On Tractable Representations of Binary Neural Networks

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Abstract

We consider the compilation of a binary neural network’s decision function into tractable representations such as Ordered Binary Decision Diagrams (OBDDs) and Sentential Decision Diagrams (SDDs). Obtaining this function as an OBDD/SDD facilitates the explanation and formal verification of a neural network’s behavior. First, we consider the task of verifying the robustness of a neural network, and show how we can compute the expected robustness of a neural network, given an OBDD/SDD representation of it. Next, we consider a more efficient approach for compiling neural networks, based on a pseudo-polynomial time algorithm for compiling a neuron. We then provide a case study in a handwritten digits dataset, highlighting how two neural networks trained from the same dataset can have very high accuracies, yet have very different levels of robustness. Finally, in experiments, we show that it is feasible to obtain compact representations of neural networks as SDDs.

1 Introduction

Recent progress in artificial intelligence and the increased deployment of AI systems have highlighted the need for explaining the decisions made by such systems; see, e.g., (Baehrens et al. 2010; Ribeiro, Singh, and Guestrin 2016b; Ribeiro, Singh, and Guestrin 2018; Lipton 2018; Shih, Choi, and Darwiche 2018b; Ignatiev, Narodytska, and Marques-Silva 2019b; Darwiche and Hirth 2020). For example, one may want to explain why a classifier decided to turn down a loan application, or rejected an applicant for an academic program, or recommended surgery for a patient. Answering such why? questions is particularly central to assigning blame and responsibility, which lies at the heart of legal systems and may be required in certain contexts. The formal verification of AI systems has also come into focus recently, particularly when such systems are deployed in safety-critical applications.

We propose a knowledge compilation approach for explaining and verifying the behavior of a neural network classifier. Knowledge compilation is a sub-field of AI that studies in part tractable Boolean circuits, and the trade-offs between succinctness and tractability (Selman and Kautz 1996; Cadoli and Donini 1997; Darwiche and Marquis 2002; Darwiche 2014). By enforcing different properties on the structure of a Boolean circuit, one can obtain greater tractability (the ability to perform certain queries and transformations in polytime) at the possible expense of succinctness (the size of the resulting circuits). Our goal is to compile the Boolean function specified by a neural network into a tractable Boolean circuit that facilitates explanation and verification.

We consider neural networks whose inputs are binary (0/1) and that use step activations. Such a network would have real-valued parameters, but the network itself induces a purely Boolean function. We seek a tractable Boolean circuit that represents this function, which we obtain in two steps. First, note that neurons with step activations and binary inputs then produce a binary output—each neuron induces its own Boolean function. Using, e.g., the algorithm of (Chan and Darwiche 2003) we can obtain a tractable circuit for a given neuron’s Boolean function. The neural network then induces a Boolean circuit, although it may not be tractable. Thus, we compile this circuit into a tractable one by enforcing additional properties on the circuit until certain operations become tractable, as done in the field of knowledge compilation. We then explain the decisions and verify the properties of this circuit, as done in (Shih, Choi, and Darwiche 2018b; Shih, Choi, and Darwiche 2018a); cf. (Darwiche and Hirth 2020).

Our approach follows a recent trend in analyzing machine learning models using symbolic approaches such as satisfiability and satisfiability modulo theory; see, e.g., (Katz et al. 2017; Leofante et al. 2018; Narodytska et al. 2018; Shih, Choi, and Darwiche 2018b; Ignatiev, Narodytska, and Marques-Silva 2019a; Ignatiev, Narodytska, and Marques-Silva 2019b; Shih, Darwiche, and Choi 2019). While machine learning and statistical methods are key for learning classifiers, it is evident that symbolic and logical approaches, which are independent of any of the models parameters, are key for analyzing and reasoning about them. Our approach, based on compilation into a tractable Boolean circuit, can go beyond queries based on (for example) satisfiability, as we shall show.

This paper is organized as follows. In Section 2 we review
A neuron with a step activation function has outputs that are either 0 or 1, then this means that the inputs to all neurons are 0 or 1. Moreover, the output of the neural network is also 0 or 1. Hence, each neuron and the network itself can be viewed as a function mapping binary inputs to a binary output, i.e., a Boolean function. For each neuron, we shall simply refer to this function as the neuron’s Boolean function. When there is a single output $Y$, we will simply refer to the corresponding function as the network’s Boolean function.

## 3 From Neural Networks to Boolean Circuits

Consider a neuron with step activation function $\sigma$, inputs $I_i$ and bias $b$. The output of this neuron is simply

$$\sigma\left(\sum_i w_i \cdot I_i + b\right) = \begin{cases} 1 & \text{if } \sum_i w_i \cdot I_i + b \geq 0 \\ 0 & \text{otherwise} \end{cases}$$

As an example, consider a neuron with 3 inputs $A$, $B$ and $C$ with weights $w_1 = 1.15$, $w_2 = 0.95$ and $w_3 = -1.05$ and a bias of $-0.52$. This neuron outputs 1 iff:

$$1.15 \cdot A + 0.95 \cdot B - 1.05 \cdot C \geq 0.52$$

Treating a value of 1 as true and a value of 0 as false, we can view this neuron as a Boolean function $f(A, B, C)$ whose output matches that of the neuron, on inputs $A$, $B$ and $C$. Figure 2 highlights two logically equivalent representations of this neuron’s Boolean function. Figure 2a highlights an Ordered Binary Decision Diagram (OBDD) representation and Figure 2b highlights a circuit representation. These functions are equivalent to the sentence:

$$\neg C \land (A \lor B) \lor [C \land A \land B],$$

i.e., if $C$ is 0 then $A$ or $B$ must be 1 to meet or surpass the threshold ($\geq 0$), and if $C$ is 1 then both $A$ and $B$ must be 1.

OBDDs, as in Figure 2a, are tractable representations—they support many operations in time polynomial (and typically linear) in the size of the OBDD (Bryant 1986; Meinel

3An Ordered Binary Decision Diagram (OBDD) is a rooted DAG with two sinks: a 1-sink and a 0-sink. An OBDD is a graphical representation of a Boolean function $f$ on variables $X = \{X_1, \ldots, X_n\}$. Every OBDD node (but the sinks) is labeled with a variable $X_i$ and has two labeled outgoing edges: a 1-edge and a 0-edge. The labeling of the OBDD nodes respects a global ordering of the variables $X$: if there is an edge from a node labeled $X_i$ to a node labeled $X_j$, then $X_i$ must come before $X_j$ in the ordering. To evaluate the OBDD on an instance $x$, start at the root node of the OBDD and let $x_i$ be the value of variable $X_i$ that labels the current node. Repeatedly follow the $x_i$-edge of the current node, until a sink node is reached. Reaching the 1-sink means $x$ is evaluated to 1 and reaching the 0-sink means $x$ is evaluated to 0 by the OBDD.
and Theobald 1998; Wegener 2000). Circuits, as in Figure 2b, are not in general tractable as OBDDs, although we will later seek to obtain tractable circuits through knowledge compilation, a subject which we will revisit in more depth in Section 4. Note further that OBDDs are also circuits that are notated more compactly.\textsuperscript{4}

Our goal now is to obtain a tractable circuit representation of a given neuron. First, consider the following class of threshold-based linear classifiers.

**Definition 1.** Let \( \mathbf{X} \) be a set of binary features where each feature \( X \) in \( \mathbf{X} \) has a value \( x \in \{0, 1\} \). Let \( \mathbf{x} \) denote an instantiation of variables \( \mathbf{X} \). Consider functions \( f \) that map instantiations \( \mathbf{x} \) to a value in \( \{0, 1\} \). We call \( f \) a linear classifier if it has the following form:

\[
f(\mathbf{x}) = \begin{cases} 
1 & \text{if } \sum_{x \in \mathbf{x}} w_x \cdot x \geq T \\
0 & \text{otherwise}
\end{cases}
\]

where \( T \) is a threshold, \( x \in \mathbf{x} \) is the value of variable \( X \) in instantiation \( \mathbf{x} \), and where \( w_x \) is the real-valued weight associated with value \( x \) of variable \( X \).

Note that such classifiers are also Boolean functions. The following result, due to (Chan and Darwiche 2003), gives us a way of obtaining a tractable circuit representing the Boolean function of such classifiers.

**Theorem 1.** A linear classifier in the form of Equation 2 can be represented by an OBDD of size \( O(2^n) \) nodes, which can be computed in \( O(n2^n) \) time.

(Chan and Darwiche 2003) further provided an algorithm to obtain the result of Theorem 1, although much more efficiently than what the bounds suggest. It was originally for compiling naive Bayes classifiers to Ordered Decision Diagrams (ODDs). However, this algorithm applies to any classifier of the form given by Equation 2, which includes naive Bayes classifiers, but also logistic regression classifiers, as well as neurons with step activation functions (Elkan 1997).

Compiling a linear classifier such as a neuron or a naive Bayes classifier is NP-hard (Shih, Choi, and Darwiche 2018a), which scaled only to dozens of features, in contrast to the preliminary work of (Choi et al. 2019), which scaled only to hundreds of features, using the algorithm of (Chan and Darwiche 2003).

Now that we can compile each neuron into a (tractable) Boolean circuit, the whole neural network will then induce a Boolean circuit as illustrated in Figure 3. That is, for the given neural network in Figure 3a, each neuron is compiled into a Boolean circuit as in Figure 3b. The circuits for neurons are then connected according to the neural network structure, leading to the Boolean circuit in Figure 3c, where the circuit of each neuron is portrayed as a block.

Using the algorithm of (Chan and Darwiche 2003), the Boolean circuit that we obtain from a neuron is tractable. The network’s Boolean circuit, that we construct from the Boolean circuits of the neurons, may not be tractable however. To use the explanation and verification techniques proposed in (Shih, Choi, and Darwiche 2018b; Shih, Choi, and Darwiche 2018a), we require a tractable circuit; cf. (Darwiche and Hirth 2020). We next show how to obtain such a circuit using tools from the field of knowledge compilation.

4 Tractability via Knowledge Compilation

In this section, we provide a short introduction to the domain of knowledge compilation, and then show how we can compile a neural network into a tractable Boolean circuit.

We follow (Darwiche and Marquis 2002), which considers tractable representations of Boolean circuits, and the trade-offs between succinctness and tractability. In particular, they consider Boolean circuits of and-gates, or-gates and inverters, but where inverters only appear at the inputs (hence the inputs of the circuit are variables or their negations). This sub-class of circuits is called Negation Normal Form (NNF) circuits. Any circuit with and-gates, or-gates and inverters can be efficiently converted into an NNF cir-
circuit while at most doubling its size.

By imposing properties on the structure of NNF circuits, one can obtain greater tractability (the ability to perform certain operations in polytime) at the possible expense of succinctness (the size of the resulting circuit). To help motivate this trade-off, consider Figure 4, which highlights the containment relationship between four complexity classes. The “easiest” class is \(NP\), and the “hardest” class is \(PP^{NP}\) (Oztok, Choi, and Darwiche 2016). The canonical problems that are complete for each class all correspond to queries on Boolean expressions. One popular computational paradigm for solving problems in these classes is to reduce them to the canonical problem for that class, and to compile the resulting Boolean expressions to circuits with the appropriate properties. For example, (Oztok, Choi, and Darwiche 2016) shows how to solve \(PP^{NP}\)-complete problems by reduction to MajMajSAT queries on a specific tractable class of Boolean circuits.

Consider now a property on NNF circuits called decomposability (Darwiche 2001a). This property asserts that the sub-circuits feeding into an and-gate cannot share variables. An NNF circuit that is decomposable is said to be in Decomposable Negation Normal Form (DNNF). In a DNNF circuit, testing whether the circuit is satisfiable can be done in time linear in the size of the circuit. Another such property is determinism (Darwiche 2001b). This property asserts that for each or-gate, if the or-gate outputs 1 then exactly one of its input is 1. A DNNF circuit that is also deterministic is called a d-DNNF. The circuit in Figure 2b is an example of a d-DNNF circuit. In a d-DNNF circuit, counting the number of assignments that satisfy the circuit can be done in time linear in the size of the circuit, assuming the circuit also satisfies smoothness (Darwiche 2001b). Hence, with these first two properties, we can solve the canonical problems in the two “easiest” classes illustrated in Figure 4.

A more recently proposed class of circuits is the Sentential Decision Diagram (SDD) (Darwiche 2011; Xue, Choi, and Darwiche 2012; Choi and Darwiche 2013). SDDs are a subclass of d-DNNF circuits that assert a stronger form of decomposability, and a stronger form of determinism. SDDs subsume OBDDs and are exponentially more succinct (Bova 2016). SDDs support polytime conjunction and disjunction. That is, given two SDDs \(\alpha\) and \(\beta\), there is a polytime algorithm to construct another SDD \(\gamma\) that represents \(\alpha \land \beta\) or \(\alpha \lor \beta\). Further, SDDs can be negated in linear time.

These polytime operations allow a simple algorithm for compiling a Boolean circuit with and-gates, or-gates and inverters into an SDD. We first obtain an SDD for each circuit input. We then traverse the circuit bottom-up, compiling the output of each visited gate into an SDD by applying the corresponding operation to the SDDs of the gate’s inputs.

SAT and MajSAT can be solved in linear time on SDDs. Further properties on SDDs allow the problems E-MajSAT and MajMajSAT, the two hardest problems illustrated in Figure 4, to be also solved in time linear in the size of the SDD (Oztok, Choi, and Darwiche 2016). In our experiments, we compiled the Boolean circuits of neural networks into standard SDDs as this was sufficient for efficiently supporting the explanation and verification queries we are interested in.

### 5 On the Robustness of Classifiers

While neural networks have become ubiquitous in machine learning and artificial intelligence, it is also increasingly apparent that neural networks learned in practice can be fragile. In particular, they can be susceptible to misclassifying an instance after small perturbations have been applied to it (Szegedy et al. 2013; Goodfellow, Shlens, and Szegedy 2014; Moosavi-Dezfooli, Fawzi, and Frossard 2016). Next, we show how compiling a neural network into a tractable circuit can give one the ability to analyze the robustness of a neural network’s decisions.

We consider first the robustness of a binary classifier’s decision to label a given instance 0 or 1. We consider the following question: how many features do we need to flip from 0 to 1 or 1 to 0, before the classifier’s decision flips? That is, we consider the robustness of a given instance as the closest instance of the opposite label, by Hamming distance.

**Definition 2** (Instance-Based Robustness). Consider a Boolean classification function \(f : \{0, 1\}^n \rightarrow \{0, 1\}\) and a given instance \(x\). The robustness of the classification of \(x\) by \(f\), denoted by \(r_f(x)\), is defined as follows. If \(f\) is a trivial function (true or false), then \(r_f(x) = \infty\). Otherwise,

\[
r_f(x) = \min_{x' \neq f(x)} d(x, x')
\]

where \(d(x', x)\) denotes the Hamming distance between \(x'\) and \(x\), i.e., the number of variables on which \(x\) and \(x'\) differ.

This notion of robustness was considered before by (Shih, Choi, and Darwiche 2018a), who also assumed binary (or

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Footnotes:

1. For more on this paradigm, see http://beyondnp.org.
2. For a video tutorial on this paradigm, “On the role of logic in probabilistic inference and machine learning,” see https://www.youtube.com/watch?v=xRxP2Wj4kuA
3. Counting how many assignments satisfy a given circuit allows us to tell whether a majority of them satisfy the circuit (MajSAT).
4. If \(s\) and \(t\) are the sizes of input SDDs, then conjoining or disjoining the SDDs takes \(O(s + t)\) time, although the resulting SDD may not be compressed (Van den Broeck and Darwiche 2015).
5. In our case study in Section 6, we used the open-source SDD package available at http://reasoning.cs.ucla.edu/sdd/.
Algorithm 1 model-robustness(f)

input: A classifier’s Boolean function f
output: The (positive) model-based robustness mr(f)

main:
1: M, h1 ← 0, f
2: for k from 2 to n do
3: h_k ← \bigwedge_{x}((h_{k-1}|x \land h_{k-1}|\bar{x})
4: f_{k-1} ← h_{k-1} \land \neg h_k
5: M ← M + (k - 1) \cdot \text{model}_\text{count}(f_{k-1})
6: end for
7: M ← M + n \cdot \text{model}_\text{count}(h_n) \{ since f_n \equiv h_n \}
8: return M

categorical) features. Other notions of robustness are discussed in (Leofante et al. 2018), for real-valued features.

Given a classification function f, we refer to an instance x as being k-robust if r_f(x) = k, i.e., it takes k flips of the features to flip the classification. In general, it is intractable to compute the robustness of a classification, unless P=NP. Consider the following decision problem:

**D-ROBUST:** Given function f, instance x, and integer k, is r_f(x) \geq k?

**Theorem 3.** D-ROBUST is coNP-complete.

Given a tractable circuit (in particular, an OBDD), this question can in fact be answered in time linear in the size of the circuit (Shih, Choi, and Darwiche 2018a).\(^{11}\) We employ the algorithm given by (Shih, Choi, and Darwiche 2018a) in Section 6, in our case studies.\(^{12}\)

Next, rather than consider the robustness of just one classification, we can consider the average robustness of a classification function, over all possible inputs. In other words, we consider the expected robustness of a classifier, under a uniform distribution of its inputs.

**Definition 3 (Model-Based Robustness).** Consider a Boolean classification function f : \{0, 1\}^n \rightarrow \{0, 1\}. The model robustness of f is defined as:

\[ mr(f) = \frac{1}{2^n} \sum_x r_f(x) \]

Let f be the classification function whose robustness we want to assess. If f(x) = 1 we refer to x as a positive instance; otherwise f(x) = 0 and we refer to x as a negative instance. We propose Algorithm 1 for computing the model robustness of a classifier over all positive instances (the robustness of negative instances can be computed by invoking Algorithm 1 on function \(-f\)).\(^{13}\)

Our algorithm is based on computing the set of functions h_k, which are the Boolean functions representing all positive instances x that have robustness k or higher. That is, h_k represents all instances x where f(x) = 1 and where r_f(x) \geq k. First, h_1 = f. For k = 2 we have:

\[ h_2 = \bigwedge_x(f|x \land f|\bar{x}) \]

where f|x denotes the conditioning of f on value x, i.e., the function that we would obtain by setting X to true (replace every occurrence of x with true, and in the case of f|\bar{x}, replace X with false). Say that x is an instance of f|x \land f|\bar{x}, and thus f(x) = 1 and f(x) remains 1 no matter how we set X. By taking the conjunction across all variables X, we obtain all instances x whose output would not flip after flipping any single feature X. Next, consider the robustness of the instances of h_2. Some of these instances x will become 1-robust with respect to h_2. These instances are in turn 2-robust with respect to the original function f. More generally, we can compute h_k from h_{k-1}:

\[ h_k = \bigwedge_x(h_{k-1}|x \land h_{k-1}|\bar{x}) \]

We can now compute the functions f_k representing all of the k-robust examples of f, via:

\[ f_k = h_k \land \neg h_{k+1}. \]

The model count of f, denoted by model_count(f), is the number of instances x satisfying a Boolean function f. We can then compute the model robustness of f by:

\[ mr(f) = \frac{1}{2^n} \sum_{k=1}^{n} \text{model}_\text{count}(f_k) \cdot k. \]

Consider now the most robust instances of a function f.

**Definition 4 (Maximum Robustness).** Consider a Boolean classification function f : \{0, 1\}^n \rightarrow \{0, 1\}, where f is non-trivial. The maximum robustness of f is defined as:

\[ \max r_f = \max_x r_f(x). \]

Note that the instances x of h_k is a subset of the instances of h_{k-1}, as computed in Algorithm 1. Hence, the model count of h_k will decrease as we increase k. At a large enough k, then h_{k+1}, and hence also f_{k+1}, will have no models and will equal false. At this point, we know k is the maximum robustness, and we can stop Algorithm 1 early.

\(^{11}\)The robustness of an instance y, x can be computed by the following recurrence, which recurses on the structure of an OBDD:

\[ r_f(y, x) = \min\{r_f(y, 1) + r_f(y, 0)\} \]

where r_f(y) = 0 if f is false and r_f(y) = \infty if f is true.

\(^{12}\)Since computing robustness is coNP-complete, we can also apply SAT solvers to this task. For a given k, we can determine if r_f(x) \leq k by first encoding the set of instances within a distance of k away from x as a CNF formula \(\phi\), using a standard encoding. We then encode the value of f(x) and the neural network’s classification function as a CNF formula \(\Delta\), using a technique similar to that by (Narodytska et al. 2018). The formula \(\phi \land \Delta\) is then satisfiable iff r_f(x) \leq k. Finally, we iterate over all possible values of k (or perform binary search), so the instance-based robustness is just the smallest value of k such that r_f(x) \leq k (i.e., \(\phi \land \Delta\) is SAT).

\(^{13}\)Recently, (Baluta et al. 2019) proposed an approach for estimating robustness using approximate model-counting, with PAC-style guarantees. Their approach scaled to 10 \times 10 digits datasets; our exact approach scales to 16 \times 16 digits datasets in Section 6.
Moreover, the largest non-\( f_k \) gives us the set of examples that are the most robust (requires the most number of features to flip).\(^{14}\)

Finally, we observe that model-based robustness appears to be computationally more difficult than instance-based robustness. In particular, the model-robustness over positive instances can be shown to be a PP-hard problem.

**D-POS-MODEL-ROBUST:** Given function \( f \), and integer \( k \), is \( \text{mr}(f) \geq k? \)

**Theorem 4.** **D-POS-MODEL-ROBUST** is PP-hard.

To compute model-based robustness using Algorithm 1, we must be able to negate, conjoin and condition on Boolean functions, as well as compute their model count. Given a circuit represented as an SDD, operations such as negation and counting the models of an SDD can be done in time linear in the size of the SDD. Conjoining two SDDs of size \( s \) and \( t \) takes time \( O(st) \) although a sequence of conjoin operations may still take exponential time, as in Algorithm 1.

### 6 A Case Study

We next provide a case study in explaining and verifying a convolutional neural network via knowledge compilation.

#### 6.1 (Binary) Convolutional Neural Networks

In our case study, we consider binary convolutional neural networks (binary CNNs).\(^{15}\) That is, if we assume binary inputs and step activations, then the outputs of all neurons are binary, and the output of the network itself is also binary. Hence a binary CNN represents a Boolean function. We can construct a Boolean circuit representing a binary CNN, and then compile it to a tractable one as described in Section 4.

Our binary CNNs contain three types of layers:

- **convolution + step layers:** a convolution layer consists of a set of filters, that can be used to detect local patterns in an input image. Typically, a ReLU unit is applied to the output of a filter. In a binary CNN, we assume step activations (whose parameters are trained first using sigmoid activations, then replacing them with step activations);

- **max-pooling layers:** a max-pooling layer can be used to reduce the dimension of an image, helping to reduce the overall computational and statistical demands. In a binary CNN, if the inputs of a max-pooling layer is 0 or 1, then the “max” reduces to a logical “or”;

- **fully-connected layers:** if the inputs are binary and if we use step activations, then each neuron represents a Boolean function, as in Section 3.

\(^{14}\)Note that if \( f \) is a non-trivial Boolean function, then \( f_x \) must be false. Suppose \( f_x \) were not false, and that \( x \) is an instance of \( f \). This means we can flip any and all variables of \( x \), and it would always be an example of \( f \). This implies that \( f \) must have been true, and hence a trivial function.

\(^{15}\)A number of binary variations of neural networks have been proposed in the literature. The XNOR-Networks of (Rastegari et al. 2016) are another binary variation of CNNs, which also assumes binary weights. The binarized neural networks (BNNs) of (Hubara et al. 2016) have binarized parameters and activations. In work closely related to ours, (Narodytska et al. 2018) studied the verification of BNNs, using SAT solvers, as discussed in Section 1.

![Figure 5: A correctly classified digit-0 and digit-1 from the test set (first row), the corresponding PI-explanations (second row, gray striped regions represent “don’t care’s”), and the corresponding fooling images (third row).](image)

**Figure 5:** A correctly classified digit-0 and digit-1 from the test set (first row), the corresponding PI-explanations (second row, gray striped regions represent “don’t care’s”), and the corresponding fooling images (third row).

#### 6.2 Experimental Setup

We consider the USPS digits dataset of handwritten digits, consisting of 16 \( \times \) 16 pixel images, which we binarized to black and white (Hull 1994). Here, we performed binary classification using different pairs of digits. We first trained a CNN using sigmoid activations, using TensorFlow. We replaced the sigmoid activations with step activations, to obtain a binary CNN that we compiled into a tractable circuit. In particular, we compiled the binary CNN into a Sentential Decision Diagrams (SDD). We shall subsequently provide analyses of the binary CNN, via queries on the SDD.

More specifically, we created two convolution layers, each with stride size 2. We first swept a 3 \( \times \) 3 filter on the original 16 \( \times \) 16 image (resulting in a 7 \( \times \) 7 grid), followed by a second 2 \( \times \) 2 filter (resulting in a 3 \( \times \) 3 grid). These outputs were the inputs of a fully-connected layer with a single output. We did not use max-pooling as the dimension was reduced enough by the convolutions. Finally, we optimized a sigmoid cross-entropy loss using the Adam optimizer.

#### 6.3 Explaining Decisions

We consider how to explain why a neural network classified a given instance positively or negatively. In particular, we consider prime-implicant explanations (PI-explanations), as proposed by (Shih, Choi, and Darwiche 2018b); see also (Ignatiev, Narodytska, and Marques-Silva 2019a; Darwiche and Hirth 2020). Say that an input image \( x \) is classified...
6.4 Explaining Model Behavior

To explain the network’s behavior as a whole (and not just per instance), we provide two visualizations of how each pixel contributes to the classification decision: a marginal grid and a unateness grid. Figure 6a is a marginal grid, which highlights the marginals of the output neuron, i.e., the probability that each pixel is white given that the output of the network is digit-1. In general, it is intractable to compute such marginals, which naively entails enumerating all $2^{256}$ possible input images and then checking the network output.

If we can compile a neural network’s Boolean function into a tractable circuit, like an SDD, then we can compute such marginals in time linear in the size of the circuit.

In Figure 6a, red pixels correspond to marginals greater than $\frac{1}{2}$, and redder pixels are closer to one. Blue pixels correspond to marginals less than $\frac{1}{2}$, and bluer pixels are closer to zero. The grid intensities have been re-scaled for clarity. Not surprisingly, we find that if the output of the network is high (indicative of a digit-1), then it is somewhat more likely that the pixels in the middle are set to white.

Figure 6b is a unateness grid, which identifies pixels that sway the classification in one direction only. Red pixels are positively unate (monotone), so turning them from off to on can only flip the classification from digit-0 to digit-1. Blue pixels are negatively unate, i.e., turning them from off to on can only flip the classification from digit-1 to digit-0. Black pixels are ignored by the network completely. Finally, gray pixels do not satisfy any unateness property. In general, determining whether an input of a Boolean function is unate/monotone or unused are computationally hard problems. In tractable circuits such as SDDs, they are queries that can be performed in time polynomial in the circuit size.

In Figure 6b, the majority of pixels are unate (monotone), suggesting that the overall network behavior is still relatively simple. We also observe that there are many unused pixels on the right and bottom borders, which can be explained by the lack of padding (i.e., given the filter size and stride length, no filter takes any of these pixels as inputs). There is another block of unused pixels closer to the middle. On closer inspection, we find that these pixels are unique to one particular filter in the second convolution layer (no other filter depends on their values). In the tractable circuit of the output neuron, we find that the circuit does not essentially depend on the output of this filter. Thus, the output of the network does not depend on the values of any of these pixels. Note that deciding whether an input of a neuron is unused is an NP-hard problem. However, given a tractable circuit such as an SDD, this question can be answered in time linear in the size of the circuit.

We emphasize a few points now. First, this (visual) analysis is enabled by the tractability of the circuit, which allows marginals to be computed and unate pixels to be identified efficiently. Second, the analysis also emphasizes that the network is not learning the conceptual differences between a digit-0 and a digit-1. It is identifying subsets of the pixels that best differentiate between images of digit-0 and digit-1 from the training set with high accuracy. This perhaps explains why it is sometimes easy to “fool” neural networks, which we demonstrated in Figure 5.

6.5 Analyzing Classifier Robustness

Next, we provide a case study in analyzing CNNs based on their robustness. We consider the classification task of discriminating between a digit-1 and a digit-2. First, we trained two CNNs with the same architectures (as described earlier), but using two different parameter seeds. We achieved...
98.18% (Net 1) and 96.93% (Net 2) testing accuracies. The SDD of Net 1 had 1,298 nodes and a size of 3,653. The SDD of Net 2 had 203 nodes and a size of 440. Net 1 obtained a model-robustness of 11.77 but Net 2 only obtained a robustness of 3.62. For Net 2, this means that on average, 3.62 pixel flips are needed to flip a digit-1 classification to digit-2, or vice versa. Moreover, the maximum-robustness of the Net 1 was 27, while that of Net 2 was only 13. For Net 1, this means that there is an instance that would not flip unless you flipped (the right) 27 pixels. These are two networks which are similar in terms of accuracy (differing by only 1.25%), but very different when compared by robustness.

Figure 7 further highlights the differences between these two networks by the level of robustness $k$. On the $x$-axis, we increase the level of robustness $k$ (up to the max of 27), and on the $y$-axis we measure the proportion of instances having robustness $k$, i.e., we plot $2^{-\text{node_count}(f_k)}$, as in Section 5. Clearly, the first network is able to more robustly classify a larger number of instances. Given two networks with comparable accuracies, we clearly prefer the one that is more robust, as it would be more resilient to adversarial perturbations and to noise. When we compute the average instance-based robustness of testing instances, Net 1 obtains an average of 4.47, whereas Net 2 obtains a lower average of 2.61, as expected.

Next, we consider in more depth Net 2, which again had a test set accuracy of 96.93%. First, we visualize the most robust and the least robust instances of the CNN. Figures 8a & 8b depict an example of a most robust digit-1 and digit-2, from the testing set. Similarly Figures 8c & 8d depict an example of a least robust digit-1 and digit-2, both having robustness 1. For these latter two instances, it suffices to flip a single pixel in each image, for the classifier to switch its label. These perturbations are given in Figures 8e & 8f. Finding training examples that have low-robustness can help finding problematic or anomalous instances in the dataset, or otherwise indicate weaknesses of the learned classifier. Finding training examples that have high-robustness provides an insight into which instances that the classifier considers to be prototypical of the class.

7 Experiments

In this section, we empirically evaluate our approach for compiling a neural network into an SDD. First, we take a given neural network trained from data, and encode it as an NNF, as described in Section 3. Next, we compile this NNF into an SDD, using the simple circuit compiler described in Section 4. We consider binary CNNs learned from a binarized MNIST dataset, downsampled to $14 \times 14$, from $28 \times 28$. Experiments were run on a Linux system with a 2.40GHz Intel i7-7560U CPU and access to 16GB RAM. The CNN has 196 inputs, a $4 \times 4$ filter with stride 4 leading to 9 hidden nodes, and one fully-connected layer. We minimized a sigmoid cross-entropy loss with an Adam optimizer. To speed up training and testing, we only used 1,024 examples from each set; note that the algorithm to compile a neural network to SDD does not need to see the training set.

Table 1 summarizes our results, across all pairs $(i, j)$ of digits. First, we observe that the neural networks we trained generally had high accuracy. Next, we see that across all pairs, the node count and edge count of the compiled SDDs

We used a few additional optimizations in our experiments. First, we labeled each NNF node by its maximum distance from the output. We then compiled the NNF nodes by depth, deepest first. This helps control the scope of the sub-functions that need to be maintained. Next, we invoked SDD minimization relatively aggressively, any time the number of live SDD nodes exceeded 215. Finally, the initial vtree used for compilation was taken from the final vtree of a previously compiled neural network.

The circuit compiler is available open-source at https://github.com/art-ai/nnf_compiler
In this paper, we proposed a knowledge compilation approach for explaining and verifying the behavior of a neural network. We considered in particular neural networks with 0/1 inputs and step activation functions. Such networks have neurons that correspond to Boolean functions. The network itself also corresponds to a Boolean function, which represents how a neural network labels an input feature vector with a class. We showed how to compile the Boolean function of each neuron and the network itself into a tractable circuit, and into an Sentential Decision Diagram (SDD) in particular. Further, we developed new queries and algorithms for analyzing the robustness of a Boolean function. In a case study, we explained and analyzed the robustness of binary convolutional neural networks (binary CNNs) for classifying handwritten digits. Finally, in our experiments, we showed that it is indeed feasible to compile neural networks with over a hundred features into SDDs.

A Proof of Theorem 2

Consider a neuron with inputs $X_1, \ldots, X_n$. Setting the inputs $X_1, \ldots, X_i$ results in a smaller sub-classifier (or sub-neuron) over inputs $X_{i+1}, \ldots, X_n$. No matter how we set the inputs $X_1, \ldots, X_i$ the resulting sub-classifier is identical (has the same weights) except for the threshold being used. Two different settings of inputs $X_1, \ldots, X_i$ may lead to identical sub-classifiers with the same threshold. Say we set variables from $X_1$ to $X_n$. There are at most $2W$ possible valid thresholds, so there are at most $2nW$ possible sub-classifiers that we can see while setting variables.

Consider an $n \times W$ matrix $A$ where cell $A[i][j]$ is associated with the sub-classifier where variable $X_i$ is about to be set, and where $j$ is the threshold being used. If $X_i$ is set to 1, we obtain the sub-classifier at $A[i+1][j] + w_j$ where $w_j$ is the (integer) weight of feature $X_i$. If $X_i$ is set to 0, we obtain the sub-classifier at $A[i+1][j]$. Each cell $A[i][j]$ thus represents an OBDD node for the corresponding sub-problem, whose hi- and lo-children are known. We add an $(n+1)$-th layer where every sub-classifier with threshold below 0 is $\perp$, and where every sub-classifier at or above 0 is $\top$. The root of the original neuron’s OBDD is then found at $A[1][T]$, which we can extract and reduce if needed.

The size of matrix $A$ bounds the size of the OBDD to $O(nW)$ nodes. Further, it takes constant time to populate each entry, and hence $O(nW)$ time to construct the OBDD.

Finally, we note that the above construction also follows the proof of Theorem 1 given by (Chan and Darwiche 2003), based also on identifying equivalence classes of sub-classifiers. Thus, we can view Theorem 2 as a tightening of the bounds of Theorem 1 for a special case (integer weights).
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