On Neural Network Equivalence Checking Using SMT Solvers

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Abstract. Two pretrained neural networks are deemed (approximately) equivalent if they yield similar outputs for the same inputs. Equivalence checking of neural networks is of great importance, due to its utility in replacing learning-enabled components with (approximately) equivalent ones, when there is need to fulfill additional requirements or to address security threats, as is the case when using knowledge distillation, adversarial training, etc. In this paper, we present a method to solve various strict and approximate equivalence checking problems for neural networks, by reducing them to SMT satisfiability checking problems. This work explores the utility and limitations of the neural network equivalence checking framework, and proposes avenues for future research and improvements toward more scalable and practically applicable solutions. We present experimental results, for diverse types of neural network models (classifiers and regression networks) and equivalence criteria, towards a general and application-independent equivalence checking approach.

Keywords: Neural network · Equivalence checking · Verification · SMT

1 Introduction

Equivalence checking is the problem of checking whether two given artifacts (e.g. digital circuits, programs, etc.) are equivalent in some sense. Equivalence checking is standard practice in the domain of hardware design and the EDA industry [27,31,33,38]. There, digital circuits are subject to successive transformations for optimization and other purposes, and it is important to ensure that each successive design preserves the functionality of (i.e., is functionally equivalent to) the original.

In this paper, we are interested in the problem of equivalence checking for neural networks (NNs). For two pretrained NNs of different architectures, or of the same architecture with different parameters, the problem is to check whether they yield similar outputs for the same inputs. Contrary to equivalence checking for digital circuits, where strict functional equivalence is typically desired, similar outputs does not necessarily mean identical outputs in the case of NNs. As we shall see, the exact definition
of equivalence depends on the application and NNs at hand (e.g. classifier, regression, etc.). Therefore, we consider both strict and approximate equivalences in this paper.

The equivalence checking problem for NNs is not only fundamental, intellectually interesting, and challenging. It is also motivated by a series of concerns similar to those motivating equivalence checking in the EDA industry, as well as recent developments in machine learning technology. The objective is to ensure that the smaller network is in some sense equivalent or approximately equivalent to the original one. Specifically, one application area is neural network compression [8]. Different compression techniques exist, e.g. knowledge distillation, pruning, quantization, tensor decomposition; see surveys in [8, 26, 29]. Knowledge distillation [15] is the process of transferring knowledge from a large neural network to a smaller one that may be appropriate for deployment on a device with limited computational resources. Another related application area includes the techniques widely known under the term regularization [21], which aim to lower the complexity of NNs in order to achieve better performance. In other cases, NNs used in systems with learning-enabled components [9] may have to be updated for a number of reasons [30]; for example, security concerns such as the need to withstand data perturbations (e.g. adversarial examples), or possibly incomplete coverage of the neural network’s input domain. In the context of NN verification, several abstraction methods are often employed, for instance in order to reduce the complexity of the verification problem, e.g. see [3]. In all the aforementioned cases, the original and resulting NNs need to be functionally comparable in some way. A number of cases where equivalence checking for neural networks arise are also discussed in [19, 28].

This paper presents the first, to our knowledge, systematic study of the equivalence checking problem for NNs, using a Satisfiability Modulo Theory (SMT) [5] approach. We define several formal notions of (approximate) equivalence for NNs, present encodings of the corresponding NN equivalence checking problems into satisfiability checking problems, and describe experimental results on examples of varying complexity.

In particular, the contributions of this paper are the following:

- We define several formal equivalence checking problems for neural networks based on various strict and approximate equivalence criteria that may each be appropriate for different neural network applications.
- We reduce the equivalence checking problem to a logical satisfiability problem using an SMT-based encoding. The approach is sound and complete in the sense that the two given NNs are equivalent iff the resulting SMT formula is unsatisfiable.
- We present a prototype implementation and experimental results including (i) sanity checks of our SMT-based encoding, and (ii) checks showing the equivalence and non-equivalence, as well as checking the scalability of SMT solvers for three diverse neural network applications covering the cases of classifiers (including the well-known MNIST dataset), as well as regression models.

The rest of this paper is organized as follows. Section 2 provides a formal definition of NN models. Section 3 presents diverse equivalence criteria for the wide range of common NN applications and formally defines the equivalence checking problem. Section 4 presents our SMT-based encoding for reducing equivalence checking to a logical satisfiability problem. Section 5 includes the experimental results. In Sect. 6, we review the related work and in Sect. 7 we provide our concluding remarks.
2 Preliminaries: Neural Networks

2.1 Notation

The set of real numbers is denoted by $\mathbb{R}$. The set of natural numbers is denoted by $\mathbb{N}$. Given some $x \in \mathbb{R}^n$ and some $i \in \{1, \ldots, n\}$, $x(i)$ denotes the $i$-th element of $x$.

2.2 Neural Networks

In general, a neural network (NN) can be defined as a function:

$$ f : I \rightarrow O $$

(1)

where $I \subseteq \mathbb{R}^n$ is some input domain with $n$ features and $O \subseteq \mathbb{R}^m$ an output domain.

For a NN image classifier, we typically have $I = [0, 255]^n \subseteq \mathbb{N}^n$ and a labeling function $L : \mathbb{R}^m \rightarrow \mathbb{N}$ that maps each $y \in O$ to some label $l \in \mathbb{N}$. For NNs solving regression problems, we have $I \subseteq \mathbb{R}^n$ and no labeling function.

The above definition of NNs is purely semantic. Concretely, a NN consists of layers of nodes (neurons), including one hidden layer ($H$) or more, beyond the layers of input ($I$) and output ($O$) nodes. Nodes denote a combination of affine value transformation with an activation function, which is typically piecewise linear or nonlinear. Value transformations are weighted based on how nodes of different layers are connected, whereas an extra term called bias is added per node. Weights ($W$) and biases ($b$) for all nodes are the NN’s parameters and their values are determined via training.

Since every layer is multidimensional we use vectors and/or matrices to represent all involved operations. Let $x \in \mathbb{R}^{1 \times n}$ be the matrix denoting some $x \in I$. For a hidden layer with $r$ nodes, $H^{1 \times r}$ represents the output of this hidden layer. Assuming that the hidden and output layers are fully connected, we denote with $W^{(1)} \in \mathbb{R}^{n \times r}$ the hidden layer weights and with $b^{(1)} \in \mathbb{R}^{1 \times r}$ the biases associated with its nodes. Similarly, the output layer weights are denoted by $W^{(2)} \in \mathbb{R}^{r \times m}$, where $m$ refers to the number of output layer nodes, and $b^{(2)} \in \mathbb{R}^{1 \times m}$ denotes the corresponding biases. Then, the output $y = f(x)$ of the NN is given by $y \in \mathbb{R}^m$ where $y$ is computed as:

$$ H = \alpha(x \cdot W^{(1)} + b^{(1)}) $$

(2)

$$ y = \alpha'(H \cdot W^{(2)} + b^{(2)}) $$

(3)

where $\alpha(\cdot), \alpha'(\cdot)$ are the activation functions (e.g. sigmoid, hyperbolic tangent, etc.) applied to the vectors of the hidden and output layers element-wise. A common activation function is the Rectified Linear Unit (ReLU), which is defined, for $\chi \in \mathbb{R}$, as:

$$ ReLU(\chi) = \begin{cases} 
\chi, & \text{if } \chi \geq 0 \\
0, & \text{otherwise}
\end{cases} $$

(4)
Another example is the hard tanh function [10] (used in the experiments of Sect. 5) that typically serves as the output layer activation function of NNs trained for regression. For $\chi \in \mathbb{R}$, hardtanh is defined as:

$$\text{HardTanh}(\chi) = \begin{cases} 
1, & \text{if } \chi > 1 \\
-1, & \text{if } \chi < -1 \\
\chi, & \text{otherwise}
\end{cases} \quad \text{(5)}$$

**Multiple Hidden Layers:** The NN definition provided above is easily generalised to multiple hidden layers $H, H', H'', \ldots$. We consider that weights and biases for all layers and nodes are fixed, since we focus on equivalence checking of NNs after training.

**Example 1.** Consider a simple feedforward NN with two inputs, two outputs, and one hidden layer with two nodes (Fig. 1). The selection of the weights and biases is done randomly, the activation function of the hidden layer is ReLU and there is no activation function for the output layer. For this example, Eq. (2) takes the form:

$$\begin{bmatrix} x_1 \\
x_2 \end{bmatrix} \cdot \begin{bmatrix} W_{11} & W_{12} \\
W_{21} & W_{22} \end{bmatrix} + \begin{bmatrix} b_1^{(1)} \\
b_2^{(1)} \end{bmatrix} = \begin{bmatrix} x_1 \\
x_2 \end{bmatrix} \cdot \begin{bmatrix} -2 & 1 \\
1 & 2 \end{bmatrix} + \begin{bmatrix} 1 \\
1 \end{bmatrix}$$

$$= \begin{bmatrix} -2 \cdot x_1 + x_2 + 1 & x_1 + 2 \cdot x_2 + 1 \end{bmatrix}$$

Denote the result of the affine transformation of the NN’s hidden layer by:

$$\begin{bmatrix} z_1 \\
z_2 \end{bmatrix} = \begin{bmatrix} -2 \cdot x_1 + x_2 + 1 & x_1 + 2 \cdot x_2 + 1 \end{bmatrix} \quad \text{and}$$

$$\mathbf{H} = \begin{bmatrix} h_1 \\
h_2 \end{bmatrix} = \begin{bmatrix} \text{ReLU}(z_1) \\
\text{ReLU}(z_2) \end{bmatrix}$$

The output $y$ of the NN from Eq. (3) is:

$$y = \begin{bmatrix} h_1 \\
h_2 \end{bmatrix} \cdot \begin{bmatrix} 2 & -1 \\
-1 & -2 \end{bmatrix} + \begin{bmatrix} b_1^{(2)} \\
b_2^{(2)} \end{bmatrix} = \begin{bmatrix} 2 \cdot h_1 - h_2 + 2 & -h_1 - 2 \cdot h_2 + 2 \end{bmatrix}$$

### 3 Strict and Approximate Equivalences for Neural Networks

In this section, we present various equivalence relations for NNs and we formulate the equivalence checking problem. Similar equivalence notions appeared recently in [19, 28].
3.1 Strict Neural Network Equivalence

Strict NN equivalence is essentially functional equivalence:

**Definition 1 (Strict NN Equivalence).** For two neural networks \( f : I \to O \) and \( f' : I \to O \), we say that they are strictly equivalent, denoted \( f \equiv f' \), if and only if:

\[
\forall x \in I, f(x) = f'(x)
\]  
(6)

Strict NN equivalence is a true equivalence relation, i.e., it is reflexive (\( f \equiv f \) for any \( f \)), symmetric (\( f \equiv f' \) iff \( f' \equiv f \)), and transitive (\( f \equiv f' \) and \( f' \equiv f'' \) implies \( f \equiv f'' \)).

However, strict NN equivalence can be a very restrictive requirement. For example, if we have two classifiers we may want to consider them equivalent if they always select the same top output class, even if the remaining output classes are not ordered in the same way. This motivates us to consider the following approximate notions of equivalence. These approximate “equivalences” need not be true equivalences, i.e., they may not satisfy the transitivity property (although they are always reflexive and symmetric).

3.2 Approximate Neural Network Equivalences Based on \( L_p \) Norms

As usual, we assume that \( O \subseteq \mathbb{R}^m \). Let \( \|y\|_p = \text{norm}_p(y) \) denoting the \( L_p \)-norm of vector \( y \in O \), for \( \text{norm}_p : O \to \mathbb{R} \) with \( p = 1, 2, \infty \). For two vectors \( y, y' \in O \), if \( p = 1 \) we obtain the Manhattan norm, \( L_1(y, y') = \|y - y'\|_1 = \sum_{i=1}^{m}|y(i) - y'(i)| \), which measures the sum of differences between the two vectors. For \( p = 2 \), we refer to the Euclidean distance \( L_2(y, y') = \|y - y'\|_2 = (\sum_{i=1}^{m}|y(i) - y'(i)|^2)^{1/2} \). Finally, for \( p = \infty \), the \( L_\infty \) distance measures the maximum change to any coordinate:

\[
L_\infty(y, y') = \|y - y'\|_\infty = \max(|y(1) - y'(1)|, \ldots, |y(m) - y'(m)|). \]  
(7)

Then, we define the following notion of approximate equivalence:

**Definition 2 ((\( p, \epsilon \))-approximate equivalence).** Consider two neural networks \( f : I \to O \) and \( f' : I \to O \), \( \text{norm}_p : O \to \mathbb{R} \), and some \( \epsilon > 0 \). We say that \( f \) and \( f' \) are \((p, \epsilon)\)-approximately equivalent, denoted \( f \sim_{p, \epsilon} f' \), if and only if:

\[
\forall x \in I, \quad \|f(x) - f'(x)\|_p < \epsilon
\]  
(8)

It can be seen that the relation \( \sim_{p, \epsilon} \) is reflexive and symmetric.

3.3 Approximate Neural Network Equivalences Based on Order of Outputs

NN classifiers work essentially by computing output values and then mapping them to specific classes. Two such networks may be considered equivalent, if they always produce the same order of outputs, even though the output values might not be the same. For example, consider two classifiers \( f \) and \( f' \) over three possible output classes. Suppose that, for a given input, \( f \) produces \((0.3, 0.5, 0.2)\) and \( f' \) produces \((0.25, 0.6, 0.15)\). We may then consider that for this input the outputs of \( f \) and \( f' \) are equivalent, since
they have the same order, namely, 2, 1, 3 (assuming vector indices start at 1). If this happens for all inputs, we may want to consider \( f \) and \( f' \) (approximately) equivalent.

To capture the above notion of approximate equivalence, we introduce the function:

\[
\text{argsort}_m : \mathbb{R}^m \to \mathcal{Z}_m, \text{ for } m \in \mathbb{N}
\]

where \( \mathcal{Z}_m \subseteq \{1, 2, 3, \ldots, m\}^m \) is the set of permutations of indices of the \( m \) elements. For a given \( s \in \mathbb{R}^m \), \( \text{argsort}_m(s) \) returns the permutation that sorts \( s \) in decreasing order. Thus, \( \text{argsort}_3(0.3, 0.5, 0.2) = \text{argsort}_3(0.25, 0.6, 0.15) = (2, 1, 3) \). If two vector values are equal, \( \text{argsort} \) orders them from lower to higher index. This ensures determinism of the \( \text{argsort} \) function, e.g., \( \text{argsort}_3(0.3, 0.4, 0.3) = (2, 1, 3) \).

**Definition 3 (Top-k argsort equivalence).** Suppose \( O \subseteq \mathbb{R}^m \). Consider two neural networks \( f : I \to O \) and \( f' : I \to O \), and some \( k \in \{1, \ldots, m\} \). We say that \( f \) and \( f' \) are top-k argsort equivalent, denoted \( f \approx_k f' \), if and only if

\[
\forall x \in I, \forall i \in \{1, \ldots, k\}, \left(\text{argsort}_m(f(x))\right)(i) = \left(\text{argsort}_m(f'(x))\right)(i)
\]

Top-k argsort equivalence requires the first \( k \) indices of the argsort of the outputs of \( f \) and \( f' \) to be equal. It is a true equivalence (reflexive, symmetric, and transitive).

A special case of top-k argsort equivalence is when \( k = 1 \). We call this argmax equivalence, with reference to the argmax function that returns the index of the maximum value of a vector, e.g., \( \text{argmax}(0.3, 0.5, 0.2) = \text{argmax}(0.25, 0.6, 0.15) = 2 \).

**Definition 4 (argmax equivalence).** Consider the same setting as in Definition 3. We say that \( f \) and \( f' \) are argmax equivalent iff \( f \approx_1 f' \).

### 3.4 Hybrid \( L_p \)-argsort Equivalences

Approximate NN equivalences based on \( L_p \) norms may not respect the order of outputs, e.g., with \( \epsilon = 1 \), the output vectors \((1, 2)\) and \((2, 1)\) may be considered equivalent, even though the order is reversed. On the other hand, argsort and argmax based equivalences respect the order of outputs but may allow too large differences to be acceptable: the output vectors \((90, 7, 3)\) and \((40, 35, 25)\) both have the same order of outputs, but if the numbers are interpreted as confidence levels, we may not wish to consider them equivalent, due to the large discrepancy between the respective confidence values.

This discussion motivates the need for an equivalence, called hybrid \( L_p – \text{argsort} \) equivalence, which considers both the order of outputs and their differences in value.

**Definition 5 (Hybrid top-k argsort equivalence).** Suppose \( O \subseteq \mathbb{R}^m \). Consider two neural networks \( f : I \to O \) and \( f' : I \to O \), and some \( k \in \{1, \ldots, m\} \). Consider also \( \| \cdot \|_p : O \to \mathbb{R} \), and some \( \epsilon > 0 \). We say that \( f \) and \( f' \) are \((p, \epsilon)\)-approximately and top-k argsort equivalent iff \( f \sim_{p, \epsilon} f' \) and \( f \approx_k f' \), i.e., they are both \((p, \epsilon)\)-approximately equivalent and top-k argsort equivalent.

Specializing to \( k = 1 \) yields the following hybrid equivalence:
Definition 6 (Hybrid argmax equivalence). Consider the same setting as in Definition 6. We say that $f$ and $f'$ are $(p, \epsilon)$-approximately and argmax equivalent iff $f \sim_{p,\epsilon} f'$ and $f \approx_1 f'$.

Definition 5 could be generalized further to involve different norms for each $i$-th element of the output vector, as well as a different bound $\epsilon_i$ for each $i \in \{1, \ldots, m\}$. We refrain from presenting such a generalization explicitly here, for the sake of simplicity.

3.5 The Neural Network Equivalence Checking Problem

Definition 7 (NN equivalence checking problem). Given two (trained) neural networks $f$ and $f'$, and given a certain NN equivalence relation $\simeq \in \{\equiv, \sim_{p,\epsilon}, \approx_k\}$, and parameters $p, \epsilon, k$ as required, the neural network equivalence checking problem (NNECP) is to check whether $f \simeq f'$.

3.6 Discussion of Application Domains for the Above Equivalence Relations

Strict equivalence is a true equivalence relation, but it might be impractical for realistic networks and numerical errors. Approximate equivalences can find several applications. For example, $(p, \epsilon)$-equivalence can be used for multi-output learning problems [40]; specifically for i) regression problems where the goal is to simultaneously predict multiple real-valued output variables [6], and ii) classification tasks to ensure that the NN output values associated with every label are close to each other with respect to some $L_p$-norm. Approximate equivalences based on the order of outputs can be useful for classification. Top-1 accuracy is an established evaluation metric. For problems with hundreds of classes, e.g. ImageNet [11], it is common practice to present the top-5 accuracy along with top-1 accuracy when benchmarking. Top-$k$ accuracy captures if any of the top $k$ highest values of the output prediction vector is assigned the correct label. As such, it could be interesting to check if two NNs are equivalent using the top-$k$ argsort equivalence. This equivalence could be important for Hierarchical Multi-label Classification [37], a classification task where the classes are hierarchically structured and each example may belong to more than one class simultaneously [7].

4 Neural Network Equivalence Checking Using SMT Solvers

Our approach to solving the NNECP is to reduce it to a logical satisfiability problem. The basic idea is the following. Suppose we want to check whether $f \simeq f'$, for two NNs $f : I \to O$ and $f' : I \to O$ and a given NN equivalence relation $\simeq$. We proceed as follows: (1) encode $f$ into an SMT formula $\phi$; (2) encode $f'$ into an SMT formula $\phi'$; (3) encode the equivalence relation $f \simeq f'$ into an SMT formula $\Phi$ such that $f \simeq f'$ iff $\Phi$ is unsatisfiable; (4) check, using an SMT solver, whether $\Phi$ is satisfiable: if not, then $f \simeq f'$; if $\Phi$ is satisfiable, then $f$ and $f'$ are not equivalent, and the SMT solver might provide a counterexample, i.e., an input violating the equivalence of $f$ and $f'$.

This idea is based on the fact that the negation of $f \simeq f'$ can be encoded as a formula which asserts that there is $x \in I$ and $y, y' \in O$, such that $y = f(x), y' = f'(x)$,
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Fig. 2. Complete Neural Network Scheme for GAN generated inputs

with $y$ and $y'$ not satisfying the equivalence conditions imposed by $\simeq$. For example, for the case of strict NN equivalence, checking whether $f \equiv f'$ amounts to checking:

$$\neg \left( \exists x \in I, y \in O, y' \in O, \ y = f(x) \land y' = f'(x) \land y \neq y' \right)$$

This in turn amounts to checking that: $y = f(x) \land y' = f'(x) \land y \neq y'$ is unsatisfiable.

In this case, we have $\phi := y = f(x)$, $\phi' := y' = f'(x)$, and $\Phi := \phi \land \phi' \land y \neq y'$.

We proceed to provide the details of building $\phi$ and $\phi'$ for given NNs, as well as $\Phi$ for the NN equivalence relations defined earlier. We note that although we present the SMT encoding of a single NN, our method is general and allows the two NNs to have different internal architectures (e.g., number and type of hidden layers, etc.).

4.1 Encoding Neural Networks as SMT Formulas

**Input Variables.** From Eq. (2), the input of a NN $f$ is a vector $x = [x_1, \ldots, x_n] \in \mathbb{R}^{1 \times n}$. The SMT formula $\phi$ encoding $f$ will have $n$ input variables, denoted as $x_1, \ldots, x_n$.

**Encoding Input Bounds.** Sometimes, the inputs are constrained to belong in a certain region. For example, we might assume that the input lies between given lower and upper bounds. In such cases, we can add input constraints as follows:

$$\bigwedge_{j=1}^{n} l_j \leq x_j \leq u_j$$  \hspace{1cm} (10)

with $l_j, u_j \in \mathbb{R}$ denoting the lower and upper bounds for the domain of input $x_j$.

**Encoding Other Input Constraints.** Often, we may only care about inputs that are “meaningful”, e.g. if we want to preserve equivalence only for “reasonable” photos of human faces, or “reasonable” pictures of handwritten digits. Encoding such input constraints can be difficult. After all, if we had a precise way to encode such “meaningfulness” as a formal mathematical constraint, we may not need NNs in the first place.

One way to address this fundamental problem is by using generative NNs [14]. The idea is depicted in Fig. 2. The output of the generative network $g$ is fed into $f$ and $f'$ that we wish to test for equivalence. The generative network $g$ models the input constraints, e.g. the output of $g$ may be pictures of human faces. Let $N$ denote the
complete network consisting of the connection of all three \( g, f, f' \), plus the equivalence constraints. We encode \( N \) as an SMT constraint and check for satisfiability. An example to satisfiability is an input \( x \) of \( g \) such that \( f(g(x)) \) and \( f'(g(x)) \) differ in the sense of the given equivalence relation. Then, \( g(x) \) provides a counterexample to the equivalence of \( f \) and \( f' \). Moreover, \( g(x) \) has been generated by \( g \), therefore it belongs by definition to the set of input constraints modeled by \( g \) (e.g., \( g(x) \) is a picture of a human face).

**Internal Variables.** For each hidden layer, we associate the *internal variables* \( z_i \) for the affine transformation, and the internal variables \( h_i \) for the activation function.

**Constraints Encoding the Affine Transformations.** Consider a single hidden layer of \( f \) with \( r \) nodes. Then, from the affine transformation of Eq. (2), we derive the constraints:

\[
\bigwedge_{j=1}^{r} \left( z_j = \sum_{k=1}^{n} x_k W_{kj}^{(1)} + b_{j}^{(1)} \right)
\]  

(11)

**Constraints Encoding the ReLU Activation Function.** If the activation function is ReLU, then its effect is encoded with the following constraints:

\[
\bigwedge_{j=1}^{r} (z_j \geq 0 \land h_j = z_j) \lor (z_j < 0 \land h_j = 0)
\]  

(12)

**Constraints Encoding the Hard tanh Activation Function.** If the activation function is the hard \( \tanh \), then its effect is encoded with the following constraints:

\[
\bigwedge_{j=1}^{r} (z_j \geq 1 \land h_j = 1) \lor (z_j \leq -1 \land h_j = -1) \lor (-1 < z_j < 1 \land z_j = h_j)
\]  

(13)

**Other Activation Functions.** The constraints described so far include atoms of the linear real arithmetic theory [20] that most SMT-solvers can check for satisfiability through decision procedures of various degrees of efficiency. Encoding other activation functions, like \( \tanh \), \( \text{Sigmoid} \), and \( \text{Softmax} \), can be problematic as they include nonlinear and exponential terms that most SAT/SMT cannot handle. A workaround is to opt for “hard” versions of these activation functions, as it is done in [1, 10]. In [24], \( \text{Softmax} \) is replaced by a piecewise linear function called \( \text{Sparsemax} \).

**Multiple Hidden Layers and Output Layer.** The constraints Eq. (11–13) are generalized to multiple hidden layers, say \( H, H', \ldots \) (with \( r, r', \ldots \) nodes, respectively).

The NN encoding is completed with the constraints for the output layer that are derived, for \( y \in \mathbb{R}^m \) from Eq. (3), as previously.
Example 2 (cont. of example 1). We assume that there are input constraints, i.e. $0 \leq x_1 \leq 1$ and $0 \leq x_2 \leq 1$ and we derive the SMT constraints for the NN of Fig. 1. For the affine transformation, we obtain $z_1 = -2 \cdot x_1 + x_2 + 1$ and $z_2 = x_1 + 2 \cdot x_2 + 1$. For the activation functions, we add the constraints $\{(z_1 \geq 0 \land h_1 = z_1) \lor (z_1 < 0 \land h_1 = 0)\}$, encoding $h_1 = ReLU(z_1) = \max(0, z_1)$ and $\{(z_2 \geq 0 \land h_2 = z_2) \lor (z_2 < 0 \land h_2 = 0)\}$, for $h_2 = ReLU(z_2) = \max(0, z_2)$. Finally, we add the output constraints $y_1 = 2 \cdot h_1 - h_2 + 2$ and $y_2 = -h_1 - 2 \cdot h_2 + 2$. The resulting SMT formula is

$$\phi := \{0 \leq x_1 \leq 1 \land 0 \leq x_2 \leq 1 \land z_1 = -2x_1 + x_2 + 1 \land (z_1 \geq 0 \land h_1 = z_1) \lor (z_1 < 0 \land h_1 = 0)\} \land z_2 = x_1 + 2x_2 + 1 \land (z_2 \geq 0 \land h_2 = z_2) \lor (z_2 < 0 \land h_2 = 0)\} \land y_1 = 2 \cdot h_1 - h_2 + 2 \land y_2 = -h_1 - 2 \cdot h_2 + 2$$

4.2 Encoding of the Equivalence Relation

As mentioned at the beginning of this section, to check the equivalence of two NNs $f$ and $f'$, we need to generate, first, their encodings $\phi$ and $\phi'$ (Sect. 4.1), and then, the encoding of the (negation of the) equivalence relation. The latter encoding is described next. We assume that $f$ and $f'$ have the same number of outputs $m$, and we let $y = (y_1, ..., y_m)$ and $y' = (y'_1, ..., y'_m)$ denote their respective output variables.

Strict Equivalence Checking. Strict equivalence (c.f., Definition 1) requires that $y = y'$. To reduce this verification problem to a satisfiability problem, we encode the negation of the above constraint, more specifically:

$$\bigvee_{i=1}^{m} y_i \neq y'_i$$  \hspace{1cm} (14)

($p$, $\epsilon$)-Approximate Equivalence Checking. ($p$, $\epsilon$)-approximate equivalence (c.f., Definition 2) requires that $\|y - y'\|_p < \epsilon$. Again, we encode the negation:

- for $p = 1$,
  $$\sum_{i=1}^{m} |y_i - y'_i| \geq \epsilon$$  \hspace{1cm} (15)

- for $p = 2$, it would be expected to be
  $$\left(\sum_{i=1}^{m} |y_i - y'_i|^2\right)^{\frac{1}{2}} \geq \epsilon$$

which involves the square-root function that yields an undecidable constraint. Instead, our encoding takes the form,

$$u = \sum_{i=1}^{m} |y_i - y'_i|^2 \land u = v \cdot v \land v \geq 0 \land v \geq \epsilon$$  \hspace{1cm} (16)
argmax Equivalence Checking. This equivalence type (c.f., Definition 4) requires that \( \text{argmax}(y) = \text{argmax}(y') \). Again, we wish to encode the negation, i.e., \( \text{argmax}(y) \neq \text{argmax}(y') \). This can be done by introducing the macro \( \text{argmaxis}(y, i, m) \) which represents the constraint \( \text{argmax}(y) = i \), assuming the vector \( y \) has length \( m \). Then, \( \text{argmax}(y) \neq \text{argmax}(y') \) can be encoded by adding the constraints below:

\[
\bigvee_{i, i' \in \{1, \ldots, m\}, i \neq i'} \text{argmaxis}(y, i, m) \land \text{argmaxis}(y', i', m) \tag{18}
\]

where \( \text{argmaxis} \) is defined as follows:

\[
\text{argmaxis}(y, i, m) := (\bigwedge_{j=1}^{i-1} y_i > y_j) \land (\bigwedge_{j=i+1}^{m} y_i \geq y_j) \tag{19}
\]

For example, for \( m = 2 \), we have:

\[
\begin{align*}
\text{argmaxis}(y, 1, 2) &= y_1 \geq y_2 \quad \text{argmaxis}(y', 1, 2) = y'_1 \geq y'_2 \\
\text{argmaxis}(y, 2, 2) &= y_2 > y_1 \quad \text{argmaxis}(y', 2, 2) = y'_2 > y'_1
\end{align*}
\]

and the overall constraint encoding \( \text{argmax}(y) \neq \text{argmax}(y') \) becomes:

\[
(y_1 \geq y_2 \land y_2 > y'_1) \lor (y_2 > y_1 \land y_1 \geq y'_2)
\]

Example 3 (cont. example 2). For the NN \( f \), we have obtained the formula \( \phi \). Now assume that there is a second NN \( f' \) that has the same number of inputs and outputs as \( f \). We define as \( y' \) the outputs of \( f' \) and the constraints are SMT encoded via \( \phi' \). The complete SMT formula \( \Phi \) for the different equivalence relations is:

\[
\begin{align*}
\Phi_{\text{strict}} &:= \{ \phi \land \phi' \land \bigvee_{i=1}^{m} y_i \neq y'_i \} \\
\Phi_{(1, \epsilon)-\text{approx}} &:= \{ \phi \land \phi' \land \sum_{i=1}^{m} |y_i - y'_i| \geq \epsilon \} \\
\Phi_{(2, \epsilon)-\text{approx}} &:= \{ \phi \land \phi' \land u = \sum_{i=1}^{m} |y_i - y'_i|^2 \land u = v \cdot v \land v \geq 0 \land v \geq \epsilon \} \\
\Phi_{(\infty, \epsilon)-\text{approx}} &:= \{ \phi \land \phi' \land \bigvee_{i=1}^{m} |y_i - y'_i| \geq \epsilon \} \\
\Phi_{\text{argmax}} &:= \{ \phi \land \phi' \land \bigvee_{i, i' \in \{1, \ldots, m\}, i \neq i'} \text{argmaxis}(y, i, m) \land \text{argmaxis}(y', i', m) \}
\end{align*}
\]
Algorithm 1 introduces an implementation in the Z3 SMT solver\(^1\) for argmax, which in our experiments showed better scalability behaviour when compared with the straightforward implementation of the aforementioned encoding for argmax.

**Algorithm 1:** Pseudo-code of argmax implementation in Z3

```plaintext
Require: Vector \( y \) of length \( m \)
Ensure: \( \text{argmax}(y) \)

\( y_{\text{max}} \leftarrow y(m) \)
\( i_{\text{max}} \leftarrow m \)

for \( i = m - 1 \) to \( i = 1 \) step -1 do
  if \( y(i) > y_{\text{max}} \) then
    \( y_{\text{max}} \leftarrow y(i) \)
  end if
  if \( y(i) = y_{\text{max}} \) then
    \( i_{\text{max}} \leftarrow i \)
  end if
end for

return \( i_{\text{max}} \)
```

**Hybrid Equivalence Checking.** The encoding of the hybrid equivalence relations in Sect. 3.4 consists of combining the corresponding constraints of the \( (p, \epsilon) \)-approximate equivalence and the argsort/argmax equivalence with a logical conjunction.

### 4.3 Optimizing the Encoding

The encoding presented so far is not optimal in the sense that it uses more SMT variables than strictly necessary. Many internal variables can be eliminated and replaced by their corresponding expressions in terms of other variables. In particular, the \( z_i \) variables encoding the affine transformations (as in Eq. 11) and the \( h_i \) variables for encoding the activation function can be easily eliminated.

### 5 Experimental Results

In this section, we report the results of experiments on verifying the equivalence of two NNs. We have used the SMT solver Z3 to check the satisfiability of all constraints that encode NN equivalence. The experiments were conducted on a laptop with a 4-core 2.8 GHz processor and 12 GB RAM. Our problems concern with NNs of different sizes, for checking their equivalence, with respect to the equivalence relations of Sect. 3. We focus on two main categories of supervised learning problems, i) classification (two case studies), and ii) regression (one case study). The source code of the implementation of the NNECP for the equivalence encoding of Sect. 4 is provided online\(^2\).

---

1. https://z3prover.github.io/api/html/.
2. https://github.com/hariselef/NNequiv_Experiments.
Bit-Vec Case Study – Classification: A bit vector (Bit-Vec) is a sequence of bits. We consider that the inputs of our NN classifier are 10-bit vectors and the targets (labels) are either True (1) or False (0). The models we check for equivalence are Feed-Forward Multi-Layer Perceptrons and we focus on two architectures. In the first case, there is a single hidden layer, while in the second, there are two hidden layers; NNs have the same number of nodes per layer. We experimented with 8 different models per architecture and for each model we increased step-wise the number of nodes per layer. NNs have been trained with the objective to “learn” that for a vector with 3 or more consecutive 1s, the output label is True and the output label is False otherwise.

MNIST Case Study – Classification: The second use case is the popular MNIST dataset on image classification. MNIST contains 70,000 grayscale images, from which 60,000 are for training and the rest for testing the models’ performance. The size of images is 28 × 28 (pixels), and every pixel value is a real in the range [0, 1]. We experimented with the same two architectures used for the Bit-Vec NNs and 5 models for each of them.

Automotive Control – Regression: For the regression case study, the goal is to use NNs that approximate the behaviour of a Model Predictive Controller, which has been designed for an automotive lane keeping assist system. The dataset contains 10,000 instances with six features representing different system characteristics obtained using sensors, along with the resulting steering angle that the car should follow (target). More details for the case study that we have reproduced can be found in Mathworks website.

5.1 Sanity Checks

The main goals of this set of experiments are: i) to ensure that our prototype implementation for equivalence checking does not have any bugs (sanity checks) and ii) to conduct a scalability analysis of the computational demands for NNs of increasing complexity when they are checked for equivalence, with the criteria of Sect. 3.

To this end, we verified the equivalence of two identical NNs, for two different architectures, both for the BitVec case study and the MNIST. The results are shown in Tables 1, 2 for the BitVec case study and in Tables 3, 4 for the MNIST. We report the number of nodes per hidden layer, the number of trainable parameters and the total number of variables in the formula generated for the SMT solver. For the BitVec experiments and for each equivalence relation, tables show the average time in seconds over 10 runs for the SMT solver to verify the equivalence of the identical NNs (standard deviation in all cases was less than 3%). For the MNIST experiments, we report the same results, but all sanity checks were conducted only once, since these experiments took more time to complete. In all cases, the SMT solver returned UNSAT, which correctly indicates that the two NNs are equivalent, as expected.

https://www.mathworks.com/help/reinforcement-learning/ug/imitate-mpc-controller-for-lane-keeping-assist.html.
Table 1. Sanity check for the BitVec case study - 1st Architecture; all equivalences are true, i.e. all SMT formulas are \textit{UNSAT}; the values in columns 4–8 show the computational time in seconds.

| # nodes per layer | # params | # SMT variables | Strict Equiv. | $L_1$ Equiv. | $L_2$ Equiv. | $L_\infty$ Equiv. | Argmax Equiv. |
|-------------------|----------|----------------|---------------|-------------|-------------|-----------------|--------------|
| 10                | 132      | 498            | 0.06          | 0.07        | 0.06        | 0.07            | 0.06         |
| 20                | 262      | 978            | 0.1           | 0.1         | 0.09        | 0.1             | 0.1          |
| 35                | 457      | 1698           | 0.17          | 0.17        | 0.14        | 0.17            | 0.17         |
| 50                | 652      | 2418           | 0.23          | 0.24        | 0.21        | 0.24            | 0.23         |
| 100               | 1302     | 4818           | 0.44          | 0.45        | 0.40        | 0.45            | 0.45         |
| 150               | 1952     | 7218           | 0.61          | 0.63        | 0.57        | 0.62            | 0.65         |
| 200               | 2602     | 9618           | 0.84          | 0.85        | 0.75        | 0.85            | 0.84         |
| 300               | 3902     | 14418          | 1.23          | 1.25        | 1.1         | 1.25            | 1.25         |

Table 2. Sanity check for the BitVec case study - 2nd Architecture; all equivalences are true, i.e. all SMT formulas are \textit{UNSAT}; the values in columns 4–8 show the computational time in seconds.

| # nodes per layer | # params | # SMT variables | Strict Equiv. | $L_1$ Equiv. | $L_2$ Equiv. | $L_\infty$ Equiv. | Argmax Equiv. |
|-------------------|----------|----------------|---------------|-------------|-------------|-----------------|--------------|
| 5                 | 97       | 378            | 0.04          | 0.04        | 0.04        | 0.04            | 0.04         |
| 10                | 242      | 938            | 0.1           | 0.09        | 0.08        | 0.09            | 0.1          |
| 15                | 437      | 1698           | 0.15          | 0.15        | 0.14        | 0.16            | 0.15         |
| 20                | 682      | 2658           | 0.24          | 0.24        | 0.20        | 0.23            | 0.23         |
| 30                | 1322     | 5178           | 0.4           | 0.39        | 0.37        | 0.39            | 0.42         |
| 40                | 2162     | 8498           | 0.62          | 0.62        | 0.58        | 0.63            | 0.63         |
| 50                | 3202     | 12618          | 0.87          | 0.91        | 0.85        | 0.88            | 0.92         |
| 60                | 4442     | 17538          | 1.17          | 1.2         | 1.21        | 1.16            | 1.23         |

Table 3. Sanity check for the MNIST case study - 1st Architecture; all equivalences are true, i.e. all SMT formulas are \textit{UNSAT}; the values in columns 4–8 show the computational time in seconds.

| # nodes per layer | # params | # SMT variables | Strict Equiv. | $L_1$ Equiv. | $L_2$ Equiv. | $L_\infty$ Equiv. | Argmax Equiv. |
|-------------------|----------|----------------|---------------|-------------|-------------|-----------------|--------------|
| 10                | 7960     | 32424          | 2.5           | 2.53        | 2.2         | 2.63            | 2.67         |
| 30                | 23860    | 95624          | 7.52          | 7.73        | 6.3         | 7.63            | 7.5          |
| 50                | 39760    | 158824         | 12.2          | 12.4        | 10.4        | 12.8            | 12.4         |
| 100               | 79510    | 316824         | 24.5          | 24.3        | 21.9        | 25              | 24.6         |
| 200               | 159010   | 632824         | 48.4          | 55.1        | 44.8        | 48.8            | 48.2         |
| 300               | 238510   | 948824         | 74            | 74          | 74          | 62.4            | 73           |
| 500               | 397510   | 1580824        | 121           | 124         | 110         | 128             | 119          |
| 750               | 596260   | 2370824        | 182           | 193         | 167         | 203             | 182          |
| 1000              | 795010   | 3160824        | 241           | 247         | 220         | 257             | 256          |
| 1300              | 1033510  | 4108824        | 314           | 336         | 283         | 331             | 321          |
| 1700              | 1351510  | 5372824        | 420           | 434         | 394         | 435             | 437          |
| 2000              | 1590010  | 6320824        | 467           | 512         | 483         | 492             | 508          |
Table 4. Sanity check for the MNIST case study - 2nd Architecture; all equivalences are true, i.e. all SMT formulas are *UNSAT*; the values in columns 4–8 show the computational time in seconds.

| # nodes per layer | # params | # SMT variables | Strict Equiv. | $L_1$ Equiv. | $L_2$ Equiv. | $L_{\infty}$ Equiv. | Argmax Equiv. |
|------------------|----------|-----------------|---------------|-------------|-------------|-----------------|---------------|
| 10               | 8070     | 32864           | 2.7           | 2.7         | 2.3         | 2.54            | 2.57          |
| 30               | 24790    | 99344           | 7.55          | 7.86        | 6.7         | 7.5             | 7.5           |
| 50               | 42310    | 169024          | 13.2          | 12.9        | 11.0        | 13.7            | 12.9          |
| 100              | 89610    | 357224          | 26.5          | 27.5        | 24.9        | 26              | 27.7          |
| 200              | 199210   | 793624          | 58.7          | 62.2        | 50.6        | 61.6            | 64.4          |
| 300              | 328810   | 1310024         | 99            | 100         | 90          | 99              | 101           |
| 500              | 648010   | 2582824         | 194           | 194         | 167         | 192             | 192           |
| 750              | 1159510  | 4623824         | 334           | 340         | 298         | 354             | 349           |
| 1000             | 1796010  | 7164824         | 524           | 530         | 514         | 523             | 560           |
| 1300             | 2724810  | 10874024        | 797           | 779         | 784         | 836             | 857           |
| 1700             | 4243210  | 16939624        | 1225          | 1161        | 1359        | 1237            | 1223          |
| 2000             | 5592010  | 22328824        | 1435          | 1530        | 2837        | 1549            | 1581          |

5.2 Equivalence Checking

In the second set of experiments, we perform equivalence checking between NNs of different architectures. The solver will return *UNSAT* if the NNs are equivalent or *SAT* if they are not. This allows us to gain insight into the efficiency and the scalability bounds of the proposed encoding for both possible outcomes. We expect that when the two NNs are not equivalent (*SAT*) the solver is quite likely to return a counterexample shortly. A time limit of 10 min was set for the solver to respond and when this did not happen the end result was recorded as a “timeout”.

**Experiments with NN Classifiers.** A series of experiments focused on the equivalence checking for NN classifiers, i.e. those trained for the BitVec and MNIST case studies. The pairs of NNs that were compared consisted of the two NN architectures that were also used for the sanity checks (Sect. 5.1). Thus, the first pair of NNs includes the NN referred in the first line of Table 1 and the NN referred in the first line of Table 2, and so on. For the BitVec equivalence checking experiments, Table 5 summarizes the obtained results, for all equivalence relations apart from the $(2, \epsilon)$-approximate equivalence, which takes much more time than the set time limit and the results for two pairs of NNs are shown separately in Table 7. For each pair of NNs in Tables 5 and 7, the answer of the SMT solver is reported (*SAT* or *UNSAT*) along with the time that it took to respond. For the $\epsilon$-approximate equivalences, we also note the $\epsilon$ values, for which the NN equivalence was checked. The reason for using relatively big values for $\epsilon$ is that the NNs do not have a nonlinear activation function in the output layer, e.g. sigmoid, and there was no way to guarantee that the outputs would scale in the same value ranges. The term MME, in some cells of the tables, stands for Maximum Memory Exceeded and is the reason for which the solver fails to respond, when not having reached the time limit of 10 min. Table 6 (and Table 7 for $(2, \epsilon)$-approximate equivalence) report the corresponding results, for the MNIST case study.
When the outcome of equivalence checking is SAT, the solver returns a counterexample (NN input) that violates the equivalence relation. If the input space is finite, it may be possible to obtain all counterexamples, as in the BitVec case study, for which we found two counterexamples of $\text{argmax}$ equivalence for the NNs of the pair \textit{model$_1$} vs \textit{model$_2$}. The NN predictions for all possible inputs were then tested and it was confirmed that the two counterexamples are the only ones that violate $\text{argmax}$ equivalence. Beyond seeing them as an extra sanity check, the counterexamples of equivalence checking may be useful, toward improving the NN robustness. However, we have not yet developed a systematic way to utilize them for this purpose. For most applications, as is the case in MNIST, it may not be feasible to obtain all possible counterexamples, due to the size of their input space. Moreover, often there is no easy way to limit the counterexample search to only “meaningful” inputs. This is the case in the MNIST case study, where the most common counterexample in the equivalence checking

\begin{table}[h]
\centering
\caption{Equivalence checking for the BitVec case study}
\begin{tabular}{|c|c|c|c|c|c|c|}
\hline
Model Pairs & \# SMT variables & Input & Internal & Output & $L_1 > 5$ & $L_{\infty} > 10$ & $\text{argmax}$ Equiv. \\
\hline
\textit{model$_1$} vs \textit{model$_2$} & 10 & 424 & 4 & SAT/0.042 s & UNSAT/35 s & UNSAT/48 s & SAT/0.23 s \\
\textit{model$_1$} vs \textit{model$_2$} & 10 & 944 & 4 & SAT/0.075 s & SAT/0.20 s & UNSAT/157 s & SAT/0.4 s \\
\textit{model$_3$} vs \textit{model$_2$} & 10 & 1630 & 4 & SAT/0.124 s & UNSAT/385 s & UNSAT/531 s & UNSAT/182 s \\
\textit{model$_4$} vs \textit{model$_2$} & 10 & 2524 & 4 & SAT/0.19 s & SAT/245 s & Timeout & SAT/86 s \\
\textit{model$_5$} vs \textit{model$_2$} & 10 & 4984 & 4 & SAT/0.35 s & Timeout & MME/509 s & SAT/240 s \\
\textit{model$_6$} vs \textit{model$_2$} & 10 & 7844 & 4 & SAT/0.5 s & Timeout & MME/568 s & SAT/450 s \\
\textit{model$_7$} vs \textit{model$_2$} & 10 & 11104 & 4 & SAT/0.75 s & Timeout & MME/588 s & Timeout \\
\textit{model$_8$} vs \textit{model$_2$} & 10 & 15964 & 4 & SAT/1.13 s & Timeout & Timeout & Timeout \\
\hline
\end{tabular}
\end{table}

\begin{table}[h]
\centering
\caption{Equivalence checking for the MNIST case study}
\begin{tabular}{|c|c|c|c|c|c|c|}
\hline
Model Pairs & \# SMT variables & Input & Internal & Output & $L_1 > 5$ & $L_{\infty} > 10$ & $\text{argmax}$ Equiv. \\
\hline
\textit{mnist$_1$} vs \textit{mnist$_2$} & 784 & 31840 & 20 & SAT/2.1 s & SAT/44 s & SAT/42 s & SAT/41 s \\
\textit{mnist$_1$} vs \textit{mnist$_2$} & 784 & 96680 & 20 & SAT/6.2 s & SAT/16 s & SAT/17 s & SAT/17 s \\
\textit{mnist$_3$} vs \textit{mnist$_2$} & 784 & 163120 & 20 & SAT/10.3 s & SAT/28 s & SAT/28 s & MME/230 s \\
\textit{mnist$_4$} vs \textit{mnist$_2$} & 784 & 336220 & 20 & SAT/21 s & SAT/56 s & SAT/ 57 s & SAT/54 s \\
\textit{mnist$_5$} vs \textit{mnist$_2$} & 784 & 712420 & 20 & SAT/45 s & SAT/120 s & SAT/120 s & SAT/118 s \\
\hline
\end{tabular}
\end{table}

\begin{table}[h]
\centering
\caption{Equivalence checking on BitVec and MNIST under $L_2$ $\epsilon$-approximate equivalence}
\begin{tabular}{|c|c|c|c|c|c|}
\hline
Model Pairs & \# SMT variables & Input & Internal & Output & $L_2 > 1$ & $L_2 > 10$ \\
\hline
\textit{model$_1$} vs \textit{model$_2$} & 10 & 424 & 4 & SAT/35 s & UNSAT/1494 s \\
\textit{model$_1$} vs \textit{model$_2$} & 10 & 944 & 4 & SAT/105 s & UNSAT/2793 s \\
\textit{mnist$_1$} vs \textit{mnist$_2$} & 784 & 31840 & 20 & MME/15436 s & - \\
\hline
\end{tabular}
\end{table}
experiments was an input vector filled with the value 0.5, which corresponds to a grayscale image whose pixels have all the same color, i.e. it is not a digit.

**Experiments with Regression NNs.** In another case study, we focused on NNs that serve as controllers in lane keeping assistant systems. Table 8 presents the details for the features and the outputs of the regression NNs for this case, as well as the valid value ranges. The pairs of NNs that were checked for equivalence consist of different versions of the same NN, produced through varying the number of epochs, for which the model was trained before being verified. We experimented with three versions of the NN controller trained for 30, 35 and 40 epochs. The argmax equivalence is meaningless, since there is only one output variable. Additionally, for the same reason, the results in Table 9 refer only to the $(1, \epsilon)$-approximate equivalence, since the various $L_p$ norms are indistinguishable, when they are applied to scalar values.

**Experiments with Weight Perturbations.** Table 10 reports the results of a set of experiments with a NN for MNIST, in which we have randomly altered the values of some weights before checking the equivalence with the original NN. In this way, since it is very likely to have a pair of equivalent NNs, the solver is forced to search for almost all possible inputs before reaching the UNSAT result. We observe that when having altered two weights (out of 7960) the solver reaches the 10 min timeout.

---

**Table 8.** Regression Problem Input Characteristics – Constraints

| Type/Parameter | Answer/Value | Remarks |
|----------------|--------------|---------|
| output/target  | $[-1.04, 1.04]$ | steering angle $[-60, 60]$ |
| input range $x_1$ | [-2,2] | $v_x$ (m/s) |
| input range $x_2$ | [-1.04, 1.04] | rad/s |
| input range $x_3$ | [-1,1] | m |
| input range $x_4$ | [-0.8, 0.8] | rad |
| input range $x_5$ | [-1.04, 1.04] | $u_0$ (steering angle) |
| input range $x_6$ | [-0.01,0.01] | $\rho$ |

**Table 9.** Equivalence checking for the Regression NNs

| Model Pairs | # SMT variables | Strict Equivalence | $L_1 > 0.5$ |
|-------------|-----------------|--------------------|--------------|
| MPC,30 vs MPC,35 | 6 17912 2 | SAT/1.95 s | Timeout |
| MPC,30 vs MPC,40 | 6 17912 2 | SAT/1.97 s | Timeout |
| MPC,35 vs MPC,40 | 6 17912 2 | SAT/1.98 s | Timeout |
Table 10. Equivalence checking with weight perturbations on the MNIST case study

| Model   | # SMT variables | # weight changes | Value range | $L_1 > 5$ | $L_\infty > 10$ | Argmax Equiv. |
|---------|----------------|-----------------|-------------|-----------|----------------|---------------|
| mnist_1 | 784            | 20              | $1 \times 10^{-1} - 1 \times 10^{-6}$ | UNSAT/30 s | UNSAT/30 s     | Timeout       |
| mnist_1 | 784            | 20              | $1 \times 10^{-1} - 1 \times 10^{-6}$ | Timeout   | Timeout        | Timeout       |

6 Related Work

Verification of NNs for various kinds of properties, such as safety, reachability, robustness, is of fast-growing interest, due to the many, often critical applications, in which NNs are employed. The authors of [23] present several algorithms for verifying NNs and classify them into three categories: reachability-based, optimization-based, and search-based. Typically, SMT-based approaches belong to the latter category. Two comprehensive surveys that include the verification of NNs using SMT solvers are given in [22] and [16]. An extensive survey of methods for the verification and validation of systems with learning enabled-components, not only NNs, is given in [39]. The equivalence checking problem for NNs is different from other verification problems for NNs: (a) in robustness verification, the goal is to check whether the output of a NN remains stable despite perturbations of its input; (b) for input-output verification of a NN, the goal is to check whether for a given range of input values, the output of the NN belongs in a given range of output values.

Other works on the equivalence of NNs are [28] and [19,35]. [28] only considers the case of strict equivalence where the outputs of the two networks must be identical for all inputs. We also define notions of approximate equivalence, as we believe strict equivalence is often too strong a requirement. [28] is also based on a SAT/SMT based encoding of the equivalence checking problem, but the overall approach is applicable only to a specific category of NNs, the so-called binarized NNs [2,17] that are not widely used in many different real-life applications. Approximate NN equivalence checking is also studied in [19,35], but their approach is based on mixed-integer linear programming (MILP) instead of SMT encoding. [19] applies the solution only to restricted regions of the input space, within a radius around the training data, whereas [35] introduces an abstraction-based solution. None of these works allows checking of hybrid equivalence.

The work in [30] focuses on the relationship between two NNs, e.g. whether a modified version of a NN produces outputs within some bounds relative to the original network. A “differential verification” technique is proposed consisting of a forward interval analysis through the network’s layers, followed by a backward pass, which iteratively refines the approximation, until having verified the property of interest. Differential verification is related to equivalence checking, but it is actually a different problem.

In [32], the authors adopt abstractions of the input domain using zonotopes and polyhedra, along with an MILP solver for verifying properties of NNs. An SMT-based verification method for a single NN is also presented in [18], whose applicability is limited only to NNs with ReLU activation functions. Finally, an interesting symbolic representation targeting only piecewise linear NNs is the one presented in [34].
7 Conclusions

In this work, we examined a series of formal equivalence checking problems for NNs, with respect to equivalence relations that can be suitable for various applications and verification requirements. We provided an SMT-based verification approach, as well as a prototype implementation and experimental results.

In our future research plans, we aim to explore whether the equivalence checking problem can be encoded in existing verification tools for NNs (e.g. Reluplex [18], ERAN [32], α−β Crown [36,41,42], VNN competition [4]) through the parallel composition of the two networks that are to be compared. An interesting prospect is to extend our approach towards finding the smallest $\epsilon$, for which two NNs become equivalent.

As additional research priorities, we also intend to explore the scalability margins of alternative solution encodings, including the optimized version of the current encoding (as described in Sect. 4.3) and to compare them with the MILP encoding in [19]. Lastly, it may be also worth exploring the effectiveness of techniques applied to similar problems from other fields, like for example the equivalence checking of digital circuits [12,13,25]. In this context, we may need to rely on novel ideas toward the layer-by-layer checking of equivalence between two NNs.

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