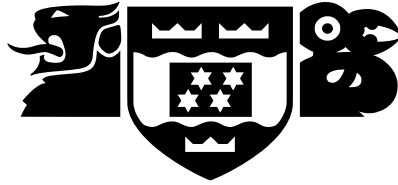


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Logical Neural Networks: Opening the black box

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Abstract

The growing popularity of Artificial Neural Networks is driving the development of systems that are not only accurate but have a decision making process that can be defended. The report develops a novel neural network architecture which builds in an interpretable structure. Experiments on the MNIST dataset showed these models have statistically equivalent performance to Multi Layer Perceptron Networks with a more interpretable learned model.

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Chapter 1

Introduction

Artificial Neural Networks (ANN's) are commonly used to model supervised learning problems. A well trained ANN can generalize well but it is difficult to interpret how the network is operating. This issue with interpretation makes ANNs like a black-box. This report aims to alleviate this problem by formalizing and developing a novel neural network architecture.

1.1 Motivation

The number of situations in which ANN systems are used is growing. This has lead to an increasing interest in systems which are not only accurate but also provide a means to understand the logic use to derive their answers [4]. Interest in interpretable systems is driven by the variety of situations that utilize ANNs where incorrect or biased answers can have significant effects on users.

Ensuring a system is Safe and Ethical are two things which depending on the application are important to verify. If an ANN was able to provide its reasoning for giving a specific output then defending actions made by the system would be a more feasible task [4].

In the context of safety a Machine Learning (ML) system often can not be tested against all possible situations, as it is computationally infeasible to do so. If accessible, the logic contained inside the model could be used to verify that the system will not take any potentially dangerous actions.

It is also important to consider the implications of an ANN being biased towards a protected class of people. A paper published in 2017 demonstrated that standard machine learning algorithms trained over text data learn stereotyped biases [3]. An ANN trained with the intent to be fair could result in a system which discriminates because of biases in the data used to train it.

Another pressure causing the development of interpretable ML systems is changing laws. In 2018 the European Union (EU) General Data Protection Regulation (GDPR or "right to explanation") will come into affect. The GDPR will require algorithms which profile users based on their personal information be able to provide "Meaningful information about the logic involved" [10]. This law would effect a number of situations where ML systems are used. For example banks, which use ML systems to make loan application decisions [5].

Using a number of simulated data researchers trained an ANN to compute the probabil-

ity of loan repayment [5]. The simulated data consisted of white and non-white individuals, both groups with the same probability of repayment. As the proportion of white to non-white individuals in the data set increased the ANN became less likely to grant loans to non-white individuals. This is a statistical phenomenon called uncertainty bias. This artificial situation demonstrates the effect biased data could have on an ANN.

The argument thus far has established that being able to defend or verify the decisions made by ANNs is not just an interesting academic question. It would allow for the creation of potentially safer and fairer ML systems. They provide a means to verify that not only correct decisions are made but they are made for justifiable reasons. The GDPR gives a monetary motivation to use interpretable systems and breaches of the regulation will incur fines [5].

1.2 Solution

To address the problems laid out thus far we improved upon a probability based network architecture called Logical Neural Networks (LNNs) which yield a simpler trained model [8].

Existing methods for interpreting ANNs are post-hoc algorithms to extract some meaning from standard ANN's. The approach presented in this report builds interpretability into the ANN through a structure based off logical functions. This report presents a formal foundation for LNNs through the following stages.

1. Motivate the concept that Logical Neural Networks are built from (Chapter 2).
2. Motivate and derive at a very specific case of Logical Neural Networks called Logical Normal Form Networks (Chapter 3).
3. Discuss the performance, generalization and interpretation capabilities of Logical Normal Form Networks (Chapter 3).
4. Discuss the situations where Logical Normal Form Networks can be applied (Chapter 4)
5. Generalise Logical Normal Form Networks to Logical Neural Networks (Chapter 5).
6. Derive modifications to the Logical Neural Network architecture to improve accuracy (Chapter 5)
7. Evaluate the modified Logical Neural Network structure (Chapter 6)
8. Demonstrate the possible use cases of Logical Neural Networks (Chapter 7).

Following the development of Logical Neural Networks they are evaluated on the MNIST data base and compared against standard Multi-Layer Perceptron Networks. It will be demonstrated that LNNs make interpretation a simpler task without sacrificing performance.

Chapter 2

Background

This chapter presents concepts related to the study conducted in this report. After each idea is introduced and discussed the relation to this work is explored.

2.1 Interpretability

To create a system that is interpretable it is necessary to have an understanding of what it means to interpret a model and how its interpretation might be evaluated. Interpretability of Machine Learning systems has been defined as "*the ability to explain or to present in understandable terms*" [4] which is ambiguous.

Situations where interpretability is important

How evaluation of interpretable systems might be carried out

2.1.1 Relation to Solution

2.2 Rule Extraction

A survey in 1995 focuses on rule extraction algorithms [1], identifying the reasons for needing these algorithms along with introducing ways to categorise and compare them.

There are three categories that rule extraction algorithms fall into [1]. An algorithm in the **decompositional** category focuses on extracting rules from each hidden/output unit. If an algorithm is in the **pedagogical** category then rule extraction is thought of as a learning process, the ANN is treated as a black box and the algorithm learns a relationship between the input and output vectors. The third category, **electic**, is a combination of decompositional and pedagogical. Electic accounts for algorithms which inspect the hidden/output neurons individually but extracts rules which represent the ANN globally [12].

To further divide the categories two more distinctions are introduced. One measures the portability of rule extraction techniques, i.e. how easily can they be applied to different types of ANN's? The second is criteria to assess the quality of the extracted rules, these are accuracy, fidelity, consistency, comprehensibility [1].

1. A rule set is **Accurate** if it can generalize, i.e. classify previously unseen examples.

2. The behaviour of a rule set with a high **fedelity** is close to that of the ANN it was extracted from.
3. A rule set is **consistent** if when trained under different conditions it generates rules which assign the same classifications to unseen examples.
4. The measure of **comprehensibility** is defined by the number of rules in the set and the number of literals per rule.

One rule extraction algorithm presented in 2000 by Tsukimoto is able to extract boolean rules from ANNs in which neurons have monotonically increasing activations, such as the sigmoid function [13]. The algorithm can be applied to problems with boolean or continuous inputs however only the boolean case will be considered here.

Each neuron is written as a boolean operation on its inputs, this is done in the following manner. Consider a neuron m in an MLPN with n inputs, construct a truth table, T , with n inputs. Let $f_i (i \in [0, 2^n])$ represent the activation of m when given row i as input and define $r_i = \bigwedge_{j=1}^n l_j$, the conjunction of all literals in the row i in T , e.g. if $n = 2$ then for row $(1, 0)$ $r_i = x_1 \wedge \neg x_2$. The approximation of m is given by

$$\bigvee_{i=1}^{2^n} g_i \wedge r_i \quad (2.1)$$

where g_i is given by

$$g_i = \begin{cases} 1 & \text{if } f_i \geq \frac{1}{2} \\ 0 & \text{if } f_i < \frac{1}{2} \end{cases}$$

By starting with the first hidden layer and progressing through the network an expression for the network can be extracted. Figure 2.1 shows an algorithm for extracting rules from an MLPN.

```

1 function extractRulesMLPN(network)
2   prev_expressions = network.inputs
3   for layer in network
4     expressions = {}
5     patters = all input patters for layer
6     for each neuron (n) in layer
7       exp = And(Or({ literals(p), p ∈ patters n(p) > ½ })))
8       expressions.add(substitute prev_expressions into exp)
9
10    prev_expressions = expressions

```

Figure 2.1: Rule Extraction Algorithm presented in [13]

The algorithm presented in figure 2.1 is exponential time in terms of n . A polynomial time algorithm is also presented but deriving it is beyond the scope of this report.

These rule extraction algorithms are all post-hoc operations. They do not place many restrictions on the structure of ANN they are applied to, resulting with complicated algorithms. The solution developed in this report builds intepretability into the ANN structure with the goal of simpler and more intuitive algorithms to interpret knowledge.

2.2.1 Relation to Solution

These surveys provide a framework for evaluating the rules extracted using a particular technique. The solution developed in this report allows for rule extraction in some situations. By introducing this content the reader is familiar with this approach to evaluating extracted rule sets.

Rule extraction algorithms make up a large portion of the current methods to interpret knowledge inside an ANN.

2.3 Noisy Neurons

Multi-Layer Perceptron Networks (MLPNs) are universal function approximators and as such can achieve a high accuracy across a broad range of problems. There are many equivalent weight representations of an MLPN which give the same solutions, this makes interpreting the network difficult [8]. By restricting the possible relationships between a neurons inputs and outputs to be a single function then only the relevance of each feature needs to be inferred. Consequently the problem interpretation becomes easier. The two functions OR and AND are easy to understand, which is a good reason to pick them over other functions.

In 2016 the concept of Noisy-OR and Noisy-AND neurons [8] were derived from the Noisy-OR relation [11], a concept in Bayesian Networks developed by Judea Pearl. A Bayesian Network represents the conditional dependencies between random variables in the form of a directed acyclic graph.

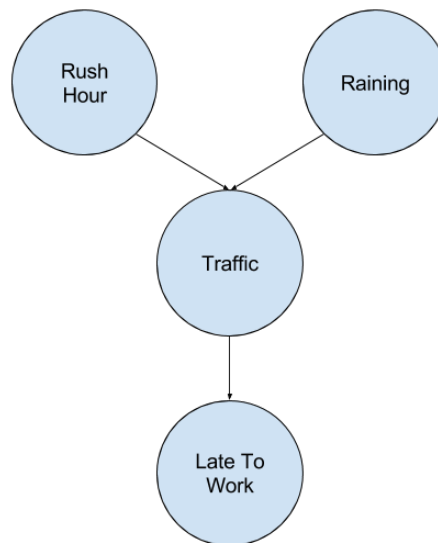


Figure 2.2

Figure 2.2 is a Bayesian network. It demonstrates the dependency between random variables "Rush Hour", "Raining", "Traffic", "Late To Work". The connections show dependencies i.e. Traffic influences whether you are late to work, and it being rush hour or raining influences whether there is traffic.

Consider a Bayesian Network with a node D and S_1, \dots, S_n being D 's parents. In other words S_i influences the node D . Each S_i is independent from all others. The relationship

between D and its parents is defined as if $S_1 \text{ OR } \dots \text{ OR } S_n$ is true then D is true. Let ϵ_i be the uncertainty that S_i influence D , then $P(D = 1 | S_1 = 1, \dots, S_n = 1)$ can be defined as Equation 2.2.

$$P(D = 1 | S_1 = 1, \dots, S_n = 1) = 1 - \prod_{i=1}^n \epsilon_i \quad (2.2)$$

Equation 2.2 shows the noisy or relation. In the context of a neuron the inputs x_1, \dots, x_n represent the probability that inputs $1, \dots, n$ are true. The output of a neuron as conditionally dependent on its inputs, in terms of a Bayesian Network the x_i 's is a parent of the neuron. Each ϵ_i is the uncertainty as to whether x_i influences the neurons output. How can weights and inputs be combined to create a final activation value for the neuron? First consider a function $f(\epsilon, x)$ which computes the irrelevance of input x . Some conditions [8] that can be placed on f are given in the following list.

1. $\epsilon = 1$ means that $f(\epsilon, x) = 1$
2. $x = 1$ means that $f(\epsilon, x) = 1$
3. Monotonically increasing in ϵ and decreasing in x . Let $f(x, \epsilon) = \epsilon^x$. The definitions for Noisy-OR and Noisy-AND gates can now be given.

The function $f(\epsilon, x)$ is 1 (i.e x is irrelevant) if x does not influence the output ($\epsilon = 1$) essentially cancelling these irrelevant inputs out in a AND or OR. The noisy activations can therefore be a logical function over $f(\epsilon_{x_i}, x_i)$ for all i .

Definition 2.3.1. A **Noisy-OR** Neuron has weights $\epsilon_1, \dots, \epsilon_n \in (0, 1]$ which represent the uncertainty that corresponding inputs $x_1, \dots, x_n \in [0, 1]$ influence the output. The activation of a Noisy-OR Neurons is given in Equation 2.3.

$$a = 1 - \prod_{i=1}^p (\epsilon_i^{x_i}) \cdot \epsilon_b \quad (2.3)$$

Definition 2.3.2. A **Noisy-AND** Neuron has weights $\epsilon_1, \dots, \epsilon_n \in (0, 1]$ which represent the uncertainty that corresponding inputs $x_1, \dots, x_n \in [0, 1]$ influence the output. The activation of a Noisy-AND Neurons is given in Equation 2.4

$$a = \prod_{i=1}^p (\epsilon_i^{1-x_i}) \cdot \epsilon_b \quad (2.4)$$

Both these parametrisations reduce to discrete logic gates when there is no noise, i.e. $\epsilon_i = 0$ for all i .

2.3.1 Relation to Solution

The noisy neurons are the building blocks for the two network architectures present in this report. Without an understanding of these concepts it would be difficult to understand the motivations for the solution developed.

2.4 Logical Normal Form Networks

2.4.1 CNF & DNF

A boolean formula is in Conjunctive Normal Form (CNF) if and only if it is a conjunction (and) of clauses. A clause in a CNF formula is given by a disjunction (or) of literals. A literal is either an atom or the negation of an atom, an atom is one of the variables in the formula.

Consider the boolean formula $\neg a \vee (b \wedge c)$, the CNF is $(\neg a \vee b) \wedge (\neg a \vee c)$. In this CNF formula the clauses are $(\neg a \vee b)$, $(\neg a \vee c)$, the literals used are $\neg a, b, c$ and the atoms are a, b, c .

A boolean formula is in Disjunctive Normal Form (DNF) if and only if it is a disjunction (or) of clauses. A DNF clause is a conjunction (and) of literals. Literals and atoms are defined the same as in CNF formulas.

Consider the boolean formula $\neg a \wedge (b \vee c)$, the DNF is $(\neg a \wedge b) \vee (\neg a \wedge c)$.

2.4.2 CNF & DNF from Truth Table

Given a truth table representing a boolean formula, constructing a DNF formula involves taking all rows which correspond to True and combining them with an OR operation. To construct a CNF one combines the negation of any row which corresponds to False by an OR operation and negates it.

Theorem 2.4.1. The maximum number of clauses in a CNF or DNF formula is 2^n

Proof. Assume the goal is to find the CNF and DNF for a Boolean formula B of size n , for which the complete truth table is given. The truth table has exactly 2^n rows.

First assume a CNF is being constructed, this is achieved by taking the OR of the negation of all rows corresponding to False, the NOT operation leaves the number of clauses unchanged. At most there can be 2^n rows corresponding to False, consequently there are at most 2^n clauses in the CNF.

A similar argument shows that the same holds for DNF. □

2.4.3 Definition of Logical Normal Form Networks

In 1996 a class of networks called Logical Normal Form Networks [6] (LNFNs) were developed. Focusing on learning the underlying CNF or DNF for a boolean expression which describes the problem. The approach relies on a specific network configuration along with restriction the function space of each neuron, allowing them to only perform an OR or AND on a subset of their inputs. Such OR and AND neurons are called Disjunctive and Conjunctive retrospectively. If the trained network is able to achieve a low enough accuracy then rules can be extracted from the network in terms of a Boolean CNF or DNF expression [6].

The algorithm which extracts rules from LNFNs would be Electic and certainly is not Portable as the algorithm is specific to the LNFN architecture. It is not possible to further classify the rule extraction algorithm as the research developing it lacks any experimental

results. Justification is also missing making the LNFNs difficult to reproduce.

2.4.4 Relation to Solution

2.5 Logical Neural Networks

ANN's containing of Noisy-OR and Noisy-AND neurons are called Logical Neural Networks [8] (LNN's). If the network consists of only Noisy neurons then it a pure LNN. ANNs containing a mix of logical and standard activations where shown to not yield interpretable models and also have lower performance, consequently when LNNs are referred to it will always be in the context of Pure LNNs.

2.5.1 Relation to Solution

Chapter 3

Foundation of Logical Normal Form Networks

Consider the set of binary classification problems which have boolean inputs. Consider some problem p in this set, with X_p and Y_p being the examples and targets retrospectively. Let B_p be the set of all boolean functions which take an $x \in X_p$ and take it to either a 1 or 0. Then finding the optimal boolean function to solve the problem p corresponds to expression 3.1 which is simply the function f with the smallest cross entropy loss.

$$\arg \min_{f \in B_p} - \sum_{0 \leq i \leq |X_p|} (Y_{p_i} \cdot \log f(X_{p_i})) + ((1 - Y_{p_i}) \cdot \log(1 - f(X_{p_i}))) \quad (3.1)$$

How might a interpretable network architecture that can learn these functions be constructed? The following facts will be helpful, any boolean function has a unique Conjunctive and Disjunctive Normal Form (CNF & DNF), both the CNF and DNF are described by the boolean operations NOT, OR and AND, in a CNF or DNF a not can only occur on a literal and the maximum number of clauses in a CNF or DNF is 2^n where n is the number of inputs.

One option is to use a standard Multi-Layer Perceptron Network (MLPN). MLPNs have been shown to be universal function approximators but are not interpretable. Learning the CNF or DNF of the optimal function is an equivalent problem. For now consider the problem of learning the CNF. This can be done with hidden layer of size k and an output layer with a single neuron. The hidden neurons only need to perform the OR operation on a subset of inputs. The output layer only need perform an AND of a subset of the hidden neurons.

Using Noisy-OR and Noisy-AND (See Section 2.3) such a network can be constructed. Noisy neurons can not compute the not of inputs so the input layer must be modified to include the negation of each input. Figure 3.1 is the structure that has been derived.

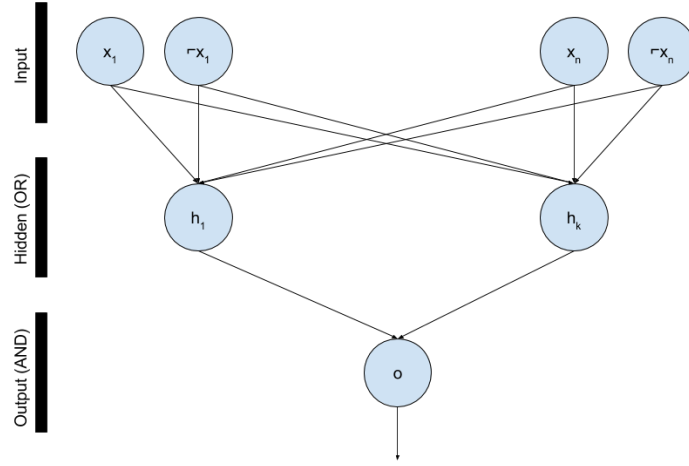


Figure 3.1: Network Archecture for Learning CNF

By the same logic a network architecture for learning the DNF can be derived, the hidden layer consists of ANDs and the output of a single OR. These networks for learning CNF and DNF formulae are a new derivation of Logical Normal Form Networks (LNFNs) [6], the difference being Noisy neurons are used instead of the previously derived Conjunctive and Disjunctive neurons. Definitions of CNF Networks, DNF Networks and LNFNs are now given.

Definition 3.0.1. A **CNF-Network** is a three layer network where neurons in the hidden layer consist solely of Noisy-OR's and the output layer is a single Noisy-AND.

Definition 3.0.2. A **DNF-Network** is a three layer network where neurons in the hidden layer consist solely of Noisy-AND's and the output layer is a single Noisy-OR.

Definition 3.0.3. A **LNF-Network** is a DNF or CNF Network

It must also be determined how many hidden units the LNFN will have, it is known that 2^n , n being the number of atoms, is an upper bound on the number of clauses needed in a CNF and DNF formula (see Theorem 2.4.1).

Theorem 3.0.1. Let T be the complete truth table for the boolean formula B . Let L be an LNFN, if L has 2^n hidden units then there always exists a set of weights for L which correctly classifies any assignment of truth values to atoms.

Proof. Let T be the truth table for a boolean function B . The atoms of B are x_1, \dots, x_n . T has exactly 2^n rows. Construct an LNFN, L , in the following manner. L has 2^n hidden units and by definition L has one output unit. The inputs to L are i_1, \dots, i_{2n} where i_1, i_2 represent $x_1, \neg x_1$ and so on. Let $\epsilon_b = 1$ for every neuron.

Let h_k denote hidden unit k . h_k has the weights $\epsilon_{k,1}, \dots, \epsilon_{k,2n}$, where $\epsilon_{k,m}$ represents input i_m 's relevance to the output of h_k . Similarly the output unit o has weights μ_1, \dots, μ_{2^n} where μ_m represents the relevance of h_m to the output of o .

Assume L is a DNF Network. Starting from row one of the table T , to row 2^n . If row a corresponds to False then set $\mu_a = 1$ (i.e. hidden node a is irrelevant), otherwise the row corresponds to True, then $\mu_a = Z$, where Z is a value close to 0 (any weight for a Noisy neuron cant be exactly 0). For each $\epsilon_{a,m}$ if the corresponding literal occurs in row a of the

truth table then $\epsilon_{a,m} = Z$ other wise $\epsilon_{a,m} = 1$.

Claim: For some assignment to the atoms of B, $x_1 = v_1, \dots, x_n = v_n$ where $v_i \in \{0, 1\}$. Then $L(i_1, \dots, i_{2n}) = B(x_1, \dots, x_n)$.

Assume $B(x_1, \dots, x_n) = 1$ for the assignment $x_1 = v_1, \dots, x_n = v_n$ corresponding to row a of T. Then if i_k is not considered in row a then $\epsilon_{a,k} = 1$ and if it is present then $i_k = 1$. The output of h_a is given by

$$\begin{aligned} &= \prod \epsilon_{a,m}^{1-i_m} \\ &= Z^{\sum_{i_k=1} (1-i_k)} \\ &= Z^0 \end{aligned}$$

Demonstrating that $\lim_{Z \rightarrow 0} \text{Out}(h_a) = \lim_{Z \rightarrow 0} Z^0 = 1$. Consider the activation of o , it is known that $\mu_a = Z$ consequently $\lim_{Z \rightarrow 0} \mu_a^{h_a} = \lim_{Z \rightarrow 0} Z^1 = 0$, therefore

$$\lim_{Z \rightarrow 0} \text{Out}(o) = 1 - \prod_{m=1}^{2^n} \mu_m^{h_m} \quad (3.2)$$

$$= 1 - 0 = 1 \quad (3.3)$$

Therefore $L(i_1, \dots, i_{2n}) = 1$. Alternatively if $B(x_1, \dots, x_n) = 0$ then no hidden neuron will have activation 1, this can be demonstrated by considering that any relevant neuron (i.e. corresponding $\mu \neq 1$) will have some input weight pair of $i_m \epsilon_m$ such that $\epsilon_m^{i_m} = 0$. Consequently it can be said that for all m $\mu_m^{h_m} = \mu_m^0 = 1$, therefore the output unit will give 0, as required.

Now assume that L is a CNF Network. The weights can be assigned in the same manner as before, except rather than considering the rows that correspond to True the negation of the rows corresponding to False are used. If a row a corresponds to True then $\mu_a = 1$, otherwise $\mu_a = Z$ and for any literal present in the row then the input to L which corresponds to the negated literal has weight Z , all other weights are 1.

Claim: For some assignment to the atoms of B, $x_1 = v_1, \dots, x_n = v_n$ where $v_i \in \{0, 1\}$. Then $L(i_1, \dots, i_{2n}) = B(x_1, \dots, x_n)$.

In this configuration it must be shown that every hidden neuron fires when the network is presented with a variable assignment which corresponds to True and there is always at least one neuron which does not fire when the assignment corresponds to False. Assume for a contradiction that for a given assignment $B(x_1, \dots, x_n) = 1$ but $L(i_1, \dots, i_{2n}) = 0$. Then there is at least one hidden neuron which does not fire. Let h_a be such a neuron. Consequently for any input weight combination which is relevant $\epsilon_{a,m}^{i_m} = 1$, so $i_m = 0$ for any relevant input. Let i_{r_1}, \dots, i_{r_k} be the relevant inputs then $i_{r_1} \vee \dots \vee i_{r_k} = \text{False}$, so $\neg(\neg i_{r_1} \wedge \dots \wedge \neg i_{r_k}) = \text{False}$, a contradiction as then $B(x_1, \dots, x_n)$ would be False.

Now assume for a contradiction $B(x_1, \dots, x_n) = 0$ but $L(i_1, \dots, i_{2n}) = 1$. Then there exists some h_a with output 1 where it should be 0. Consequently there exists at least one input/weight pair with $\epsilon_{a,m}^{i_m} = 1$ that should be 0. Let i_{r_1}, \dots, i_{r_k} be all the relevant inputs, at least one relevant input is present i_r . Consequently $i_{r_1} \vee \dots \vee i_{r_k} = \text{True}$, therefore $\neg(\neg i_{r_1} \wedge \dots \wedge \neg i_{r_k}) = \text{True}$, a contradiction as then $B(x_1, \dots, x_n)$ is True.

□

Theorem 3.0.1 provides justification for using 2^n hidden units, it guarantees that there at least exists an assignment of weights yielding a network that can correctly classify each item in the truth table.

3.1 Noisy Gate Parametrisation

The parametrisation of Noisy gates require weight clipping, an expensive operation. A new parametrisation is derived that implicitly clips the weights. Consider that $\epsilon \in (0, 1]$, therefore let $\epsilon_i = \sigma(w_i)$, these w_i 's can be trained without any clipping, after training the original ϵ_i 's can be recovered.

Now these weights must be substituted into the Noisy activation. Consider the Noisy-OR activation.

$$\begin{aligned}
a_{or}(X) &= 1 - \prod_{i=1}^p (\epsilon_i^{x_i}) \cdot \epsilon_b \\
&= 1 - \prod_{i=1}^p (\sigma(w_i)^{x_i}) \cdot \sigma(b) \\
&= 1 - \prod_{i=1}^p \left(\left(\frac{1}{1 + e^{-w_i}} \right)^{x_i} \right) \cdot \frac{1}{1 + e^{-b}} \\
&= 1 - \prod_{i=1}^p ((1 + e^{-w_i})^{-x_i}) \cdot (1 + e^{-w_i})^{-1} \\
&= 1 - e^{\sum_{i=1}^p -x_i \cdot \ln(1 + e^{-w_i}) - \ln(1 + e^{-b})} \\
&\text{Let } w'_i = \ln(1 + e^{-w_i}), \quad b' = \ln(1 + e^{-b}) \\
&= 1 - e^{-(W' \cdot X + b')}
\end{aligned}$$

From a similar derivation we get the activation for a Noisy-AND.

$$\begin{aligned}
a_{and}(X) &= \prod_{i=1}^p (\epsilon_i^{1-x_i}) \cdot \epsilon_b \\
&= \prod_{i=1}^p (\sigma(w_i)^{1-x_i}) \cdot \sigma(w_b) \\
&= e^{\sum_{i=1}^p -(1-x_i) \cdot \ln(1 + e^{-w_i}) - \ln(1 + e^{-b})} \\
&= e^{-(W' \cdot (1-X) + b')}
\end{aligned}$$

Concisely giving equations 3.4, 3.5

$$a_{and}(X) = e^{-(W' \cdot (1-X) + b')} \quad (3.4)$$

$$a_{or}(X) = 1 - e^{-(W' \cdot X + b')} \quad (3.5)$$

The function taking w_i to w'_i is the soft ReLU function which is performing a soft clipping on the w_i 's.

3.2 Training LNF Networks

Using equations 3.5 and 3.4 for the Noisy-OR, Noisy-AND activations retrospectively allows LNFNs to be trained without the need to clip the weights.

Provide a discussion as to why single example training works best

Training the networks on all input patterns at the same time lead to poor learning, whereas training on a single example at a time had significantly better results.

The ADAM Optimizer is the learning algorithm used, firstly for the convenience of an adaptive learning rate but also because it includes the advantages of RMSProp which works well with on-line (single-example) learning [7], which LNFNs respond well to.

Preliminary testing showed that LNFN's are able to learn good classifiers on boolean gates, i.e. NOT, AND, NOR, NAND, XOR and Implies. It is also possible to inspect the trained weights and see that the networks have learnt the correct CNF or DNF representation.

3.3 LNF Network Performance

How do LNFNs perform against standard perceptron networks which we know to be universal function approximators. Two different perceptron networks will be used as a benchmark

1. One will have the same configuration as the LNFNs, i.e. 2^n hidden neurons.
2. The other has two hidden layers, both with N neurons.

The testing will consist of selecting 5 random boolean expressions for $2 \leq n \leq 9$ and training each network 5 times, each with random initial conditions. Figure 3.2 shows a comparison between all 4 of the networks and figure 3.3 shows just the LNFN's.

Re Run Performance Comparison Experiment

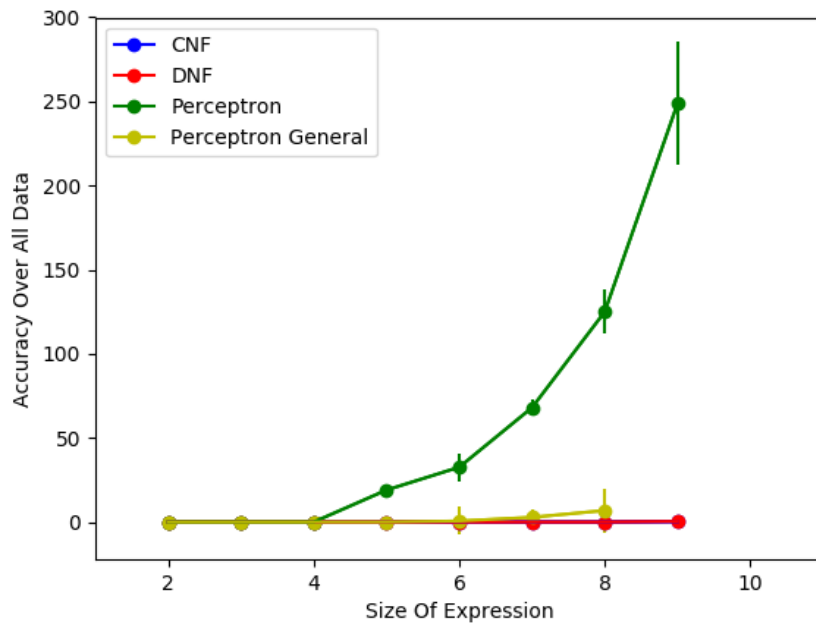


Figure 3.2

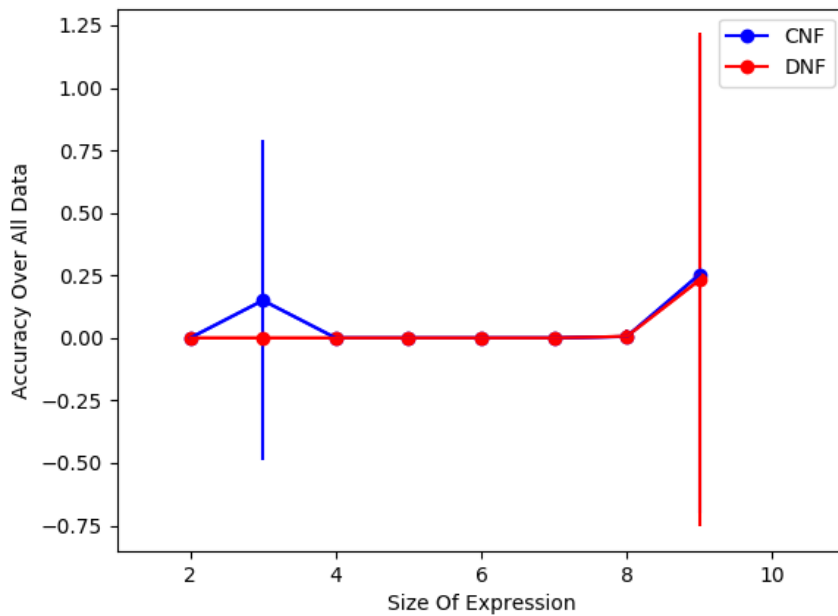


Figure 3.3

Figure 3.2 shows that neither of the perceptron networks perform as well as the LNF Networks as n increases. Figure 3.3 shows on average there are no statistically significant differences between the CNF or DNF networks. What is not present in Figure 3.3 is that sometimes the CNF network consistently out performs the DNF and visa versa, theoretically both should be able to learn any boolean expression.

What causes some expressions to be harder to learn for one type of LNFN compared to another?

3.4 LNF Network Generalization

These networks are able to perform as well as standard perceptron networks but so far they have been trained on a complete data set, in practice this will almost never be the case. Standard ANN's are widely used because of their ability to generalize, for LNFN's to be useful they must also be able to generalize.

Re Run Performance Comparison Experiment

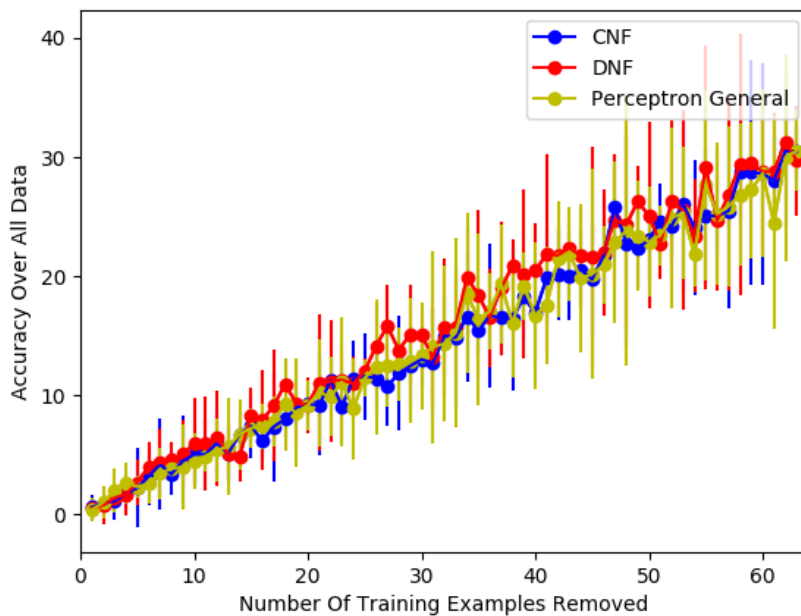


Figure 3.4

Figure 3.4 shows a comparison between the generalization ability of CNF, DNF and Perceptron networks. The graph shows the performance over all training data when successively removing elements from the training set. It demonstrates that the CNF and DNF networks generalize as well as the perceptron networks when trained over boolean problems with 6 inputs, this trend continues as n increases up to 9. Training LNFNs on boolean problems with more than 9 inputs is too expensive.

3.5 LNF Network Rule Extraction

Given the logical nature of LNFNs, is it possible to extract boolean rules. Consider the weights for a logical neuron $W = \{w_1, \dots, w_n\}$, These can be converted to $\epsilon_i = \sigma(w_i)$ where $\epsilon_i \in [0, 1]$ and represents the relevance input x_i has on the neurons output.

To extract meaningful rules from the network using $\{\epsilon_1, \dots, \epsilon_n\}$ it is important that at the conclusion of training each $\epsilon_i \approx 1$ or $\epsilon_i \approx 0$. If this is the case then it is possible to interpret

the neuron as a purely logical function, say that the neuron in question was a Noisy-OR, then the neuron can be seen as performing a logical OR on all the inputs with corresponding $\epsilon \approx 0$.

Conjecture 3.5.1 is the foundation of the following rule extraction algorithm, it was derived from experimental evidence by training LNFNs over complete truth tables and inspecting the weights. Ideally Conjecture 3.5.1 would be proved, but that is out of scope for this report.

Conjecture 3.5.1. For an LNFN network trained on a binary classification problem with boolean inputs, as the loss approaches 0 (i.e. the correct CNF or DNF has been found) the weights $\{w_1, \dots, w_n\}$ approach ∞ or $-\infty$, consequently each ϵ_i approaches 0 or 1.

The Algorithm displayed in figure 3.5 extracts rules from CNFNs, it takes the output weights (ow) and hidden weights (hw) as input and outputs the a boolean expression. A similar algorithm can be derived for DNFNs, it is omitted but can be obtained by simply switching the logical operations around.

```

1 atoms = {x1, ¬x1, ..., xn, ¬xn}
2
3 function extractRulesCNFN(ow, hw)
4   ow = σ(ow)
5   hw = σ(hw)
6   relvHidden = [hw[i] where ow[i] := 0]
7
8   and = And([])
9   for weights in relvHidden
10     or = Or([atoms[i] where weights[i] := 0])
11     and.add(or)
12
13   return and

```

Figure 3.5: Rule Extraction Algorithm (for CNFN)

In practice many clauses in the extracted expression contain redundant terms, i.e. clauses that are a tautology or a duplicate of another, filtering these out is not an expensive operation.

Section 3.4 discusses the generalization capabilities of LNFNs compared to MLPNs and shows that they are statistically equivalent. How does training over incomplete truth tables effect the generalization of extracted rules and what factors could influence this?

Consider B to be the set of all boolean problems with n inputs. What is the cardinality of B , there are 2^n rows in the truth table and 2^{2^n} ways to assign true/false values to these rows, each way corresponding to a different boolean function, consequently $|B| = 2^{2^n}$. So consider some $b \in B$ represented by 2^n rows of a truth table, removing one row from the training data means there are now two possible functions that could be learnt, one where the removed row corresponds to true and the other to false. As more rows are removed this problem is compounded, if m rows are taken then there are 2^m possible functions.

When constructing a CNF or DNF from a truth table as discussed in Section 2.4.2, in the case of CNF only the rows corresponding to false are considered and for the DNF only rows corresponding to true. Despite the fact that if m rows are removed from the training set then there are 2^m possible functions that could represent the partial truth table, learning the CNF and DNF may alleviate some of the issues caused by it, another possibility is to combine the CNF and DNF formulas to create a better rule set.

Figure 6.40 shows how the rule set of an CNFN generalizes as examples are removed, figure 3.7 shows the same but for DNFs.

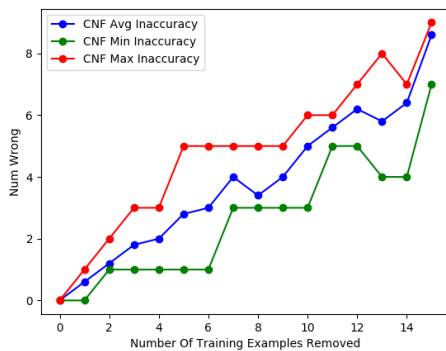


Figure 3.6

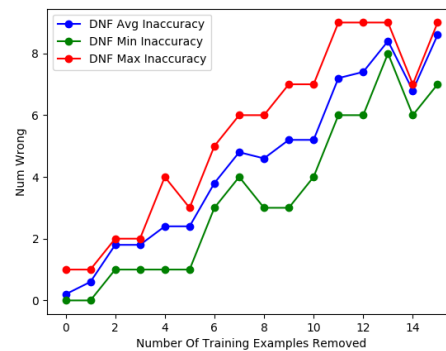


Figure 3.7

In figures 6.40 & 3.7 the training examples which are removed get randomly selected, how is the performance effected if the removed examples are chosen more carefully. In the next experiment only examples corresponding to false are removed and the resultant training set is given to a DNFN.

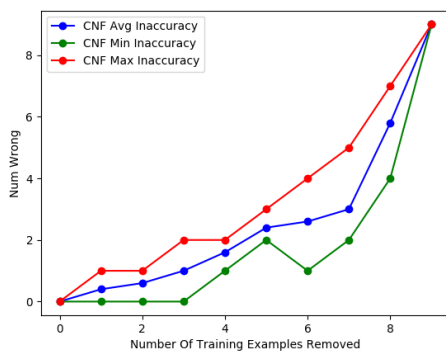


Figure 3.8

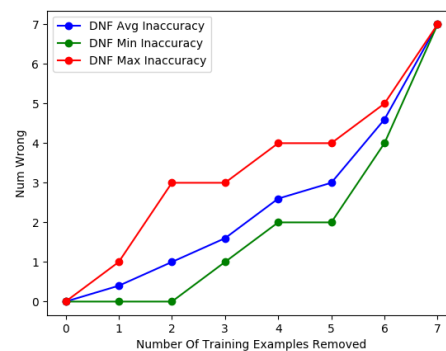


Figure 3.9

Figures 3.8 & 3.9 demontrait CNFNs and DNFNs trained over partial data retrospectively. In the case of CNFNs only true entries of the truth table are removed and for the DNFNs only false entries. For the most part the minimum line is lower however the average line is roughly the same, this would indicate that while the choice of examples removed has an effect initial conditions have a more significant influence on the generalization performance.

Chapter 4

Investigation of Logical Normal Form Networks

The LNFNs presented in Chapter 3 have only been shown to be applicable when learning boolean truth tables. This chapter investigates extending LNFNs to support multi class classification problems and continuous feature spaces.

4.1 Multi-class Classification

Extending an ANN to support multi class classification is achieved by adding more output neurons, one for each class. The value output neuron i can be considered the probability of class i . The networks output is now a vector representing the class distribution.

For example if given a problem with 3 classes then 1, 0, 0, 0, 1, 0 and 0, 0, 1 represent class 1, 2 and 3 retrospectively. The LNFN would have 3 output neurons, each representing a bit in the output vector. During the training process if the true class of an example was 1 then the desired output vector would be 1, 0, 0.

This process of converting a categorical variable to a binary string is known as **One-Hot Encoding**

Definition 4.1.1. An LNFN to solve a k class classification problem is unchanged apart from the number of output neurons which is k .

4.1.1 Evaluation

The Lenses problem [9] is multi class and contains a natural rule system making it an ideal problem for evaluating LNFNs. Each example has four features, three are binary and one categorical (of size 3). Applying One-Hot encoding to the categorical variable yields a set of instances each with length 6.

The LNFN will be evaluated against an MLPN with a two layer structure where the layer width are $2 \cdot n$ and n respectively.

The performance of the two classifiers will be compared using Leave-One-Out (LOE) Cross-Validation. The structure of the MLPN differs in the number of hidden layers/units, there are two hidden layers, one with $2 \cdot n$ hidden units and the other with n

Re Run Experiments

	Error Rate	Error Rate CI (95%)
CNF Net	-	-
DNF Net	-	-
PCEP Net	-	-

Table 4.1: Network Performance On Lenses Problem

Table 4.1 demonstrates that the CNF & DNF Networks perform comparably to an MLPN as the confidence intervals for the errors overlap.

Now that the LNFN network has three output neurons it should be possible to extract three rules describing each of the classes. Consider that each problem instance is of the following form $\{a, b, c, d, e, f\}$ where a, b, c, d, e, f are all atoms. f refers to the *tear production rate* being normal or reduced if $f = \text{False}$ or True retrospectively. Giving a description of the other atoms is not beneficial as they refer to medical terms which are unimportant.

The following rules have been extracted from a CNFN after being trained over the complete Lenses data set. Any duplicate clause or Tautology has been filtered out, the resultant extracted formula has also been manually simplified (so they can be displayed and understood better).

- Class 1: $(a \vee b \vee e) \wedge (a \vee \neg d) \wedge (c \vee e) \wedge f$
- Class 2: $(a \vee b \vee \neg c \vee d) \wedge \neg e \wedge f$
- Class 3: $(\neg a \vee b \vee c \vee \neg f) \wedge (a \vee \neg d \vee e \vee \neg f) \wedge (\neg b \vee c \vee d \vee \neg f) \wedge (d \vee \neg e \vee \neg f)$

Immediately it is possible to find useful information about this problem that was not obvious before. For example $\neg f = \text{True} \implies \text{Class 3}$, or *if the tear reduction rate is reduced then do not fit contact lenses*.

The DNFN might be more applicable as the rules will be more insightful. Each clause in the formulas represents a situation where the class is true. The formulae extracted from the DNFN confirm the previous knowledge extracted, $\neg f = \text{True} \implies \text{Class 3}$.

- Class 1: $(a \wedge \neg b \wedge \neg c \wedge e \wedge f) \vee (\neg a \wedge \neg d \wedge e \wedge f)$
- Class 2: $(\neg c \wedge \neg e \wedge f) \vee (c \wedge d \wedge \neg e \wedge f)$
- Class 3: $(\neg a \wedge \neg b \wedge c \wedge \neg d) \vee (\neg a \wedge d \wedge e) \vee \neg f$

Table 4.2 demontres the performance of extracted rules over the Lenses dataset.

Re Run Experiments

	Rule Error Rate	Rule Error Rate CI (95%)
CNF Net	-	-
DNF Net	-	-

Table 4.2

4.2 Features with Continuous Domains

The input features to an LNFN are probabilities, as such they are allowed to be continuous but must be in the range $[0, 1]$. Consider an abstractive benchmark problem such as the Iris data set [9]. An option would be to normalize all the variables to force them into the expected range $[0, 1]$. The values of all the features after normalization are compatible with an LNFN, but consider the meaning, these normalized features do not represent probabilities.

Forgetting the fact that the features do not represent probabilities and comparing the performance of an LNFN to a MLPN over the Lenses data set shows poor performance of the Logical network. The LNFN converges to a solution with a loss of 96.932, poor performance when compared to a perceptron network that can achieve loss of 0.0.

Inspecting the class prediction of each reveals that for a problem instance that has a true class of Iris-virginica or Iris-versicolor then LNFN sometimes predicts multiple classes, this leads to the belief that these networks have issues with learning problems that are not linearly separable as the two classes which an LNFN has trouble differentiating between are not linearly separable.

Not only did this result in poor performance but normalization is a crude way to apply this logical model to a situation where it does not make sense to apply it. The inputs of an LNFN should be interpretable as probabilities. Normalizing the values in the Iris data set gives values in the 0 to 1 range but you can't think of them as probabilities.

Have another experiment to show this

The experiments conducted showed LNFNs can be applied to continuous problems but only in the situation where each input variable can be thought of as a probability.

Chapter 5

Logical Neural Networks

There are two key issues with LNFNs. Firstly the number of hidden units becomes unfeasible as the number of inputs increases. Secondly if the problem size is small enough and the network can be trained the volume of hidden neurons allows for the possibility to memorise the input data.

Using what has been learnt about LNFNs the class of Logical Neural Networks (LNNs) can be defined.

Definition 5.0.1. A Logical Neural Network is an ANN where each neuron has a noisy activation.

LNNs have a more flexible structure, allowing for deeper networks and hidden layers with a variable number of hidden neurons. The current LNN model has been shown to have poor performance when compared to a Multi-Layer Perceptron Network [8]. An LNN, consisting of Noisy-OR hidden units and Noisy-AND outputs, was shown to perform worse than an MLPN.

There are two key issues caused by removing the restrictions imposed by the LNFN definition (Definition 3.0.3) which must be addressed

1. Noisy neurons do not have the capacity to consider the presence of the negation of an input. This was a problem for LNFNs as well, however given that only the negations of atoms need to be considered to learn a CNF or DNF it was easily fixed by presenting the network with each atom and its negation. The problem can not be solved so easily for LNNs. A boolean formula can not always be represented by only AND and OR gate, i.e the set of operations $\{AND, OR\}$ is not functionally complete.
2. Another problem faced by LNNs that are not restricted to be either a CNFN or DNFN is that the structure of the network will have a higher impact on whether the problem can be learnt.

Resolving Issue 1 involves making our operation set functionally complete, this requires the *NOT* operation. There are two ways to include the *NOT* operation in the LNNs, one is to simply augment the inputs to each layer appending so it receives the input and its negation. Another is to derive a parametrisation of Noisy gates which can learn to negate inputs. However both these have no way to enforce mutual exclusivity between an input and its negation.

5.1 Modified Logical Neural Network

5.1.1 Connections Between Layers & Parameters

Figure 5.1 provides a new structure for the connections between the lectures.

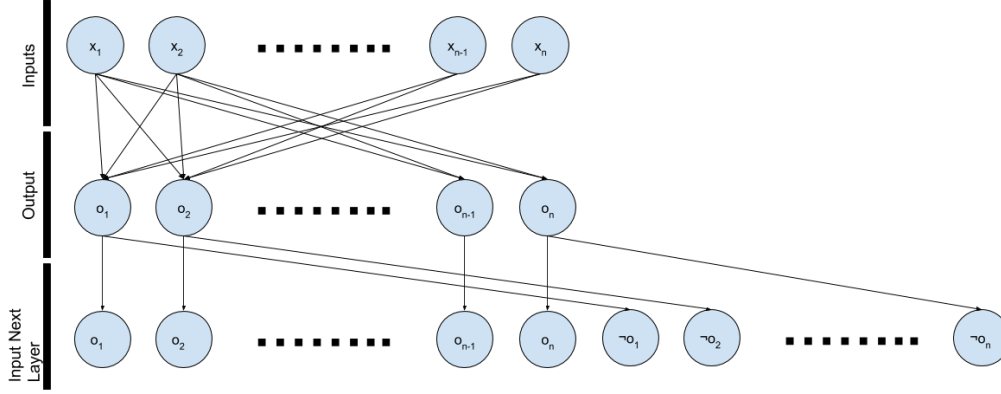


Figure 5.1

Figure 5.1 shows the new LNN structure which includes an implicit NOT operation. The input to each layer consists of the true output of the previous plus the negated output from the last layer. If a layer has 20 outputs then there are 40 inputs to the following layer.

5.1.2 Softmax Output Layer

The softmax function takes a vector of real values to a vector of values in the range $[0, 1]$ that equal 1 when summed. The softmax function highlights the difference between the maximum and smaller values by increasing this difference. It is used in multiclass classification to generate a probability distribution over the different outcomes and promote mutual exclusivity between the different classes.

The old LNN structure does not include a Softmax layer as the output layer. A traditional Softmax layer would not be effective as the neuron outputs are limited to the range $[0, 1]$. Figure 5.2 shows an example of the softmax function on probabilities, instead of highlighting the difference between 0.1 and 0.9 the resulting vector has the values closer together.

$$A = \{0.1, 0.9\}$$

$$\text{SoftMax}(A) = \left\{ \frac{e^{0.1}}{e^{0.1} + e^{0.9}}, \frac{e^{0.9}}{e^{0.1} + e^{0.9}} \right\}$$

$$\cong \{0.29, 0.71\}$$

Figure 5.2: Demonstration of Softmax on probabilities

Consider the following vector of probabilities $P = \{p_1, \dots, p_n\}$ where p_i is the probability the given example belongs to class i . Then define $p'_i = \frac{p_i}{\sum_j p_j}$, performing this action to generate a vector P' where each of the classes are mutually exclusive. This operation can be

thought of as a "Logical Softmax".

Adding a "Logical Softmax" may guarantee mutual exclusivity of each classes but will it cause the network to be less interpretable? Consider that without with no softmax then the network outputs directly represent the probabilities that the input vector is class k given the parameters. Once the "Logical Softmax" has been introduced then it becomes less clear what the non softmaxed probabilities represent. The softmax introduces a dependency between the output neurons of the network which might cause a decrease in interpetability. This is a question which will be explored during experimentation with the modified LNN architecture.

5.2 Weight Initialization

This new structure is a super set of LNFNs, it should be possible to create and train an CNFN or DNFN with the modified LNN, however this is not the case. There are many more weights in the network now. The current weight initialization technequic causes the output to saturate and nothing is able to be learnt when there exist to many neurons in the network. Before proceeding to experiment with the modified LNN a method to initialize the weights must be developed.

Deriving a Distribution For The Weights Before a weight initialization algorithm can be derived good learning conditions must be identified. Ideally the output of each neuron would be varied for each training example, i.e. $y \sim U(0,1)$. Each training example $X = \{x_1, \dots, x_n\}$ has each component $x_i \in (0,1]$, it will be assumed that $x_i \sim U(0,1)$. If the input vectors and output of each neuron are both distributed $U(0,1)$ then the input to any layer is distributed $U(0,1)$, based on this fact it can be argued that the weight initialization is the same for both Noisy-OR and Noisy-AND. Recall the activations for Noisy neurons

$$a_{AND}(X) = e^{-(w_1(1-x_1)+\dots+w_n(1-x_n))}$$

$$a_{OR}(X) = 1 - e^{-(w_1x_1+\dots+w_nx_n)}$$

Consider a random variable g , if $g \sim U(0,1)$ then $1 - g \sim U(0,1)$ also holds. Consequently, if $x_i \sim U(0,1)$ then $1 - x_i \sim U(0,1)$, also $e^{-z} \sim U(0,1)$ then $1 - e^{-z} \sim U(0,1)$. It is therefore enough to consider $e^{-(w_1x_1+\dots+w_nx_n)}$ when deriving the initialization method for each w_i .

Strictly speaking each $w_i = \log(1 + e^{w_i'})$ (as derived in Section 3.1) however for the purposes of this initialisation derivation it will be assumed that $w_i \in (0\infty]$.

Given that $y = e^{-z} U(0,1)$, a first step is to determine the distribution of z .

Theorem 5.2.1. If $y \sim U(0,1)$ and $y = e^{-z}$, then $z \sim \exp(\lambda = 1)$

Proof. Consider that $y = e^{-z}$ can be re written as $z = -\log(y)$.

$$\begin{aligned}
F(z) &= P(Z < z) \\
&= P(-\log(Y) < z) \\
&= P\left(\frac{1}{Y} < e^{-z}\right) \\
&= P(Y \geq e^{-z}) \\
&= 1 - P(Y \leq e^{-z}) \\
&= 1 - \int_0^{e^{-z}} f(y) dy \\
&= 1 - \int_0^{e^{-z}} 1 dy \\
&= 1 - e^{-z}
\end{aligned}$$

Therefore $F(z) = 1 - e^{-\lambda z}$ where $\lambda = 1$. Consequently $z \sim \exp(\lambda = 1)$ \square

The problem has now been reduced to find how w_i is distributed given that $z \sim \exp(\lambda = 1)$ and $x_i \sim U(0, 1)$. The approach taken is to find $E[w_i]$ and $var(w_i)$.

$$\begin{aligned}
E[z] &= E[w_1 x_1 + \dots + w_n x_n] \\
&= E[w_1 x_1] + \dots + E[w_n x_n] \text{ (independence)} \\
&= E[w_1]E[x_1] + \dots + E[w_n]E[x_n] \\
&= n \cdot E[w_i]E[x_i] \text{ (i.i.d)} \\
&= n \cdot E[w_i] \cdot \frac{1}{2} \\
1 &= \frac{n}{2} \cdot E[w_i] \\
E[w_i] &= \frac{2}{n}
\end{aligned}$$

$$\begin{aligned}
var(z) &= var(w_1 x_1 + \dots + w_n x_n) \\
&= var(w_1 x_1) + \dots + var(w_n x_n)
\end{aligned}$$

$$\begin{aligned}
var(w_i x_i) &= (E[w_i])^2 var(x_i) + (E[x_i])^2 var(w_i) + var(w_i) var(x_i) \\
&= \frac{4}{n^2} \cdot \frac{1}{2} + \frac{1}{4} \cdot var(w_i) + var(w_i) \cdot \frac{1}{12} \\
&= \frac{1}{3n^2} + \frac{1}{3} var(w_i)
\end{aligned}$$

Consequently the variance can be found by the following

$$\begin{aligned}
1 &= n \cdot \left[\frac{1}{3n^2} + \frac{1}{3} \text{var}(w_i) \right] \\
3 &= \frac{1}{n} + n \cdot \text{var}(w_i) \\
3n &= n^2 \text{var}(w_i) \\
\text{var}(w_i) &= \frac{3}{n}
\end{aligned}$$

From the above arguments $E[w_i] = \frac{2}{n}$ and $\text{var}(w_i) = \frac{3}{n}$. These values need to be fitted to a distribution that weights can be sampled from. Based on our initial assumptions this distribution must also generate values in the interval $[0, \infty]$. Potential distributions are Beta Prime, Log Normal.

Fitting To Log Normal A LogNormal distribution has two parameters μ and σ^2 , by the definition of lognormal $E[w_i] = \frac{2}{n} = e^{\mu + \frac{\sigma^2}{2}}$ and $\text{var}(w_i) = \frac{3}{n} = [e^{\sigma^2} - 1] \cdot e^{2\mu + \sigma^2}$. Consequently

$$\begin{aligned}
\frac{2}{n} &= e^{\mu + \frac{\sigma^2}{2}} \\
\log\left(\frac{2}{n}\right) &= \mu + \frac{\sigma^2}{2} \\
\log\left(\frac{4}{n^2}\right) &= 2\mu + \sigma^2
\end{aligned}$$

From here this can be substituted into the other formula to give

$$\begin{aligned}
\frac{3}{n} &= [e^{\sigma^2} - 1] \cdot e^{2\mu + \sigma^2} \\
&= [e^{\sigma^2} - 1] \cdot e^{\log(\frac{4}{n^2})} \\
&= [e^{\sigma^2} - 1] \cdot \frac{4}{n^2} \\
3n &= 4 \cdot e^{\sigma^2} - 4 \\
\frac{3n + 4}{4} &= e^{\sigma^2} \\
\sigma^2 &= \log \frac{3n + 4}{4}
\end{aligned}$$

Finally this substituted back gives the mean

$$\begin{aligned}
\log\left(\frac{4}{n^2}\right) &= 2\mu + \log \frac{3n + 4}{4} \\
2\mu &= \log\left(\frac{4}{n^2}\right) - \log \frac{3n + 4}{4} \\
\mu &= \frac{1}{2} \cdot \log \frac{16}{n^2(3n + 4)}
\end{aligned}$$

Giving the parameters for the log normal distribution below

$$\sigma^2 = \log \frac{3n+4}{4} \quad (5.1)$$

$$\mu = \frac{1}{2} \cdot \log \frac{16}{n^2(3n+4)} \quad (5.2)$$

Weight Initialization for LNNs Through experiments the weights sampled from a Log Normal distribution perform better than when sampled from a Beta Prime distribution. The algorithm for weight initialization can now be given but first consider that each weight that is sampled from the Log Normal distribution has the following property $w \sim LN$, $w = f(w')$ where w' can be any real value, consequently to obtain the initial weights each w must be inversely transformed back to the space of all real numbers.

```

1  function constructWeights(size):
2       $w_i \sim LN$  (for i = 0 to size)
3      return  $f^{-1}(\{w_0, \dots\})$ 

```

Figure 5.3: Weight Initialization Algorithm for LNNs

Based on experimental evidence the following Conjecture 5.2.1 can be made. Ideally a formal argument would be given, however this is out of scope for this project.

Conjecture 5.2.1. If the problem is boolean and the loss is "small enough" then similarly to LNFNs rules can be extracted directly from the weights.

The LNN structure is significant when it comes to the learnability of problems so conjectures 5.2.1 allow for determining whether a network configuration is correct.

Chapter 6

Evaluation Of Logical Neural Networks

To evaluate Logical Neural Networks their performance and interpretability are explored. There are **FILL IN** criteria that will be used for this evaluation.

1. Performance comparison between the old and new Logical Neural Network Structures.
2. Performance comparison between Multi Layer Perceptron Network.
3. Performance comparison between networks with and without Logical Softmax.
4. Comparison of interpretability between MLPNs and new and old LNNs

Through out the evaluation of LNNs the following questions concerning the affects of the two new components of LNNs will be discussed.

1. Does the modified LNN structure yield trained models with better performance than a Multilayer Perceptron Network and an LNN without the modified structure? This is without using the Logical Softmax Operation.
2. Does the modified LNN structure with a Logical Softmax yield better results than the modified structure without LSO.
3. How does the new structure effect interpretability of LNN models.
4. How does the Logical SoftMax affect the interpretability of LNN models.

6.1 Performance of Logical Neural Networks

To evaluate the performance of Logical Neural Networks (LNNs) a number of different configurations will be trained over the MNIST dataset. Given the problem is MNIST the number of input neurons will be 784 and number of output neurons will be 10. The number of training epochs will be 30.

Each experiment running on the new LNN architecture will be performed with and without an LSM

1. **(OR \rightarrow AND) Old Architecture:** This will consist of 30 hidden OR neurons.
2. **(OR \rightarrow AND) Architecture:** Same as 1 but with the new LNN architecture

3. **(AND \rightarrow OR) Architecture:** 30 hidden and neurons
4. **(OR \rightarrow AND \rightarrow AND) Architecture:** 60 Or neurons, 30 AND neurons
5. **(OR) Architecture:**
6. **(AND) Architecture:**
7. **(AND) Old Architecture:**

Results Each network is trained 30 to average the results over different initial conditions, significance tests are also conducted by creating a 95% confidence interval. The error rates displayed in Table 6.2 are on the MNIST testing data.

Network Config	Error Rate	Error Rate CI	Error Rate (with SM)	Error Rate CI (with SM)
60 \rightarrow 30	0.034	(0.031, 0.038)	0.035	(0.030, 0.040)
30	0.046	(0.042, 0.050)	0.045	(0.041, 0.050)
N/A	0.085	(0.085, 0.085)	0.084	(0.084, 0.084)

Table 6.1: Results of experiments with Sigmoid models

Network Config	Error Rate	Error Rate CI	Error Rate (LSM)	Error Rate CI (LSM)
(OR \rightarrow AND) Old	0.105	(0.098, 0.115)	0.048	(0.043, 0.052)
(OR \rightarrow AND)	0.088	(0.079, 0.094)	0.042	(0.039, 0.046)
(AND \rightarrow OR)	0.098	(0.073, 0.141)	?	?
(OR \rightarrow AND \rightarrow AND)	0.053	(0.046, 0.060)	0.032	(0.029, 0.036)
(OR)	0.382	(0.381, 0.384)	0.334	(0.331, 0.336)
(AND)	0.137	(0.135, 0.139)	0.076	(0.075, 0.079)
(AND) Old	0.312	(0.311, 0.314)	0.111	(0.109, 0.114)

Table 6.2: Results of experiments with Logical Neural Network models

By examining the following conclusions can be made

1. *New LNN Architecture Gives Better Performance Than the Old:* The confidence intervals for test set performance do not overlap for Archetctures **(OR \rightarrow AND) Old** and **(OR \rightarrow AND)** (without LSM). This can also be observed from Archetctures **(AND) Old** and **AND**.
2. *Adding A LSM Improves Performance:* Every LNN using the new architecture gets a statistically significant performance increase when a LSM is added.

The experemnts show that both the new archetcture and LSM give a stistically signif-
icant improvement in peformance. From observing **(OR \rightarrow AND) Old** and **(OR \rightarrow AND)**
(with LSM) it is possible to see that when a LSM is added then the change in archetcture
does not introduce an increase in peformance. However the oposite is true when comparing
the **(AND)** and **(AND) Old** networks.

6.2 Interpretability of Logical Neural Networks

There are two cases of interpretability. In the situation where input and outputs are discrete interpretability becomes Rule Extraction. The other situation is where the inputs are continuous.

6.2.1 Discrete Case (Rule Extraction)

To assess the rule extraction of LNNs the Tic Tac Toe problem will be the benchmark [9]. This problem involves classifying tic-tac-toe endgame boards and determining whether 'x' can win. There are 9 categorical attributes, representing each cell of the board, each cell can have 'x', 'o' or 'b' for blank.

The purpose of this application is to demonstrate the rule extraction capabilities of LNN's

This gives a total of 27 attributes, if using an LNN then the hidden layer would consist of 134217728 neurons, an intractable number, if the computer did not run out of memory then computing the gradients would be very slow.

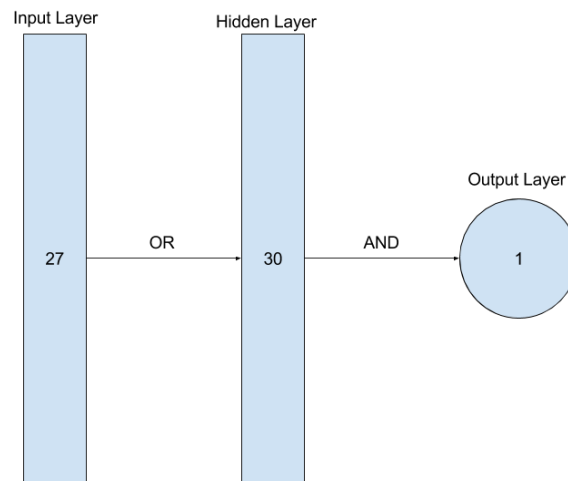


Figure 6.1

There are a total of 958 instances, 70% of which will be used for training, the rest for testing. Using the new LNN with the structure described in Figure 6.1 (using 30 hidden OR neurons) is able to achieve an error rates displayed in Table 6.3. The experiment is averaged over 30 runs

	Net Error Rate	Net Error Rate CI	Rule Error Rate	Rule Error Rate CI
Training	0.0035	(0.0035, 0.0035)	0.0000	(0.0000, 0.0000)
Testing	0.0015	(0.0015, 0.0015)	0.0259	(0.0104, 0.0451)

Table 6.3: Results of experiments with Logical Neural Networks on the Tic Tac Toe problem

What about the performance of the same network but swap around the activations? It was conjectured that networks of this form have poor learning [8] but with these new LNNs

it might not be true any more. Changing the configuration so that the AND activation is before the OR obtains a result which is better than the previous, shown in Tabel 6.4.

	Net Error Rate	Net Error Rate CI	Rule Error Rate	Rule Error Rate CI
Training	0.0035	(0.0035, 0.0035)	0.0000	(0.0000, 0.0000)
Testing	0.0015	(0.0015, 0.0015)	0.0038	(0.0, 0.0139)

Table 6.4: Results of experiments with Logical Neural Networks on the Tic Tac Toe problem on a AND - OR Network

It can be concluded that the conjecture saying that an LNN with an AND-OR configuration does not learn no longer holds.

Evaluation of LNN Rules

The rule extraction algorithm given in Figure 3.5 is an eclectic algorithm as this category describes algorithms that examine the network at the unit level but extract rules which represent the network as a whole. The algorithm is not portable as it can only be applied to networks with the LNN architecture.

Finally what is the quality of the rules extracted from LNN, this is measured by the Accuracy, Fedelity, Consistency and Comprehensibility [1].

1. **Accurate:** As demonstrated experimentally the extracted rules are able to generalise well to unseen examples.
2. **Fedelity:** The experiments show that the rules perform very similar to the network they where extracted from.
3. **Consistency:** Through the previous experements the extracted rules from each interation only had 8% overlap between the ones which where incorrectly classified. This was found by taking the average proportion of the ones incorrectly classified over one interation compared to all iterations.
4. **Comprehensibility:** The upper limit of the size of the rules is related to the number of layers and neurons. The OR AND model obtains a complex set of rules, in total 35 of the OR clauses are considered by the output neuron. On the otherhand the AND OR model only utilizes 11. The structure also contributes to the comprehensibility of the rules. For instance each clause in the AND OR rules represent a situation where the rule set is true.

6.2.2 Continuous Case

In the continous case extracting boolean rules is not possible as each input no longer represents a boolean but rather a degree of truth. In terms of MNIST, being able to construct an image representing how relevant each input feature is to each of the possible output neurons would allow visual verification that the network has learnt something interesting.

Determining the influence that the inputs to a layer have on the outputs of the layer is trivial. The definition of weights from one layer to another directly correspond to how much influence the corresponding input has. Computing the influence that a neuron has across layers is not so simple.

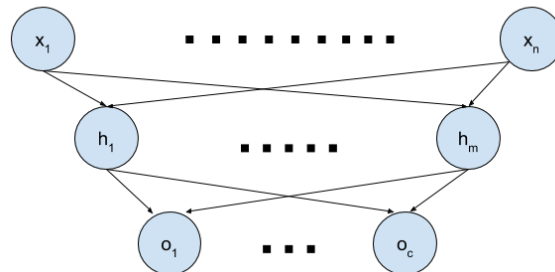


Figure 6.2: Example Network

Consider the problem of trying to determine how each x_i effects each o_j . This is quivalent to trying to find ϵ'_i in the following equation. Note that exponent on each ϵ refers to the neuron it belongs to

$$(\epsilon'_i)^{x_i} = \prod_{k=0}^m (\epsilon_m^{o_j})^{\prod_{b=0}^n (\epsilon_b^{h_k})^{x_b}}$$

This new ϵ is dependent on all the other x_i 's, not just the one of interest. Consequently it is only possible to directly compute the effects of the input features on the first layer of hidden neurons.

Without the possibility of computing the output neurons as direct functions of the input features another method to interpret the knowledge inside the LNN is needed. Consider the case of a LNN with 1 hidden layer. The approach will be to compute all the hidden neurons as function of the inputs, then using the weights from the hidden neurons to outputs rank the most important hidden neurons for each classification.

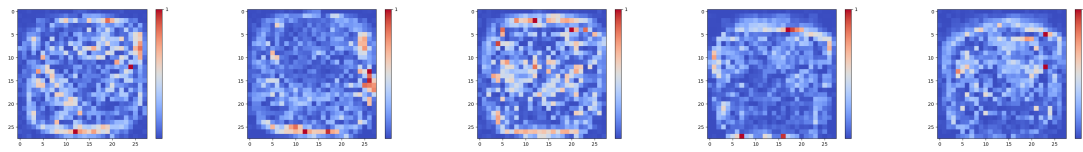
Intepretability will be assessed by comparing various MNIST models using the new architecture again each other but also the original LNN model. Part of this assment will be to determine what effects the LSM has on the model interpretation.

To compare the intepretability of the old and new architectures aingle layer AND model will be used, this model has been shown to have a high accuracy and it is simpler to interpret as it does not contain any hidden layers.

An attempt will be made to interpret some multi layer models as these get better performance and therefore are more practical to use.

No Hidden Layer Networks

Sigmoid Network In the depictions of weights from a sigmoid network the blue represents a negative value and the red represents are positive weights. The features do not appear to represent any intepretable features of the digits.



Digit 0

Digit 2

Digit 4

Digit 7

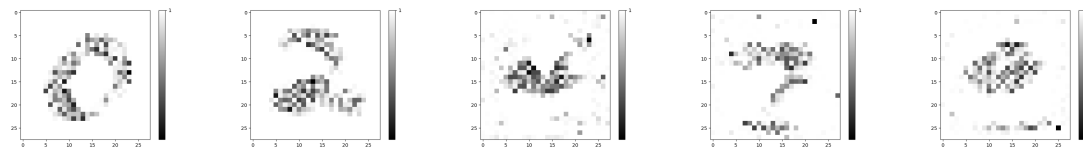
Digit 9

Figures representing the output neurons of a sigmoid neural network with no hidden layers

AND Network Old Architecture (With and With Out LSM) The network without an LSM is using the pixels which occur in all representations of each digit. On the other hand the network with an LSM is using the average border to achieve its classifications. Both models are interpretable as it is possible to understand the logic used in their decision making.

Each of the models describe the problem in a different way, uncovering different information. The model without an LSM shows describes what is common between every drawing of that digit. The model with an LSM demonstrates which parts of each digit vary the most and what parts are reasonably confident.

The one benefit that the model with an LSM has over the other is that more of the output neurons look to visually represent the digit they are supposed to classify.



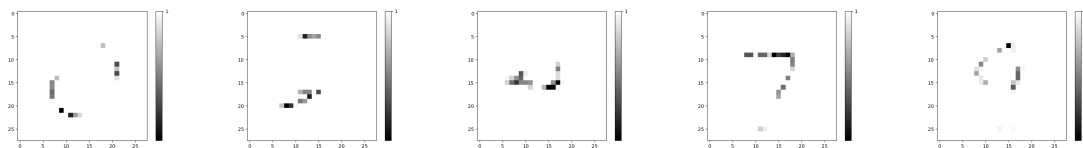
Digit 0

Digit 2

Digit 4

Digit 7

Digit 9



Digit 0

Digit 2

Digit 4

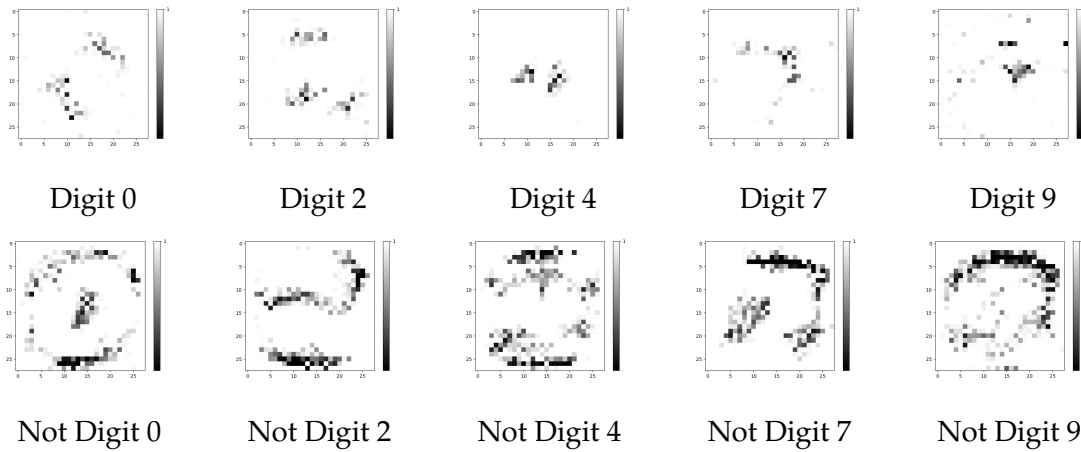
Digit 7

Digit 9

Figures representing the weighted connections between the inputs and outputs in an AND network with the old architecture. Top row is with an LSM and bottom row is without an LSM

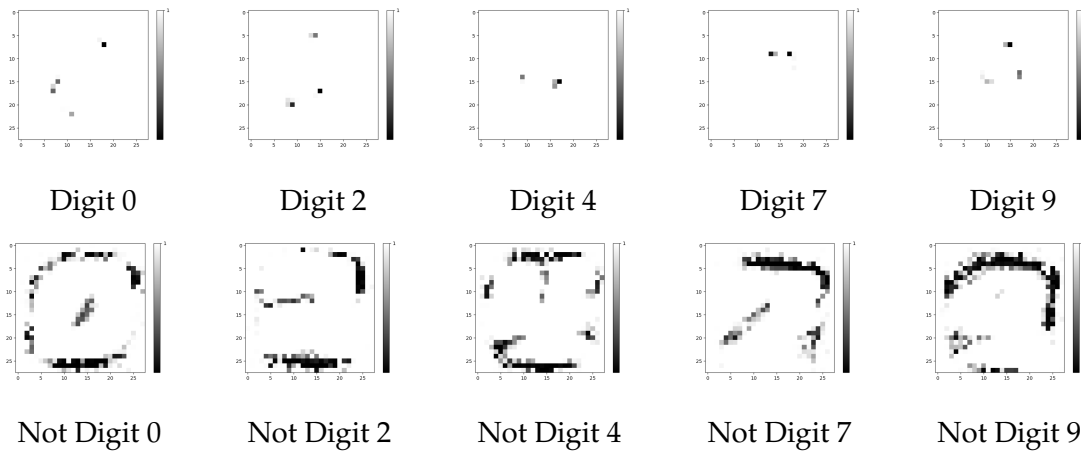
AND Network (With LSM) The top row of images represent positively weighted inputs and the bottom row represents the negatively weighted inputs.

These weights are providing two sets of information. The inputs which are positively weighted are the pixels that occur in many of the representations of the digit. Negatively weighted inputs represent the border of the digit, if pixels on this border are present then the neuron is less likely to be active. Using the classification of 0 as an example. The network does not like pixels in the middle as the center of a zero should be empty. The outer circle represents the border of the average 0, if these pixels are present then it's less likely to be a zero as most instances of a 0 do not have pixels present there.



Figures representing the weighted connections between the inputs and outputs for an AND network with an LSM. The top row shows the pixels that when present contribute to the classification as the digit while the bottom row shows the pixels which when they are not present contributes to the classification

AND Network (With out LSM) This appears to be performing classification in the same way as to the AND Net with an LSM. However there is a key difference, this network has much harder boundaries compared to the softer and nosier boundaries for the AND network with LSM.



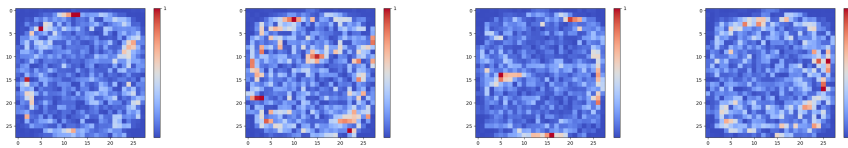
Conclusion of Intepretability for LNNs with No Hidden Layer The logical soft max introduces more noise into the weights but do not diminish the intepretability of the system. Using the new structure (i.e. adding nots of inputs) appears to change the means of which the LNN classifies the digits. Without the nots the network positively weight the pixels which make-up the filling of the digits. On the other hand when the nots are added the network negatively weights pixels sitting just outside the border of the average digit.

Compared to the Sigmoid network the LNNs are more intepretable as it is possible to make determinations about how the network is making its classification decisions. Based on this experemental evedence it is possible to conclude that in the context of LNNs with no hidden layers the new LNN archecture and LSM improve the intepretability.

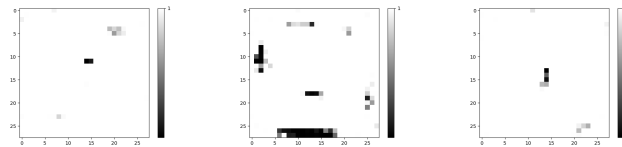
Single Hidden Layer Networks

Interpreting these multilayer models is a more difficult task as the hidden layer introduces dependencies between the inputs when considering how they influence the classification. To test the interpretability of these networks assume the goal is to verify that the digit 1 is being classified in a sensible way. With each network the hidden neurons which have the most influence on the classification be 1 will be displayed.

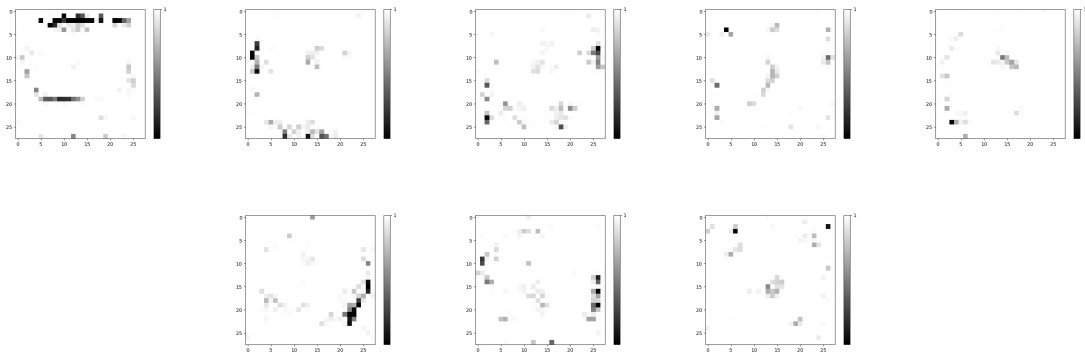
Sigmoid Network The hidden features learnt by the Sigmoid Network do not appear to represent any meaningful information about the digit 1.



OR \rightarrow AND Network Old Structure (With Out LSM) When considering that these hidden features represent an OR of the inputs it can be seen how they might makeup a 1. The first and last appear to be the stem of the 1 where as the middle one contains a dark bar at the bottom which could be the base.



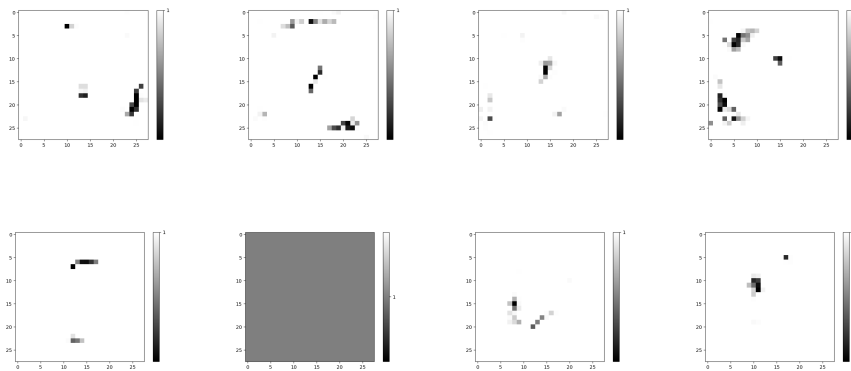
OR \rightarrow AND Network Old Structure (With LSM) In a similar fashion of the OR AND Network without an LSM these features are not clearly representative of a 1. Moreover these features generally do not place a lot of emphasis on any particular input features.



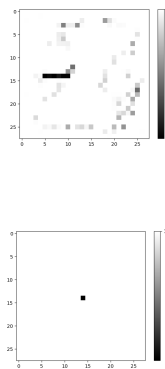
With LSM

OR → AND Network (With Out LSM) This network is running on the new architecture and as such each feature has two "channels", one representing the inputs that feature positively likes and the other the inputs which are negatively liked (i.e. neuron is more active when these inputs are not present).

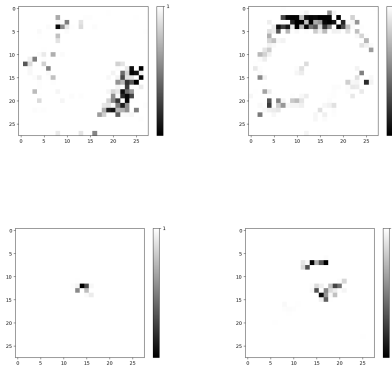
The features below represent the ones which if present contribute to the classification being a 1. These features are sparse and place a high weight on the inputs which they like.



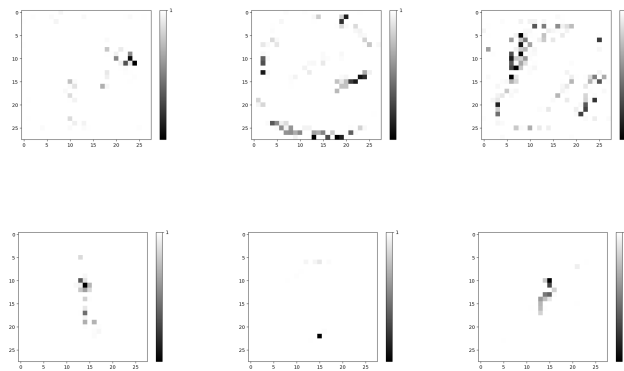
The following feature contributes to the classification of being a 1 if its not present. This would appear to represent the outer border of what could be a 1.



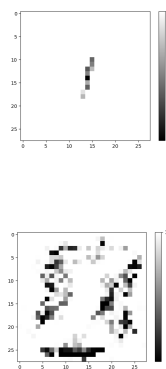
OR \rightarrow AND (With LSM) The features extracted from this network do not appear to correspond to a 1, not in a way which is immediately interpretable. Below are the features which are positively weighted towards a 1.



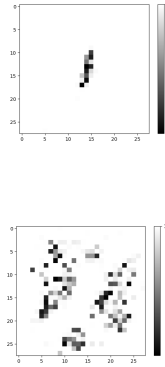
The following features are the ones which are negatively weighted towards being a 1.



AND \rightarrow OR Model (With Out LSM) This network has a small number of features associated with each classification. In terms of the classifying the digit 1 there is only 1 hidden features. This feature appears to classify a 1 by positively liking the stem of a 1 and disliking the anything outside the average 1.



AND \rightarrow OR Model (With LSM) Similarly to the AND OR Model with out the LSM this model appears to positively like the inputs on the stem of a 1 and dislike any pixle outside the average border of a 1.



Conclusion of Intepretability for LNNs with No Hidden Layer The results of the experiments show that in the context of multi layer adding an LSM introduces more noise into the feature maps. And similarly to before the sigmoid weights do not appear to relate to digit 1 in any meaningful way.

Results

From the above experiments and discussions the following conclusions can be made

1. *Adding Nots Improves Intepretability:* Using the new structure with nots allows the network to place a greater emphasis on the presence or absence of various pixles. Without the Nots not many of inputs are of great importance, rather many have a relatively small relevance.
2. *Adding an Logical Soft Max does not hinder the intepretability (on the new architecture):* By comparing the two different network architectures with and without an LSM it is possible to see that the intepretability is not directly effected and the features representing the classification of the digit 1 are not significantly changed.
3. *Intepretability of Network is Heavily Dependent on Structure:* As shown through the previous examples the OR \rightarrow AND networks harder to interpret than the AND \rightarrow OR architecture.

6.3 Summary Of Logical Neural Network Evaluation

Each of the Logical Neural Networks with a Logical Soft-Max has been shown to have either statistically equivalent or better performance than the corresponding Multi-Layer Perceptron Network. The addition of a Logical Soft-Max gives around a 50% increase in performance. The new structure does not appear to make a statistically significant difference in the peformance of LNNs.

By assessing the intepretability of LNNs it was found that the new structure (adding NOTs) promotes a more intuitive learnt representation and inclusion of an LSM does not

hinder the interpretability but does increase the noise in the weights.

Using the new LNN structure and LSM yields more interpretable models with an increased performance.

Chapter 7

Application to Auto Encoders

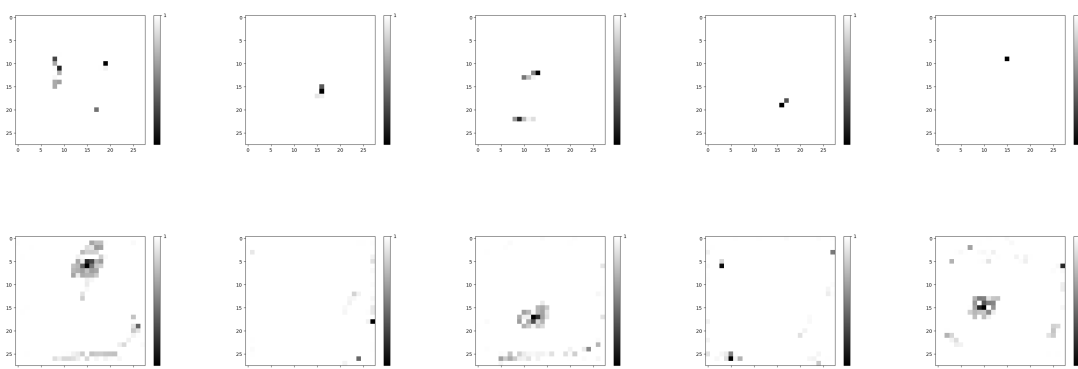
Auto encoders [2] are a network architecture which aim to take the input to some reduced feature space and then from this feature space back to the original input with the smallest error. The case where there is one linear layer doing the encoding and decoding is called **Linear Autoencoder**, this architecture corresponds to performing Principle Component Analysis (PCA) on the data.

For some data sets, such as MNIST, PCA is not an effective way to reduce the dimensions of the data **NEED CITATION**. For this reason Logical Autoencoders are proposed (Definition 7.0.1) as an alternative means to lower the dimensions of a dataset.

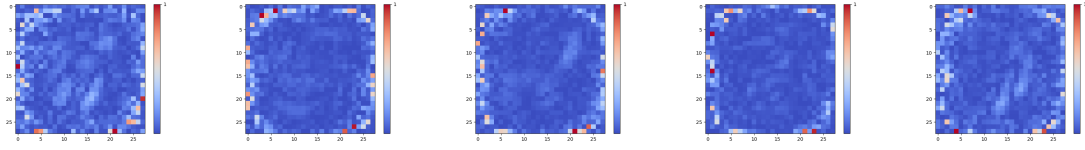
Definition 7.0.1. A **Logical Autoencoder** is an Autoencoder where the encoder and decoder are LNNs

The experiments carried out will be to compress the MNIST feature space (784 dimensions) into 10 dimensions using different Auto encoder architectures. The accuracy and interpretability of the features will be explored. Each model was trained for 30 epochs

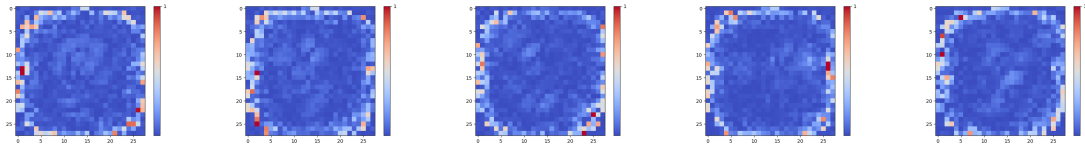
Result of Logical Auto Encoder (LoAE) A logical auto encoder, consisting of a single AND layer for both the encoder and decoder, was able to compress the feature space to 20 dimensions and achieve a Mean Square Error (MSE) of 20.55 on the training set and 20.22 on the testing set.



Result of Linear Auto Encoder (LAE) A linear auto encoder obtained an MSE of 21.34 on the training and 21.25 on the test data.



Result of Sigmoid Auto Encoder (SAE) A sigmoid autoencoder achieved an MSE of 14.43 on the training data and 14.25 on the testing data.



Discussion While the results show that the Sigmoid Auto Encoder (AE) outperforms the Logical one this is an example of how Logical Neural Networks can be applied to different situations in Machine Learning where the goals are different from classification. The features learnt by the Logical AE are sparse and possibly interpretable as each one can be viewed as a logical AND of the input features.

A Logical Auto Encoder provides a means to trade off between the interpretability of the model and the performance.

Chapter 8

Conclusion

The growing number of situations where Artificial Neural Networks (ANNs) are used is driving the development of interpretable models. Being able to defend an ANNs decision can protect users from unsafe or ethically biased systems and protect companies utilizing such systems from breaching EU regulations.

This report derived modifications for the LNN structure giving them statistically equivalent performance to standard Multi-Layer Perceptron Networks and improving the interpretability of the learnt models. Consequently this report has shown that LNNs are a suitable alternative to Multi Layer Perceptron Networks, obtaining an interpretable model and without sacrificing accuracy. LNNs are however limited in the domains to which they can be applied.

By observing the weights of LNNs trained over the MNIST data set it was possible to determine what input features contributed to each classification and verify that the logic learnt was "sensible". The experimentation also revealed a limitation of LNNs, obtaining an interpretable model is not as simple as using any LNN. Interpretability depends on the choice and order of the logical activations. A future study might aim to demonstrate interpretability by using LNNs to learn a variety of problems and then perform user studies on domain experts. The motivation behind LNNs is to allow verification of decisions, a person whose job is to grant or deny bank loans should be able to interpret an LNN trained to perform such a task.

Beyond applications to classification tasks Logical Neural Networks were applied to Auto Encoders. While the performance of Logical Auto Encoders was worse than standard Sigmoid Auto Encoders it demonstrates the flexibility of LNNs and the range of situations where they can be applied.

Perhaps the biggest limitation of LNNs comes down to interpreting multi layer logical neural networks. It is possible to directly extract the influence each input feature has on the outputs in LNNs with no hidden layers. However hidden layers introduce dependencies between input features making it difficult to find a direct influence of inputs on the outputs. Because of this limitation any future work which can develop better ways to interpret these models would increase the power of LNNs.

This report has provided a formal foundation for Logical Neural Networks and shown their ability to not only learn accurate but also interpretable models. While limitations have been identified this does not diminish potential of LNNs but rather provides avenues to increase their application.

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