

Comprehending Neural Networks

via Translation to And-Inverter Graphs

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Part I

Introduction

Abstract This thesis gives a novel algorithm \mathcal{N} that helps users understand neural networks by abstraction to and-inverter graphs (AIGs). I find that AIGs are more comprehensible than neural networks due to their conciseness. For small neural networks, \mathcal{N} consistently creates AIG abstractions with perfect accuracy. However, translating large neural networks to AIGs introduces the memorization versus generalization problem. Here, memorization elicits noise and reduces the comprehensibility of the AIG. To extract generalization, I tested an ensemble of AIGs over separate neural networks. Illustrating this highly accurate AIG ensemble as a single AIG is a promising next step to creating concise, generalized, and accurate neural network abstractions.

Format This thesis is divided into five parts: introduction (Part I), background (Part II), methods (Part III), results (Part IV), and the appendix (Part V). Part I gives a summary of the thesis. Part II clarifies definitions and surveys related work. The fine details of my work are presented in Part III. Part IV gives a conclusion and suggests future work. Finally, refer to Part V for a reminder of common abbreviations, mathematical symbols, and other definitions.

Purpose This thesis was funded by the AFRL Research Grant FA8650-20-F-1956 with co-directors Dr. Robert Ball and Joshua Jensen, M.S. to research explainable artificial intelligence. Furthermore, this thesis coincided with my ambition to understand complex structures, create novel algorithms, research the philosophies of comprehension, and further artificial intelligence.

Chapter 1

Introduction

1.1 Background Summary

Neural networks (NNs) are powerful machine learning techniques, yet they are exceptionally difficult to understand due to their intricate structure. From the many techniques analyzing neural networks [3, 4], three generic categories are derived: decompositional, eclectic, and pedagogical.

Decompositional techniques consider individual weights, activation functions, and the finer details of the network. For example, learning each node in the neural network is a decompositional technique.

On the other hand, a pedagogical approach learns by an oracle or teacher—allowing a relatively facile change in underlying machine learning structures. For example, a simple pedagogical approach may be a decision tree whose training inputs are fed into a neural network, and the decision tree’s learned class values are the output of the neural network. This simple pedagogical approach can easily transition from the neural network black box to another machine learning algorithm.

Finally, eclectic approaches consider the neural networks as a gestalt—a figure whose sum (big picture) is more valuable than the individual parts (details). Namely, the eclectic approach combines the decompositional and pedagogical approaches. An example of an eclectic approach is directing a learning algorithm over neural nodes (decompositional) while omitting inputs negligible to the final product (pedagogical). In this paper, I take an eclectic approach with localized learning of each neuron (a decompositional technique) with directions given by the latter layers (partly pedagogical).

1.2 A Comprehensible Medium

In Chapter 4, I argue that a comprehensible structure must be concise and that AIGs are more concise than neural networks. As such, this thesis understands neural networks via translation to AIGs.

AIGs AIGs (And-Inverter Graphs) are formally verifiable (provable with formal methods) and legacy white box structures. The AIG is a directed, acyclic graph that consists of an input layer, a finite or null amount of intermediate layers, and an output layer. Besides the input nodes, every node in an AIG is binary and performs logical conjunction upon its two in-edges. Additionally, every edge in an AIG can invert inputs (perform a logical NOT), hence the term “And-Inverter Graph”.

Software Fortunately, open-source implementations of AIGs with active maintenance already exist. I use Mockturtle from the EPFL’s Logic Synthesis Library [5] to translate the intermediate representation (a network of lookup tables) to an AIG. Additionally, I use Brayton and Mischenko’s ABC software [1] to simplify and visualize the AIGs.

1.3 Neural Networks Considered

As described in Chapter 2, neural networks have many forms. This thesis will only consider a subset of all possible neural networks.

Types Allowed The intended neural network is a feed-forward, sequentially layered, fully connected, multi-layer perceptron (a traditional neural network). Meaning if and only if some node A is in a layer i (a hidden layer), then each node in layer i-1 has a directed edge ending at A and A begins a directed edge to a node if and only if the node is in layer i+1.

Formal Definition Let the transition set be δ and each sequential layer be expressed as L_i . Then this algorithm allows any neural network with the property

$$i \in L_{l-1}, j \in L_l \longleftrightarrow (i \rightarrow j) \subseteq \delta$$

for any output or hidden layer L_l .

If a neural network meets the requirements above except for being fully connected, one can create pseudo-edges with a weight of zero for it to become a fully connected neural network.

1.4 Converting Neural Networks to AIGs

This section describes how I convert neural networks to a network of sum of products (SoP) that is easily translated to an AIG.

Definitions Let the traversal over the neural network be called \mathcal{N} (Algorithm 4), the optimized binary decision tree that approximates activation functions (Section 2.1) be \mathcal{B} (Section 8.2), and the network of SoPs be \mathcal{T} . The feature space is already binarized (Section 10.2.1) and the neural network is trained.

Decision Tree (\mathcal{B}) Traditional decision trees that use information gain or Gini impurity are too powerful and computationally expensive than what is required. I present \mathcal{B} —a linear and optimized binary decision tree that accurately finds the SoP for a neural node. See Section 7.2 and Section 7.3 for details on the activation functions \mathcal{B} can approximate. Furthermore, \mathcal{B} had the same predictions as the traditional decision trees for these activation functions (see Section 6.4). Since \mathcal{B} creates the network of SoPs \mathcal{T} ad hoc, \mathcal{B} is never stored.

Complexity \mathcal{B} is in $\Omega(n)$ and $O(2^n)$ with an average of $O(2^{0.5n})$ where n is the amount of in-degree weights for the given node (Chapter 9). Cook’s Theorem states that the Boolean satisfiability problem is NP-complete [6]. Since \mathcal{B} is a type of Boolean satisfiability, placing \mathcal{B} in P space would be an unlikely and phenomenal feat. However, \mathcal{B} still managed to get an impressive average-case complexity. Note: after I created \mathcal{B} , Shi et al. found an older algorithm that computes what \mathcal{B} does in $O(2^{0.5n}n)$ time [7].

Parsing (\mathcal{N}) \mathcal{N} traverses the neural layers in reverse—from the output layer (L_n) to the first hidden layer (L_1). Traversing L_i before L_{i-1} allows any negligible nodes in L_{i-1} to be skipped entirely. Nodes within a layer are independent of each other and can be naïvely parallelized. Each neural node is only parsed over once (and possibly skipped).

Translation Summarized Succinctly, \mathcal{N} parses over the neural network in reverse and employs \mathcal{B} to find the sum of products as needed. Then an AIG is produced.

1.5 Reasoning and Results

Comprehensibility The esoteric nature of the neural network is due to the complexity of and vast amount of nodes, weights, summations, multiplications, and activation functions. Since AIGs are simpler and more concise than neural networks, they are relatively comprehensible. In Chapter 4, I provide further analysis on comprehensibility considering the overall complexity of the neural network and how interpretable the basis (input names and values) is.

Practicality and Results \mathcal{N} successfully translated simple neural networks to concise AIGs with perfect accuracy. However, the translation of large neural networks suffered from the memorization versus generalization problem and elicited noise. Future work of an AIG ensemble to reintroduce generalization is investigated in Section 10.3. A concise and accurate AIG provides another tool for machine learning experts to use in debugging, analyzing, and understanding the complex neural networks and their corresponding data. Notably, AIGs cannot abstract some functions found by neural networks enough to be comprehensible as some functions are inherently complex and difficult to understand.

Part II

Background

Chapter 2

Neural Networks

Traditional neural networks train on a data set containing inputs and classifications (supervised learning). After training, the neural network predicts classifications for new inputs.

Neural networks in machine learning originated from the McCulloch and Pitts paper that modeled how neurons might work [8]. A major milestone of the neural network was overcoming the XOR problem which was solved by backpropagation (discovered by [9] and solved by [10]). See [11] for a survey on the theory of neural networks and [12] for a survey on deep neural network architectures and their applications.

2.1 Structure

A lack of formal definitions for neural networks hindered formal proofs in the neural network's early decades. E. Fiesler gave a flexible hierarchical and a universal mathematical definition to give the field a solid and formal foundation [13]. Below is a summary of his hierarchy with some added research.

- **Topology**
 - **Framework**
 - * **Number of clusters** (i.e. layers or slabs). Layers and slabs are both subsets of neurons with the same hierarchical level, however, layers are ordered while slabs need not be. Not enforcing order means that the neurons in a slab can be rearranged.

- * Number of neurons in each cluster
- Inter-connection scheme
 - * Connection types
 - **Interlayer connections** are connections between adjacent layers and are the most common connection type.
 - **Intralayer connections** connect neurons of the same layer. A self-connection is a type of intralayer connection where the neuron connects to itself.
 - **Supralayer connections** connect a neuron to a layer that is neither adjacent nor in the same layer.
 - * **Connectivity** defines how dense the connections are among the neurons. A fully interlayered-connected network is commonly shortened as a fully connected network—this thesis will use this shorthand version. A plenary neural network is a neural network with all possible connections in the interlayer, intralayer, and supralayer domains.
 - * **Symmetry versus asymmetry.** A symmetric connection uses the same weight for both directions (i.e backpropagation and forward feeding). An asymmetric connection uses one weight for both directions.
 - * **Order.** Higher-order connections combine the outputs of several neurons as a single input—usually by multiplication. Specifically, a higher-order connection that combines N outputs is called an N^{th} -order connection. Furthermore, the highest-order connection determines the order of the entire network. Most neural networks are first order.

- Constraints

- **Weight value range** is the set of values an output may be amplified or diminished by.
- **Local threshold value range** holds the values allowed for an offset for each neuron’s activation. This is often perpetuated with a bias node (neuron) at each hidden layer.
- **Activation range** is the set of values a neuron may output.

- Initial state

- **Initial weights.** These should be created with random numbers to break symmetry which mitigates the potential null space. Intuitively, allowing the initial weights to be in a substantial subset of the weight value range would further rupture symmetry; however, larger initial weights may result in exploding values during propagation [14].
- **Initial local thresholds.** The bias nodes can be set with heuristically chosen constants (often the constant equals one). The weights attached to the bias node are chosen as described for initial weights.
- **Initial activation functions.** Commonly, the initial activation functions are unchanged throughout the training process.
- **Transition functions** update the state of the neural network.
 - **Activations functions** (neuron functions) translate the inputs of a neuron to its respective output given some function $a(x)$.
 - **Learning rules** dictate how weights will be updated.
 - * **Cost functions** (also called loss functions or error functions) determine the magnitude of a penalty given a miss. A correct prediction suffers no penalty [14].
 - * **Optimizer functions** use the cost found in the cost function to update the weights.
 - **Clamping functions** decide if a neuron will consider incoming information.
 - **Ontogenetic functions** change the neural network’s topology.

Neural Networks Considered This thesis will focus on the most common neural networks. Specifically, they will be fully interlayered-connected, symmetric, first-order neural networks with some finite amount of layers and nodes. The networks are trained on a binary data set so binary cross-entropy will be the loss function. The Adam optimizer (a stochastic gradient-based optimization algorithm [15]) is used throughout this thesis unless mentioned otherwise. Despite training on a binary data set, the activation functions are real-valued. The types of activation functions recommended are discussed in Section 7.3 and Section 7.2. The initial weights are randomly initialized to

small values. Bias nodes with a value of one are used in every layer except the output layer unless stated otherwise. Activation functions will not change over time. Furthermore, the clamping and ontogenetic functions will not be considered.

Feedforward Some examples in this thesis use matrix notation to describe part of the feedforward process. Simply, \vec{x} is the vector of inputs and \vec{w} is the vector of weights. Furthermore, $\vec{x} \cdot \vec{w}^T = \theta$ where θ is the dependent variable for some activation function f . For example, when computing the activation function $f(\theta)$ for H_1 in Figure 2.1, $\vec{w} = (X_1 \rightarrow H_1, X_2 \rightarrow H_1, bias_node \rightarrow H_1) = (4.4638, -4.4073, -2.6025)$ and $\vec{x} = (X_1, X_2, 1)$. So if $X_1 = X_2 = 0$, then $\theta = -2.6025$ and H_1 will output $f(-2.6025)$.



Figure 2.1

2.2 Types of Activation Functions

Identity Function The identity or linear activation function is $f(x) = cx$ where c is a predefined constant. If a neural network is filled with identity activation functions, it can only discriminate linearly separable data (see Figure 2.2 for an example). The linear function is sometimes used for the output neuron to allow a prediction of any real number (given the constraints of the system).

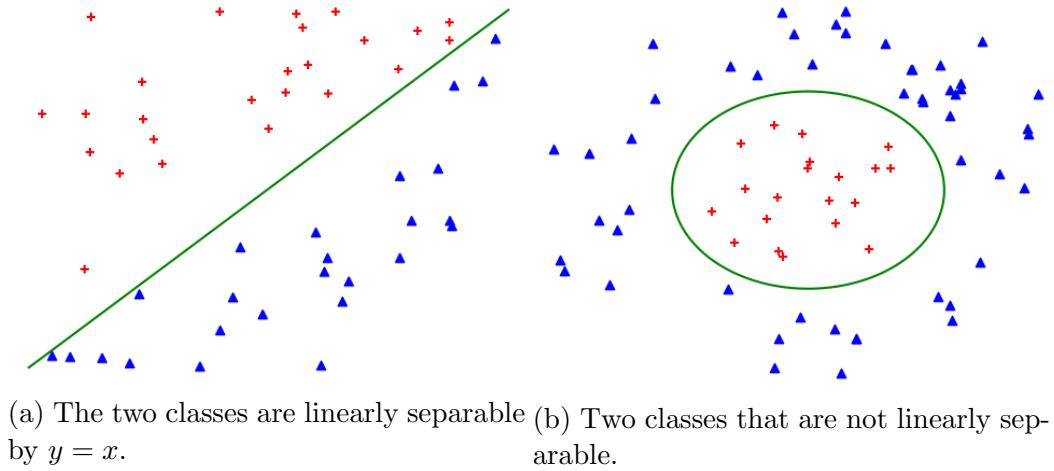


Figure 2.2

ReLU The Rectified Linear Unit function (ReLU) is $f(x) = \max(0, x)$. ReLU is the simplest nonlinear activation function and is commonly used in deep learning for its simple derivatives [14]. To remedy the loss of information in the $\max(0, x)$ cast, leaky ReLUs ($f(x) = \max(cx, x)$ for $0 < c < 1$) are a similar function that still allow negative values to propagate. Swish is a differentiable function similar to the ReLU [16].

Sigmoids Sigmoid functions take the shape of an “s” and are commonly used for binary classification. Examples of sigmoid activation functions and their output range (\mathcal{R}) include

- $f(x) = \frac{1}{1+e^{-x}}$. $\mathcal{R} \in (0, 1)$, exclusively.
- $f(x) = \tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$. $\mathcal{R} \in (-1, 1)$, exclusively.

- $f(x) = 1.7159 \tanh(\frac{2x}{3})$. $\mathcal{R} \in (-1.7159, 1.7159)$, exclusively.

Since the hyperbolic tangent (\tanh) can be computationally expensive, LeCun et al. recommend using $f(x) = 1.7159 \tanh(\frac{2x}{3})$ which allows for an approximation with a ratio of polynomials [17]. Symmetric or odd sigmoids (sigmoid functions that do not change when reflected across the line $y = -x$) often converge faster than the logistic function $f(x) = \frac{1}{1+e^{-x}}$ [18]. This is partially due to symmetric sigmoids allowing negative activations. In neuroscience, positive and negative activations are called inhibitory and excitatory, respectively. As negative activations can help neural networks, inhibitory neurons help the human cortex [19].

Softmax While sigmoid functions can be described as a probability distribution over a binary classification, softmax activations give a probability distribution over n classifications. Essentially, each class is given a log probability similar to the logistic function above. Each log probability is then normalized by dividing the log probability by the sum of all log probabilities. By performing normalization, all probabilities in the vector sum up to one [14] (see Algorithm 1 for an algorithmic description). After the softmax is computed, the input with the highest probability is predicted.

Algorithm 1: The softmax function.

Input: \vec{a} , the input array.
Output: P , an array of probabilities.
forall $a_i \in a$ **do**

$$\quad \left| P[i] \leftarrow \frac{e^{a_i}}{\sum_{a_j \in a} e^{a_j}};$$

return P

Summary of the Common Activation Functions

$$\text{ReLU: } f(x) = \begin{cases} x, & \text{if } x > 0, \\ 0, & \text{if } x \leq 0. \end{cases}$$

$$\text{Leaky ReLU: } f(x) = \begin{cases} x, & \text{if } x > 0, \\ cx, & \text{if } x \leq 0. \end{cases}$$

$$\text{Swish : } f(x) = \frac{x}{1 + e^{-x}}$$

$$\text{Logistic: } f(x) = \frac{1}{1 + e^{-x}}$$

$$\tanh: f(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$$

$$\text{Softmax: } \max(P) \text{ for } P(a_i \in Z) = \frac{e^{a_i}}{\sum_{a_j \in Z} e^{a_j}}$$

Since Keras allows many of these [activation functions](#), custom activation functions, and granular control and inspection of neural networks, Keras (with the Tensorflow backend) is used to create neural networks throughout this thesis. which also allows custom activation functions. More research on activation functions can be found in [20].

Chapter 3

Graphs

3.1 Graphs

Graphs are abstract data types from graph theory that are defined as the pair (V, E) , where

- V is a set of vertices (or states).
- E is a set of edges (transitions between vertices). Edges may be directed (one-way) or undirected (two-way).

Circuits Circuits are specialized types of graphs where each node is called a gate and computes some function. Formally, a circuit is a triple (M, L, G) , where

- M is a set of values.
- L is a set of gate functions (or labels) that maps n-ary input to a single output: $M^i \mapsto M$.
- G is a directed acyclic graph labeled with L .

AIGs And-Inverter Graphs (AIGs) are Boolean circuits with

- $M = \mathbb{B} = \{0, 1\}$.
- $L = \{AND, NOT\}$.

- G is finite.

Despite AIGs being structurally inefficient at a hardware level, AIGs excel in abstractions with their effective manipulations of complex Boolean functions and simple design. This thesis is only concerned with comprehensibility so the abstraction is essential, and any hardware inefficiency is irrelevant. Furthermore, simplification and visualization of AIGs have been implemented in free software such as “ABC: An academic industrial-strength verification tool” [1].

MIGs Formally, Majority-Inverter Graphs (MIGs) are Boolean circuits with

- $M = \mathbb{B} = \{0, 1\}$.
- $L = \{MAJ, NOT\}$, where MAJ is the majority gate.
- G is finite.

MIGs were introduced in 2014 with two basis operations: majority and inversion. According to Amarú et al., a set of five primitive transformations creates a complete axiomatic system. By definition, a complete axiomatic system can prove any valid statement in the theory true or false. Therefore, the five primitive transformations allow a simple traversal of the entire MIG representation space. On average, MIG optimization reduces the logic levels by 18% when compared to AIGs optimized by the state-of-the-art ABC tool [1]. Furthermore, Amarú et al. proved MIGs to be a superset of AIGs [21].

While the reduced levels of MIGs would make the graph more concise than AIGs, majority gates are not as intuitive as and/or gates to some people.

AOIGs And-Or-Inverter Graphs (AOIGs) are Boolean circuits with

- $M = \mathbb{B} = \{0, 1\}$.
- $L = \{AND, OR, NOT\}$.
- G is finite.

AIGs use De Morgan's law

$$\neg(\neg a \wedge \neg b) = a \vee b$$

to illustrate an OR. While AIGs may require more NOTs than an AOIG, the optimized AOIG has the same amount of nodes as an optimized AIG for any Boolean formula.

Comprehensibility As discussed in Chapter 4, comprehensibility can be defined as conciseness. From this, it stands to reason that MIGs are more comprehensible than AIGs. Furthermore, conciseness can be improved by converting subgraphs in the MIG to OR or AND nodes if doing so does not increase the total amount of nodes. Future work can investigate the comprehensibility of Majority-And-Or-Inverter Graphs further. See Amarú et al.'s work for information on how conversion may be done [21].

BDDs Binary Decision Diagrams (BDDs) are rooted, directed, acyclic graphs that consist of terminal and binary decision nodes (see Figure 3.1). BDDs were used by Shi et al. to illustrate activation functions that were converted to step functions [7]. Future work may investigate if BDDs are more comprehensible than AIGs.

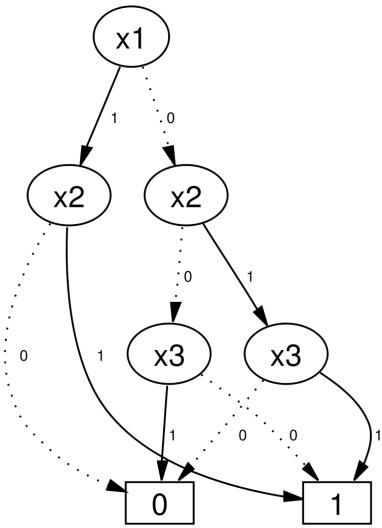


Figure 3.1: A binary decision diagram (BDD) for $f(x_1, x_2, x_3) = \neg(x_1x_2x_3) + x_1x_2 + x_2x_3$. This picture is from [Wikipedia](#).

3.2 ABC Software

This thesis uses ABC software [1] to illustrate and simplify AIGs. See Figure 3.2 for an example and below for the legend.

Legend for ABC's AIG

- Inputs: up-right triangles (\triangle).
- Outputs: upside-down triangles (∇).
- AND gates: oval nodes (\circ).
 - Labels: ABC labels nodes numerically; the numbers have no logical value.
- NOT gates: a dashed arrow ($--\rightarrow$).

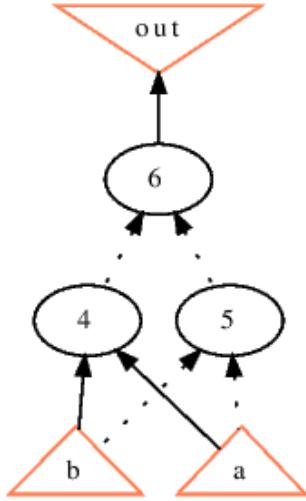


Figure 3.2: An AIG for the XOR function: $\text{out} = \neg ab \vee \neg ba$.

- Transitions: an arrow that is solid for transitions without a NOT gate (\rightarrow) and dashed for transitions with a NOT gate ($--\rightarrow$).

File Formats To write AIGs to the disk, I used the AIGER format (a highly-compressed format intended for AIGs) [22] with the Python library pyAiger [23] when coding in Python. However, writing AIGER files is not implemented in EPFL’s library (a C++17 library for logic synthesis) [5]. In C++17, I used the BENCH format (a public format that can encode AIG equivalents) [24] since it produced the smallest file size of the intersection between what EPFL’s library could write and ABC [1] could read.

ABC Commands ABC has a simple command-line integration with the “-c” option—example: “abc -c ‘commands_here’”. After the file (that encodes the AIG) was written, I ran a bash script with the below command to read the file, translate it into an AIG, refactor (simplify) the AIG, and then finally illustrate the AIG.

```
abc -c "read ${file}; strash; refactor; show;"
```


Chapter 4

Comprehension

In this chapter, comprehension is analyzed and quantified. Later, I show that an AIG is more comprehensible than a neural network due to its conciseness (fewer nodes, fewer transitions, and simpler functions). Finally, some tips on understanding the AIG are given.

4.1 Understanding

A Complete Understanding Comprehension is a loaded term, yet the strongest form of comprehension can be expressed well by parts of Descartes’ “Rules for the Direction of the Mind” [25]. Essentially, one must intuit each basic fact (input) before understanding the relations among the inputs. Furthermore, this extends to relationships of relationships: one must intuit the first-order relationships before understanding second-order relationships. Descartes’ philosophy on comprehension is a bottom-up approach (start from the primitives and work to the more abstract).

First-Order Logic (FOL) In formal logic, FOL is defined as quantifying over propositional logic with the existential or universal quantifiers. However, this thesis defines first-order relationships as the innermost relationship to be understood, and n^{th} -order relationships are relationships of the $(n - 1)^{th}$ -order ones.

Nth-Order Relationship Example

$$\phi = (a \wedge b) \wedge (\neg c \wedge b)$$

Here, the zeroth-order relationships are the atomic values a , b , and c . First-order relationships are $a \wedge b$ and $\neg c \wedge b$. The entire property, ϕ , is a second-order relationship. This definition is not strict. For example, one could consider the NOT operator as another level; I just use n^{th} -order relationships to loosely articulate how nested a relationship is.

A General understanding While a complete understanding is optimal, a disciplined intuition may be impractical in cases with a high-order relationship. For example, consider the unary operator “meta”. “meta” transcends its operand using self-reference so “cognition” (thinking) would become “meta-cognition” (thinking about thinking). Extending this concept to n^{th} -order meta-cognition (thinking about $(n-1)$ -order meta-cognition), it is time-consuming to intuit each lower-order meta-cognition, but our understandings of “cognition” and “meta” give us a general feel for what an n^{th} -order meta-cognition would mean¹. This arching principle (or pattern) is articulated using mathematical induction in Section 4.1.

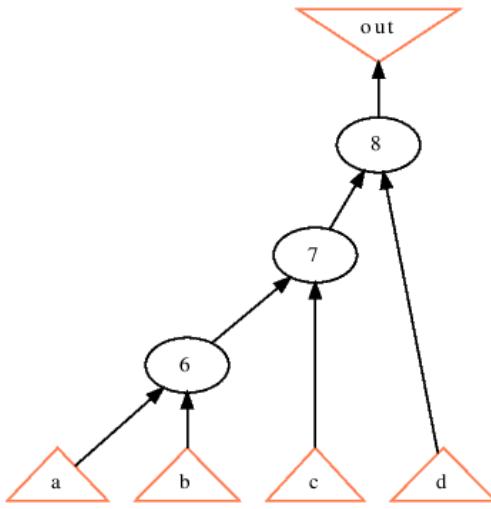
1. Basis step: The initial (first-order) state of n^{th} -order meta-cognition is meta-cognition. Since cognition (zeroth-order) means thinking and “meta” is a self-referential operator, meta-cognition means to think about thinking.
2. Induction step: N^{th} -order meta-cognition is thinking about $(N - 1)^{th}$ -order meta-cognition.

Figure 4.1: Understanding n^{th} -order meta-cognition using a type of “arching principle” called mathematical induction.

AIG Example Consider a Boolean function that is the conjunction of all its atoms (example in Figure 4.2a). For people that have previously intuited the conditional of universal truth (i.e. all elements must be true), they

¹Following the argument that metascience applies reflectively to itself [26], one can argue that metacognition encompasses n^{th} -order metacognition since metacognition is a type of cognition. However, assume that is not the case for this example.

can quickly understand this graph. For others, the graph can be understood using mathematical induction (see Figure 4.2b).



(a) AIG for $\text{out} = a \wedge b \wedge c \wedge d$.

1. Basis step: a must be true and the first-order relationship $a \wedge b$ must be true.
2. Induction step: traversing the graph, the $(n - 1)^{\text{th}}$ -order relationship and the n^{th} -order relationship must be true.

(b) Understanding Figure 4.2a by mathematical induction.

Figure 4.2: Understanding an AIG that represents the universal truth conditional.

Boolean Logic Example Consider the property ϕ over the atoms `fight` (to contend in physical conflict) and `flight` (to flee from physical conflict):

$$\phi = (\text{fight} \wedge \neg\text{flight}) \vee (\neg\text{fight} \wedge \text{flight})$$

After reading the inputs' definitions, start by understanding the innermost relations.

- $\neg\text{flight}$ must mean “to not flee from physical conflict.”
- $\neg\text{fight}$ must mean “to not contend in physical conflict.”

Next, we intuit the two conjunctions.

- $(\text{fight} \wedge \neg\text{flight})$: to contend in physical conflict and to not flee from physical conflict.

- ($\neg \text{fight} \wedge \text{flight}$): to not contend in physical conflict and to flee from physical conflict.

Finally, apply the final disjunction and understand ϕ is satisfied in one of two scenarios: 1) where one fights and does not flee, or 2) where one does not fight and flees.

4.2 Quantifying Comprehensibility

This section begins with a basic definition of comprehensibility and extends that definition to allow the comprehensibility of similar graphs to be determined without human subjects. Later, the comprehensibility of a neural network is contrasted with the AIG.

Basic Definition: comprehensibility scales by the inverse of the average time it takes one to understand it (e.g. $\frac{1}{1 \text{ second}}$ is larger and more comprehensible than $\frac{1}{100 \text{ seconds}}$).

Conditional Conclusion: If each input, relation, and output of two graphs take approximately equal time to intuit, then the graph with more inputs, relations, and outputs is less comprehensible. Additionally, if the graph with more inputs, relations, and outputs also takes longer to intuit each part, then this graph is still less comprehensible than the other.

Derived Definition This definition allows us to quickly determine how understandable an AIG is to another. While I will not explicitly calculate the formula in every AIG, know that when I contrast the comprehensibility of graphs that satisfy the above condition, I will use the derived definition

$$\text{Comprehensibility} = \frac{1}{\|I\| + \|R\| + \|O\|}$$

where $\|I\| + \|R\| + \|O\|$ is the sum of the magnitudes of inputs, relations, and outputs.

Future Work If one takes Descartes' bottom-up approach, then the number of nodes and transitions should convey comprehensibility as seen in the

derived definition. However, recall from Figure 4.2a that a top-down approach may be quicker than and elicit approximately the same understanding as a bottom-up approach. I will leave ideas such as this to future work for a comprehensive quantification of comprehension.

AIG versus Neural Network If one were to attempt intuition of a traditional and neural network, each activation function would be seen as a classifier with some real-valued range for some weighted inputs. Analogous to earlier terms, each neural node in the first hidden layer is a first-order relationship and each node in the n^{th} layer is an n^{th} -order relationship. For hidden sigmoid activation functions, this relationship is the probability that the given set of weighted $(n - 1)^{th}$ -order relations indicate some intermediary binary classification.

Furthermore, intuiting a trained neural network would require people to intuit each activation function, $(n - 1)^{th}$ -order relation, each bias constant and weight vector, multiplication, and addition over the real numbers. In contrast, AIGs have fewer distractions and simpler gates—people must simply understand the inputs, AND-gates, and NOT-gates over Boolean values. \mathcal{B} (Section 8.2.2) optimizes away negligible inputs and the bias constant so \mathcal{B} produces an AIG with strictly fewer relations and simpler transitions.

See Section 3.1 and Chapter 2 for the definitions of AIGs and neural networks respectively.

4.3 Inputs

Understanding Inputs Consider if Figure 4.2a stood for some fictional female’s (Ashley’s) preference in men where (a, b, c, d) stood for (confident, humble, masculine, gentle). To cultures where masculine is antonymous with gentle or for people who believe that confidence cannot coexist with humility, Figure 4.2a would make no sense to them despite its simplicity. In this case, no structure can help the individual understand what is being articulated—the inputs must be better defined or understood.

Reducing Inputs Additionally, Ashley may have considered confidence to be a trait of masculinity (\therefore confidence \subseteq masculinity). Now, the input basis is not optimized for comprehension (it is not minimized) since the information was duplicated in the confidence and masculinity axes. Future work

can investigate the optimal ways to reduce the input space while remaining comprehensible.

Dimension Reduction While there exist dimension reduction techniques such as PCA (see Figure 4.3) that reduce the input space, these techniques may not be facilely understandable. For example, PCA casts m inputs into n components ($PCA : i^m \mapsto c^n$ for $m \geq n$) by combining information from inputs and omitting other information. Each component in the component-space is likely to be more difficult to understand than each input.

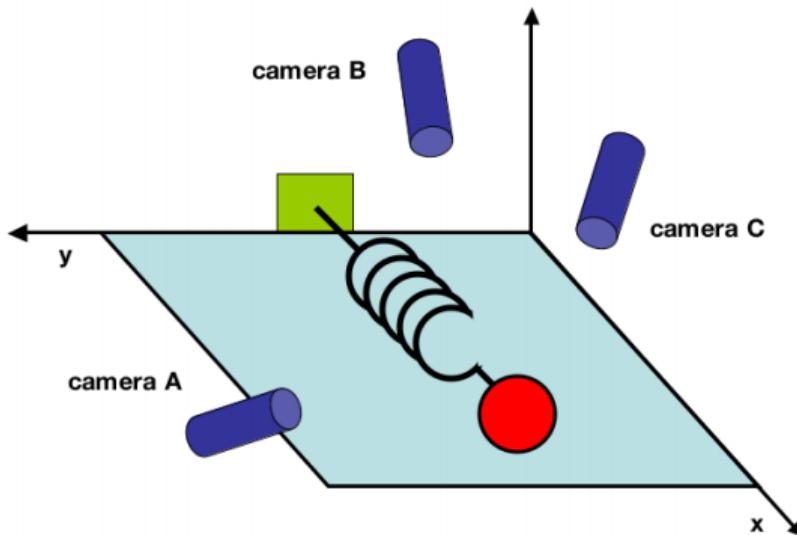


Figure 4.3: Shlen's PCA tutorial used this example of data duplication [27]. Only one camera is needed to predict the spring's position at any given time, yet multiple cameras are giving us variants of the same data. Dimension-reduction techniques such as PCA help alleviate duplicated information such as this.

Many Inputs

While comprehension is possible by unconscious or conscious means, both ways are impractical for a human to learn large data sets or intricate graphs.

Unconscious Comprehension Consider MNIST [28]: this problem is to predict hand-written digits using numerous pixel values. One might reason that since humans can decipher digits given by dots, people can also interpret a digit from a series of numeric dot values. As shown by BrainPort (a computer to brain interface that sends signals to a blind person’s tongue from a camera allowing them to see [29]), it may be possible for our unconscious minds to reorganize the relationships seen by numeric pixel values to visualize a digit, but for the sake of facile comprehension, this is eccentric and difficult [29, 30]. Furthermore, cognitive psychologists have coined this type of learning as “implicit learning” which our conscious mind cannot fully acknowledge nor articulate [31]. Even if one could intuit large data sets this way, the person could not articulate the findings to another.

Conscious Comprehension As for our conscious brain, we can only hold a small, finite amount of information in our working memory at a time [32]. Intuiting a concept means that the concept is stored into a longer-term portion of our memory from our working memory, and this process takes time for each concept to be stored. Therefore, there exist concepts with such intricacy that will take too much time to be realistically intuited.

Patterns However, a multitude of inputs, relations, and outputs does not necessitate complexity. If one can recognize groups or patterns in the mass of information, some understanding can be elucidated. For example, the numerous pixels in the MNIST input space can be understood by aligning shaded pixels (not numeric values) as the original images. Then one can correlate lines and curves from the original data to pixel values in the data set.

Patterns via Machine Learning Alternatively, one can employ a convolutional neural network (CNN) to highlight patterns of massive data. Given many inputs, CNNs learn patterns independent of location and create a feature-map of these patterns. One can then learn which features are associated with which types of curves and/or lines. Tools such as saliency masks can help humans understand the patterns learned [3].

4.4 Tips and Further Reading

Tips Understanding the entire AIG may still be a daunting task—even taken one relationship at a time. For the more complex AIGs, it may be better to consider individual sequences as they come about. Realize that a zero input to AND forces that gate to become zero, no matter what the other input is. Since this other variable is considered a “don’t care”, you can skip all nodes which create the “don’t-care” variable for this input sequence. See Theorem 10.2.2 for an example.

Final Notes The user must understand that the AIG model is an abstraction of the neural network that approximates the possibly biased data set. According to Descartes’, believing in false relationships makes one less knowledgeable than if one did not know any relationship exists [25].

Further Reading Human comprehension is at the intersection of several subjects including philosophy, cognitive psychology, neuroscience, anthropology, and more. An emergent field called “cognitive science” attempts to unite computer science and mathematical models with these many subjects. Furthermore, machine learning and artificial intelligence attempt to capture comprehension using mathematical models. For those interested in truth and axioms, I recommend reading Tarski’s theories of truth and satisfiability [33] and Gödel’s incompleteness theorems [34]. While Tarski argued that truth is problematic, but the satisfaction of properties are obtainable, this thesis uses truth as defined in a Boolean context. For philosophies of comprehension and cognitive systems, there exists associationism [35] and connectionism [36,37] among many others. For more research into self-referential logic and paradoxes, investigate Alan Turing’s work in [38]. To research interactions and strategies among two or more agents, read into game theory [39–41].

Chapter 5

Other Influential Works

A major problem in converting neural networks to a Boolean structure is the memorization versus generalization problem. Boolean structures such as AIGs are logical structures that are commonly used for memorization. One of the few works done that elicited generalization from logical operations (specifically factoring) is “Learning and Memorization” by Chatterjee [42]. Later, Brudermueller et al. used LogicNet and random forests to mitigate the memorization problem when converting neural networks to AIGs [2]. After I had completed the \mathcal{B} and \mathcal{N} algorithms (Section 8.2.2 and Algorithm 4), Shi et al. [7] published a paper that used Chan and Darwiche’s algorithm [43] to solve the problem \mathcal{B} does in $O(2^{0.5n}n)$ time.

5.1 Chatterjee

Lookup tables (LUTs) save previously calculated results in an array-structure. For Boolean functions, an N-bit LUT has a fan-in of N and 2^N possible entries. Chatterjee arranged LUTs in successive layers to mimic a fully connected neural network. However, unlike a neural node in a fully connected neural network, each LUT only receives inputs from a random subset of the previous layer of LUTs during training. This is done to mitigate complexity and has precedents in deep-learning architectures such as convolutional neural networks. Chatterjee describes these random inputs as a memorization process with noise. Furthermore, each LUT is globally trained on the entire network’s output (helping elicit generalization).

In related work, Chatterjee and Mishchenko discover clues on how neural

networks generalize (not by brute-force but by finding common patterns) while illustrating how circuit-based simulations can detect overfitting [44].

While parsing the neural network in \mathcal{N} , I took the idea of global training from LogicNet (see Algorithm 4). However, the final algorithm for \mathcal{N} was not a traditional machine learning technique since there was no explicit training. To consider the final output, I created \mathcal{N} to parse the neural network in reverse. This allowed \mathcal{N} to skip negligible neural nodes and to prevent islands in the final AIG.

5.2 Brudermueller et al.

In 2020, Brudermueller et al. published an article contrasting three pipelines (see Figure 5.1) that converted neural networks to AIGs using ABC [2]. To binarize the inputs, Brudermueller et al. simply cast the numbers into their binary representations.

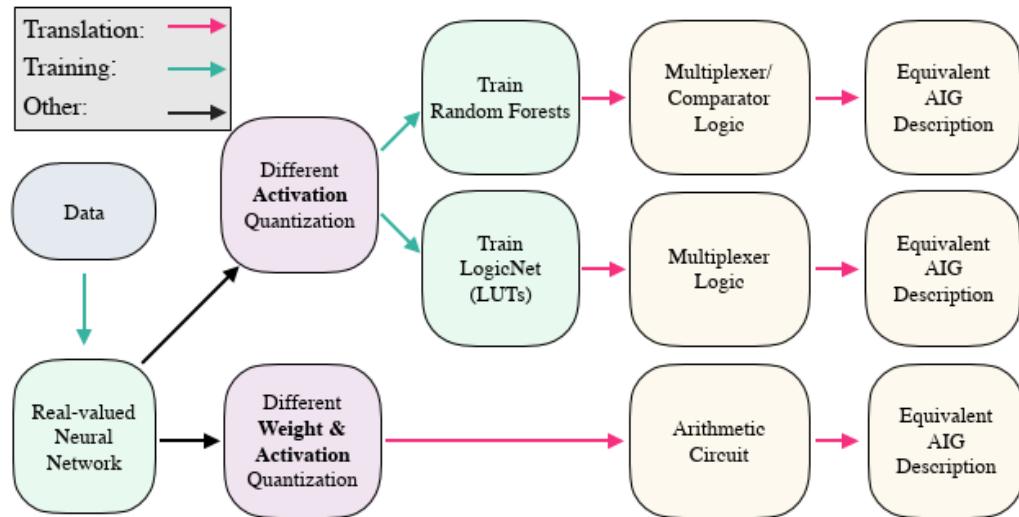


Figure 5.1: The pipelines contrasted in Brudermueller et al. [2].

In their direct translation, the researchers directly create an arithmetic circuit using multipliers, comparators, adders, multiplexers, and shifters. Each input and weight is allowed m bits, clipping and binning is done throughout their activation function circuit to keep inputs and weights at m bits. They found this pipeline elicited noise and the AIGs were less accurate than

the pipelines that used dependency elimination ad-hoc (throughout the circuit) (see Section 4.3 of [2]).

The other two pipelines tested included random forests and LogicNet. For each of these pipelines, the outputs of each activation node were trained on the global activation to eliminate “unimportant” features or relations. In contrast, I realized these “unimportant” features or relations were likely tentative or developing relationships of the neural network and Section 10.3 suggests an ensemble of neural networks to and-inverter graphs would also elicit generalization. Future work can discover which way is more effective.

While Brudermueller et al. note that there is little work done on using logical operations to find generalization, one article that researches this topic is “Learning and Memorization” by Chatterjee [42]. Here, Chatterjee used factoring to elicit generalization. Furthermore, these simplified structures allow one to test the sensitivity of the inputs.

5.2.1 ABC and AIGs

AIGs The idea to use an AIG (which can represent any Boolean function) as the comprehensible output came from Brudermueller et al. Furthermore, freely-available software called “ABC” can take AIGs as input and provide powerful transformations such as redundancy removal to make the AIG more comprehensible [1].

Satisfiability The Boolean satisfiability problem (SAT) asks if there exists a set of inputs (given some restraints) that invokes a true output. SAT solvers can have $O(n)$ complexity—where n equals the number of variables [45–47]. Fortunately, ABC includes an SAT solver called MiniSAT [1] which can be used to test the properties of AIGs abstracted from neural networks. Additionally, AIGs are formally verifiable (properties of AIGs can be proven or disproven).

5.3 Shi et al.

In “On Tractable Representations of Binary Neural Networks”, Shi et al. [7] trained a neural network with sigmoid activations which were later transformed into step activations to allow an easier translation to an ordered binary decision diagram (OBDD or BDD) [7]. For BDDs, variable ordering

is essential to create the most concise BDD. Furthermore, this paper connected finding the truth table of a neural node with an analogous problem Chan and Darwiche had solved with $O(2^{0.5n}n)$ complexity [43]. While Shi et al. also convert activation functions to a binary step function based on some threshold, I extend this research by exploring which activation functions are best suited for the binary function cast in Section 7.2. Shi et al. partially overlap the novel work I had done and came out after I had completed much of my experiments.

Part III

Methods

Part III articulates the work and thoughts that went into compiling an AIG from a neural network. Chapter 6 shows a prototype created in Python using Keras sequential neural models, Sklearn’s decision tree, and other Python tools which empirically produced an AIG with a ludicrous $O(5^n)$ time complexity. Chapter 7 recognizes the extensive computation time required to elicit the XORNN (XOR Neural Network) prototype and lays the groundwork for an optimized binary decision tree (\mathcal{B}) in Chapter 8. Chapter 8 also defines how the network is parsed (\mathcal{N}). Finally, Chapter 10 introduces AIG construction with real data sets—including those with “don’t-care” variables. Chapter 9 in Part IV gives supporting evidence that \mathcal{B} reduced the worst-case complexity to $O(2^n)$ and the average case to $O(2^{0.5n})$.

Chapter 6

XORNN

This chapter investigates neural networks that can solve the XOR problem as a prototype to construct AIGs. Efficient algorithms and other examples are introduced in Chapter 8 and Chapter 10 respectively.

6.1 Definitions

XOR Definition For the prototype, I used the simple, nonlinear data set XOR. Formally, XOR can be defined as $f(a, b) = (a \vee b) \wedge \neg(ab)$. $f(a, b)$ gives us this truth table for XOR (Table 6.1).

Table 6.1

a	b	$f(a, b)$
0	0	0
0	1	1
1	0	1
1	1	0

XOR Problem The simplest neural network that can solve the nonlinear, XOR problem poised by Minsky and Papert [9] requires three layers. The first layer (the input layer) is composed of two input nodes and one bias node. The second layer (a hidden layer) has two nodes and one bias node.

The final layer (the output layer) is a single node. The hidden nodes and the output node are equipped with the sigmoid activation function.

XORNN defined Let AllXORNN be the set of all neural networks that perfectly fit the XOR data set and have the topology as described above and as visualized in Figure 6.1. A specific neural network in AllXORNN is referred to as XORNN. An initialized neural network will be trained on the data found in Table 6.1; if 100% accuracy is obtained, the neural network becomes a XORNN. Since all possibilities of the XOR data set are known and trained upon, perfect accuracy is attainable and generalization is not a concern—that is, XORNN cannot be overfitted. However, I found that XORNN’s created with the code given in Section 6.2.1 often reached a local minimum of 75% accuracy for at least a million epochs. If the neural network had less than 100% accuracy after about 5000 epochs, it was better to simply reset the weights and start again.

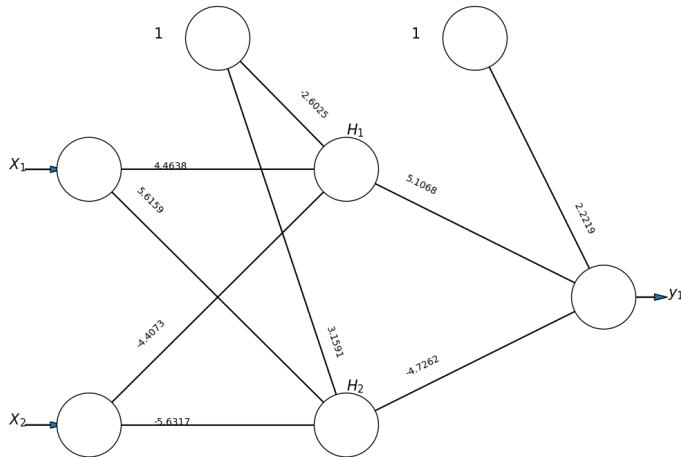


Figure 6.1: Every XORNN has the same topology—only the weights differ.

6.2 Creating XORNNS

This section highlights how XORNNS are efficiently made. Efficiency is important since the more XORNNS that are produced, the larger our sample data is.

6.2.1 XORNN Code

The pseudo-code in Algorithm 2 surveys how a XORNN is created—the corresponding Python script is in Section 6.2.1. An example of the boundaries drawn by a XORNN is given in Figure 6.2. Section 6.2.2 explains how and why this algorithm was refined.

Algorithm 2: Pseudocode for the Python script in Section 6.2.1.

Output: XORNN

for $i = 0 \dots 49$ **do**

- Initialize an XOR neural network (XORNN) with the topology illustrated in Figure 6.1.
- Train XORNN on the XOR data set (Table 6.2).
- if** *Accuracy is 100%* **then**
- return** *XORNN*

throw “A XORNN could not be produced. Statistically, this is unlikely to occur given 50 attempts.”

return

Review of the Python libraries used in Section 6.2.1.

- Keras is an API for creating neural networks with the user’s choice of Theano or Tensorflow for the backend.
- NumPy is advertised as “[t]he fundamental package for scientific computing.” NumPy provides high-level functions to manipulate C-style arrays.
- Scikit-learn (also called sklearn) is a general machine learning library with a broad choice of machine learning algorithms and metrics to measure these algorithms.

Python code corresponding to Algorithm 2.

```
import numpy as np
from keras.models import Sequential
from keras.layers import Dense
from sklearn import metrics

def create_xor_nn(numEpochs=5000, numAttempts=50):
    inputs, outputs = np.array([[0,0],[0,1],[1,0],[1,1]])
    , np.array([0,1,1,0])
    #build a new neural net (with new random weights) and
    #train it until the neural net can reach 100%
    #accuracy.
    #Gives up after numAttempts=50 tries.
```

```

#Most of the time, three or fewer tries are needed.
for _ in range(numAttempts):
    #Create a sequential neural network model with
    Keras
    xorModel = Sequential()
    #Dense() is a Keras object for a fully connected
    layer
    #the first add() includes the input layer and the
    first hidden layer
    xorModel.add(Dense(2, input_dim=len(inputs[0]),
                      activation='sigmoid'))
    xorModel.add(Dense(1, activation='sigmoid'))
    xorModel.compile(
        loss='binary_crossentropy', optimizer='adam', metrics
        =['binary_accuracy'])
    )

#train the neural net
history = xorModel.fit(inputs, outputs, epochs=
    numEpochs, verbose=0)
predictions = xorModel.predict_classes(inputs)
accuracy = metrics.accuracy_score(predictions,
                                    outputs)
print("Accuracy: ", accuracy)
#stop trying for new neural networks once we
achieve perfect accuracy
if accuracy == 1:
    break
if accuracy != 1:
    #Statistically, this error is very unlikely given
    50 attempts.
    raise RuntimeError('A XORNNS was not produced after'
                       ' ' + str(numAttempts) + ' attempts.')
return xorModel

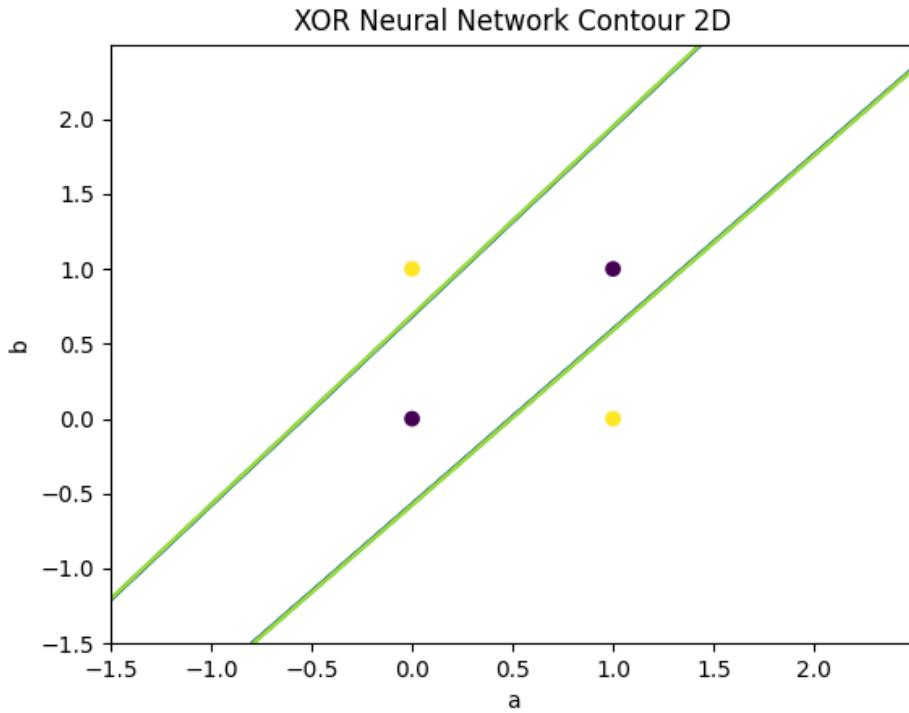
xorModel = create_xor_nn()
#once we create the model, we can save it for
persistence across sessions

```

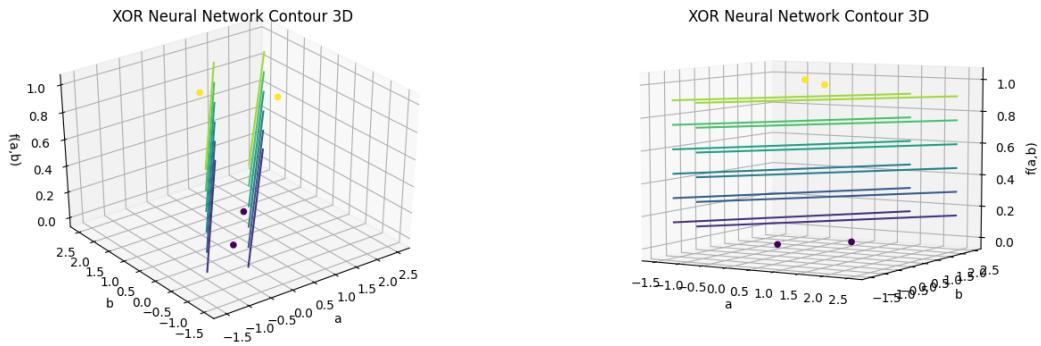
```
saveToThisPath = '/tmp/xor.kerasModel'  
xorModel.save(saveToThisPath, overwrite=True,  
    include_optimizer=True)
```

After saving our XORNN as done above, we can load the saved model with this script:

```
import keras  
loadedXor = keras.models.load_model('filePathHere')
```



(a) A 2D contour plot of XORNN predictions with the XOR data set plotted. The slope is so steep, all of the contour lines have agglomerated together.



(b) A 3D contour plot of the same XOR neural network in Figure 6.2a.

(c) A side view of Figure 6.2b.

Figure 6.2: Graphs of a XORNN boundary (lines) compared with the XOR data set (dots).

6.2.2 Rationale for Algorithm 2

Local Minima As illustrated in Figure 6.3, I discovered that the neural networks with suboptimal accuracy after 5000 epochs would often remain suboptimal for at least 1,000,000 epochs. To remedy being stuck in this local minima, I reinitialized the neural network with random weights after 5000 epochs. Future work can investigate if there is an epoch threshold where suboptimal NNs will never become a XORNN and the basis of original weights that elicit this phenomenon.

Degeneracy Figure 6.3 shows that a few XORNNs' accuracies decreased (therefore losing status as a XORNN) as the epochs surpassed 50,000. 64.4% of all NNs were XORNNs at 50,000 epochs while 100,000 epochs only yielded XORNNs 58.4% of the time. With the Adam optimizer algorithm (refer to Section 2.1 for a review on optimizer functions and other neural network components), neural networks were consistently found to remain in a local minimum about 42% of the time. Preliminary results indicate that the SGD (stochastic gradient descent) optimizer which Adam was based on also stalls in these local minima. The code in Section 6.2.1 was created with this experiment in mind.

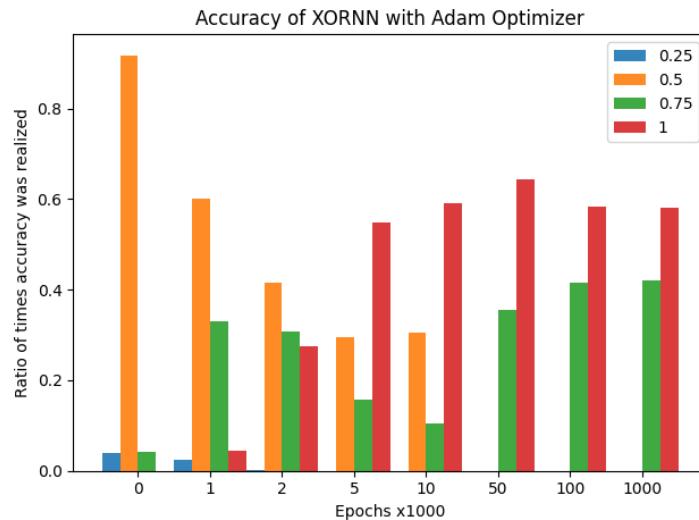


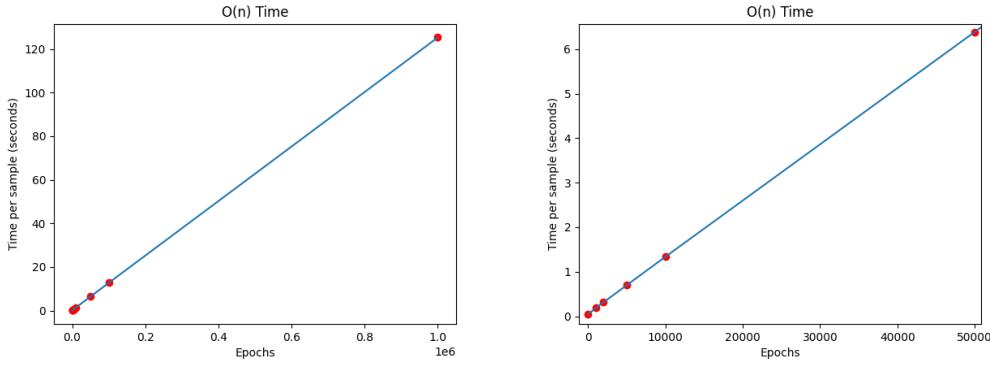
Figure 6.3: The accuracy is differentiated by color. Epochs 0 through 100,000 had 500 samples each. 1,000,000 epochs had 100 samples. No sample was reused and tested with the code in Section 6.2.1.

6.2.3 Time Creating XORNN

Experiments were done with six threads on a six-core Intel i5-9600K CPU and aggregated into Figure 6.4. To prevent threads from obtaining the same pseudo-random weights, a short lock guarded the critical section that initialized weights with a random seed. This lock and child-process spawn times were negligible compared to the training time of the model.

GPU Training GPU training was not implemented due to the small size of the matrices. GPUs excel at multiplying large matrices. And matrix size increases proportionally to the number of nodes in the fully connected neural network. My XORNN topology (Figure 6.1), with a total of seven nodes, trains slower on an RTX 2070 with CUDA than on the Intel i5-9600K CPU.

CPU-Level Parallelism While implementing CPU-level parallelism, I found Keras' backend Theano was throttled by Theano's locks and switched to the Tensorflow backend to solve the throttling problem.



- (a) The training time is linear with the number of epochs.
(b) Figure 6.4a zoomed in by omitting the two largest epochs.

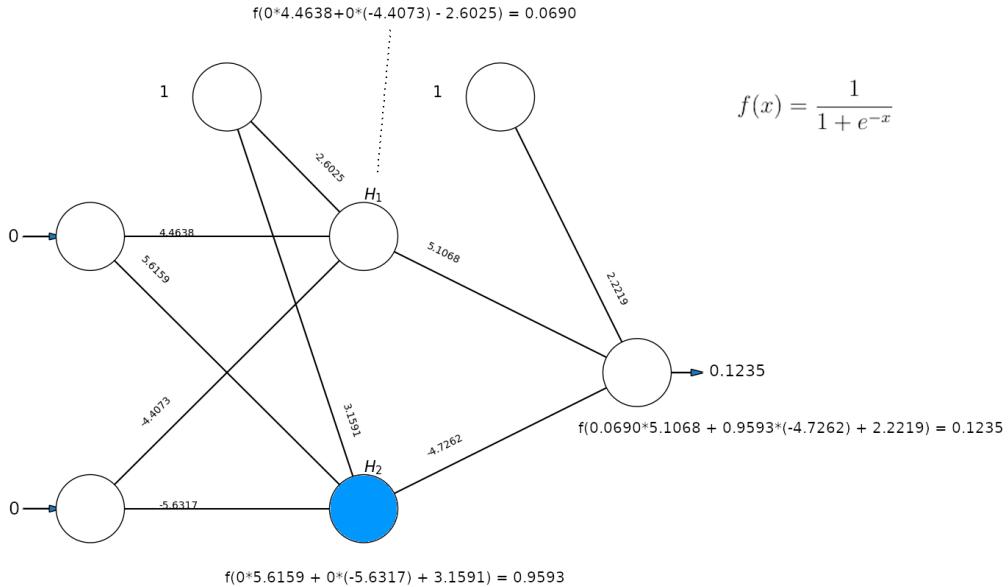
Figure 6.4

6.3 Understanding XORNN

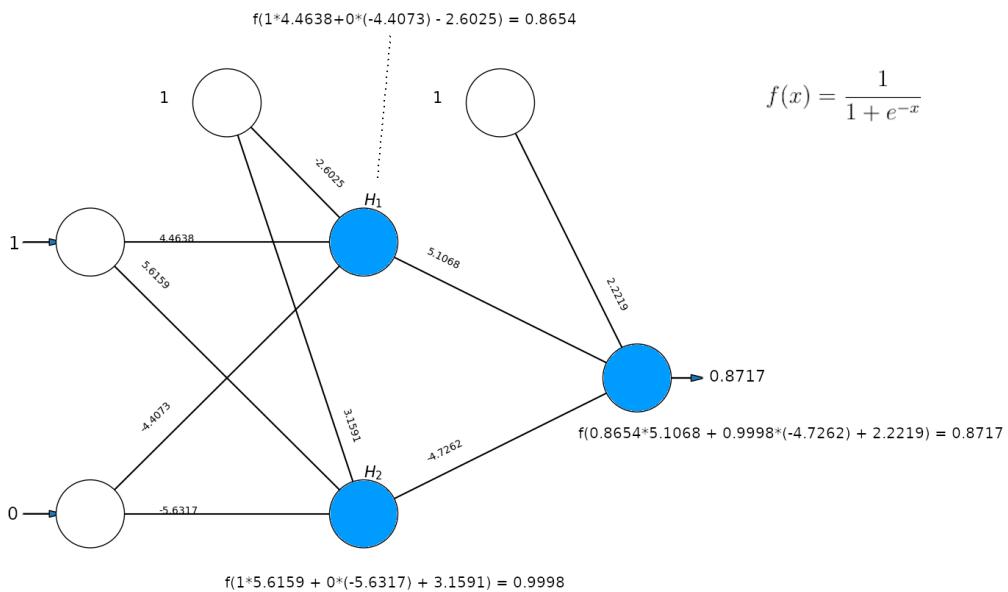
To gain a better understanding of the rule extraction techniques, let us exhaustively traverse and illustrate the XOR data set with a specific XORNN in Figure 6.5. Using the activation function $f(x) = \frac{1}{1 + e^{-x}}$, the blue nodes indicate an activation greater than 0.5. Table 6.2 converts Figure 6.5 into a more comprehensible truth table.

Table 6.2: The logic of the XORNN in Figure 6.5.

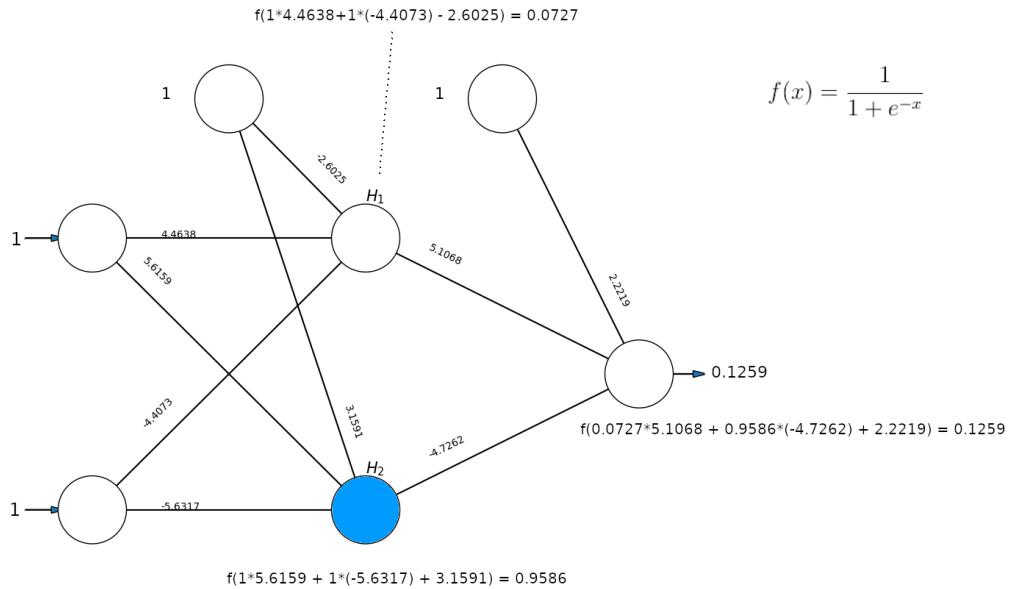
x_1	x_2	$h_1(x_1, x_2)$	$h_2(x_1, x_2)$	$out(h_1, h_2)$
0	0	0	1	0
1	0	1	1	1
1	1	0	1	0
0	1	0	0	1



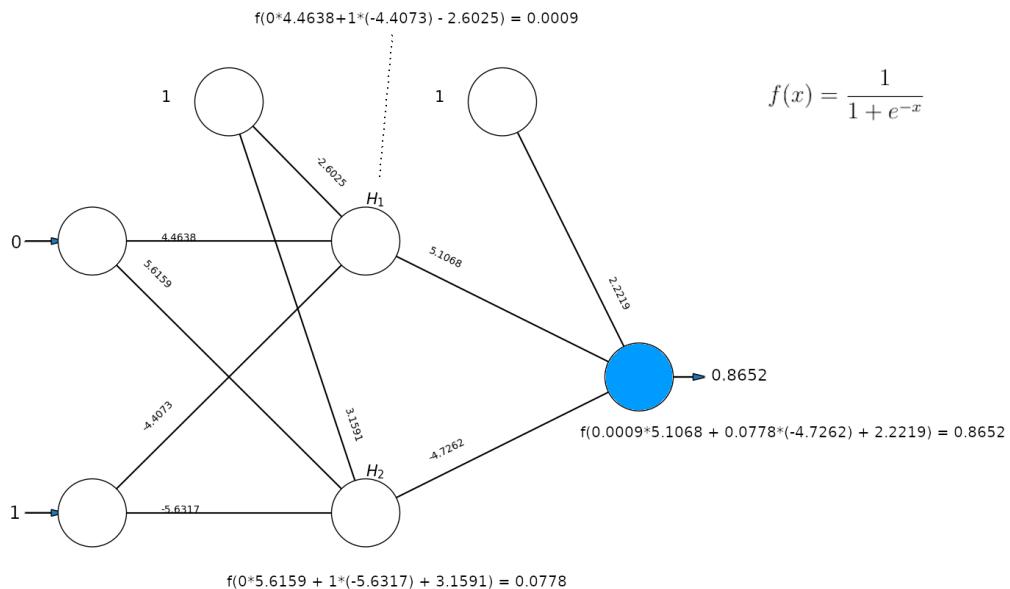
(a) A walkthrough with inputs = {0,0}.



(b) A walkthrough with inputs = {1,0}.



(c) A walkthrough with inputs = {1,1}.



(d) A walkthrough with inputs = {0,1}.

Figure 6.5: Exhaustive walkthroughs of a XORNN.

6.4 Learning XORNN

This section investigates using a network of decision trees (called XORD) to approximate a XORNN.

6.4.1 Creating a Decision Tree Network

Tree Graphs The tree graphs in this section use sklearn's [48] built-in graphing function which uses Graphviz [49] and several other libraries. Consider the optimal decision tree for the XOR data set as illustrated in Figure 6.6. Each of the parent (white) nodes contain 5 lines of text. The first line is the conditional of the node that dictates which branch to take (left is true and right is false). The second line shows the Gini impurity of the conditional. The third line represents the number of samples the node was given at this point, and the fourth line shows how many samples of each class were given. Finally, the last line is the tree's best guess of a class given its current path. The color of the nodes signifies the class prediction.

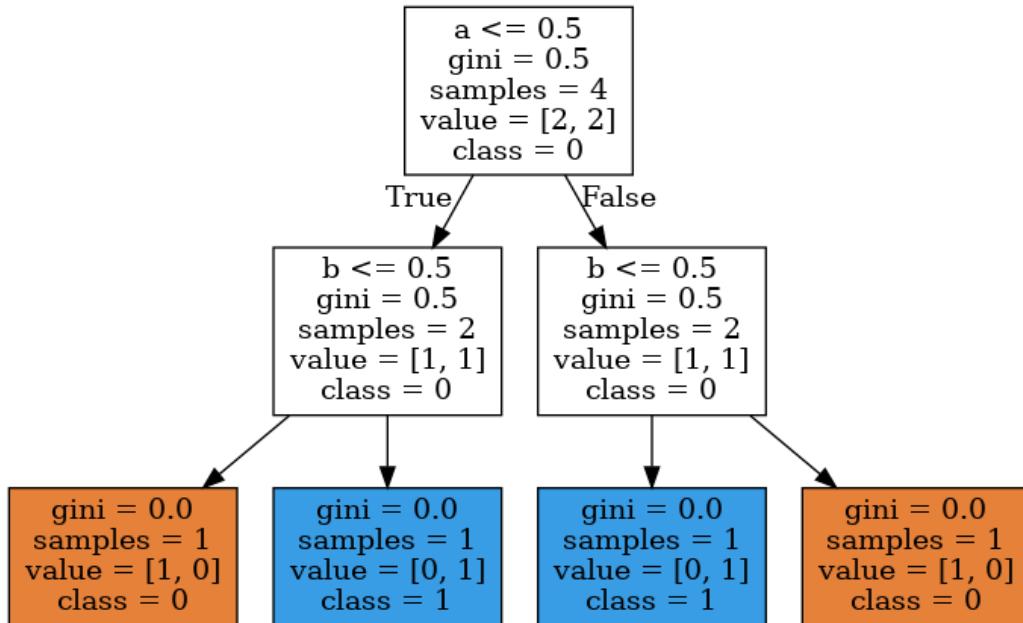


Figure 6.6: The optimal decision tree for the XOR data set created with Sklearn [48].

Learning the Neural Nodes To approximate and extract logic from a XORNN, a simple decompositional technique is employed: learn each node with a decision tree then layer the decision trees according to their respective nodes (see Figure 6.7). Finally, Section 6.5 analyzes the logic of the decision-tree network.

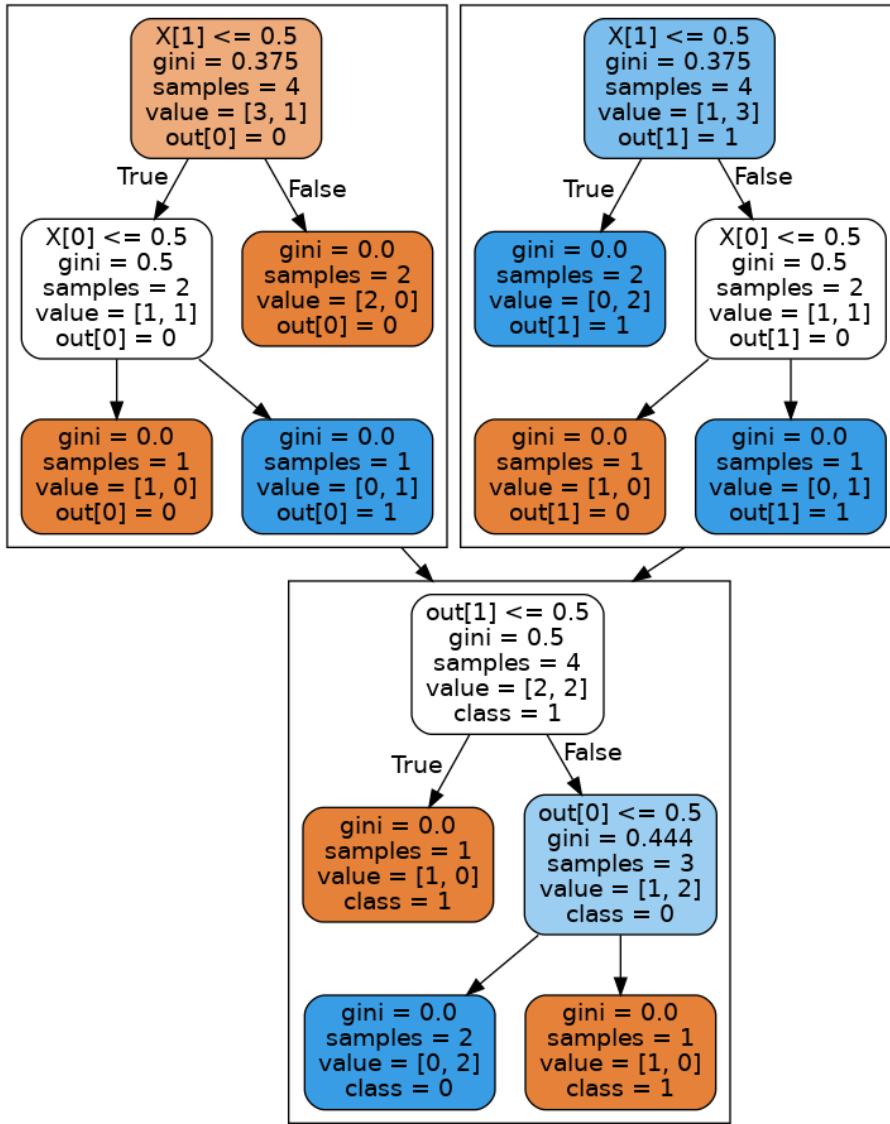


Figure 6.7: A decision tree network learned from the binarized activations of the XORNN pictured here Figure 6.5. The top left decision tree learned the activation from node H_1 , the top right decision tree's activation function was from H_2 , and the final decision tree at the bottom represents the activation from the output node. As one can see, this decision tree network requires reorganizing to be shown as Figure 6.6.

6.5 Understand the Decision Tree Network

This section translates Figure 6.7 to a Python function by nesting the conditionals of the decision tree. After the Python code is tested to correctly model Figure 6.7, I convert the Python to Boolean algebra to prove it correctly approximates XORNN and the XOR data set.

XORD to Python Since all inputs in the decision tree are binary, it is known that “ $x[1] \leq 0.5$ ” means “ $x[1] == 0$ ” and “ $x[1] > 0.5$ ” means “ $x[1] == 1$ ”. After this realization, I recreated the conditionals in my Python code below.

```
def xord(x):
    #initialize the output node's input to impossible
    #values
    out = [-1,-1]
    #H1 (Hidden node 1) (also the top-left decision tree)
    #produces x[0] (here we call it out[0]) for the
    #out node
    if x[1] == 0: #gini = 0.375
        if x[0] == 0: #gini = 0.5
            out[0] = 0 #samples = 1
        else:
            out[0] = 1 #samples = 1
    else:
        out[0] = 0 #samples = 2

    #H2 (top-right decision tree) produces out[1]
    if x[1] == 0: #gini = 0.375
        out[1] = 1 #samples = 2
    else:
        if x[0] == 0: #gini = 0.5
            out[1] = 0 #samples = 1
        else:
            out[1] = 1 #samples = 1

    #Output node (bottom decision tree)
    if out[1] == 0: #gini = 0.5
```

```

    return 1 #samples = 1
else:
    if out[0] == 0: #gini = 0.444
        return 0 #samples = 1
    else:
        return 1 #samples = 2

#x can be any of the four data points in XOR
allInputs = [[0,0],[0,1],[1,0],[1,1]]
for x in allInputs:
    print(x, ' returned ', xord(x))

```

Running the script in Section 6.5 confirms the decision-tree network in Figure 6.7 is correct.

```

[0, 0]  returned  0
[0, 1]  returned  1
[1, 0]  returned  1
[1, 1]  returned  0

```

Conditionals to SoP Now let us simplify Figure 6.6 further by translating each if-else chain to a sum of products (SoP) (shown in my Python code below). Simply begin with the outer-most if, then create a product for each path (following the logic of each conditional). If class 1 is reached during the traversal, write the current product in the sum of products. Any paths that end with a class 0 are omitted. The final SoP will fully encompass the space of our if-else blocks. This idea of only including class 1 in the sum of products was tested to work here and implemented in \mathcal{B} in Section 8.2.

```

#Goal: change all comparisons and assignments to
      Boolean logic.

#Conjoin each conditional with each conditional within
      it.
#Add the conjunction (product) to the sum of products
      only if an assignment of True is found.
#If the False assignment is found, backtrack the
      product in a tree-like fashion.

```

```

def xord_simplified(x):
    #initialize the output node's input
    out = [False, False]
    #H1 (Hidden node 1) and top-left decision tree
    #produces out[0] for the out node's input
    out[0] = (not x[1] and x[0])
    # if not x[1]: # add not x[1] to our product
    #     if not x[0]: #add not x[0] to the product
    #         out[0] = False
    #     else: #x[0] is true #remove not x[0] and add x
    [0]
    #             out[0] = True #add our first product 'not x
    [1] and x[0]'
    # else: #x[1] is true
    #     out[0] = False

    #Begin with a new empty product with each outermost
    if block.
    #H2 and top-right decision tree produces out[1]
    out[1] = not x[1] or (x[0] and x[1])
    # if not x[1]: #product = not x[1]
    #     out[1] = True #add product.
    # else: # x[1] is true #flip the final conditional.
    product = x[1]
    #     if not x[0]: #product = x[1] and not x[0]
    #         out[1] = False
    #     else: # x[0] is true #product = x[1] and x[0]
    #         out[1] = True #SoP = not x[1] or (x[0] and
    x[1])

    #Output node and bottom decision tree
    return not out[1] or (out[0] and out[1])
    # if not out[1]:
    #     return True
    # else: #out[1] is true
    #     if not out[0]:
    #         return False
    #     else: #out[0] is true

```

```
#           return True
```

In Python, “and” operators take precedence over “or” operators, so the parentheses are not needed but help with cohesion for those less attenuated to Python’s parsing. Without comments, the function is now the following:

```
def xord_simplified(x):
    out = [False, False]
    out[0] = (not x[1] and x[0])
    out[1] = not x[1] or (x[0] and x[1])
    return not out[1] or (out[0] and out[1])
```

Identical Logic With this simplification, we can see that $\text{out}[1]$ (node H_2) and the return (output node) share the same simplified logic. Indeed, the ordered weights going into the respective nodes in Figure 6.1 share similar ratios ($3.1591 : 5.6159 : -6.6317 \approx 2.2219 : 5.1068 : -4.7262$). This is due to x being a linear function of its dependent variables which are scaled with their respective weights. This concept is further explored in Section 7.2 and brings the idea of identifying equivalent subtrees in Section 8.4.2.

Using substitution, the function is redefined below.

```
def xord_simplified(x):
    return (not (not x[1] or (x[0] and x[1]))) or ((not x
        [1] and x[0])
        and (not x[1] or (x[0] and x[1])))
```

This substitution evokes a complicated expression. Using Boolean algebra, the function is simplified to the definition of XOR below.

```
def xord_simplified(x):
    return (x[1] and not x[0]) or (not x[1] and x[0])
```

Proving the Derived Code Correct

Theorem 6.5.1. *The Python code $(\text{not } (\text{not } x[1] \text{ or } (x[0] \text{ and } x[1]))) \text{ or } ((\text{not } x[1] \text{ and } x[0]) \text{ and } (\text{not } x[1] \text{ or } (x[0] \text{ and } x[1])))$ is equivalent to $(x[1] \text{ and not } x[0]) \text{ or } (\text{not } x[1] \text{ and } x[0])$.*

Proof. Let $x[0] = a$ and $x[1] = b$. Then our return statement is:

$$\neg(\neg b + ab) + (\neg ba(\neg b + ab)) \quad (6.1)$$

Change the first product using De Morgan's laws.

$$\neg(\neg b + ab) = b \neg(ab) \quad (6.2)$$

Again, use De Morgan's laws.

$$b \neg(ab) = b(\neg a + \neg b) \quad (6.3)$$

Use the distributivity of AND over OR.

$$b(\neg a + \neg b) = b \neg a + b \neg b \quad (6.4)$$

Use a law of complementation (b and not b must be a false statement).

$$b \neg a + b \neg b = b \neg a + 0 \quad (6.5)$$

Removing the 0 of the logical sum, return the simplified first product.

$$\neg(\neg b + ab) + (\neg ba(\neg b + ab)) = b \neg a + (\neg ba(\neg b + ab)) \quad (6.6)$$

Use the distributive property on the second product.

$$(\neg ba(\neg b + ab)) = \neg b \neg ba + \neg ba ab \quad (6.7)$$

Remove clear redundancies using the laws of idempotence.

$$\neg b \neg ba + \neg ba ab = \neg ba + \neg bb \quad (6.8)$$

Use a law of complementation.

$$\neg ba + \neg bb = \neg ba + 0 \quad (6.9)$$

Remove the 0 from the logical sum and return the second product back to the original equation.

$$\neg(\neg b + ab) + (\neg ba(\neg b + ab)) = b \neg a + (\neg ba(\neg b + ab)) \quad (6.10)$$

$$= \neg ab + \neg ba \quad (6.11)$$

□

Python to AIG Using AIGER [22,23] and ABC [1], the logic of the neural network is expressed with an and-inverter graph (AIG) in Figure 6.8. See Section 3.2 for details on ABC's AIGs.

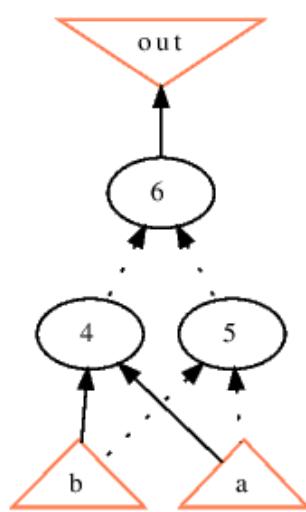
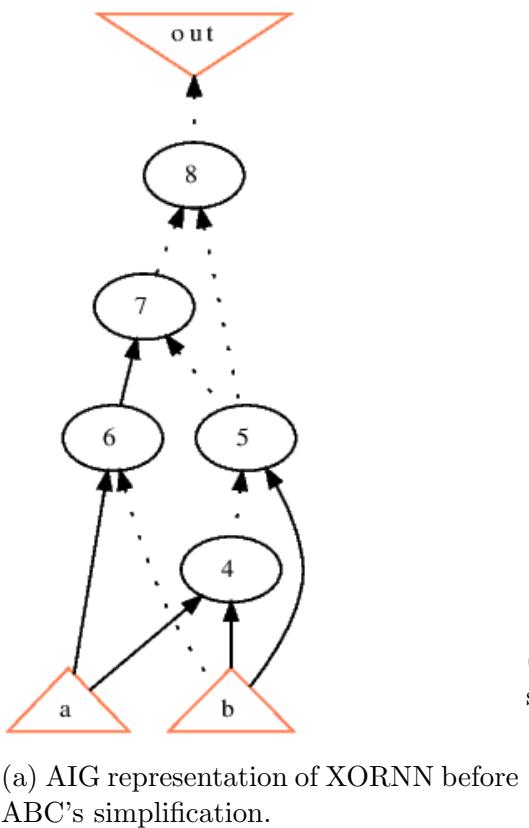


Figure 6.8: Equivalent AIG representations of XORNN.

Chapter 7

Importance

The importance of an input is the input’s influence on class prediction. While importance can be evaluated with Gini impurity or information gain, this chapter finds a more computationally efficient way to determine importance specifically for neural nodes.

Furthermore, this chapter discusses why only weights and some scalar threshold (θ_t) need to be considered in \mathcal{B} . Section 7.1 briefly discusses why weights are the “important” factor. Furthermore, Section 7.2 and Section 7.3 explains how \mathcal{B} does not have to compute the activation function.

Binarization Regarding quantization, I cast all input values (values from the initial data set) into $\{0, 1\}$. This works fine for some inputs; however, other inputs have a non-monotonic relationship with the output and too much information is lost with the 0,1 cast. In the latter case, single inputs can be read as two or more inputs which can effectively maintain information (further addressed in Section 10.2.2).

7.1 Weights

Each activation function, f has a single dependent variable, θ . θ is found by the dot product of the weight (\vec{w}) and input (\vec{x}) vectors.

Lemma 7.1.1 and Theorem 7.1.2 shows that the importance of each $x_i \in \vec{x}$ is exactly the absolute value of the corresponding $w_i \in \vec{w}$. This is the discovery that allows \mathcal{B} to skip the computationally expensive information gain or Gini impurity that are often used in decision trees.

Lemma 7.1.1. *For every $x_i \in \vec{x}$, $\frac{\delta\theta}{\delta x_i} = w_i$.*

Proof.

$$\theta = \vec{x} \cdot \vec{w}^T = w_0x_0 + w_1x_1 + \cdots + w_{n-1}x_{n-1} + 1 \times w_bb \quad (7.1)$$

$$\frac{\delta\theta(\vec{w}, \vec{x})}{\delta x_i} = w_i \quad (7.2)$$

□

Theorem 7.1.2. *The importance of $x_i \in \vec{x}$ is the absolute value of the corresponding $w_i \in \vec{w}$.*

Proof. Since each input ($x_i \in \vec{x}$) has the same range and is scaled by its respective weight (see Lemma 7.1.1) in the linear function $\theta(\vec{w}, \vec{x})$, the portion of contribution each x_i has towards θ can be found by taking the ratio of w_i to the absolute sum of all $|w| \in \vec{w}$.

$$\text{importance}(x_i) = \frac{|w_i|}{\sum_{w_j \in \vec{w}} |w_j|}$$

Removing the common denominator among all $\text{importance}(x_i) \in \text{importance}(\vec{x})$ yields:

$$\text{importance}(x_i) = |w_i| \quad (7.3)$$

□

Because of Theorem 7.1.2, \mathcal{B} sorts all weights in a given node by its absolute value then iterates from the largest (most important) to the smallest (least important).

7.2 Monotonic Functions

This thesis uses a threshold to approximate a real-valued function as a binary function. To binarize a real function into two classes, Lemma 7.2.1 can be used. The third case can be decided in the respective algorithm that is created. For example, I chose whichever value would stop \mathcal{B} from further traversal in the \mathcal{B} algorithm. Figure 7.1b provides a visual example.

Lemma 7.2.1. *Given a function $f(\theta)$ and a threshold $\alpha \in \mathcal{R}$*

$$g(\alpha, f(\theta)) = \begin{cases} 1 & f(\theta) > \alpha \\ 0 & f(\theta) < \alpha \\ 0 \vee 1 & f(\theta) = \alpha \end{cases}$$

Alternatively, one can find the independent variable θ instead of α for $f(\theta) = \alpha$. Then, any relaxed or strictly monotonic function does not need to compute f for every class decision and instead can use Lemma 7.2.2. Theorem 7.2.3 proves non-decreasing monotonic functions can use a threshold on the domain, and a similar proof can be made for non-increasing monotonic functions. See Section 7.3 for examples of non-monotonic functions that can be used.

Lemma 7.2.2. *A threshold is θ_t in the function:*

$$g(\theta_t, x) = \begin{cases} 1 & x > \theta_t \\ 0 & x < \theta_t \\ 0 \vee 1 & x = \theta_t \end{cases}$$

$0 \vee 1$ depends on the algorithm. \mathcal{B} takes whichever value renders a quicker computation (a greedy approach).

Theorem 7.2.3. *For any non-decreasing monotonic function f and any given threshold α on the dependent axis, the corresponding independent value θ_t for $f(\theta_t) = \alpha$ may be used as the threshold without any loss in accuracy. That is, $g(f(\theta_t), f(x)) = g(\theta_t, x)$. g is defined in Lemma 7.2.2.*

Proof. By definition, non-decreasing monotonic functions must satisfy the property:

$$\forall(x, y) : x \leq y \longleftrightarrow f(x) \leq f(y) \quad (7.4)$$

Therefore, if $f(\theta_t) = \alpha$, then each case in $g(\alpha, f(x))$ is identical to $g(\theta_t, x)$.

$$f(x) > \alpha \longleftrightarrow x > \theta_t \quad (7.5)$$

$$f(x) < \alpha \longleftrightarrow x < \theta_t \quad (7.6)$$

$$f(x) = \alpha \longleftrightarrow x = \theta_t \quad (7.7)$$

Therefore,

$$g(f(\theta_t), f(x)) = g(\theta_t, x) \quad (7.8)$$

□

Non-Increasing Monotonic Functions Usually, activation functions do not satisfy the *non-increasing* monotonic property:

$$\forall(x, y) : x \leq y \longleftrightarrow f(x) \geq f(y)$$

However, if an activation function does, then

$$g(\alpha, f(x)) = \neg g(\theta_t, x)) \quad (7.9)$$

since the function's slope changes from positive to negative.

7.2.1 Proving a Function is Monotonic

To prove a function is monotonic and that the logic above can therefore be applied to it, one can prove its first derivative is always non-positive or always non-negative. An example is given in Theorem 7.2.4.

Theorem 7.2.4. *One of the most common activation functions, $f(\theta) = \frac{1}{1 + e^{-\theta}}$, is a non-decreasing monotonic function.*

Proof. This is done by proving $f(\theta)$'s first derivative is always non-negative.

Using the chain rule, we find $\frac{df}{d\theta}$.

$$f(\theta) = (1 + e^{-\theta})^{-1} \quad (7.10)$$

$$\frac{df}{d\theta} = -(1 + e^{-\theta})^{-2} \cdot -e^{-\theta} \quad (7.11)$$

$$\frac{df}{d\theta} = \frac{e^{-\theta}}{(1 + e^{-\theta})^2} \quad (7.12)$$

$e^{-\theta}$ is positive since e is positive and a real-valued exponent cannot change the positivity of its base nor yield 0 from a non-zero base.

$$e^{-\theta} > 0 \quad (7.13)$$

Any square of nonzero, real-valued numbers must always yield a positive real value. To prove the denominator is nonzero, see that $1 > 0$ and $e^{-\theta} > 0$ by Equation (7.13). Since both values are positive and real, their summation must also be positive and real.

$$(1 + e^{-\theta})^2 > 0 \quad (7.14)$$

Of course, dividing a positive real number by another positive real number results in a positive real number. Therefore,

$$\frac{df}{d\theta} = \frac{e^{-\theta}}{(1 + e^{-\theta})^2} > 0 \geq 0 \quad (7.15)$$

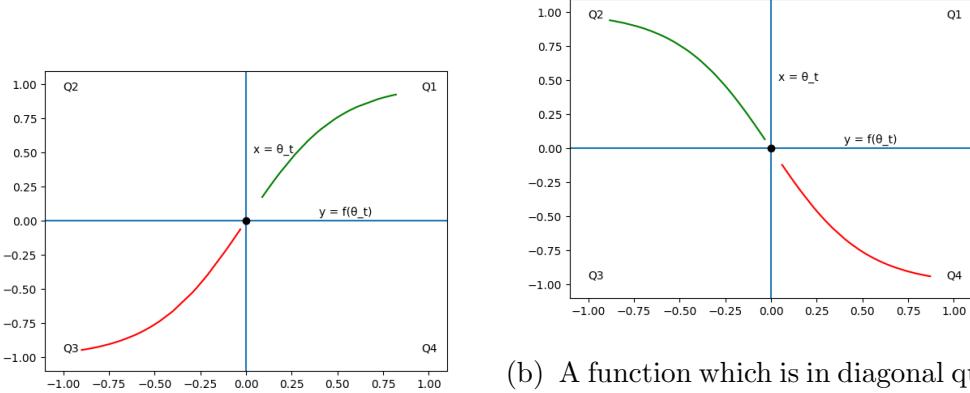
□

7.3 Generalizing to More Activation Functions

Section 7.2 relies on the monotonicity of the activation function. This section generalizes the principle of using a threshold in the domain instead of the range.

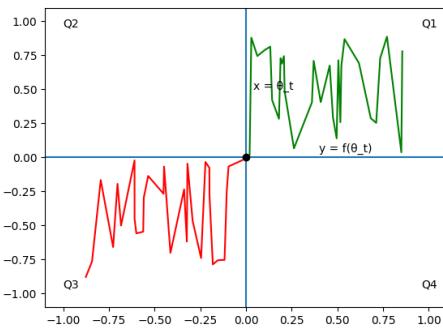
Diagonal Quadrants Using the domain to find the threshold instead of the range assumes that the range's threshold corresponds to the domain's threshold. This occurs when two perpendicular lines (one horizontal and one vertical) are drawn intersecting $(\theta, f(\theta))$ and the function only resides on the lines of or inside two diagonal quadrants (see an illustration in Figure 7.1). For monotonic functions, any threshold satisfied this property.

Decent Threshold Choices Besides satisfying the diagonal-quadrants property, a threshold must also be a “decent” choice. A formal analysis of “decent” choices for the threshold θ_t will be left for future work, but factors such as θ_t being a mean, median, point of inflection, drastic change in slope (ReLU), or an intersection with the y-axis are valid arguments that the threshold is “decent”. For odd (symmetric with respect to the origin), monotonic functions, Figure 7.2 shows a good strategy to find suitable thresholds. Figure 7.3 shows examples of finding a decent threshold for functions that are not odd. Finally, Figure 7.4 shows some uncommon activation functions where \mathcal{B} is not guaranteed to do well with.



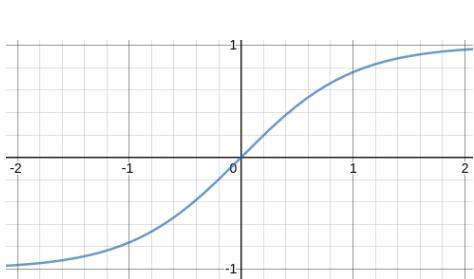
(a) A function which is in diagonal quadrants Q1 and Q3.

(b) A function which is in diagonal quadrants Q2 and Q4. Notice how the positive class (green) is for values less than θ_t . Accordingly, \mathcal{B} must flip which products (summations of weights) which are considered true and false (see Section 7.2).

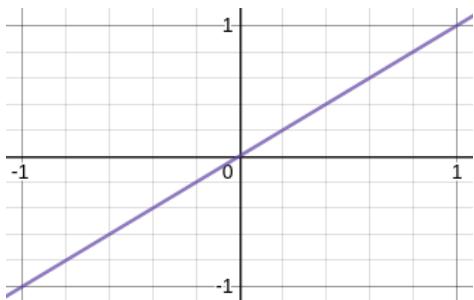


(c) The function does not need to be monotonic.

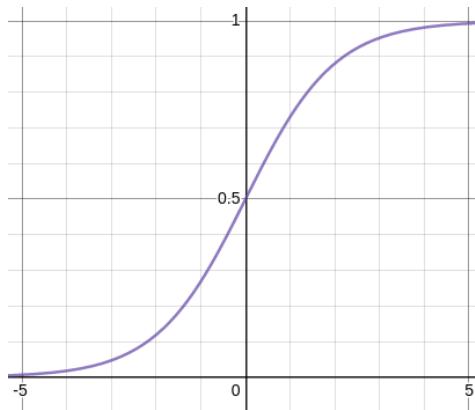
Figure 7.1: Examples of graphs which satisfy the diagonal quadrants property.



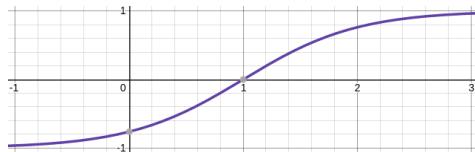
(a) In $\tanh(\theta) = \frac{2}{1+e^{-2\theta}} - 1$,
 $(a, b) = (0, 0)$ so $\theta_t = 0$.



(c) The identity function $f(\theta) = \theta$
has $(a, b) = 0$ and $\theta_t = 0$.

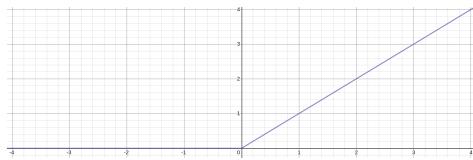


(b) In $\frac{1}{1+e^{-\theta}}$, $(a, b) = (0, 0.5)$ so
 $\theta_t = 0$.

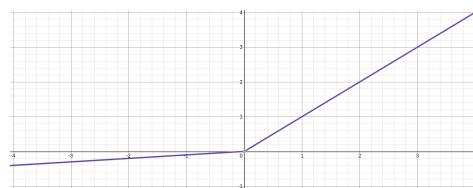


(d) Most activation functions center around $\theta = 0$. This function $\tanh(\theta-1)$ is a translation of $\tanh(\theta)$ which yields $(a, b) = (1, 0)$ and $\theta_t = 1$. While not recommended as an activation function, this example is to illustrate the uncommon case of $\theta_t \neq 0$.

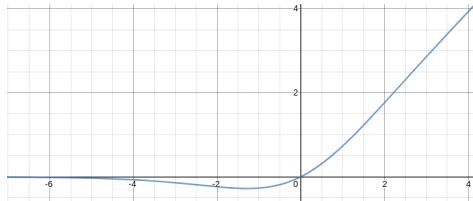
Figure 7.2: If a monotonic function $f(\theta)$ can be translated to an odd function by a constant pair (a, b) in $f(\theta - a) + b$, then $f(\theta)$ has a suitable threshold at $\theta_t = a$.



(a) For the ReLU activation function $f(\theta) = \max(0, x)$, we see a drastic change in slope at $(0, 0)$. Furthermore, ReLU was purposely designed with this sudden change at $\theta = 0$. $\theta_t = 0$ is a quality choice.

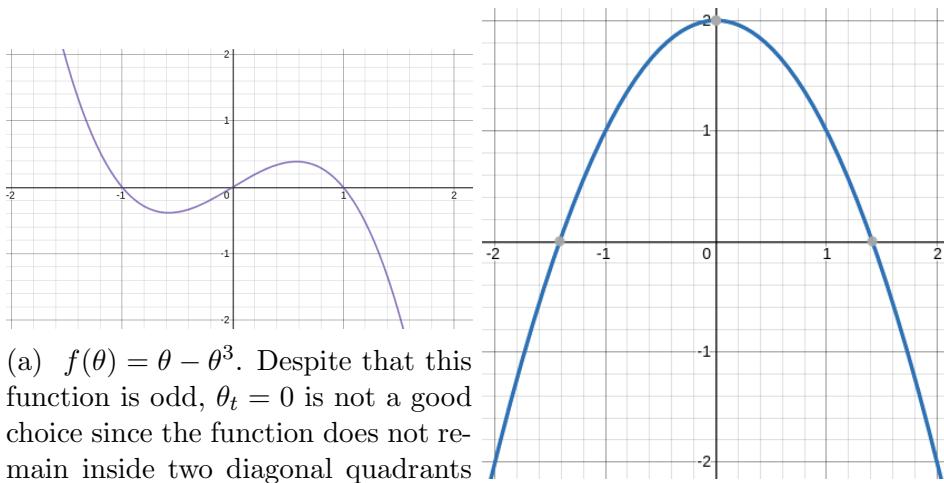


(b) The leaky ReLU activation function $f(\theta) = \max(0.1x, x)$ was made with similar intentions as ReLU. For similar reasons, $\theta_t = 0$ is a decent choice.



(c) The Swish activation function $f(\theta) = \theta \cdot \text{sigmoid}(\beta x)$ models a differentiable ReLU activation function [16]. Like ReLU, Swish has a great choice of $\theta_t = 0$.

Figure 7.3: These functions will not be odd even if translated by any constant pair. However, they still have a decent choice of $\theta_t = 0$ since the function remains one the lines of or in two diagonal quadrants.



(a) $f(\theta) = \theta - \theta^3$. Despite that this function is odd, $\theta_t = 0$ is not a good choice since the function does not remain inside two diagonal quadrants

when centered on $\theta_t = 0$. However, if the frequency of weight summations inside $-1 < \theta < 1$ is small, \mathcal{B} can still give accurate results.

(b) $f(\theta) = -\theta^2 + 2$. Even functions have no possible threshold where the function is contained in two quadrants. Therefore, even functions are unsuitable for \mathcal{B} .

Figure 7.4: Activation functions where the accuracy of \mathcal{B} will be low or conditional on the weights.

Unsuitable Activation Functions For uncommon activation functions such as Figure 7.4a, a single threshold is unsuitable. While \mathcal{B} can work with any threshold, the results will be less accurate as less of the function is contained within two diagonal quadrants. To regain the lost accuracy, a set of ranges could be implemented such as $\theta_R = \{(-\infty, -1], [0, 1]\}$; however, this would likely make \mathcal{B} more computationally expensive on average. Considering the infrequent use and impracticality of such activation functions on \mathcal{B} , I will leave them to future work.

7.4 Application to \mathcal{B}

For functions that are contained in quadrants one and three (see Figure 7.1), \mathcal{B} translates weight summations that are greater than θ_t as a product in the sum of products, and weight summations that are less than θ_t are forgotten. For functions contained in quadrants two and four, the opposite can be done.

Algorithm 3 Since each activation function has been binarized, the outputs of previous functions (\vec{x}) can be considered as a bitmask. Now \mathcal{B} searches for every possible bitmask of \vec{x} whose dot product with the weight vector \vec{w} is greater than the threshold θ_t . The domain threshold θ_t can be used instead of a range threshold because most activation functions satisfy the diagonal quadrant property for suitable choices of θ_t . Chapter 8 investigates this problem thoroughly.

Algorithm 3:

Input:

- $\vec{w} \in \mathbb{R}^n$, the weight vector.
- θ_t the threshold.

Output: $P \in \mathbb{B}^{m \times n}$ for $0 \leq m \leq 2^n$. P is a table of products that consist of every product in the sum of products which represents this given node.

```

 $P \leftarrow \emptyset$ 
/* The set  $\mathbb{B}^n$  can also be described as an n-ary Cartesian
   power of  $\{0,1\}$ .
forall  $\vec{x} \in \mathbb{B}^n$  do
  if  $\vec{x} \cdot \vec{w}^T \geq \theta_t$  then
     $P \leftarrow P \cup \vec{x}$ 
return  $P$ 

```

Chapter 8

Parsing the Neural Network

To parse the neural network, each layer must be traversed, then each node in the current layer is converted to a sum of products; finally, an AIG is constructed. First, a computationally expensive brute-force attempt is shown in Section 8.1. Next, ideas from Section 7.2 are implemented into the optimized binary decision tree (\mathcal{B}) which is presented in \mathcal{B} . \mathcal{B} converts a neural node to a sum of products (SoP) ad hoc. Next, Algorithm 7 describes the layer parsing. See Algorithm 4 for an overview of the neural network parsing and when \mathcal{B} is implemented.

Algorithm 4: A brief algorithmic description of Chapter 8.

Input: $N[1 \dots L]$ and θ_t . N is an array representing the layers of a neural network, and each layer is an array of in-degree weights. θ_t is the threshold.

Output: AIG

Let SoP be a two-dimensional table where each element is a sum of products.

forall $l_i \in N$ **do**

forall $n_j \in l_i$ **do**
 $SoP_{i,j} \leftarrow \mathcal{B}(n_j)$

$AIG \leftarrow table_sop_to_aig(SoP)$

return AIG

After the algorithm is explained, supplemental ideas and future work for \mathcal{B} are given in Section 8.4. Finally, alternative algorithms to \mathcal{B} are mentioned in Section 8.5.

	$w_1 = 3$	$w_2 = -6$	$w_3 = -2$	$w_{act} = \overrightarrow{mask}_i \cdot \vec{w} + 3$	$w_{act} \geq 0$
\overrightarrow{mask}_0	0	0	0	3	1
\overrightarrow{mask}_1	0	0	1	1	1
\overrightarrow{mask}_2	0	1	0	-3	0
\overrightarrow{mask}_3	0	1	1	-5	0
\overrightarrow{mask}_4	1	0	0	6	1
\overrightarrow{mask}_5	1	0	1	4	1
\overrightarrow{mask}_6	1	1	0	0	1
\overrightarrow{mask}_7	1	1	1	-1	0

Table 8.1: A truth table finding all 2^3 linear combinations of $\vec{w} = [3 \ -6 \ -2]$ which satisfy $w_{act} \geq 0$. 3 is the bias constant and 0 is the threshold. Section 8.5.1 gives a linear algebra implementation for this brute force approach.

8.1 Brute Force

In this section, I give an example of a brute-force for-loop approach in Algorithm 5. Examples of bitmask vectors (\overrightarrow{mask}) are illustrated in Table 8.1 where each variable is defined and $w_{act} \geq 0$ is the conditional.

Preamble for Algorithm 5 Let n = the number of dimensions in \vec{x} , $SOP = \text{false}$ be the sum of products, and P be the current product. Let \mathbb{L} be the ordinal set of layers in the neural network. Each $l \in \mathbb{L}$ is a double (W, B) where W is a matrix of weights with the ordinal of the previous layer's node found by the column number, and the current layer's node ordinal found by the row number. In other words, the weight $w_{i,j}$ in matrix W is yielded by the transition function $prev_j \rightarrow_w curr_i$. See Figure 8.1 for an illustration. B is the vector of bias weights for each node in the layer. Finally, “|” and “>>” are binary AIG operators for parallel composition and sequential composition, respectively [23].

Let the layers in NeuralNetwork be ordered as $\{1, 2, 3, \dots\}$. Since the input layer's (L_0) out-degree weights are remembered by L_1 's in-degree weights, the algorithm will extract the input layer (L_0) from the first layer (L_1) in the neural network array and its nodes will be defined as $\{node_{0,1}, node_{0,2}, \dots, node_{0,n}\}$.

Algorithm 5: Converting a neural network to an AIG with brute force and for loops.

Input:

- NeuralNetwork, a two-dimensional array of weights following Figure 8.1.
- $\theta_t \in \mathcal{D}$ of $f(x)$, the threshold (θ_t) of the activation function $f(x)$ as a domain value (\mathcal{D}). See Section 7.2 and Section 7.3 for why $\theta_t \in \mathcal{D}$.

Output: NNAIG, the AIG representation of NeuralNetwork

NNAIG $\leftarrow null$

foreach $layer_l \in NeuralNetwork$ **do**

```

    layerAIG  $\leftarrow null$ 
    /*  $\overrightarrow{row}_i$  is a row vector that consists of all in-degree
       weights (except the bias weight) for the  $i^{th}$  node in
       layer  $l$ . */
    foreach  $\overrightarrow{row}_i, bias \in layer$  do
        /* The SoP representing the  $i^{th}$  node of the  $l^{th}$  layer
           will be saved to  $node_{l,i}$  */
         $node_{l,i} \leftarrow false$ 
        /* Iterate over every possible bitmask */
        forall  $\overrightarrow{mask} \in (false, true)^{length(\overrightarrow{row})}$  do
            if  $\overrightarrow{row} \cdot \overrightarrow{mask} + bias \geq \theta_t$  then
                 $product \leftarrow true$ 
                forall  $b_i \in \overrightarrow{mask}$  do
                    /*  $node_{l-1,i}$  is the  $i^{th}$  node from the
                       previous layer. */
                    if  $b_i = 0$  then
                         $product \leftarrow product \wedge \neg node_{l-1,i}$ 
                    else
                         $product \leftarrow product \wedge node_{l-1,i}$ 
                     $node_{l,i} \leftarrow node_{l,i} \vee product$ 
             $layerAIG \leftarrow layerAIG | SoP$ 
    NNAIG  $\leftarrow NNAIG >> layerAIG$ 
return NNAIG

```

$$\begin{array}{cccc}
 prev_1 \rightarrow_w curr_1 & prev_2 \rightarrow_w curr_1 & \dots & prev_n \rightarrow_w curr_1 \\
 prev_1 \rightarrow_w curr_2 & \ddots & \ddots & \vdots \\
 \vdots & \ddots & \ddots & \vdots \\
 prev_1 \rightarrow_w curr_m & \dots & \dots & prev_n \rightarrow_w curr_m
 \end{array}$$

- (a) The layer l represented by a matrix of one-way transition functions \rightarrow_w with operands of two nodes in adjacent layers where $prev_j$ is the prior layer.

$$\begin{array}{cccc}
 w_{1,1} & w_{1,2} & \dots & w_{1,n} \\
 w_{2,1} & \ddots & \ddots & \vdots \\
 \vdots & \ddots & \ddots & \vdots \\
 w_{m,1} & \dots & \dots & w_{m,n}
 \end{array}$$

- (b) A simplified version of Figure 8.1a. For consistency with matrix notation, weights are labeled as $w_{curr_i, prev_j}$.

Figure 8.1

8.2 Binary Decision Tree (\mathcal{B})

The classes of neural nodes are true, false, and mixed. For example, a neural node with all positive weights must always be true (hence the class “true”). However, many nodes are in the mixed class since they may be true or false. \mathcal{B} determines each neural node’s class and proceeds to find the sum of products if the node is in the mixed class. If the node is true or false, \mathcal{B} labels it as such in $\Theta(n)$ time. Otherwise, \mathcal{B} has an average complexity of $O(2^{0.5n})$ and a worst-case complexity of $O(2^n)$ (see Chapter 9).

During the node’s parsing, \mathcal{B} keeps track of which node in the previous layer was considered in this sum of products. If every node in the current layer does not use some node X from the previous layer, then X is given a “negligible” class. The parsing algorithm, \mathcal{N} , directs \mathcal{B} to approximate a node and skips the negligible nodes.

As proven in Section 7.1, ordering weights by importance is the same as ordering weights by the greatest absolute value—this is why \mathcal{B} sorts the weight vector. Furthermore, recall the activation function is not computed due to Section 7.2 and Section 7.3. The definition of a threshold is given in Lemma 7.2.2. Furthermore, \mathcal{B} takes advantage of knowing that trained

neural networks often have sparse weight matrices [50].

8.2.1 Order

To list the inputs from the greatest importance to the least importance I used the C++ standard library's (STL) `std::sort` which has a time complexity of $O(n \log(n))$. However, the ordinal value (position) of the weight was used to determine which node in the previous layer the weight came from. This ordinality is destroyed by sorting. To compensate, I created a simple struct called “ordinal_weight.”

```
struct ordinal_weight {
    unsigned short const ordinal;
    float const weight;
    ordinal_weight(unsigned short const o, float const w)
        : ordinal(o), weight(w){}
    inline bool absGreaterThan(ordinal_weight const& rhs)
        const{
        return std :: fabs(weight) > std :: fabs(rhs.weight);
    }
};
```

Then STL's sort function allows for an easy sort.

```
std :: sort(
    ordinalWeightsArr.begin(),
    ordinalWeightsArr.end(),
    [](ordinal_weight const& lhs, ordinal_weight const&
        rhs){
        return lhs.absGreaterThan(rhs);
    }
);
```

8.2.2 \mathcal{B} Defined

As described before, \mathcal{B} is an optimized, binary decision tree which finds the sum of products (SoP) approximating a neural node. Section 8.2.2 illustrates \mathcal{B} in pseudo-code.

To summarize, \mathcal{B} keeps track of the current summation of weights (current), the minimum possible summation (min), and the maximum possible

summation (max). If min is ever greater than or equal to zero, then any combination of future weights will yield true—therefore these weights are “don’t-cares” for this product. In the second case, if max is ever less than or equal to zero, then any combination of future weights will yield false (early termination). Finally, if neither case is true, the tree continues traversing. Note that both cases include equals in their conditional, this is the greedy approach as foreshadowed in Lemma 7.2.2.

Definitions Let π be the current path in \mathcal{B} and binaryNodeArgs be a tuple $(currentSum, maxSum, minSum, node_{l,j}, i, product, SoP, prevNodesMatter)$ where

- currentSum is the summation of weights given π .
- maxSum is the maximum possible summation of weights given π .
- minSum is the minimum possible summation of weights given π .
- $node_{l,j} = (w_0, o_0), (w_1, o_1), \dots, (w_n, o_n)$ is an array of weight_ordinal pairs (see Section 8.2.1) which consists of the in-degree weights for the j^{th} node of the l^{th} layer.
- (w_i, o_i) is the current weight_ordinal pair in $node_{l,j}$
- product is a truth array that will be updated and joined with the sum of products.
- SoP is the table of products.
- prevNodesMatter is a Boolean array which \mathcal{B} uses to tell the network parser which nodes from the previous layer were used in $node_{l,j}$.

Procedure $\text{root}(\text{node}_{l,j}, b, \theta_t)$.

Input:

- $\text{node}_{l,j} = [(w_0, o_0), (w_1, o_1), \dots, (w_n, o_n)]$, a vector of weight-ordinal pairs.
- b , a bias constant.
- θ_t , the θ -threshold (see Section 7.3).
- negligible, a Boolean variable. If $\text{node}_{l,j}$ was not used for any node in the sequential layer, \mathcal{B} , which approximates the node, is skipped entirely.
- prevNodesMatter, as described in Section 8.2.2.

Output:

- SoP , a sum of products describing $\text{node}_{l,j}$.
- prevNodesMatter is manipulated and passed by reference.

```

if negligible is true then
    return
/* Check if this node is always true or always false. */
 $b \leftarrow b - \theta_t;$ 
 $currentSum \leftarrow b;$ 
 $minSum \leftarrow b;$ 
 $maxSum \leftarrow b;$ 
for  $i \leftarrow 0 \dots n$  do
    if  $w_i \geq 0$  then
        |  $maxSum \leftarrow maxSum + w_i$ 
    else
        |  $minSum \leftarrow minSum + w_i$ 
if  $maxSum < 0$  then
    | return false
else if  $minSum \geq 0$  then
    | return true
/* Sorted by weight value. */*
 $node_{l,j} \leftarrow sort(node_{l,j});$ 
/* Initialize values */*
 $product \leftarrow true;$ 
 $SoP \leftarrow false;$ 
/* Begin the algorithm */*
 $binaryNodeArgs \leftarrow$ 
 $(currentSum, maxSum, minSum, node_{l,j}, 0, product, SoP, prevNodesMatter);$ 

if  $w_0 \geq 0$  then
    | pos_true(binaryNodeArgs);
    | pos_false(binaryNodeArgs);
else
    | neg_true(binaryNodeArgs);
    | neg_false(binaryNodeArgs);
return  $SoP$ 

```

Procedure atomize(l, o) –a name mangling function that labels each given node from the neural network.

Input:

- l , the layer number.
- o , the node's ordinal value.
- prevNodesMatter, as defined in Section 8.2.2.

Output: A unique name for $node_{l-1,o}$ to be used in labeling AIG nodes.

```
prevNodesMatter[o] ← true;
/* The ordinal value, o, is referring to the previous
   layer; hence, the name-wrangling does “l-1”.           */
return "L" + string(l-1) + "N" + string(o)
```

Procedure directions(*binaryNodeArgs*)

Input: *binaryNodeArgs*

```
i ← i + 1;
if  $w_i \geq 0$  then
    posTrue(binaryNodeArgs);
    posFalse(binaryNodeArgs);
else
    negTrue(binaryNodeArgs);
    negFalse(binaryNodeArgs);
return
```

Procedure posTrue(binaryNodeArgs). The true case of a positive weight.

Input: binaryNodeArgs
 $product \leftarrow product \wedge atomize(o_i);$
 $current \leftarrow current + w_i;$
 $minSum \leftarrow minSum + w_i;$
if $minSum \geq 0$ **then**
 | $SoP \leftarrow SoP \vee product$
else
 | directions(binaryNodeArgs)
return

Procedure posFalse(binaryNodeArgs). The false case of a positive weight.

Input: binaryNodeArgs
 $product \leftarrow product \wedge \neg atomize(o_i);$
 $max \leftarrow max - w_i;$
if $max \geq 0$ **then**
 | directions(binaryNodeArgs)
return

Procedure negTrue(binaryNodeArgs). The true case of a negative weight.

Input: binaryNodeArgs
 $product \leftarrow product \wedge atomize(o_i);$
 $current \leftarrow current + w_i;$
 $max \leftarrow max + w_i;$
if $max \geq 0$ **then**
 | directions(binaryNodeArgs)
return

Procedure negFalse(binaryNodeArgs). The false case of a negative weight.

Input: binaryNodeArgs
 $product \leftarrow product \wedge \neg atomize(o_i);$
 $min \leftarrow min - w_i;$
if $min \geq 0$ **then**
 | $SoP \leftarrow SoP \vee product$
else
 | directions(binaryNodeArgs)
return

8.2.3 Complexity

While the sum of products of a node in the worst case is exponential ($O(2^n)$) due to the Cook-Levin theorem [6], \mathcal{B} is able to have an average complexity of $O(2^{0.5n})$ (see Chapter 9) and a best-case complexity of $\Omega(n)$.

Best-Case of \mathcal{B} Consider the case where all weights and the bias are positive and the threshold is zero. \mathcal{B} will iterate over each weight (costs $\Theta(n)$) to find the maximum and minimum sums possible. Since every weight and the bias are positive, the minimum sum will be equal to the bias which is greater than zero. \mathcal{B} ends here and notes that this neural node is always true. The $O(n \times \log_2(n))$ sort nor the tree traversal are needed. Therefore, \mathcal{B} 's best case is $\Theta(n)$. See Figure 8.2b for an example.

Worst-Case of \mathcal{B} \mathcal{B} 's worst case is $O(2^n)$ and occurs when all of the weights have equal magnitudes and are as evenly distributed as possible between the positives and negatives bins (a weight vector with an odd size cannot have equal distribution between the positives and negatives). Figure 8.2a illustrates this case. However, Section 9.2.4 shows that \mathcal{B} 's worst case is still approximately twice as fast as the brute-force approach.

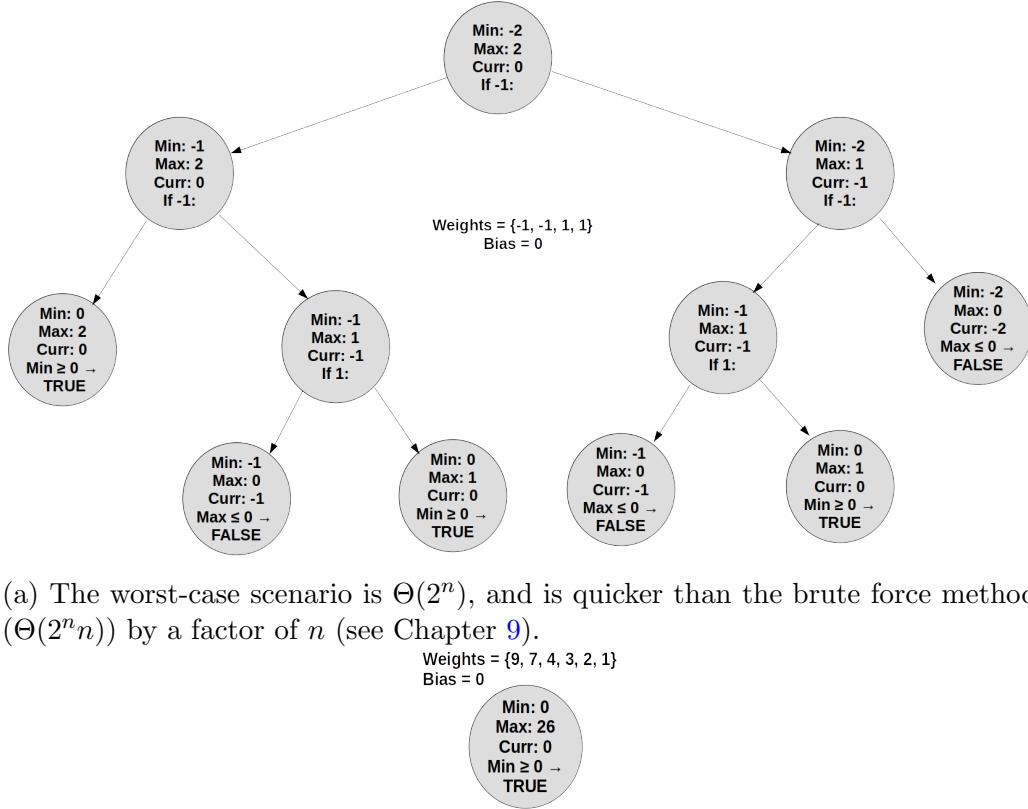


Figure 8.2: Visualization of the possible complexity extremes.

8.3 Traversing the Neural Network

The neural network's reversed traversal allows the algorithm to decide if a neural node must be predicted by \mathcal{B} as defined in \mathcal{B} or if the neural node is negligible and subsequently skipped. This is tracked by the `prevNodesMatter` argument in \mathcal{B} . Algorithm 6 describes a problematic forward traversal which calculates \mathcal{B} for every node while Algorithm 7 is the optimized reverse traversal.

Forward Traversal Algorithm 6¹ can be naïvely parallelized by node or by layer. However, Algorithm 6 can also produce islands (graph components that do not include an input node and an output node) or dead ends (a non-output node with an out-degree of zero) in the final AIG. For example, if no sum of products produced by layer 2 include $node_{1,i}$ from layer 1, then the AIG will have a dead-end representing $node_{1,i}$. An island may occur if a node is determined to be constant (always true or always false) and is negligible (not used in any SoP for the subsequent layer). Algorithm 7 modifies Algorithm 6 by omitting negligible nodes from computation and the AIG output.

Algorithm 6: Forward Traversal

Input: $NN = [l_1, l_2, \dots, l_m]$. Each $l_i \in NN$ is a vector of nodes $[node_0, node_1, \dots, node_n]$. Each $node_j \in l_i$ is a vector of weight-ordinal pairs (w_k, o_k) where o_k is the placement of w_k in the original input vector for $node_j$. The original placement signifies the associated node from the previous layer. The function $root$ is as defined in \mathcal{B} and begins \mathcal{B} .

Output: AIG approximation of the neural network.

```

for  $i = 1 \dots m$  do
    forall  $node_j \in l_i$  do
         $SoP_{i,j} \leftarrow root(node_{i,j}, bias, \theta_t);$ 
        Label the output of  $SoP_{i,j}$  as  $atomize(i, o_j);$ 
         $ParallelAIG_i \leftarrow SoP_{i,0}|SoP_{i,1}| \dots |SoP_{i,n};$ 
    endfor
     $CompleteAIG \leftarrow ParallelAIG_1 >> ParallelAIG_2 >> \dots >>$ 
     $ParallelAIG_m;$ 
return  $CompleteAIG$ 

```

Reverse Traversal Algorithm 7 reduces the computation needed by omitting the negligible neural nodes which also prevents dead ends and islands.

¹Recall that “|” and “>>” are binary operators that take AIG as operands and denote parallel and sequential compositions, respectively [23].

Algorithm 7: \mathcal{N} : Reverse traversal

Input: $NN = [l_1, l_2, \dots, l_m]$ as described in Algorithm 6.

Output: AIG approximation of the neural network.

Let $length(l_i)$ return the number of nodes in l_i ;

$DoCurrentInputsMatter \leftarrow [true_0, true_1, \dots, true_{length(l_m)}]$;

for $i = m, m - 1, \dots, 1$ **do**

$DoPrevInputsMatter \leftarrow [false_0, false_1, \dots, false_{length(l_{i-1})}]$;

forall $node_{i,j} \in l_i$ **do**

$SoP_{i,j} \leftarrow$

$root(node_{i,j}, bias, \theta_t, DoCurrentInputsMatter[j], DoPrevInputsMatter);$

$DoCurrentInputsMatter \leftarrow DoPrevInputsMatter;$

$ParallelAIG_i \leftarrow SoP_{i,0}|SoP_{i,1}| \dots |SoP_{i,n};$

$CompleteAIG \leftarrow ParallelAIG_1 >> ParallelAIG_2 >> \dots >>$

$ParallelAIG_m$;

return $CompleteAIG$

8.4 Additional Ideas

8.4.1 Maximum Tree Depth

To reduce the worst case complexity, a maximum depth (d) can be enforced. The worst-case complexity will become $O(2^d)$ and the average case will be $O(2^{0.5n})$ (recall n is the size of the weight array) if $d > 0.5n$ else the average complexity will be $O(2^d)$. However, the maximum depth will give some loss in accuracy for instances which \mathcal{B} would normally surpass d .

Maximum tree depth has been implemented in the source code for \mathcal{B} .

Recall the XORNN from Chapter 6 was only composed of three layers. If we change the first two layers from two to ten inputs, the average amount of nodes in the decision trees increases exponentially. In Figure 8.3a, no maximum depth is enforced. However, the optimal solution's depth cannot exceed the size of the previous layer (10 in this case); the proof is in Chapter 7 and \mathcal{B} enforces this concept.

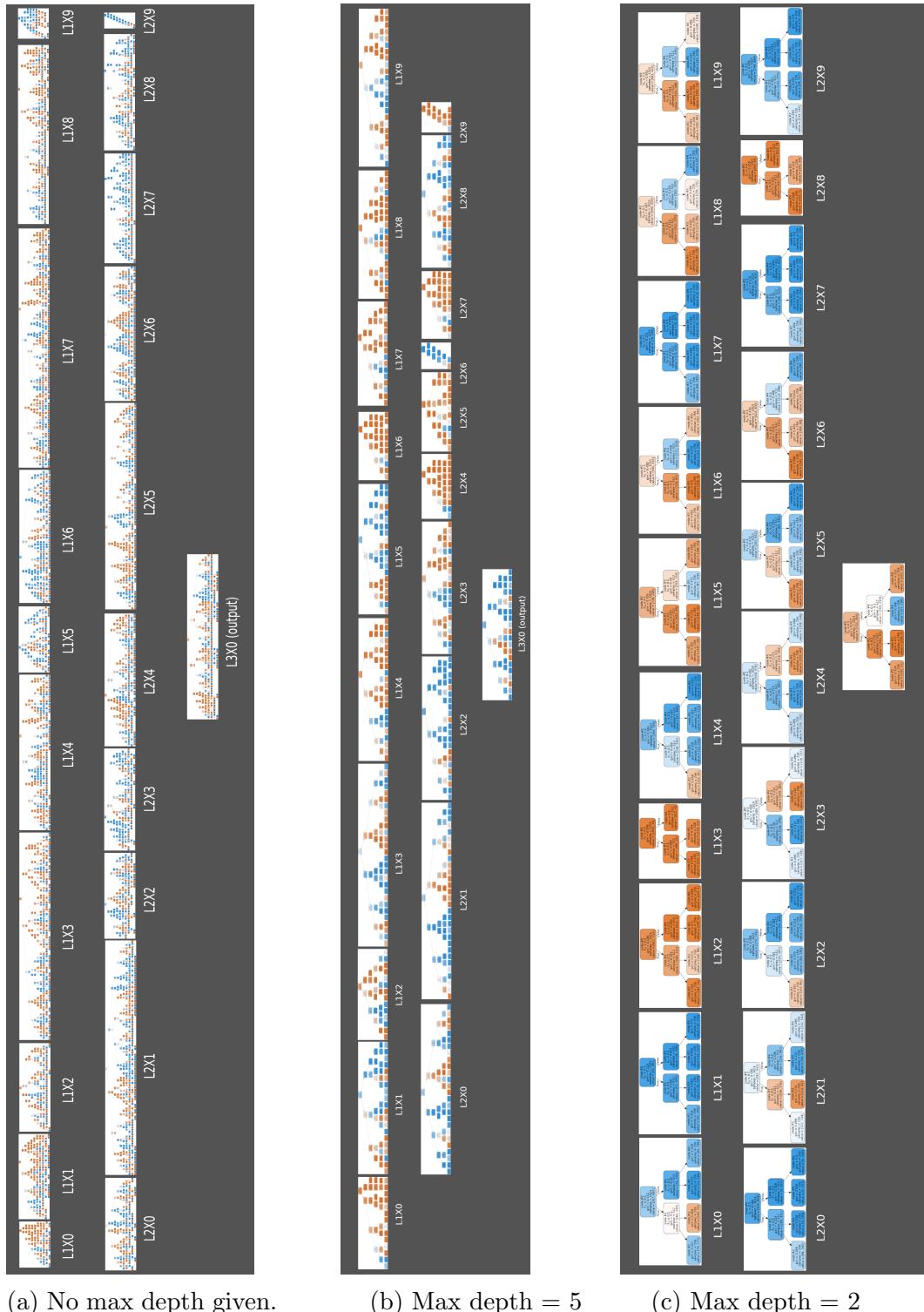


Figure 8.3: Three decision tree networks each representing a 10-10-10-1 (inputs, hidden layer 1, hidden layer 2, output) layered neural network. The input layer is inserted into the first layer of decision trees, then the network proceeds through the layers in the same fashion a neural network predicts input—the only difference being \mathcal{B} is now the activation function.

8.4.2 Subtrees and Dynamic Programming

Since $\theta = \vec{x} \cdot \vec{w}^T$ is a linear combination, coefficients (weights) with similar ratios and positivity yield similar activations. This causes some subtrees in \mathcal{B} to be identical. Future work may determine how to recognize these repeated structures.

8.5 Alternatives

8.5.1 Linear Algebra

Alternatively, linear algebra could be used to obtain the sum of products for a node. Below is the Python source code that can be used to compute an entire layer (all input weight sizes are the same since the network is fully connected).

```
import numpy as np
from itertools import product
sizeOfPrevLayer = 10
sizeOfThisLayer = 1
#columns are the weights from the previous layer to the
#ith (row) node of the current layer
weights = np.random.uniform(-10, 10, (sizeOfPrevLayer,
    sizeOfThisLayer))
inputs = np.asarray(list(product([0,1], repeat=
    sizeOfPrevLayer))) #2^n possibilities
outputs = np.matmul(inputs, weights) >= 0
#Construct truth tables by concatenating inputs and
#outputs. A layer of nodes expressed as a layer of
#sum of products can be derived from this.
...
```

The iterative algorithm of matrix multiplication places this algorithm at $\Theta(2^n \times n \times \text{sizeOfLayer})$. However, Raz that proved the lower bound for matrix multiplications of two **square** matrices is $\Omega(n^2 \log_2 n)$ [51]. Currently, there exists no algorithm with this low complexity—Alman and Williams published the current best complexity of $O(n^{2.37286})$ in October 2020 [52].

Theorem 8.5.1. *Let s be the size of the current layer and n be the size of the weight array (equal the size of the previous layer). Then, the matrix approach has a lower bound of $\Omega(2^n n \log_2 n)$ if $n \leq s$ and $\Omega(2^n s \log_2 s)$ if $n \geq s$.*

Proof. If $n \leq s$, then let's assume the matrix product $M = 2^n \times n \cdot n \times s$ is instead $C = 2^n \times n \cdot n \times n$ which is a quicker computation than the original.

Split the left-hand side of C ($2^n \times n$) into $\frac{2^n}{n}$ submatrices each with size $n \times n$ and having no overlap. Then the product of each submatrix with the reduced RHS ($n \times n$) has a lower bound of $\Omega(n^2 \log_2 n)$ by Raz's theorem. Since there are $\frac{2^n}{n}$ submatrices, C is therefore in

$$\Omega\left(\frac{2^n}{n} n^2 \log_2 n\right) = \Omega(2^n n \log_2 n)$$

Since M is more computationally expensive than C , M is also in $\Omega(2^n n \log_2 n)$.

Alternatively, $n > s$. Like the prior proof, I reduce M to a less expensive C matrix. Let $C = 2^n \times s \cdot s \times s$.

Following the same logic as before, split $2^n \times s$ into $\frac{2^n}{s}$ submatrices. Then, C is in

$$\Omega(2^n n \log_2 n)$$

Since M is more computationally expensive than C , M is also in $\Omega(2^n n \log_2 n)$. \square

Corollary 8.5.1.1. *With a worst-case complexity of $O(2^n)$ per node, \mathcal{B} is still more computationally efficient when computing an entire layer $O(s \times 2^n)$ than the theoretical optimal algorithm for the linear algebra approach of $\Omega(2^n n \log_2 n)$.*

8.5.2 A Table-Based Approach

First and foremost, this algorithm has a worse memory complexity and average time complexity than \mathcal{B} . This approach attempted to exploit tables to reduce the worst case of $O(2^n)$ to $O(2^{0.5n}n)$ which occurs when the weights are approximately equal in absolute value and distribution of positive and negative weights. Unfortunately, this algorithm's time complexity is $\Theta(2^n n)$ and the memory complexity is in $\Omega(2^{\frac{n}{2}} n)$ and $O(2^n n)$. In comparison, \mathcal{B} has a time and space complexity of $\Omega(n)$ to $O(2^n)$ with an average of $O(2^{0.5n})$ (see the complexity of nodes in Section 9.1).

This algorithm was appealing due to the potential $\Omega(2^{\frac{n}{2}})$ memory-bound (see Table 8.2) and the binary search shown in step 4. This algorithm's best-case occurs exactly in the worst cases of \mathcal{B} and was intended to only be used in those cases.

Step 0: Begin with a set of weights, W .

Step 1: Divide W into sorted negative and positive bins; negligible weights (0 plus or minus the machine epsilon or greater if the user desires) can be omitted. This step is done in $\Theta(n)$.

Step 2: For each possible bitmask in both bins, calculate and remember the respective subsum (can be done by matrix multiplication Section 8.5.1). This step is in $\Omega(2^{0.5n} n \log_2 n)$ if the negative and positive bins are equal in size and $\Omega(2^n n \log_2 n)$ on the other extreme.

Step 3: Sort both bins. If step 3a can be done, this step will be a constant $O(1)$, else it will take $\Omega(2^{n/2} \times \log_2(2^{n/2}) = \Omega(2^{n/2}n)$ and $O(2^n n)$.

Step 3a: Depending on the data set, the sort may be done inherently in step 2. For both bins, if the sum of the two smallest (in absolute value) is greater than or equal to the greatest absolute value of that same bin, a bitmask pattern as done in Table 8.2 can be done to produce a completely sorted array. In NEG from Table 8.2, the two smallest absolute values are $\{-1, -0.9\}$ and the greatest absolute value is -1.1 . Now, $|-1 + -0.9| \geq |-1.1|$ so this set of weights can be sorted inherently. Omitting the negligible weights in step 1 allows more sets to be inherently sorted given this bitmask pattern. Furthermore, this algorithm was planned to only occur when the weights have approximately equal absolute values. These cases often allow for step 3a.

Algorithm 8: Step 4. See Table 8.2 for an example.

Input:

- POS, a bin of subsums for all possible positive weights with the respective bitmask table.
- NEG, a bin of subsums for all possible negative weights with the respective bitmask table.

Output: NodeSoP. A sum of products explaining the current node.

```

if sizeof(NEG) > sizeof(POS) then
    bins  $\leftarrow$  POS
    binl  $\leftarrow$  NEG
else
    bins  $\leftarrow$  NEG
    binl  $\leftarrow$  POS
NodeSop  $\leftarrow$  False
foreach (Bitmaski, subsumi)  $\in$  bins do
    Bitmaskn  $\leftarrow$  BinarySearch(binl, subsumi) /* BinarySearch
        returns the bitmask that corresponds to the subsum
        which is the closest absolute value in binl that is
        smaller than subsumi */
    if Bitmaskn is null then
         $\downarrow$  continue
    foreach Bitmaskj  $\in$  Bitmask1 . . . Bitmaskn do
        product  $\leftarrow$  bins(Bitmaski)  $\cup$  binl(Bitmaskj)
        NodeSop  $\leftarrow$  NodeSop  $\vee$  product
return NodeSop

```

Analysis of Algorithm 8 Let s be the size of bin_s and l be the size of bin_l where $0 \leq s \leq 2^{\frac{n}{2}}$, $2^n \geq l \geq 2^{\frac{n}{2}}$, and $s \times l = 2^n$. Finding each $Bitmask_n$ in step 4 is in $O(s \log_2(l))$ which has the worst case when $s = l$. In terms of n , this makes the complexity $O(2^{\frac{n}{2}} \log_2(2^{\frac{n}{2}})) = O(2^{\frac{n}{2}}n)$ to find each $Bitmask_n$. Unfortunately, adding each lower bitmask in the inner loop makes the algorithm $O(sl) = O(2^n)$.

Algorithm 8 Example In Table 8.2, $subsum_s$'s (POS bin) first subsum s_1 is zero which is paired with Bitmask1. Searching the NEG bin for the

absolute value closest to s_1 and still less than s_1 yields Bitmask1, therefore Bitmask1 of POS unioned with Bitmask1 of NEG yields a total summation greater than or equal to zero—therefore this combination is a product in the sum of products representing the node (SoP_{node}). $subsum_s$'s second subsum s_2 is 1 (Bitmask2) which finds the closest, smaller absolute value in NEG bin at Bitmask2 so Bitmask2 of NEG unioned with Bitmask2 of POS is also a product in SoP_{node} . Additionally, each BitmaskN in NEG below Bitmask2 unioned with Bitmask2 of POS is also in SoP_{node} —here that only includes Bitmask1 of NEG. So far, $SoP_{node} = 000000 + 001001 + 000001$ where the 000000 comes from the iteration of Bitmask1 in POS, and 001001 + 000001 comes from Bitmask2 in NEG.

To assert correctness (not needed in the algorithm—only for human understanding), add the respective subsums for each product in the SoP_{node} obtained so far:

$$\begin{aligned} 000000 &\rightarrow NEG(000) + POS(000) = 0 + 0 = 0 \geq 0 \\ 001001 &\rightarrow NEG(001) + POS(001) = -0.9 + 1 = 0.1 \geq 0 \\ 000001 &\rightarrow NEG(000) + POS(001) = 0 + 1 = 1 \geq 0 \end{aligned}$$

Table 8.2: An example of step two in Section 8.5.2 with the set of weights being {1.2,1.1,1,-1.1,-1,-0.9} and the bias constant $B = 0$.

Weights	NEG			Negative Subsums BitmaskN·NEG+B	POS			Positive Subsums BitmaskN·POS+B
	-1.1	-1	-0.9		1.2	1.1	1	
Bitmask1	0	0	0	0	0	0	0	0
Bitmask2	0	0	1	-0.9	0	0	1	1
Bitmask3	0	1	0	-1	0	1	0	1.1
Bitmask4	1	0	0	-1.1	1	0	0	1.2
Bitmask5	0	1	1	-1.9	0	1	1	2.1
Bitmask6	1	0	1	-2	1	0	1	2.2
Bitmask7	1	1	0	-2.1	1	1	0	2.3
Bitmask8	1	1	1	-3	1	1	1	3.3

Conclusion This algorithm was promising because of the binary search in Algorithm 8 and only computing $2^{0.5n}$ subsums in the best case. However, even if we assume the best matrix algorithm possible for the best case in step

2 ($\Omega(2^{0.5n}n \log_2 n)$) and a constant sort in step 3, step 4 will still make this algorithm's optimal scenario $O(2^n)$. The memory and time complexities of this algorithm are worse than \mathcal{B} .

Chapter 9

Empirical Complexity of \mathcal{B}

This chapter compares \mathcal{B} 's average complexity, worst-case complexity, and the alternative brute force's complexity in time and space. The average complexity was derived by performing many simulations on \mathcal{B} with a random array of weights with a uniform distribution. The empirical evidence is found by doing three regression fits: 2^{bn} , $a \times 2^{bn}$, and $a \times 2^n$ where a and b are the constants to be found in the regression fits and n is the independent variable being tested (n is either the number of nodes or the time spent).

Future work can investigate the nature of neural network nodes and how close a uniformly-random distribution properly represents the average neural node. All regression fits were done with the SciPy Python library.

Notably, the computational time spent for \mathcal{N} (the parsing algorithm that employs \mathcal{B} many times) to approximate a neural network was dwarfed when comparing the time spent to construct the AIG using Mockturtle [5]. All experiments here only considered \mathcal{N} .

9.1 Node Complexity

This section is the best empirical evidence for \mathcal{B} 's average case of $O(2^{0.5n})$ and \mathcal{B} 's worst-case being $\theta(2^n)$.

\mathcal{B} only needs to remember the current path being traversed (memory of $O(n)$), but the sum of products remembered for \mathcal{N} scales with \mathcal{B} 's. Therefore, the memory complexity of \mathcal{B} is its total nodes whose complexities are found to be in $O(2^n)$ with an average of $O(2^{0.5})$.

9.1.1 Average Node Complexity

After analyzing Figure 9.1, we see the best-fit regression for $a \times 2^n$ is the worst fit of the three regression functions. The other two regressions ($a \times 2^{bn}$ and 2^{bn} for $b \approx 0.5$) are the better fits for the data.

Table 9.1: Average node complexities of \mathcal{B}

Node Type	2^{bn}	$a \times 2^{bn}$	$a \times 2^n$
Leaves	$\approx 2^{4.743 \times 10^{-1}n}$	$\approx 1.870 \times 10^{-1} \times 2^{5.269 \times 10^{-1}n}$	$\approx 4.362 \times 10^{-8} \times 2^n$
Parents	$\approx 2^{4.956 \times 10^{-1}n}$	$\approx 6.184 \times 10^{-1} \times 2^{5.107 \times 10^{-1}n}$	$\approx 8.548 \times 10^{-8} \times 2^n$
Total Nodes	$\approx 2^{5.085 \times 10^{-1}n}$	$\approx 7.859 \times 10^{-1} \times 2^{5.160 \times 10^{-1}n}$	$\approx 1.291 \times 10^{-7} \times 2^n$

Percent Increases In Figure 9.2, the percentage increase from the average amount in the weight size prior is shown in a scatterplot. Since 10,000 out of the possible $c \times 2^n$ samples were used for each weight size, there is an increasing variance as the weight array gets larger—increasing the samples in proportion to the exponentially increasing possibilities would likely reduce the change in variance. However, this would cause sampling to be exponentially more expensive on an already exponential algorithm.

In Figure 9.2, the median and means all show an approximate increase of 40%, which indicates the average case is approximately $O(1.4^n)$. This validates the average case of $O(2^{0.5n})$ since

$$2^{0.5n} = (2^{0.5})^n \approx 1.4^n$$

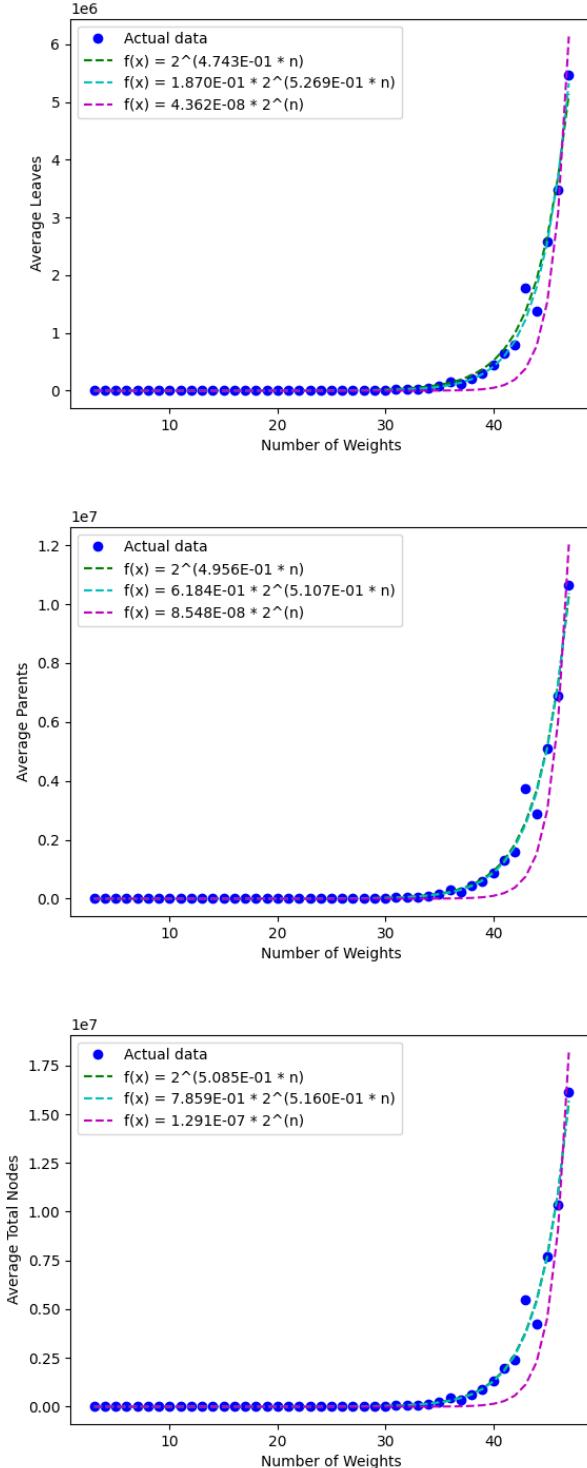


Figure 9.1: Scatter plots of \mathcal{B} 's average nodes with regression fits from Table 9.1.

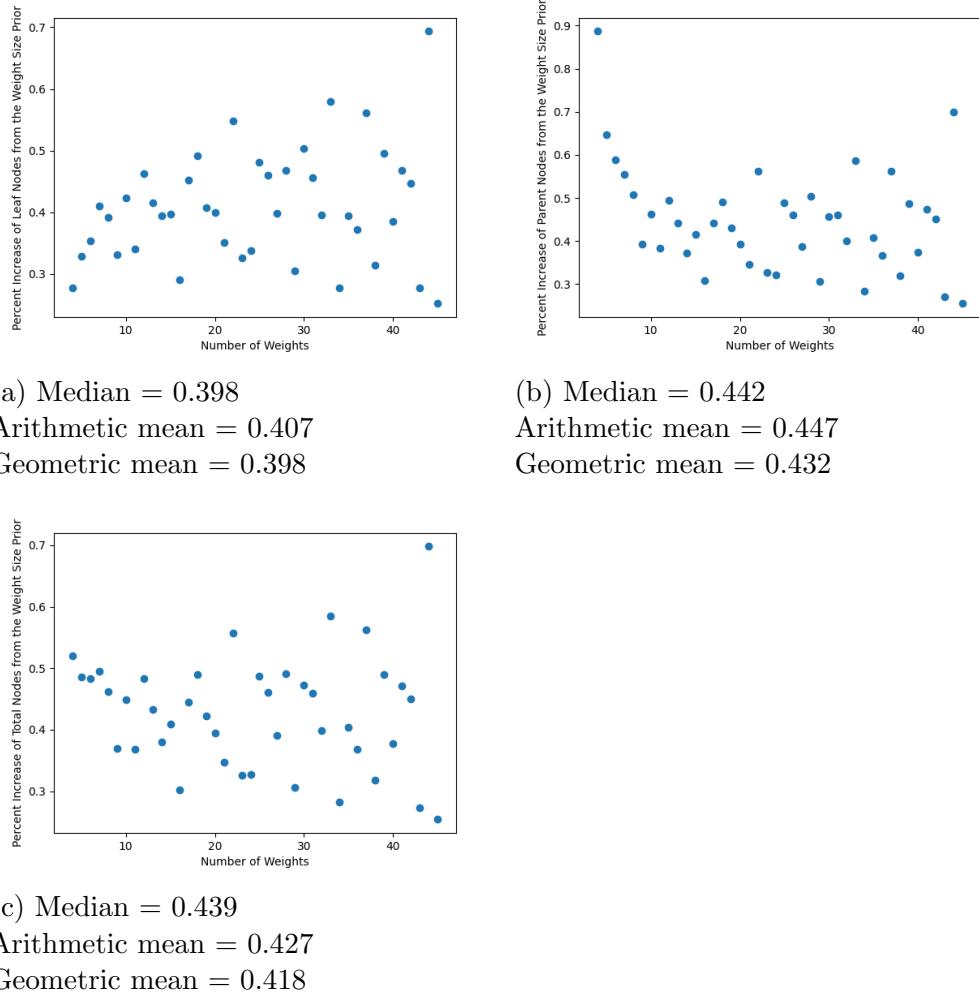


Figure 9.2: The average increases for the average node complexity using 10,000 samples for each weight. A value of 0.439 for weight_n means that n was 1.439 times greater than weight_{n-1}.

9.1.2 Worst-Case Node Complexity

Regression fits for the worst-case are shown in Table 9.2. The empirical evidence in Figure 9.3 strongly supports the theoretical analysis for \mathcal{B} 's worst case of $O(2^n)$. In Figure 9.4, we can see alternating increases (odd versus even weight array sizes). Despite the odd sizes being a smaller increase from the prior even size than vice versa, both appear to be asymptotic between 0.95 and 1 which indicates the complexity is $O(2^n)$.

Table 9.2: Worst-case complexities

Node Type	2^{bn}	$a \times 2^{bn}$	$a \times 2^n$
Leaves	$\approx 2^{8.615 \times 10^{-1}n}$	$\approx 1.098 \times 10^{-1} \times 2^{9.813 \times 10^{-1}n}$	$\approx 7.770 \times 10^{-2} \times 2^n$
Parents	$\approx 2^{8.976 \times 10^{-1}n}$	$\approx 2.927 \times 10^{-1} \times 2^{9.642 \times 10^{-1}n}$	$\approx 1.509 \times 10^{-1} \times 2^n$
Total Nodes	$\approx 2^{9.201 \times 10^{-1}n}$	$\approx 3.988 \times 10^{-1} \times 2^{9.699 \times 10^{-1}n}$	$\approx 2.286 \times 10^{-1} \times 2^n$

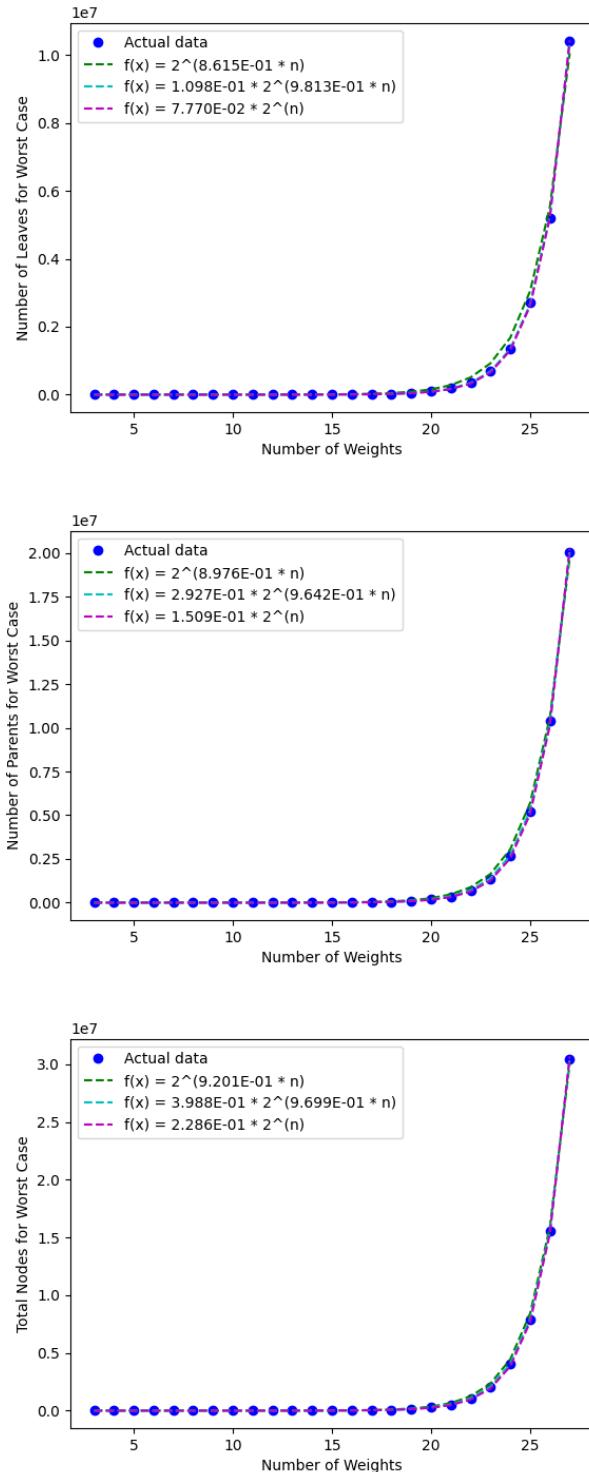


Figure 9.3: Scatter plots of \mathcal{B} 's node count in the worst-case with regression fits from Table 9.2.

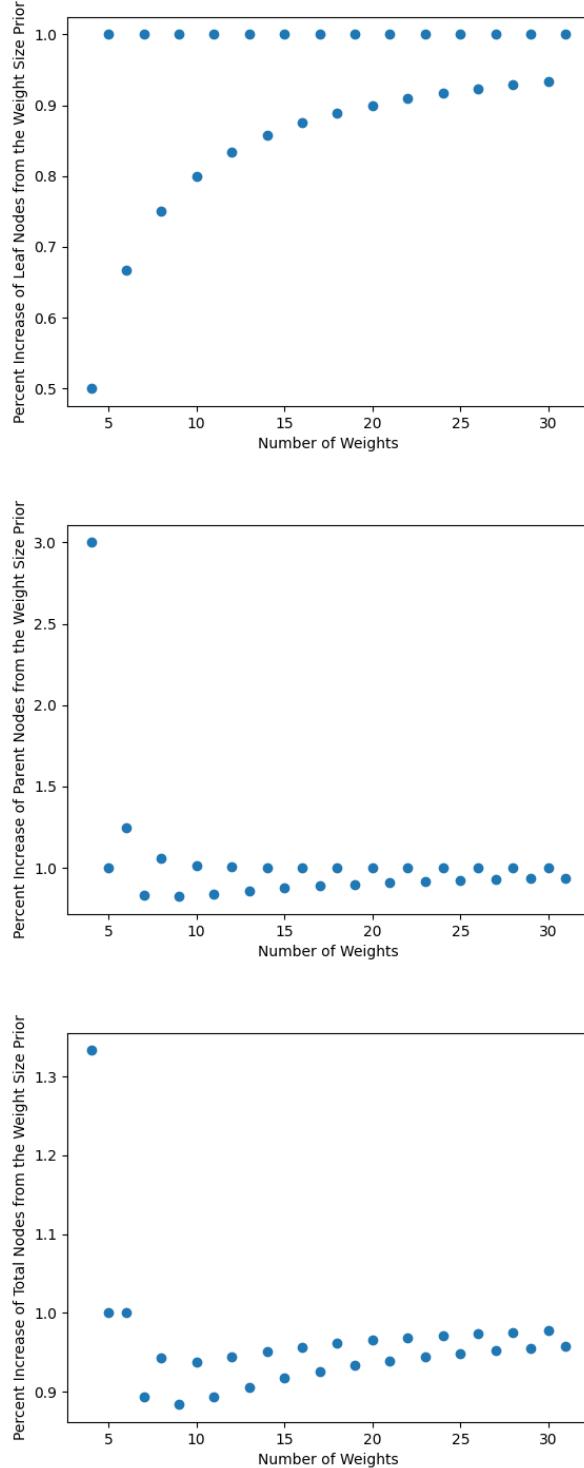


Figure 9.4: The percentage increase for the worst case. Following the structure of Figure 9.2, a value of 1.0 for weight_n means that weight_n had twice the amount of nodes as weight_{n-1} .

9.1.3 Exhaustive Case

The exhaustive version of \mathcal{B} would be a binary tree that does not terminate early (see more information about \mathcal{B} in Section 8.2.2). By enabling early termination, the amount of total nodes in the worst case is about $\frac{1}{9}$ of the exhaustive traversal of the tree. The exhaustive traversal ($O(2^n)$) is also faster than the brute-force approach ($O(2^n n)$) (see Section 9.2.3). Table 9.3 illustrates the speedup of \mathcal{B} 's worst cases over the exhaustive cases. The speedup (represented as percents) was found using the coefficient a from the $a \times 2^n$ complexities in Table 9.2.

Table 9.3: The exact node complexity if \mathcal{B} always calculated every possibility (exhaustive case).

Node Type	Exhaustive Case	Percent of \mathcal{B} 's Worst-case Node Complexities
Leaf	2^n	1287%
Parent	$2^n - 1$	663%
Total Nodes	$2^{n+1} - 1$	875%

9.2 Time Complexity

These results further validate complexities hypothesized in Section 9.1 and give the brute force's complexity as a point of reference.

9.2.1 Average Time Complexity

Table 9.4 and Figure 9.5 use a uniformly random distribution to approximate the average case of \mathcal{B} . The problem of the average-case complexity here coincides with the average amount of minterms needed to express the linear combinations.

Table 9.4

Percentile	2^{bn}	$a \times 2^{bn}$	$a \times 2^n$
10th	$\approx 2^{3.270 \times 10^{-1}n}$	$\approx 6.754 \times 10^{-4} \times 2^{5.577 \times 10^{-1}n}$	$\approx 4.252 \times 10^{-10} \times 2^n$
25th	$\approx 2^{3.502 \times 10^{-1}n}$	$\approx 1.429 \times 10^{-2} \times 2^{4.845 \times 10^{-1}n}$	$\approx 8.438 \times 10^{-10} \times 2^n$
50th	$\approx 2^{3.766 \times 10^{-1}n}$	$\approx 1.224 \times 10^{-2} \times 2^{5.154 \times 10^{-1}n}$	$\approx 1.964 \times 10^{-9} \times 2^n$
75th	$\approx 2^{4.033 \times 10^{-1}n}$	$\approx 7.447 \times 10^{-4} \times 2^{6.295 \times 10^{-1}n}$	$\approx 4.743 \times 10^{-9} \times 2^n$
90th	$\approx 2^{4.384 \times 10^{-1}n}$	$\approx 2.043 \times 10^{-3} \times 2^{6.326 \times 10^{-1}n}$	$\approx 1.439 \times 10^{-8} \times 2^n$

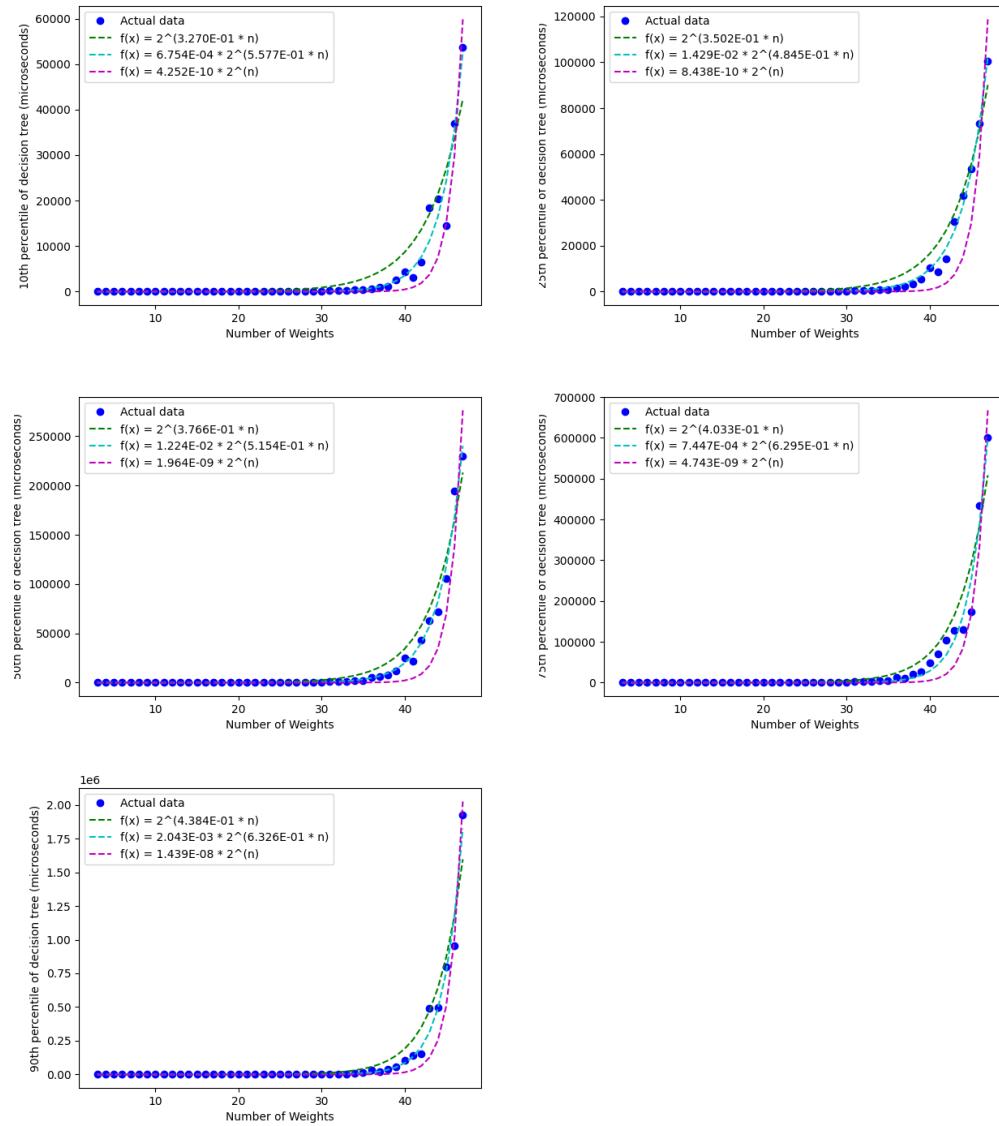


Figure 9.5: Scatter plots of recorded times for \mathcal{B} 's average case (random weights were used) with regression fits from Table 9.4.

9.2.2 Worst-Case Time Complexity

Table 9.5 and Figure 9.6 use weight arrays where each element has the same absolute value and the distributed between positive and negative bins are done as evenly as possible. Figure 9.6 shows that regressions of about 2^n were the best fit. This confirms \mathcal{B} 's worst case of $O(2^n)$.

Table 9.5

Percentile	2^{bn}	$a \times 2^{bn}$	$a \times 2^n$
10th	$\approx 2^{7.316 \times 10^{-1}n}$	$\approx 5.530 \times 10^{-3} \times 2^{1.014n}$	$\approx 7.188 \times 10^{-3} \times 2^n$
25th	$\approx 2^{7.317 \times 10^{-1}n}$	$\approx 5.394 \times 10^{-3} \times 2^{1.016n}$	$\approx 7.206 \times 10^{-3} \times 2^n$
50th	$\approx 2^{7.319 \times 10^{-1}n}$	$\approx 5.347 \times 10^{-3} \times 2^{1.016n}$	$\approx 7.226 \times 10^{-3} \times 2^n$
75th	$\approx 2^{7.321 \times 10^{-1}n}$	$\approx 5.413 \times 10^{-3} \times 2^{1.016n}$	$\approx 7.251 \times 10^{-3} \times 2^n$
90th	$\approx 2^{7.325 \times 10^{-1}n}$	$\approx 6.205 \times 10^{-3} \times 2^{1.009n}$	$\approx 7.299 \times 10^{-3} \times 2^n$

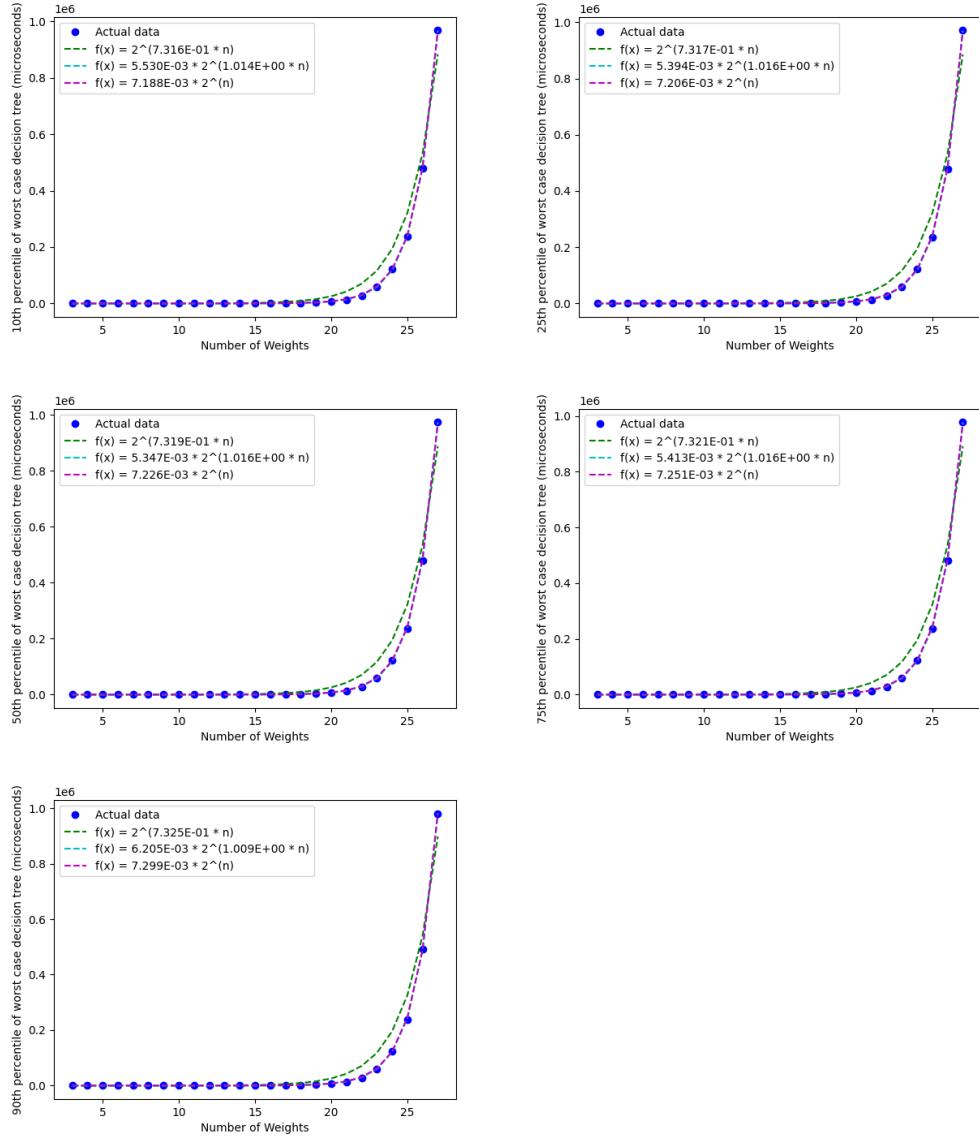


Figure 9.6: Scatter plots of times recorded for \mathcal{B} 's worst-case with regression fits from Table 9.5.

9.2.3 Brute-Force Complexity

Table 9.6 and Figure 9.7 approximates the complexity of a brute-force solution. The brute force solution is a simple recursive program that iterates over all 2^n mask possibilities as shown in Section 9.2.3 and Section 9.2.3. Following the logic from Section 8.5.1, this algorithm has a complexity of $O(2^n n)$. However, the regressions are done in the same manner as the prior regressions were done as a control.

Procedure initializeBruteForce

Input: n , the number of weights.

Output: productTable , a sum of products describing the random weight array created.

```

/* Initialize random array.                                */
randArr ← array(value=random_double, size=n);
initMask ← array(value=false, size=n);
productTable ← ∅;
/* Let  $\theta_t = 0$  for this pseudocode.                  */
if  $\text{initMask} \cdot \text{randArr}^T > \theta$  then
    productTable ← productTable ∪ initMask;
bruteForceIter(randArr, productTable, initMask, 0);
return productTable

```

Procedure bruteForceIter

Input:

- randArr: an array of random weight values.
- productTable: the table of products.
- currentMask: the current bitmask.
- maskIter: tracks the current position in currentMask to update.

Output: Updates the productTable which is passed by reference.

```

if maskIter = currentMask.size() then
    return
    bruteForceIter(randArr, sopTable, currentMask, maskIter + 1);
    currentMask[maskIter] = true;
    if currentMask · randArrT > 0 then
        productTable ← productTable ∪ currentMask;
    bruteForceIter(randArr, productTable, currentMask, maskIter + 1);
return

```

Table 9.6

Percentile	2^{bn}	$a \times 2^{bn}$	$a \times 2^n$
10th	$\approx 2^{8.833 \times 10^{-1}n}$	$\approx 3.381 \times 10^{-1} \times 2^{9.468 \times 10^{-1}n}$	$\approx 1.362 \times 10^{-1} \times 2^n$
25th	$\approx 2^{8.867 \times 10^{-1}n}$	$\approx 3.824 \times 10^{-1} \times 2^{9.430 \times 10^{-1}n}$	$\approx 1.444 \times 10^{-1} \times 2^n$
50th	$\approx 2^{8.947 \times 10^{-1}n}$	$\approx 5.058 \times 10^{-1} \times 2^{9.347 \times 10^{-1}n}$	$\approx 1.656 \times 10^{-1} \times 2^n$
75th	$\approx 2^{9.057 \times 10^{-1}n}$	$\approx 7.014 \times 10^{-2} \times 2^{1.061n}$	$\approx 1.998 \times 10^{-1} \times 2^n$
90th	$\approx 2^{9.086 \times 10^{-1}n}$	$\approx 6.508 \times 10^{-2} \times 2^{1.068n}$	$\approx 2.099 \times 10^{-1} \times 2^n$

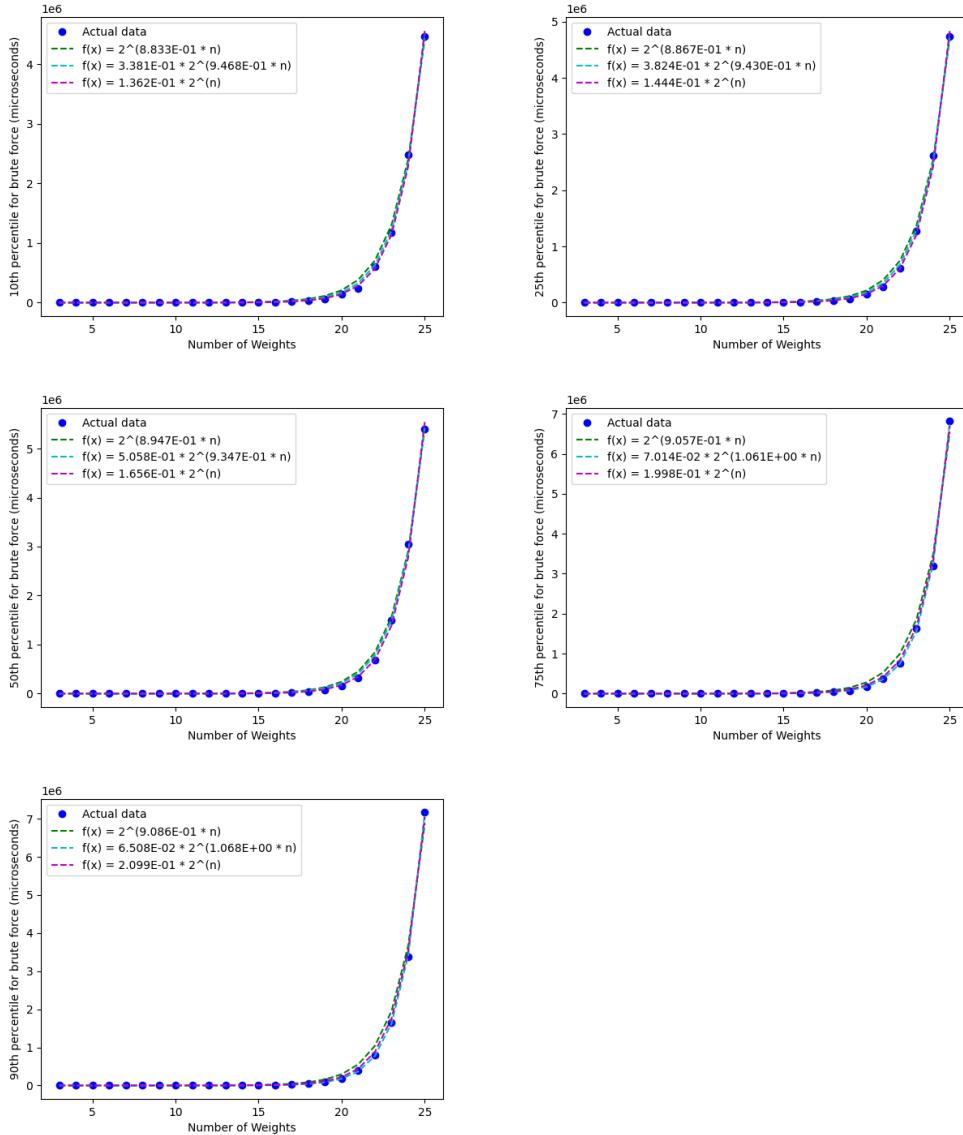


Figure 9.7: Scatter plots of the times recorded using the brute force approach with regression fits from Table 9.6.

9.2.4 Average, Worst, and Brute Time Ratios

While the average-case and the worst-case of \mathcal{B} and the brute force algorithm all have different complexities ($O(2^{0.5n})$, $O(2^n)$, $O(2^n n)$, respectively), the ratios are shown below to give an idea of how much quicker \mathcal{B} is for weight sizes 3 through 26. These ratios will only increase in favor of \mathcal{B} for greater weight sizes.

Table 9.7: The speedups for each complexity in the form $a \times 2^n$. Note: $x : y$ is the ratio of how much faster y is than x so Worst-case:Average is the speedup of Average compared to the Worst-case.

Percentile	Worst-case:Average	Brute-force:Average	Brute-force:Worst-case
10th	1.69×10^8	3.21×10^8	1.89
25th	8.54×10^7	1.71×10^8	2.00
50th	3.68×10^7	8.43×10^7	2.29
75th	1.53×10^7	4.21×10^7	2.76
90th	5.07×10^6	1.46×10^7	2.88
Geometric Mean	3.34×10^7	7.78×10^7	2.33
Arithmetic Mean	6.24×10^7	1.27×10^8	2.36

9.3 Conclusion

I have empirically determined \mathcal{B} (defined in Section 8.2.2) to have an average complexity (in the number of nodes and amount of time) of $O(2^{0.5n})$ and a worst-case complexity (in the number of nodes and amount of time) of $O(2^n)$. In contrast, the brute-force approach has a time complexity of $\Theta(2^n n)$.

Chapter 10

Don't-Care Variables

In Boolean algebra, “don’t-cares” are variables that do not affect the output. For example, when predicting if it is going to rain tomorrow, the name of the weatherman is irrelevant and is considered a “don’t-care variable”.

Determining don’t-care variables is important in reducing the number of nodes that are represented in the final AIG, which is important in this thesis for the end goal of comprehensibility.

10.1 Red is Stop

First, let’s begin with a simple Boolean function. I use an example of the colors in a standard traffic light: red, yellow, and green. In this example, the yellow and green lights as input are irrelevant or ignored by the neural network—two don’t-care variables. Although I use three inputs, of which two are ignored, my point is to illustrate that any number of inputs can be ignored by a neural network if they do not contribute to the output and are thus “don’t-care variables.”

RYG RYG is a simple function with two don’t-care variables:

$$RYG(R, Y, G) = \neg R$$

In other words, the function RYG takes in the input of R, Y, and G as input, but Y and G are irrelevant to the output of the neural network, which simply returns the negation of R. As such, Y and G are don’t-care variables. Table 10.1 shows how a neural network can discover this relationship (simplified

with \mathcal{N}). See Figure 10.1a for the AIG representation of this table. Next, ABC further simplifies the function to Figure 10.1b.

Table 10.1: Every row is a product in the sum of products for each of the neural nodes trained on the RYG function in a $3 \times 2 \times 1$ (excluding biases) neural network. The nodes are named as $L\#X\#$ where the $\#$ after L is the layer number and the $\#$ after X is the node number of the layer. The input layer is L1. Since each node in L1 is activated when the input it represents is 1, L1 is boring and is not given a table.

L2X1			L2X2			L3X1	
r	y	g	r	y	g	L2X1	L2X2
0	-	-	0	-	0	1	-
						0	1

Theorem 10.1.1 translates Table 10.1 into the Boolean logic equivalent. Furthermore, Theorem 10.1.1 shows that \mathcal{N} was able to optimize away the y don't-care variable but not the g don't-care variable. Using simplification logic, we see that \mathcal{N} gave a correct formula and that g can be optimized away.

\mathcal{N} can only optimize away don't cares that are immediately discarded in the next layer. Logic synthesis from ABC's simplification tool removes don't-care variables that are not immediately apparent [1]. See Table 10.1 for an illustration.

Theorem 10.1.1. *\mathcal{N} 's approximation of the neural network (shown in Table 10.1) is equivalent to RYG.*

Proof. First, convert Table 10.1 to Boolean functions.

$$L2X1 = \neg r \tag{10.1}$$

$$L2X2 = \neg r \neg g \tag{10.2}$$

$$L3X1 = L2X1 \vee \neg L2X1 \wedge L2X2 \tag{10.3}$$

Using substitution then simplification,

$$L3X1 = \neg r \vee \neg(\neg r) \wedge \neg rg \tag{10.4}$$

$$= \neg r \vee r \neg rg \tag{10.5}$$

$$= \neg r \vee 0 \tag{10.6}$$

$$= \neg r \tag{10.7}$$

□

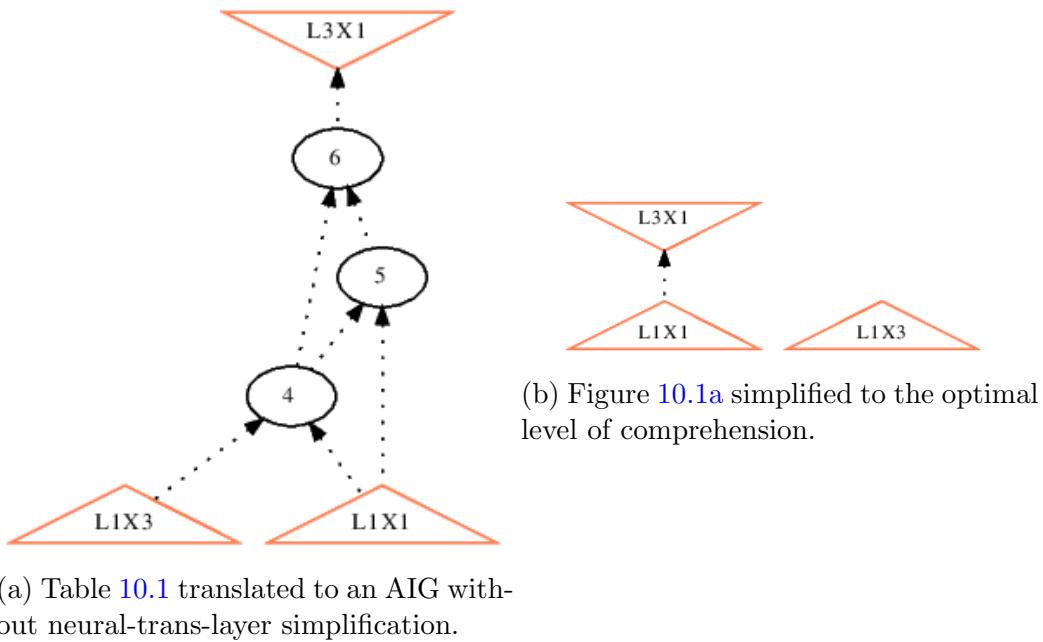


Figure 10.1: AIGs derived from Table 10.1. L1X1 is red and L1X3 is green. \mathcal{N} was able to optimize away L1X2 (yellow). This serves as a secondary proof that Table 10.1 is equivalent to RYG.

Table 10.1 shows the finished AIG that shows that the single input (L1X1 or “R”) is the only input needed and results in its negated input.

Discussion Interestingly, the neural network allowed for an impossible case of $\neg r \wedge r$ in one of the products (see Equation (10.5)). This opens the door for future work in \mathcal{B} . Perhaps the scenario is possible before the binarization and this quasi impossibility could be used to achieve a better understanding of the neural network. Alternatively, this scenario is impossible and future work could help \mathcal{B} skip these impossible scenarios. Another instance of \mathcal{B} including unneeded values is seen in Section 10.2.3.

10.2 Binarization and Limitations

10.2.1 Real to Binary Inputs

Before real-valued input is used, it must be cast to a Boolean value (binarized). Algorithm 9 defines how binarization is done in this chapter.

Algorithm 9: Binarization algorithm.

Input:

- \hat{x} , some threshold.
- $I \in \mathbb{R}^n$, the set of inputs in the real domain.

Output: $I_{\text{binarized}} \in \mathbb{B}^n$.

forall $x \in I$ **do**

$$x \leftarrow \begin{cases} 0 & \text{if } x < \hat{x} \\ 1 & \text{otherwise.} \end{cases}$$

return I

Binarization Thresholds Preliminary investigations tested four methods to obtain a threshold: median, mean, K-means with one centroid (took the centroid's value), and K-means with two centroids (took the average of the two centroid values). The mean threshold appeared to give the most accurate results. Future work can further analyze this threshold.

10.2.2 Illustrating the Limitations of Algorithm 9

Two limitations are identified in this section: binarized data sets that produce all possibilities and binarized data sets which do not accurately represent the original data.

Higgs

Consider the Higgs data set (a data set from particle physics that consists of real numbers) [53]. This set is split into high-level values (produced by functions) and low-level values (basic data used to compute the high-level features). A goal with this data set is to find better functions to predict if

the given data is noise or an important signal. To do so, a neural network can be trained on the data then analyzed.

Neural Network Results After applying the binarization algorithm in Algorithm 9 with the mean threshold, I was able to get 67% accuracy and 0.67 AUC by implementing a 28X24X24X1 (size of each layer from the input layer (28) to the output layer (1)) neural network with the swish function activation (the majority class is 53%). Using real numbers and a far more intricate deep neural network, Baldi, Sadowski, and Whiteson managed to get 88% accuracy and 88 AUC in [53]. However, the AIG constructed from my 28X24X24X1 neural network (with binarized input) generated a file size too large (greater than 4GB) for ABC. So I was unable to use ABC’s simplification tools.

The loss in accuracy by binarizing the Higgs data set can be better understood by looking at the binarized Iris data set in Section 10.2.2.

A Simpler Neural Network Since the 28X24X24X1 elicited an AIG too large for ABC to simplify, I tested a simpler neural network with fewer inputs.

I used Pearson correlation on the low-level values to approximate the five most promising inputs for a simple 5X4X4X1 neural network. Upon testing, I discovered the neural network performed poorly. After analyzing the data set, I found every one of the 2^6 possible Boolean combinations was present. See Table 10.2 for an example of every Boolean combination given two inputs.

a	b	f(x)
0	0	0
0	0	1
0	1	0
1	0	0
0	1	1
1	0	1
1	1	0
1	1	1

Table 10.2: A neural network cannot learn this function when reduced to this set, yet when trained on the original set the neural network biased towards the most instances of input/output pairs.

AIGs From Uncertain Neural Networks Furthermore, the resulting AIG's approximation of the simpler neural network had varying accuracy (about 50% to 90%). This is due to the activation outputs being around the binary threshold caused by the trained neural network's uncertainty. See Section 10.3 for more research into neural network certainty and resulting AIG approximations.

Binarization Limits

Some features cannot be binarized without a sufficient loss of information. In this section I will use the historic Iris data set from the early 1900s. The Iris data set is often used in statistics and machine learning education because of the simplicity of the data set. There are three Iris species in the data set: Virginica, Setosa, and Versicolor.

For example, notice how Virginica's sepal width (orange lines) in Figure 10.2 tends to be less than Setosa's but greater than Versicolor's sepal widths. Assume we wanted to create a binary class of "yes Virginica" or "not Virginica" and binarize the respective inputs. With Algorithm 9, we are allowed one threshold (\hat{x}) for each input. Where should the \hat{x} for sepal width be? If $\hat{x} = 3$ then both 0 and 1 have approximately a $\frac{1}{3}$ chance to represent Virginica's sepal width—this makes the sepal width input useless. A better solution is to place \hat{x} between Virginica and Versicolor ($\hat{x} \approx 2.8$), then 1 will have about 50% chance of being Virginica and 0 will be not Virginica.

However, this problem is better solved if we gave sepal width more thresholds and more bits as done in Algorithm 10. Future work can expand on converting a real-valued input to multiple binary inputs (even greater than two) which can preserve essential information. Brudermueller et al. converted real-valued numbers to multiple binary inputs, but they did not minimize the number of bits needed per input [2].

Algorithm 10: Example of casting a real-valued input into multiple binary inputs.

Input:

- $I_s \in \mathbb{R}^n$, the set of all sepal width inputs.
- $\hat{x}_1 = 2.8$, the first threshold for sepal width.
- $\hat{x}_2 = 3.2$, the second threshold for sepal width.

Output: $I_{s:2-bit}$, a set representing each element in I_s as a pair of bits.

```

 $I_{s:2-bit} \leftarrow \emptyset$ 
forall  $x \in I_s$  do
  if  $x < \hat{x}_1$  then
    |  $I_{s:2-bit} \leftarrow I_{s:2-bit} \cup \{00\}$ 
  else if  $x < \hat{x}_2$  then
    |  $I_{s:2-bit} \leftarrow I_{s:2-bit} \cup \{01\}$ 
  else
    |  $I_{s:2-bit} \leftarrow I_{s:2-bit} \cup \{10\}$ 
return  $I_{s:2-bit}$ 

```

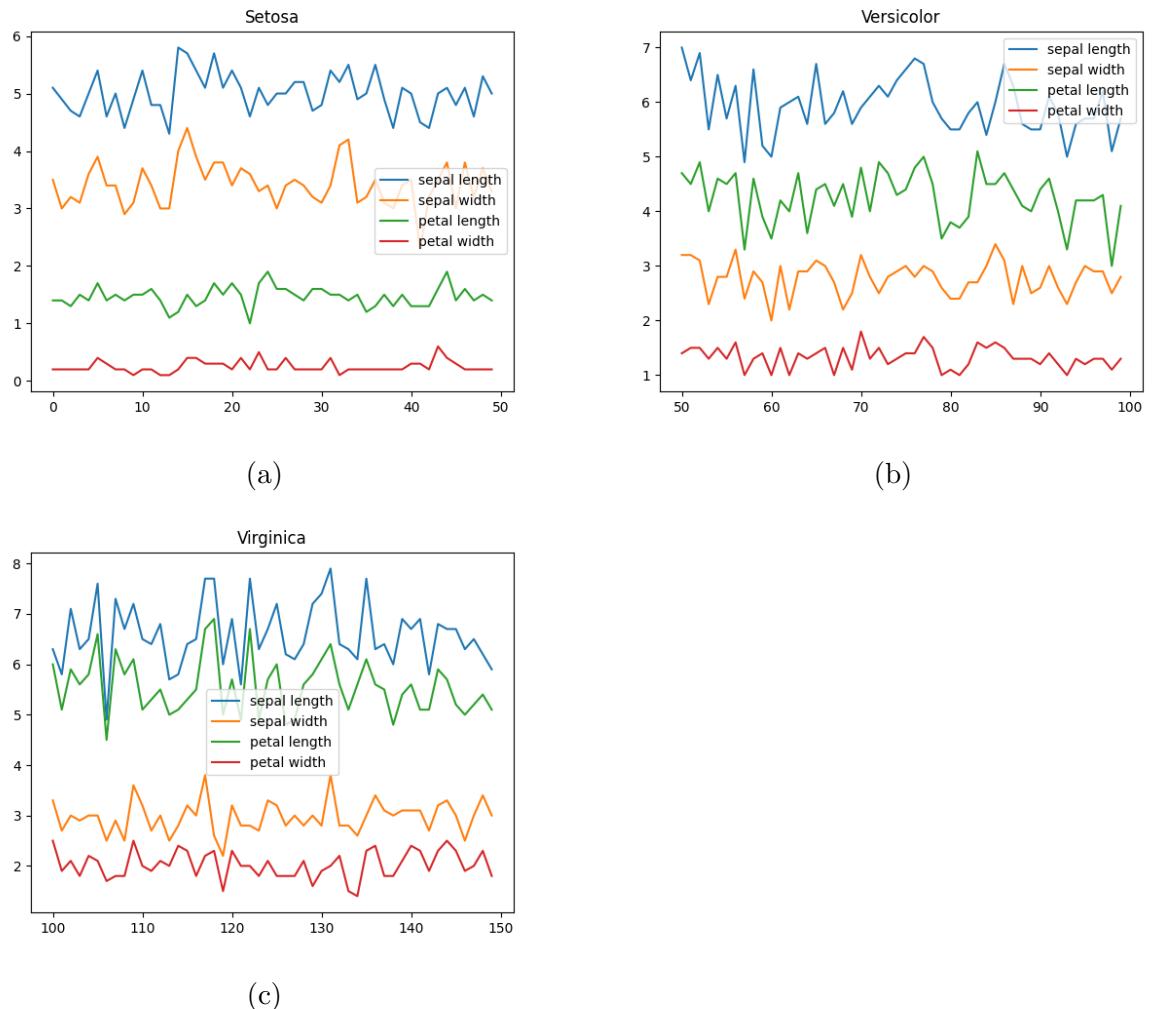


Figure 10.2: Line plots of the features for each class in the renown Iris data set.

Since Algorithm 9 cast the real-valued inputs into binary with a single pivot, the optimal data set for this algorithm consists of important inputs (inputs with the most weight in deciding classes) that are linearly separable—such as two clusters. Inputs that should not be determined by a single threshold will lose useful information (by definition) and should be discarded. This is why the future work of casting real-values to multiple bits is vital. Linearly separable relationships are the reason \mathcal{B} can binarize activation functions in Section 7.2.

Alternatively, one may train two neural networks—one that predicts Versicolor or Setosa, and the other predicts Versicolor or Virginica. To begin this second approach, copy the Iris data set into a second data set, then erase all Virginica instances from the data set for the first neural network, and all Setosa rows from the other. Now, sepal width is linearly separable in both data sets. The first neural network is explored in Section 10.2.3.

10.2.3 Versicolor or Setosa

Generalization Captured I ran a 4X2X1 (bias nodes excluded) neural network several times on the Versicolor/Setosa binarized data set with the only difference being the initial randomized weights.

I will use a quadruple (sepal length, sepal width, petal length, petal width) or (n_1, n_2, n_3, n_4) to represent the inputs of the Iris data set with an epistemological commitment of $\{0, 1, -\}$ which denotes {false, true, don't care}, respectively. Over 20 tests, the constructed AIG and the original neural network correctly predicted class 0 for inputs with $(-, -, 0, 0)$ and class 1 for inputs like $(-, -, 1, 1)$. Six of those eight possibilities were explicitly trained in the neural network (the six unique possibilities are shown in Table 10.3). Theorem 10.2.2 and Theorem 10.2.1 prove that the AIG correctly predicted these classes.

sepal length	sepal width	petal length	petal width	class
0	1	0	0	0
0	0	0	0	0
1	1	0	0	0
1	1	1	1	1
1	0	1	1	1
0	0	1	1	1

Table 10.3: All unique instances from the 100 rows left from excluding the Virginica class/feature combinations. Each input is binarized by the mean threshold (Section 10.2.1). Class 0 is Setosa and class 1 is Versicolor.

The network contains 4 logic nodes and 0 latches.

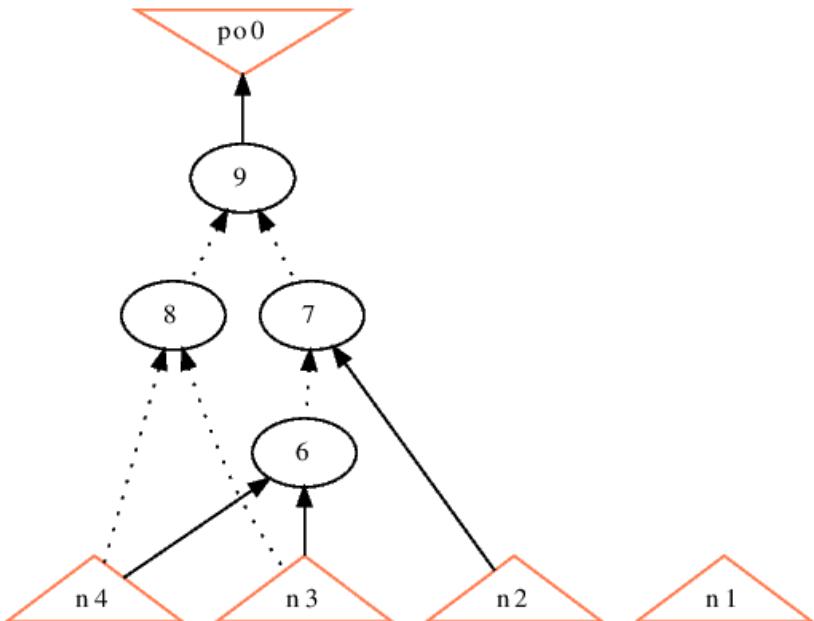


Figure 10.3: The AIG constructed by the weights given in Table 10.4; $(n_1, n_2, n_3, n_4) = (\text{sepal length}, \text{sepal width}, \text{petal length}, \text{petal width})$. From this, we can illustrate the neural network places heavy importance on homogeneous petal length/width pairs (see Theorem 10.2.1 and Theorem 10.2.2).

Theorem 10.2.1. *For the AIG in Figure 10.3, inputs that satisfy (-, -, 0, 0) must be class 0.*

Proof. Let $(n3, n4) = (0, 0)$. Then

$$Node_8 = AND(\neg n3, \neg n4) = 1 \quad (10.8)$$

In the binary AND operation, if any input is zero, then the result is zero.

$$Node_9 = AND(\neg Node_8, -) = 0 \quad (10.9)$$

The edge $Node_9 \rightarrow po0$ does not negate so

$$Node_9 = po0 \quad (10.10)$$

□

Theorem 10.2.2. *For the AIG in Figure 10.3, inputs that satisfy (-, -, 1, 1) must be class 1.*

Proof. Let $(n3, n4) = (1, 1)$. Then

$$Node_8 = AND(\neg n3, \neg n4) = 0 \quad (10.11)$$

$$Node_6 = AND(n3, n4) = 1 \quad (10.12)$$

$$Node_7 = AND(\neg Node_6, -) = 0 \quad (10.13)$$

$$Node_9 = AND(\neg Node_8, \neg Node_7) = po0 = 1 \quad (10.14)$$

□

Noise While the AIG (Figure 10.3) accurately approximated the neural network for homogeneous petal length and petal width pairs, it was incorrect for inputs that the neural network was uncertain of (heterogeneous petal length and petal width values such as (-, -, 0, 1) or (-, -, 1, 0)). Given the data set, these heterogeneous pairs seem impossible or highly unlikely. It makes sense that the AIGs could not accurately predict these values since the neural networks were not even certain about them. Future work can

```

Hidden node 1: -6.009057,2.0612597,-2.9449704,5.974104,6.9705567;
Hidden node 2: -5.9144406,1.9556314,-2.8650305,6.964409,5.840615
Output node: -12.945059,13.440295,13.615166

```

Table 10.4: An example of a 4X2X1 neural network that is certain for homogeneous sepal length/width values and uncertain for other inputs. Each of the hidden nodes's in-degree weights are ordered as bias, sepal length, sepal width, petal length, and petal width. The output node in-degree weights are ordered as bias, hidden node 1, hidden node 2.

consider the input space with \mathcal{N} and omit the neural network relationships specifically for these unlikely inputs for a simpler AIG output.

Across several tests, the resulting AIG from the 4X2X1 neural network all articulated the homogeneous sepal length/width pairs with the predicted class correctly (see two more AIG examples in Figure 10.4 and Figure 10.5). The small neural network gave this relationship priority. Subtle and developing relationships in the neural network occurred inconsistently and were often not helpful. Furthermore, removing these subtle or developing relationships will help human comprehension. Figure 10.5 shows an example of the many developing or subtle relationships a large neural network may have. To remove these subtle or developing relationships, I recommend finding an intersection of several AIGs that approximate several different neural networks (an ensemble of AIGs). Section 10.3 is the first step to finding accurate (and relatively concise) AIGs for complicated neural networks by using ensembles.

Despite that the 4X2X1 neural network was uncertain for most of the heterogeneous petal length/width inputs, Section 10.3 shows that larger neural networks have room to predict heterogeneous pairs with greater certainty and elicit AIGs that correctly approximate the neural network (with about 95% accuracy).

The network contains 5 logic nodes and 0 latches.

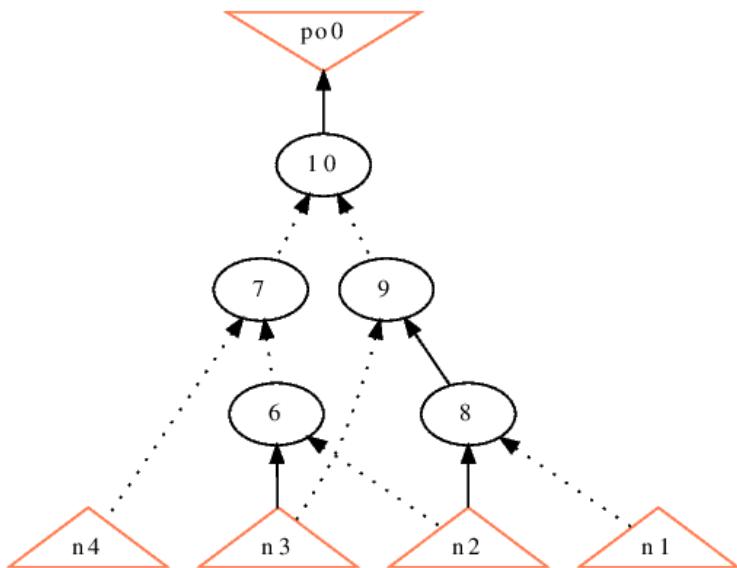


Figure 10.4: An AIG constructed from a separate neural network trained on the same data as the neural network that elicited Figure 10.3. We see that any input of homogeneous (n₃, n₄) pair is 100% accurate.

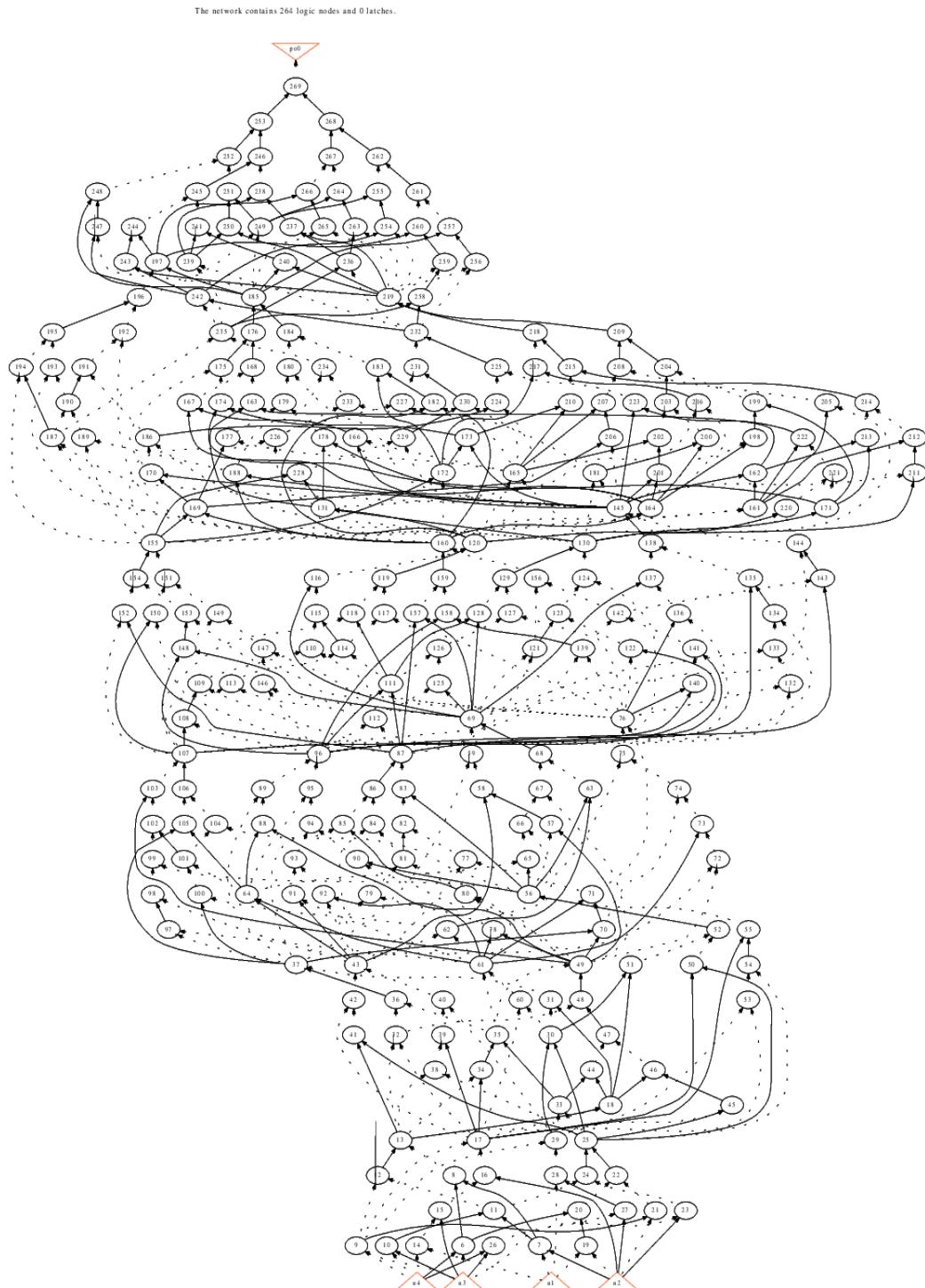


Figure 10.5: The AIG from a larger neural network ($4 \times 5 \times 5 \times 5 \times 5 \times 5 \times 1$ excluding biases) that was trained on the same data set eliciting Table 10.3. Like all other AIGs derived from neural networks trained on this data, homogeneous petal width/length pairs were perfectly construed. This AIG is more complicated due to the greater volume of subtle or developing relationships in the neural network.

10.3 Ensemble of Neural Networks and AIGs

This section investigates mitigating the memorization problem of converting a single neural network to a single AIG. Preliminary results in Section 10.3.2 show that an ensemble is highly accurate and can successfully generalize. Furthermore, I hypothesize that removing the noise from memorization (using an ensemble) can elicit a more concise and comprehensible AIG.

10.3.1 Developing and Subtle Relationships

The AIG is less accurate on input vectors when the neural network itself is uncertain. The nodes of the neural network are constantly developing relationships to minimize the network’s loss. Of course, not all developing relationships become certain—some are consistently in an uncertain state. Probing the network out of an uncertain state can be done by providing it more information (more training data). During the network’s search of relationships, some subtle relationships may find room to develop (especially in larger neural networks). These subtle relationships only slightly help with class prediction and often differ among neural networks. Removing the subtle or uncertain relationships with an ensemble would create an AIG that more accurately and comprehensibly represents the data set as seen by an ensemble of neural networks.

Figure 10.5 is an intricate AIG due to the memorization of many subtle and developing relationships found in the large neural network. In contrast, Figure 10.4 and Figure 10.3 represent smaller neural networks and fewer subtle and developing relationships that make the AIGs more comprehensible.

Since different neural networks have varying subtle and developing relationships, an intersection of logic using an ensemble can extract generalized relationships. While Section 10.2.3 shows how a 4X2X1 neural network could articulate the feature combinations for prediction, this section uses two larger neural networks (4X3X3X1 and 4X8X8X8X8X1) to produce a realistic amount of noise (more subtle or developing relationships to articulate).

10.3.2 Neural Network and AIG Ensemble Accuracy

Table 10.6 and Table 10.7 show the average predictions for both neural networks and their respective AIGs. The values in the top row are the inputs

Table 10.5: Summary for the two neural network ensembles of dimensions 4X3X3X1 (smaller) and 4X8X8X8X8X1 (larger) trained on the data set mentioned in Table 10.3.

Epochs	500	1000	2000	4000	8000
Samples	1000	1000	1000	750	500
Average AIG Accuracy (smaller)	0.9443	0.9604	0.9689	0.9740	0.9749
Average AIG Accuracy (larger)	0.9486	0.9532	0.9511	0.9517	0.9554

tested, and their columns are the average predictions from the neural network trained on X epochs (found in the leftmost column) and the average predictions from the respective AIG. These tables indicate that an ensemble of neural networks (given enough epochs) can be accurately represented by an AIG.

In Table 10.3, the quadruple (sepal length, sepal width, petal length, petal width) on the top rows correspond to the symbols NN# and AIG# which are the neural network and AIG predictions on the respective quadruple. Conforming to previous tests, the training set for these neural networks had six unique inputs that correspond to the NN1, NN2, NN3, NN5, NN6, and NN7 inputs (Table 10.3 lists these unique inputs as well). That means NN4, NN8 (the only two homogeneous petal length/width pairs not trained on), and NN9 through NN16 (the heterogeneous petal length/width pairs) were all predicted from novel input (not in the training set).

Table 10.6: This table consists of average neural network (4X3X3X1) probabilities (listed under NN#) and average AIG approximations (listed under AIG#) given an input vector (sepal length, sepal width, petal length, petal width) (in the top rows). Interestingly, the pairs (NN11, AIG11) and (NN14, AIG14) have a negative correlation while Table 10.7 has no negative correlations. The negative correlation indicates that an AIG was less likely to correctly predict the neural network for this input vector despite that the neural network gave a more certain probability. Future work may investigate why this is.

	(0,0,0,0)	(0,1,0,0)	(1,1,0,0)	(1,0,0,0)	(1,0,1,1)	(1,1,1,1)	(0,0,1,1)	(0,1,1,1)
Epochs	NN1	NN2	NN3	NN4	NN5	NN6	NN7	NN8
500	0.17	0.12	0.15	0.46	0.87	0.84	0.85	0.71
1000	0.04	0.03	0.03	0.29	0.97	0.97	0.97	0.91
2000	0	0	0	0.08	1	1	1	0.99
4000	0	0	0	0	1	1	1	1
8000	0	0	0	0	1	1	1	1
Epochs	AIG1	AIG2	AIG3	AIG4	AIG5	AIG6	AIG7	AIG8
500	0	0	0	0.53	1	1	1	0.97
1000	0	0	0	0.23	1	1	1	1
2000	0	0	0	0.08	1	1	1	1
4000	0	0	0	0.02	1	1	1	1
8000	0	0	0	0.01	1	1	1	1
	(0,0,0,1)	(0,1,0,1)	(1,1,0,1)	(1,0,0,1)	(1,0,1,0)	(1,1,1,0)	(0,0,1,0)	(0,1,1,0)
Epochs	NN9	NN10	NN11	NN12	NN13	NN14	NN15	NN16
500	0.65	0.21	0.56	0.83	0.83	0.55	0.65	0.21
1000	0.8	0.06	0.61	0.96	0.96	0.63	0.81	0.06
2000	0.92	0.01	0.68	0.99	0.99	0.68	0.92	0.01
4000	0.97	0	0.73	1	1	0.72	0.97	0
8000	0.98	0	0.72	1	1	0.73	0.98	0
Epochs	AIG9	AIG10	AIG11	AIG12	AIG13	AIG14	AIG15	AIG16
500	0.97	0.01	0.79	1	1	0.77	0.96	0.01
1000	0.96	0	0.74	1	1	0.77	0.96	0
2000	0.97	0	0.73	1	1	0.76	0.97	0
4000	0.96	0	0.73	1	1	0.71	0.95	0
8000	0.95	0	0.7	1	1	0.71	0.95	0

Table 10.7: Average neural network (4X8X8X8X8X8X1) probabilities and AIG approximations given inputs (sepal length, sepal width, petal length, petal width).

	(0,0,0,0)	(0,1,0,0)	(1,1,0,0)	(1,0,0,0)	(1,0,1,1)	(1,1,1,1)	(0,0,1,1)	(0,1,1,1)
Epochs	NN1	NN2	NN3	NN4	NN5	NN6	NN7	NN8
500	0.03	0.02	0.03	0.27	0.98	0.98	0.98	0.97
1000	0.01	0.01	0.01	0.22	1	1	1	0.99
2000	0	0	0	0.19	1	1	1	1
4000	0	0	0	0.16	1	1	1	1
8000	0	0	0	0.19	1	1	1	1
Epochs	AIG1	AIG2	AIG3	AIG4	AIG5	AIG6	AIG7	AIG8
500	0	0	0	0.68	1	1	1	1
1000	0	0	0	0.63	1	1	1	1
2000	0	0	0	0.62	1	1	1	1
4000	0	0	0	0.59	1	1	1	1
8000	0	0	0	0.56	1	1	1	1
	(0,0,0,1)	(0,1,0,1)	(1,1,0,1)	(1,0,0,1)	(1,0,1,0)	(1,1,1,0)	(0,0,1,0)	(0,1,1,0)
Epochs	NN9	NN10	NN11	NN12	NN13	NN14	NN15	NN16
500	0.95	0.03	0.8	0.98	0.98	0.79	0.95	0.03
1000	0.98	0.01	0.84	1	1	0.84	0.99	0.01
2000	0.99	0	0.82	1	1	0.82	0.99	0
4000	0.99	0	0.81	1	1	0.84	0.99	0
8000	1	0	0.82	1	1	0.81	0.99	0
Epochs	AIG9	AIG10	AIG11	AIG12	AIG13	AIG14	AIG15	AIG16
500	1	0.01	0.92	1	1	0.92	1	0.01
1000	1	0.01	0.93	1	1	0.94	1	0.02
2000	1	0.01	0.91	1	1	0.91	1	0.01
4000	0.99	0.01	0.91	1	1	0.9	1	0.01
8000	1	0.01	0.92	1	1	0.91	1	0

Figure 10.6 and Figure 10.7 shows the distribution plots of AIG accuracy compared to the neural network predictions. These figures confirm that inaccuracies are more likely to occur when the neural network is uncertain (gives probabilities close to 50%). Since more training (epochs) causes neural networks to become more certain, the more trained networks yield more accurate AIGs. This training need not be enough to overfit the data. Table 10.7 and Table 10.6 shows the neural network correctly generalizes for 4000 epochs and Table 10.5, Figure 10.7, and Figure 10.6 show 4000 epochs make the neural network certain enough to yield highly accurate AIGs.

Conclusion In conclusion, an ensemble of AIGs derived from neural networks is more accurate than any single AIG. Furthermore, an intersection of the AIGs would remove the intricacies of subtle and developing relationships—yielding a more comprehensible structure.

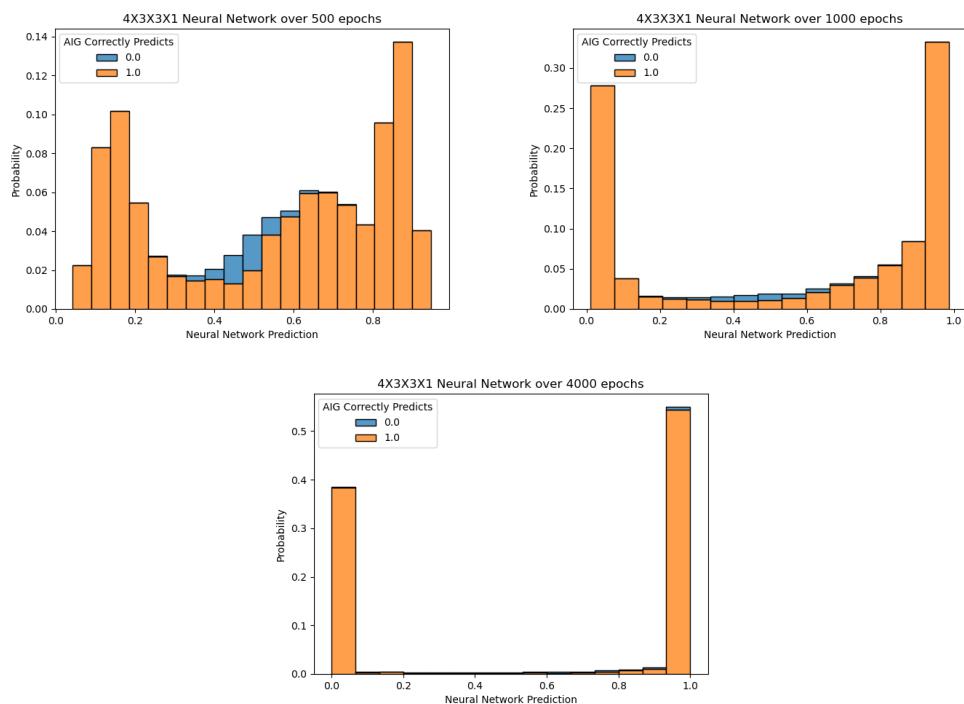


Figure 10.6: Distribution plots that shows the AIG's accuracy for all 16 inputs over all samples of the 4X3X3X1 neural network for the respective number of epochs (shown in the title). The blue color denotes the portion of incorrect AIG predictions while the orange color shows the portion of correct AIG predictions. An AIG prediction is correct if it matches the neural network prediction.

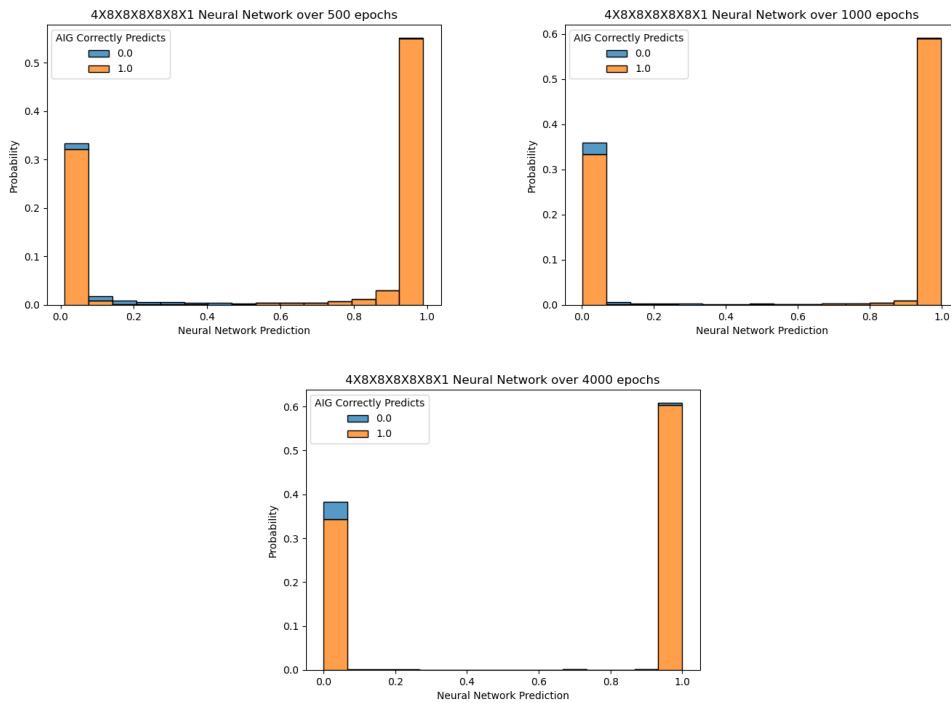


Figure 10.7: AIG approximations for the 4X8X8X8X8X1 neural network following the standards mentioned in Figure 10.6.

Part IV

Results

Chapter 11

Results and Moving Forward

11.1 Conclusion

Comprehension In Chapter 4, I found that comprehensibility scales inversely proportional to the intuitiveness and the number of states and transitions. This thesis successfully translated neural networks into a more comprehensible format (AIGs)—with some loss in accuracy.

NN to AIG Chapter 7 found that the importance of each input (to a neural node) was the absolute value of the respective weight over the absolute sum of all weights. \mathcal{B} (Section 8.2.2) exploited this idea and implemented a novel binary decision tree that computationally outperformed other decision trees for this specific problem. \mathcal{N} (Section 8.3) traversed the neural network in reverse order, skipping negligible neural nodes and implementing \mathcal{B} on other neural nodes.

Accuracy

Lossy Translations The accuracy of an AIG is found by comparing its predictions to the predictions of the neural network the AIG is approximating. The AIGs constructed by \mathcal{B} and \mathcal{N} were completely accurate on smaller neural networks that did not have room for extra noise (Chapter 6, Section 10.1). In Chapter 10, it was discovered that AIG predictions were accurate about half of the time for input vectors that the neural network had predictions at about 50% (uncertain predictions). This is likely due to the lossy abstractions of binarizing activation functions. Furthermore, these

uncertain predictions are the developing or subtle relationships produced by the neural networks.

Mitigating Accuracy Loss Due to Lossy Translations The inaccurate predictions from AIGs are mostly caused by predictions that the neural network is uncertain of. Furthermore, Section 10.3 shows that the AIGs produced by \mathcal{N} are highly accurate on average. This indicates the input vectors yielding inaccurate predictions are largely due to developing or subtle relationships (these relationships are part of memorization and not generalization). Consequently, the AIG’s inaccuracies can be mitigated with an intersection of many AIGs where each AIG approximates a separately trained neural network (Section 10.3). This ensemble method would remove the subtle or developing relationships (noise), and yield a concise AIG that highlights the important relationships.

11.2 Future Work

Pruning Unnecessary intricacies arise when neural networks are larger than needed. Pruning the neural network before, during, and/or after training will mitigate bloated graphs such as Figure 10.5. See this brief survey for more information on neural network pruning: [54].

Binary-Weight-Networks Rastegari et al. found that binary neural networks (such as Binary-Weight-Networks and XNOR-Networks) often give sufficient results even with limited precision [55]. Simplifying these neural networks to AIGs would be straight forward and likely elicit results quicker and more accurately than networks with real-valued weights. A survey on binary neural networks was published by Qin et al. in 2020 [56].

Input Space Chapter 10 shows that capturing relationships for impossible inputs can heavily complicate the end product. To remedy this, one can remove the impossible or implausible instances from the AIG’s consideration. This can be done inside of \mathcal{N} or by amending the layered sum of products produced by \mathcal{N} . The advantages of this idea could include a quicker algorithm and a more concise and accurate depiction of the neural network.

Related Work Brudermueller et al. reduced each hidden layer’s input space by using random forests or LogicNet to remove “unimportant” variables [2].

Related Work Published After my Experiments As mentioned in Section 5.3, Shi et al. [7] published an article that cited an algorithm [43] to approximate neural nodes with a time complexity better than \mathcal{B} ($O(2^{0.5n}n)$ versus $O(2^n)$). Additionally, Shi et al. mentions the fragility of neural networks and relates how robustness can be analyzed with the BDD produced by their algorithm, but they did not mention the memorization versus generalization problem cited by [2, 44] and seen in Section 10.2. In future work, I plan to investigate intersecting several AIGs from several trained neural networks to elicit generalization (see Section 10.3).

AIG Intersection Section 10.2.3 shows that the weights of neural networks could significantly differ despite that the training algorithm only differing in its initial weight values. The commonality (intersection) of the many AIGs over the trained neural networks appears to elicit generalization and are the paths that AIGs consistently and accurately represent from the original neural networks. This intersection will highlight the best relationships while omitting the more subtle or developing relationships (see Section 10.3 for supporting data). Furthermore, this intersection will cause the AIGs to be more concise which helps with comprehensibility (Chapter 4).

End Product The and-inverter graph was chosen due to its eminence in theoretical Boolean operations. Other graphs may be more readable or result in fewer nodes and transitions (e.g. majority-inverter graph ([21]) or binary decision diagrams (Section 3.1)).

Satisfiability This thesis also introduces a new algorithm to predict satisfiability given a data set. Step 1: train several neural networks; step 2: convert the several networks to a Boolean structure (perhaps with AIG intersections); finally, check for satisfiability using formal methods on the constructed structure.

Multiple Outputs One could binarize output functions such as softmax to approximate neural networks with multiple outputs. However, the AIG

or other Boolean structure may give more than one answer per input.

Part V

Appendix

Appendix A

Definitions

A.1 Abbreviations

- \mathcal{B} : the optimized, binary decision tree that approximates a neural node (Section 8.2.2).
- \mathcal{N} : the algorithm that parses the neural network with \mathcal{B} in reverse (Algorithm 7).
- NN: neural network.
- LUT: lookup table.
- SoP: sum of products.
- AIG: and-inverter graph (Section 3.1).
- MIG: majority-inverter graph (Section 3.1).
- BDD: binary decision diagram (Section 3.1).
- \mathbb{R} : the set of real numbers.
- $\mathbb{B} = \{0, 1\}$: the Boolean set.
- $L\#_1 X \#_2$: the $\#_2^{th}$ node of the $\#_1^{th}$ layer.
- $\#_1 X \#_2 X \cdots X \#_n$: the ordered dimensions (excluding bias nodes unless otherwise stated) of an n-layered neural network starting with the input

layer's size ($\#_1$). Example: 28X24X24X1 is a neural network with an input layer of size 28, two hidden layers of size 24 each, and an output layer with a size of 1.

A.2 Mathematical Symbols

- \leftarrow : assignment (read as “gets”).
- \in : is an element of (read as “in”).
- \cup : union.
- \cap : intersection.
- \wedge : and.
- \vee : or.
- \neg : not.
- \mapsto : maps to.
- \rightarrow : implies.
- \longleftrightarrow : bi-implication (read as “if and only if”).
- \forall : the universal quantifier (read as “for all”).
- \exists : the existential quantifier (read as “there exists”).
- \therefore : therefore.
- \models : models (or satisfies).

A.3 Complexity Symbols

- O : Big-O notation—the asymptotic upper bound.
- Ω : Omega notation—the asymptotic lower bound.
- Θ : Theta notation—the asymptotic upper and lower bound.

A.4 Vocabulary

- N^{th} -order relationship: a loose definition conveying how nested the relationship is (see Chapter 4).
- Satisfiability: if some structure s holds for some property ϕ , then this structure satisfies (models) the property. Formally, $s \models \phi$.

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