be applications where we use a non-linear classifier but we apply data manipulation tricks like a kernel trick to achieve a linear decision boundary. Assuming this method would work it could increase the power of our explanation of the decision making of the neural network. Another limitation is that we do not recognize a non-binary concept, a state either contains or does not contain a concept.

In this thesis we did not consider the magnitude of the direction of the gradient in our evaluation of whether our neural network was using a given concept, this was a decision made on our part but could be investigated further.

5.3 Future Work

To iterate on this research, training a neural network with greater computing power, or with a larger neural network architecture, will allow the us to hopefully achieve a super-human neural network in Breakthrough. This would give greater confidence in the learned concepts, possibly allowing for pedagogical research on the topic regarding which concepts are optimal to train people in the game environment.

The work done in this thesis was only a proof of concept of the process of explaining the internal concept a neural network uses while acting in a board game environment. Ideally, one would like to extend this work to a larger set of board games.

Additionally applying this method to a more diverse set of environments would be an interesting field of research. We envision a self driving car agent being examined with respect to a higher level concept of aggressiveness, or a mortgage agent being examined with respect to a higher level concept of gender bias.

5.4 Conclusion

The work done in this paper is only a first step in examining working agents in active environments with respect to human level concepts. If improved it could have a great impact in our trust on neural network that improve our daily lives. While the testbed for the research was a discrete game environment, there is a clear way forward to dynamic systems with discrete human level concepts. Our results show that for an agent that clearly does not achieve human level performance its actions are often selected with respect to human level concepts.

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