Abstract Neural Networks

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Abstract. Deep Neural Networks (DNNs) are rapidly being applied to safety-critical domains such as drone and airplane control, motivating techniques for verifying the safety of their behavior. Unfortunately, DNN verification is NP-hard, with current algorithms slowing exponentially with the number of nodes in the DNN. This paper introduces the notion of Abstract Neural Networks (ANNs), which can be used to soundly overapproximate DNNs while using fewer nodes. An ANN is like a DNN except weight matrices are replaced by values in a given abstract domain. We present a framework parameterized by the abstract domain and activation functions used in the DNN that can be used to construct a corresponding ANN. We present necessary and sufficient conditions on the DNN activation functions for the constructed ANN to soundly over-approximate the given DNN. Prior work on DNN abstraction was restricted to the interval domain and ReLU activation function. Our framework can be instantiated with other abstract domains such as octagons and polyhedra, as well as other activation functions such as Leaky ReLU, Sigmoid, and Hyperbolic Tangent.

Code: https://github.com/95616ARG/abstract_neural_networks

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1 Introduction

Deep Neural Networks (DNNs), defined formally in Section 3, are loop-free computer programs organized into layers, each of which computes a linear combination of the layer’s inputs, then applies some non-linear activation function to the resulting values. The activation function used varies between networks, with popular activation functions including ReLU, Hyperbolic Tangent, and Leaky ReLU [13]. DNNs have rapidly become important in a variety of applications, including image recognition and safety-critical control systems, motivating research into the problem of verifying properties about their behavior [18].

Although they lack loops, the use of non-linear activation functions introduces exponential branching behavior into the DNN semantics. It has been shown that DNN verification is NP-hard [18]. In particular, this exponential behavior scales with the number of nodes in a network. DNNs in practice have very large numbers of nodes, e.g., the aircraft collision-avoidance DNN ACAS Xu [17] has 300 and a modern image recognition network has tens of thousands [20]. The
number of nodes in modern networks has also been growing with time as more effective training methods have been found [3].

One increasingly common way of addressing this problem is to compress the DNN into a smaller proxy network which can be analyzed in its place. However, most such approaches usually do not guarantee that properties of the proxy network hold in the original network (they are unsound). Recently, Prabhakar et al. [30] introduced the notion of Interval Neural Networks (INNs), which can produce a smaller proxy network that is guaranteed to over-approximate the behavior of the original DNN. While promising, soundness is only guaranteed with a particular activation function (ReLU) and abstract domain (intervals).

In this work, we introduce Abstract Neural Networks (ANNs), which are like DNNs except weight matrices are replaced with values in an abstract domain. Given a DNN and an abstract domain, we present an algorithm for constructing a corresponding ANN with fewer nodes. The algorithm works by merging groups of nodes in the DNN to form corresponding abstract nodes in the ANN. We prove necessary and sufficient conditions on the activation functions used for the constructed ANN to over-approximate the input DNN. If these conditions are met, the smaller ANN can be soundly analyzed in place of the DNN. Our formalization and theoretical results generalize those of Prabhakar et al. [30], which are an instantiation of our framework for ReLU activation functions and the interval domain. Our results also show how to instantiate the algorithm such that sound abstraction can be achieved with a variety of different abstract domains (including polytopes and octagons) as well as many popular activation functions (including Hyperbolic Tangent, Leaky ReLU, and Sigmoid).

Outline In this paper, we aim to lay strong theoretical foundations for research into abstracting neural networks for verification. Section 2 gives an overview of our technique. Section 3 defines preliminaries. Section 4 defines Abstract Neural Networks (ANNs). Section 5 presents an algorithm for constructing an ANN from a given DNN. Section 6 motivates our theoretical results with a number of examples. Section 7 proves our soundness theorem. Section 8 discusses related work, while Section 9 concludes with a discussion of future work.

2 Motivation

DNNs are often denoted by a graph of the form shown in Figure 1a. The input node $x_1$ is assigned the input value, then the values of $h_1$ and $h_2$ are computed by first a linear combination of the values of the previous layer (in this case $x_1$) followed by some non-linear activation function. The behavior of the network is dependent on the non-linear activation function used. We will assume that the output layer with nodes $y_1$, $y_2$, and $y_3$ uses the identity activation function $I(x) = x$. For the hidden layer with nodes $h_1$ and $h_2$ we will consider two scenarios, each using one of the following two activation functions:

$$
\sigma(x) = \begin{cases} 
  x & \text{if } x \geq 0 \\
  0 & \text{otherwise}
\end{cases} \quad \phi(x) = \begin{cases} 
  x & \text{if } x \geq 0 \\
  0.5x & \text{otherwise}
\end{cases}
$$
Fig. 1: Example DNN to INN and one of many instantiations of the INN.

Using $\sigma$ as the activation function for the hidden layer, when $x_1 = 1$ we have $h_1 = \sigma(1x_1) = 1$ and $h_2 = \sigma(-1x_1) = 0$. That in turn gives us $y_1 = I(1h_1 + 1h_2) = 1$, $y_2 = I(1h_1 + 0h_2) = 1$, and $y_3 = I(0h_1 + 1h_2) = 0$.

Using $\sigma$ as the activation function for the hidden layer, when $x_1 = 1$, we have
\[
\begin{align*}
h_1 &= \sigma(1x_1) = 1 \\
y_1 &= I(1h_1 + 1h_2) = 1
\end{align*}
\]
\[
\begin{align*}
h_2 &= \sigma(-1x_1) = 0 \\
y_2 &= I(1h_1 + 0h_2) = 1 \\
y_3 &= I(0h_1 + 1h_2) = 0.
\end{align*}
\]

Using $\phi$ as the activation function for the hidden layer, when $x_1 = 1$, we have
\[
\begin{align*}
h_1 &= \phi(1) = 1 \\
y_1 &= 0.5
\end{align*}
\]
\[
\begin{align*}
h_2 &= \phi(-1) = -0.5 \\
y_2 &= 1
\end{align*}
\]
\[
\begin{align*}
y_3 &= -0.5.
\end{align*}
\]

2.1 Merging Nodes

Our goal is to merge nodes and their corresponding weights in this DNN to produce a smaller network that over-approximates the behavior of the original one. One way of doing this was proposed by Prabhakar et al. [30], where nodes within a layer can be merged and the weighted interval hull of their edge weights is taken. For example, if we merge all of the $h_i$ nodes together into a single $\mathbb{T}$ node, this process results in an Interval Neural Network (INN) shown in Figure 1b.

Intuitively, given this new INN we can form a DNN instantiation by picking any weight within the interval for each edge. We can then find the output of this DNN instantiation on, say, $x_1 = 1$. We take the output of the INN on an input $x_1$ to be the set of all such $(y_1, y_2, y_3)$ triples outputted by some such instantiated DNN on $x_1$.

For example, we can take the instantiation in Figure 1c. Using the $\sigma$ activation function, this implies $(y_1 = 1, y_2 = 1, y_3 = 0)$ is in the output set of the INN on input $x_1 = 1$. In fact, the results of Prabhakar et al. [30] show that, if the $\sigma$ activation function is used, then for any input $x_1$ we will have some assignment to the weights which produces the same output as the original DNN (although many assignments will produce different outputs — the output set is an over-approximation of the behavior of the original network).
However, something different happens if the network were using the $\phi$ activation function, a case that was not considered by Prabhakar et al. [30]. In that scenario, the original DNN had an output of $(0.5, 1, -0.5)$, so if the INN were to soundly over-approximate it there would need to be some instantiation of the weights where $y_1$ and $y_3$ could have opposite signs. But this cannot happen — both will have the same (or zero) sign as $h$!

These examples highlight the fact that the soundness of the algorithm from Prabhakar et al. [30] is specific to the ReLU activation function ($\sigma$ above) and Interval abstract domain. Their results make no statement about whether INNs over-approximate DNNs using different activation functions (such as $\phi$ above), or if abstractions using different domains (such as the Octagon Neural Networks defined in Definition 11) also permit sound DNN over-approximation.

This paper develops a general framework for such DNN abstractions, parameterized by the abstract domain and activation functions used. In this framework, we prove necessary and sufficient conditions on the activation functions for a Layer-Wise Abstraction Algorithm generalizing that of Prabhakar et al. [30] to produce an ANN soundly over-approximating the given DNN. Finally, we discuss ways to modify the abstraction algorithm in order to soundly over-approximate common DNN architectures that fail the necessary conditions, extending the applicability of model abstraction to almost all currently-used DNNs.

These results lay a solid theoretical foundation for research into Abstract Neural Networks. Because our algorithm and proofs are parameterized by the abstract domain and activation functions used, our proofs allow practitioners to experiment with different abstractions, activation functions, and optimizations without having to re-prove soundness for their particular instantiation (which, as we will see in Section 7, is a surprisingly subtle process).

3 Preliminaries

In this section we define Deep Neural Networks and a number of commonly-used activation functions.

3.1 Deep Neural Networks

In Section 2 we represented neural networks by graphs. While this is useful for intuition, in Section 4 we will talk about, e.g., octagons of layer weight matrices, for which the graph representation makes significantly less intuitive sense. Hence, for the rest of the paper we will use an entirely equivalent matrix representation for DNNs, which will simplify the definitions, intuition, and proofs considerably. With this notation, we think of nodes as dimensions and layers of nodes as intermediate spaces. We then define a layer to be a transformation from one intermediate space to another.

Definition 1. A DNN layer from $n$ to $m$ dimensions is a tuple $(W, \sigma)$ where $W$ is an $m \times n$ matrix and $\sigma : \mathbb{R} \to \mathbb{R}$ is an arbitrarily-chosen activation function.
We will often abuse notation such that, for a vector $\mathbf{v}$, $\sigma(\mathbf{v})$ is the vector formed by applying $\sigma$ to each component of $\mathbf{v}$.

**Definition 2.** A Deep Neural Network (DNN) with layer sizes $s_0, s_1, \ldots, s_n$ is a collection of $n$ DNN layers $(W^{(1)}, \sigma^{(1)}), \ldots, (W^{(n)}, \sigma^{(n)})$, where the $(W^{(i)}, \sigma^{(i)})$ layer is from $s_{i-1}$ to $s_i$ dimensions.

Every DNN has a corresponding function, defined below.

**Definition 3.** Given a DNN from $s_0$ to $s_n$ dimensions with layers $(W^{(1)}, \sigma^{(1)}), \ldots, (W^{(n)}, \sigma^{(n)})$, the function corresponding to the DNN is the function $f : \mathbb{R}^{s_0} \rightarrow \mathbb{R}^{s_n}$ given by $f(\mathbf{v}) = \mathbf{v}^{(n)}$, where $\mathbf{v}^{(i)}$ is defined inductively by $\mathbf{v}^{(0)} = \mathbf{v}$ and $\mathbf{v}^{(i)} = \sigma^{(i)}(W^{(i)}(\mathbf{v}^{(i-1)}))$.

Where convenient, we will often refer to the corresponding function as the DNN or vice-versa.

**Example 1.** The DNN $N_1$ from Figure 1a when using the $\sigma$ hidden-layer activation function, is represented by the layers $\left(\begin{bmatrix} 1 \\ -1 \end{bmatrix}, \sigma\right)$ and $\left(\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, I\right)$. The function corresponding to the DNN is given by $N_1(x_1) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \sigma\left(\begin{bmatrix} 1 \\ -1 \end{bmatrix} x_1\right)$.

### 3.2 Common Activation Functions

There are a number of commonly-used activation functions, listed below.

**Definition 4.** The Leaky Rectified Linear Unit (LReLU) \cite{he2015delving}, Rectified Linear Unit (ReLU), Hyperbolic Tangent (tanh), and Threshold (thresh) activation functions are defined:

\[
\text{LReLU}(x; c) := \begin{cases} 
  x & x \geq 0 \\
  cx & x < 0 
\end{cases}, \quad \text{ReLU}(x) := \text{LReLU}(x; 0), \\
\text{tanh} := \frac{e^{2x} - 1}{e^{2x} + 1}, \quad \text{thresh}(x; t, v) := \begin{cases} 
  x & \text{if } x \geq t \\
  v & \text{otherwise}
\end{cases}.
\]

Here LReLU and thresh actually represent families of activation functions parameterized by the constants $c, t, v$. The constants used varies between networks. $c = 0$ is a common choice for the LReLU parameter, hence the explicit definition of ReLU.

All of these activation functions are present in standard deep-learning toolkits, such as Pytorch \cite{Paszke2019}. Libraries such as Pytorch also enable users to implement new activation functions. This variety of activation functions used in practice will motivate our study of necessary and sufficient conditions on the activation function to permit sound over-approximation.
4 Abstract Neural Networks

In this section, we formalize the syntax and semantics of Abstract Neural Networks (ANNs). We also present two types of ANNs: Interval Neural Networks (INNs) and Octagon Neural Networks (ONNs).

An ANN is like a DNN except the weights in each layer are represented by an abstract value in some abstract domain. This is formalized below.

**Definition 5.** An $n \times m$ weight set abstract domain is a lattice $\mathcal{A}$ with Galois connection $(\alpha, \gamma)$ with the powerset lattice $\mathcal{P}(\mathbb{R}^{n\times m})$ of $n \times m$ matrices.

**Definition 6.** An ANN layer from $n$ to $m$ dimensions is a triple $(\mathcal{A}, \mathcal{A}, \sigma)$ where $\mathcal{A}$ is a member of the weight set abstraction $\mathcal{A}$ and $\sigma : \mathbb{R} \rightarrow \mathbb{R}$ is an arbitrarily-chosen activation function.

Thus, we see that each ANN layer $(\mathcal{A}, \mathcal{A}, \sigma)$ is associated with a set of weights $\gamma(\mathcal{A})$. Finally, we can define the notion of an ANN:

**Definition 7.** An Abstract Neural Network (ANN) with layer sizes $s_0, s_1, \ldots, s_n$ is a collection of $n$ ANN layers $(\mathcal{A}(i), \mathcal{A}(i), \sigma(i))$, where the $i$th layer is from $s_{i-1}$ to $s_i$ dimensions.

We consider the output of the ANN to be the set of outputs of all instantiations of the ANN into a DNN, as illustrated in Figure 2.

**Definition 8.** We say a DNN with layers $(\mathcal{W}(i), \sigma(i))$ is an instantiation of an ANN $T$ with layers $(\mathcal{A}(i), \mathcal{A}(i), \sigma(i))$ if each $\mathcal{W}(i) \in \gamma(T)(\mathcal{A}(i))$. The set of all DNNs that are instantiations of an ANN $T$ is given by $\gamma(T)$.

The semantics of an ANN naturally lift those of the DNN instantiations.

**Definition 9.** For an ANN $T$ from $s_0$ to $s_n$ dimensions, the function corresponding to $T$ is the set-valued function $T : \mathbb{R}^{s_0} \rightarrow \mathcal{P}(\mathbb{R}^{s_n})$ defined by $T(v) := \{g(v) \mid g \in \gamma(T)\}$.

Space constraints prevent us from defining a full Galois connection here, however one can be established between the lattice of ANNs of a certain architecture and the powerset of DNNs of the same architecture.

The definition of an ANN above is agnostic to the actual abstract domain(s) used. For expository purposes, we now define two particular types of ANNs: Interval Neural Networks (INNs) and Octagon Neural Networks (ONNs).

**Definition 10.** An Interval Neural Network (INN) is an ANN with layers $(\mathcal{A}(i), \mathcal{A}(i), \sigma(i))$, where each $\mathcal{A}(i)$ is an interval hull domain. The interval hull domain represents sets of matrices by their component-wise interval hull.

Notably, the definition of INN in Prabhakar et al. [30] is equivalent to the above, except that they further assume every activation function $\sigma(i)$ is the ReLU function.
An \( \mathbf{A}^{(1)} \), \( \mathbf{A}^{(2)} \), \( \mathbf{A}^{(3)} \) \( \sigma^{(1)} \), \( \sigma^{(2)} \), \( \sigma^{(3)} \) \( \mathbf{H}^{(1,1)} \), \( \mathbf{H}^{(1,2)} \), \( \mathbf{H}^{(1,3)} \), \( \mathbf{H}^{(2,1)} \), \( \mathbf{H}^{(2,2)} \), \( \mathbf{H}^{(2,3)} \), \( \mathbf{H}^{(j,1)} \), \( \mathbf{H}^{(j,2)} \), \( \mathbf{H}^{(j,3)} \) \( \mathbf{w}^{(1,1)} \), \( \mathbf{w}^{(1,2)} \), \( \mathbf{w}^{(1,3)} \), \( \mathbf{v}^{(1,1)} \), \( \mathbf{v}^{(1,2)} \), \( \mathbf{v}^{(1,3)} \), \( \mathbf{v}^{(2,1)} \), \( \mathbf{v}^{(2,2)} \), \( \mathbf{v}^{(2,3)} \), \( \mathbf{v}^{(j,1)} \), \( \mathbf{v}^{(j,2)} \), \( \mathbf{v}^{(j,3)} \)

**Example 2.** We first demonstrate the interval hull domain: \( \gamma_{\text{int}} \left( \left[ \begin{array}{cc} [-1,1] & [0,2] \\ [-3,-2] & [1,2] \end{array} \right] \right) = \left\{ \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} \middle| a \in [-1,1], b \in [0,2], c \in [-3,-2], d \in [1,2] \right\} \). We can thus define a two-layer INN \( f(\mathbf{v}) := [0,1] [0,1] \text{ReLU} \left( \left[ \begin{array}{cc} [-1,1] & [0,2] \\ [-3,-2] & [1,2] \end{array} \right] \mathbf{v} \right) \). We can instantiate this network in a variety of ways, for example \( g(\mathbf{v}) := [0.5,1] \text{ReLU} \left( \left[ \begin{array}{cc} 0 & 2 \\ -2.5 & 1.5 \end{array} \right] \mathbf{v} \right) \in \gamma(f) \). Taking arbitrarily \((1,1)^T\) as an example input, we have \( g((1,1)^T) = [1] \in f((1,1)^T) \). In fact, \( f((1,1)^T) \) is the set of all values that can be achieved by such instantiations, which in this case is the set given by \( f((1,1)^T) = [0,3] \).

**Definition 11.** An Octagon Neural Network (ONN) is an ANN with layers \( (\mathbf{A}^{(1)}, \mathbf{A}^{(2)}, \sigma^{(1)}) \), where each \( \mathbf{A}^{(i)} \) is an octagon hull domain \( \mathbb{R}^{n \times m} \). The octagon hull domain represents sets of matrices by octagons in the space of their components.

**Example 3.** Octagons representing a set of \( n \times m \) matrices can be thought of exactly like an octagon in the vector space \( \mathbb{R}^{n \times m} \). Unfortunately, this is particularly difficult to visualize in higher dimensions, hence in this example we will stick to the case where \( nm = 2 \).

Let \( O_1, O_2 \) be octagons such that

\[
\gamma_{\text{oct}}(O_1) = \left\{ \begin{bmatrix} a \\ b \end{bmatrix} \middle| a - b \leq 1, -a + b \leq 1, a + b \leq 2, -a - b \leq 2 \right\}
\]

\[
\gamma_{\text{oct}}(O_2) = \left\{ \begin{bmatrix} a \\ b \end{bmatrix} \middle| a - b \leq 2, -a + b \leq 3, a + b \leq 4, -a - b \leq 5 \right\}
\]
We can thus define a two-layer ONN \( f(v) := O_2 \text{ReLU} (O_1 v) \). One instantiation of this ONN \( f \) is the DNN \( g(v) := [3 \ 1] \text{ReLU} \left( \begin{bmatrix} 0.5 \\ 1.5 \end{bmatrix} v \right) \in \gamma(f) \). We can confirm that \( g(1) = [3] \in f(1) \).

We can similarly define Polyhedra Neural Networks (PNNs) using the polyhedra domain \( \mathbb{R}^{\mathbb{P}} \).

5 Layer-Wise Abstraction Algorithm

Given a large DNN, how might we construct a smaller ANN which soundly over-approximates that DNN? We define over-approximation formally below.

**Definition 12.** An ANN \( T \) over-approximates a DNN \( N \) if, for every \( v \in \mathbb{R}^n \), \( N(v) \in T(v) \).

**Remark 1.** By Definition 12 then, \( T \) over-approximates \( N \) if, for every \( v \) we can find some instantiation \( T_v \in \gamma(T) \) such that \( T_v(v) = N(v) \).

Algorithm 3 constructs a small ANN that, under certain assumptions discussed in Section 2, soundly over-approximates the large DNN given. The basic idea is to merge groups of dimensions together, forming an ANN where each dimension in the ANN represents a collection of dimensions in the original DNN. We formalize the notion of “groups of dimensions” as a layer-wise partitioning.

**Definition 13.** Given a DNN with layer sizes \( s_0, s_1, \ldots, s_n \), a layer-wise partitioning \( P \) of the network is a set of partitionings \( P(0), P(1), \ldots, P(n) \) where each \( P(i) \) partitions \( \{1, 2, \ldots, s_i\} \). For ease of notation, we will write partitionings with set notation but assume they have some intrinsic ordering for indexing.

**Remark 2.** To maintain the same number of input and output dimensions in our ANN and DNN, we assume \( P(0) = \{\{1\}, \{2\}, \ldots, \{s_0\}\} \) and \( P(n) = \{\{1\}, \{2\}, \ldots, \{s_n\}\} \).

**Example 4.** Consider the DNN corresponding to the function

\[
 f(x_1) = \begin{bmatrix} 1 \\ 1/0 \\ 0 \end{bmatrix} \text{ReLU} \left( \begin{bmatrix} -1/0 \\ 1 \end{bmatrix} x_1 \right).
\]

The layer sizes are \( s_0 = 1, s_1 = 2, s_2 = 3 \).

Hence, one valid layer-wise partitioning is to merge the two inner dimensions: \( P(0) = \{\{1\}\} \), \( P(1) = \{\{1, 2\}\} \), \( P(2) = \{\{1\}, \{2\}, \{3\}\} \). Here we have, e.g., \( P_1(0) = \{1\} \), \( P_1(1) = \{1, 2\} \), and \( P_3(2) = \{3\} \).

Our layer-wise abstraction algorithm is shown in Algorithm 3. For each layer in the DNN, we will call Algorithm 1 to abstract the set of mergings of the layer’s weight matrix. This abstract element becomes the abstract weight \( A(i) \) for the corresponding layer in the constructed ANN.

The functions PCMs and ScaleCols are defined more precisely below.

**Definition 14.** Let \( P \) be some partition, i.e., non-empty subset, of \( \{1, 2, \ldots, n\} \). Then a vector \( c \in \mathbb{R}^n \) is a partition combination vector (PCV) if (i) each component \( c_i \) is non-negative, (ii) the components of \( c \) sum to one, and (iii) \( c_i = 0 \) whenever \( i \notin P \).
Algorithm 1: $\hat{\alpha}(M, P^{in}, P^{out}, A)$

| Input: | Matrix $M$. Partitionings $P^{in}$, $P^{out}$ with $|P^{in}| = k$. Abstract domain $A$. |
| Output: | Abstract element representing all merges of $M$. |
| 1 | $S \leftarrow \{\}$ |
| 2 | $w \leftarrow (|P_1^{in}|, |P_2^{in}|, \ldots, |P_k^{in}|)$ |
| 3 | for $C \in \text{PCMs}(P^{in})$ do |
| 4 | for $D \in \text{PCMs}(P^{out})$ do |
| 5 | $S \leftarrow S \cup \{\text{ScaleCols}(D^TMC, w)\}$ |
| 6 | return $\alpha_A(S)$ |

Algorithm 2: $\hat{\alpha}_{bin}(M, P^{in}, P^{out}, A)$

| Input: | Matrix $M$. Partitionings $P^{in}$, $P^{out}$ with $|P^{in}| = k$. Abstract domain $A$. |
| Output: | Abstract element representing all binary merges of $M$. |
| 1 | $S \leftarrow \{\}$ |
| 2 | $w \leftarrow (|P_1^{in}|, |P_2^{in}|, \ldots, |P_k^{in}|)$ |
| 3 | for $C \in \text{BinPCMs}(P^{in})$ do |
| 4 | for $D \in \text{BinPCMs}(P^{out})$ do |
| 5 | $S \leftarrow S \cup \{\text{ScaleCols}(D^TMC, w)\}$ |
| 6 | return $\alpha_A(S)$ |

Algorithm 3: AbstractLayerWise($\mathfrak{A}, \Sigma)(N, P, A$)

| Input: | DNN $N$ consisting of $n$ layers $(W^{(i)}, \sigma^{(i)})$ with each $\sigma^{(i)} \in \Sigma$. Layer-wise partitioning $P$ of $N$. List of $n$ abstract weight domains $A^{(i)} \in \mathfrak{A}$. |
| Output: | An ANN with layers $(A^{(i)}, A^{(i)}, \sigma^{(i)})$ where $A^{(i)} \in A^{(i)} \in \mathfrak{A}$. |
| 1 | $A \leftarrow [\_ ]$ |
| 2 | for $i \in \{1, 2, \ldots, n\}$ do |
| 3 | $A^{(i)} \leftarrow \hat{\alpha}(W^{(i)}, P^{(i-1)}, P^{(i)}, A^{(i)})$ |
| 4 | $A$.append($\langle A^{(i)}, A^{(i)}, \sigma^{(i)} \rangle$) |
| 5 | return $A$ |

Definition 15. Given a partitioning $P$ of $\{1, 2, \ldots, n\}$ with $|P| = k$, a partitioning combination matrix (PCM) is a matrix $C = [c_1 c_2 \cdots c_k]$, where each $c_i$ is a PCV of partition $P_i$. We refer to the set of all such PCMs for a partitioning $P$ by PCMs($P$).

Definition 16. A PCM is binary if each entry is either 0 or 1. We refer to the set of all binary PCMs for a partitioning $P$ as BinPCMs($P$).

Definition 17. For an $n \times m$ matrix $M$, PCM $C$ of partitioning $P^{in}$ of $\{1, 2, \ldots, m\}$, and PCM $D$ for partitioning $P^{out}$ of $\{1, 2, \ldots, n\}$, we call $D^TMC$ a merging of $M$.

The $j$th column in $MC$ is a convex combination of the columns of $M$ that belong to partition $P_j^{in}$, weighted by the $j$th column of $C$. Similarly, the $i$th row in $D^T M$ is a convex combination of the rows in $M$ that belong to partition $P_i^{out}$. In total, the $i, j$th entry of merged matrix $D^TMC$ is a convex combination of the entries of $M$ with indices in $P_i^{out} \times P_j^{in}$. This observation will lead to Theorem 11 in Section 5.1.
Definition 18. Given a matrix $M$, the column-scaled matrix formed by weights $w_1, w_2, \ldots, w_k$ is the matrix with entries given component-wise by $\text{ScaleCols}(M, (w_1, \ldots, w_k))_{i,j} := M_{i,j}w_j$.

Intuitively, column-scaling is needed because what were originally $n$ dimensions contributing to an input have been collapsed into a single representative dimension. This is demonstrated nicely for the specific case of Interval Neural Network and ReLU activations by Figures 3 and 4 in Prabhakar et al. [30].

Example 5. Given the matrix $M = \begin{bmatrix} m_{1,1} & m_{1,2} & m_{1,3} \\ m_{2,1} & m_{2,2} & m_{2,3} \\ m_{3,1} & m_{3,2} & m_{3,3} \\ m_{4,1} & m_{4,2} & m_{4,3} \end{bmatrix}$, partitioning $\mathbb{P}^{(0)} = \{ \{1,3\}, \{2\} \}$ of the input dimensions and $\mathbb{P}^{(1)} = \{ \{2,4\}, \{1,3\} \}$ of the output dimensions, we can define a PCM for $\mathbb{P}^{(0)}$ as $C := \begin{bmatrix} 0.25 & 0 \\ 0 & 0.75 \end{bmatrix}$ and a PCM for $\mathbb{P}^{(1)}$ as: $D := \begin{bmatrix} 0 & 0.99 \\ 0.4 & 0 \\ 0 & 0.01 \\ 0.6 & 0 \end{bmatrix}$.

We can then compute the column-merged matrix $MC = \begin{bmatrix} 0.25m_{1,1} + 0.75m_{1,3} & m_{1,3} \\ m_{2,1} & m_{2,3} \\ 0.25m_{3,1} + 0.75m_{3,3} & m_{3,3} \\ 0.25m_{4,1} + 0.75m_{4,3} & m_{4,3} \end{bmatrix}$, and furthermore the column-row-merged matrix $D^TMC = \begin{bmatrix} 0.4(0.25m_{2,1} + 0.75m_{2,3}) + 0.6(0.25m_{4,1} + 0.75m_{4,3}) & 0.4m_{2,2} + 0.6m_{4,2} \\ 0.99m_{2,1} + 0.75m_{2,3} & 0.25m_{3,1} + 0.75m_{3,3} \end{bmatrix}$.

Finally, we can column-scale this matrix like so:

$$\text{ScaleCols}(D^TMC, (2, 2)) = \begin{bmatrix} 0.8(0.25m_{2,1} + 0.75m_{2,3}) + 1.2(0.25m_{4,1} + 0.75m_{4,3}) & 0.8m_{2,2} + 1.2m_{4,2} \\ 1.98(0.25m_{1,1} + 0.75m_{1,3}) + 0.02(0.25m_{3,1} + 0.75m_{3,3}) & 1.98m_{1,2} + 0.02m_{3,2} \end{bmatrix}.$$
of $W^{(i)}$, such that $(D \otimes C)R = D^T W^{(i)} C$. From this intuition, it follows that the converse to Theorem \[\text{II}\] does not hold, as every matrix $E$ cannot be decomposed into vectors $D \otimes C$ as described (i.e., not every matrix has rank 1). Hence, the convexity condition may be slightly weakened. However, we are not presently aware of any abstract domains that satisfy such a condition but not convexity.

**Example 6.** Let $W^{(i)} = \begin{bmatrix} 1 & -2 & 3 \\ 4 & -5 & 6 \\ 7 & -8 & 9 \end{bmatrix}$ and consider $\mathbb{P}^{(i-1)} = \{\{1, 2\}, \{3\}\}$ and $\mathbb{P}^{(i)} = \{\{1, 3\}, \{2\}\}$. Then we have the binary PCMs $\text{BinPCMs}(\mathbb{P}^{(i-1)}) = \left\{ \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 \\ 1 & 1 \end{bmatrix} \right\}$ and $\text{BinPCMs}(\mathbb{P}^{(i)}) = \left\{ \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 \\ 1 & 1 \end{bmatrix} \right\}$. These correspond to the column-scaled binary mergings $\left\{ \begin{bmatrix} 2 & 3 \\ 8 & 6 \end{bmatrix}, \begin{bmatrix} -4 & 3 \\ -10 & 6 \end{bmatrix}, \begin{bmatrix} 14 & 9 \\ 8 & 6 \end{bmatrix}, \begin{bmatrix} -16 & 9 \\ -10 & 6 \end{bmatrix} \right\}$.

We can take any PCMs such as $C = \begin{bmatrix} 0.75 & 0 \\ 0.25 & 0 \\ 0 & 1 \end{bmatrix}$ for $\mathbb{P}^{(i-1)}$ as well as $D = \begin{bmatrix} 0.5 & 0 \\ 0 & 1 \\ 0.5 & 0 \end{bmatrix}$ for $\mathbb{P}^{(i)}$, resulting in the scaled merging $\text{ScaleCols}(D^T W^{(i)} C, (2, 1)) = \begin{bmatrix} 3.5 & 6 \\ 3.5 & 6 \end{bmatrix}$. According to Theorem \[\text{II}\] we can write this as a convex combination of the four column-scaled binary merged matrices. In particular, we find the combination

\[
\begin{bmatrix} 3.5 & 6 \\ 3.5 & 6 \end{bmatrix} = (1.5/2)(1)(0.5)(1) \begin{bmatrix} 2 & 3 \\ 8 & 6 \end{bmatrix} + (0.5/2)(1)(0.5)(1) \begin{bmatrix} -4 & 3 \\ -10 & 6 \end{matrix} + (1.5/2)(1)(0.5)(1) \begin{bmatrix} 14 & 9 \\ 8 & 6 \end{bmatrix} + (0.5/2)(1)(0.5)(1) \begin{bmatrix} -16 & 9 \\ -10 & 6 \end{bmatrix}.
\]

We can confirm that this is a convex combination, as

\[
(1.5/2)(1)(0.5)(1)+(0.5/2)(1)(0.5)(1)+(1.5/2)(1)(0.5)(1)+(0.5/2)(1)(0.5)(1) = 1.
\]

Because we can find such a convex combination for any such non-binary merging in terms of the binary ones, and because the abstract domain is assumed to be convex, including only the binary mergings will ensure that all mergings are represented by the abstract element $A^{(i)}$.

### 5.2 Walkthrough Example

**Example 7.** Consider again the DNN from Example 4 corresponding to $f(x_1) = \begin{bmatrix} 1 & 1 \\ 1 & 0 \\ 0 & 1 \end{bmatrix} \sigma \left( \begin{bmatrix} 1 \\ -1 \end{bmatrix} x_1 \right)$, the partitioning $\mathbb{P}^{(0)} = \{\{1\}\}$, $\mathbb{P}^{(1)} = \{\{1, 2\}\}$, $\mathbb{P}^{(2)} = \{\{1\}, \{2\}, \{3\}\}$, which collapses the two hidden dimensions, and assume the abstract domains $A^{(i)}$ are all convex.

For the input layer, we have $w = (1)$, because the only partition in $\mathbb{P}^{(0)}$ has size 1. Similarly, the only binary PCM for $\mathbb{P}^{(0)}$ is $C = [1]$. However, there are two binary PCMs for $\mathbb{P}^{(1)}$, namely $D = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ or $D = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$. These correspond to the binary merged matrices $[1]$ and $[-1]$. Hence, we get $A^{(1)} = \alpha_{A^{(1)}}(\{[1], [-1]\})$, completing the first layer.
For the output layer, we have \( w = (2) \), because the only partition in \( P^{(1)} \) contains two nodes. Hence, the column scaling will need to play a role: because we have merged two dimensions in the domain, we should interpret any value from that dimension as being from both of the dimensions that were merged. We have two binary mergings, namely \([1 \ 1] \) and \([1 \ 0] \) and \([0 \ 1] \). This, after rescaling gives us \( A^{(2)} = \alpha_{A^{(2)}} \left( \left\{ \begin{bmatrix} 2 \\ 0 \\ 2 \\ 0 \\ 2 \end{bmatrix} \right\} \right) \).

In total then, the returned ANN can be written \( (A^{(1)}, \sigma), (A^{(2)}, x \mapsto x) \) or in a more functional notation as \( g(x) = A^{(2)} \sigma(A^{(1)} x) \), where in either case \( A^{(1)} = \alpha_{A^{(1)}} (\left\{ \begin{bmatrix} 1 \\ -1 \end{bmatrix} \right\}) \), and \( A^{(2)} = \alpha_{A^{(2)}} \left( \left\{ \begin{bmatrix} 2 \\ 0 \\ 2 \\ 0 \\ 2 \end{bmatrix} \right\} \right) \).

Note in particular that, while the operation of the algorithm was agnostic to the exact abstract domains \( \mathfrak{A} \) and activation functions \( \Sigma \) used, the semantics of the resulting ANN depend entirely on these. Hence, correctness of the algorithm will depend on the abstract domain and activation functions satisfying certain conditions. We will discuss this further in Section 6.

### 6 Layer-Wise Abstraction: Instantiations and Examples

This section examines a number of examples. For some DNNs, Algorithm 3 will produce a soundly over-approximating ANN. For others, the ANN will provably not over-approximate the given DNN. We will generalize these examples to necessary and sufficient conditions on the activation functions \( \Sigma \) used in order for \( \text{AbstractLayerWise}(\mathfrak{A}, \Sigma)(N, \mathbb{P}, \mathcal{A}) \) to soundly over-approximate \( N \).

#### 6.1 Interval Hull Domain with ReLU Activation Functions

Consider again the DNN from Example 7 given by \( f(x_1) = \begin{bmatrix} 1 \\ 1 \\ 0 \\ 0 \\ 1 \end{bmatrix} \) ReLU \( \left( \begin{bmatrix} 1 \\ -1 \end{bmatrix} [x_1] \right) \) and partitioning which merges the two intermediate dimensions. Using the interval hull domain in Example 7 gives the corresponding INN: \( g(x_1) = \begin{bmatrix} 2 \\ 2 \\ 0 \\ 2 \end{bmatrix} \) ReLU \( \left( \begin{bmatrix} -1 \right. \begin{bmatrix} 1 \\ -1 \end{bmatrix} \right) [x_1] \).

In fact, because the ReLU activation function and interval domain was used, it follows from the results of Prabhakar et al. that \( g \) in fact over-approximates \( f \). To see this, consider two cases. If \( x_1 > 0 \), then the second component in the hidden dimension of \( f \) will always become 0 under the activation function. Hence, \( f(x_1) = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \) ReLU \( (1 \ [x_1]) \) = \( \begin{bmatrix} 2 \\ 0 \end{bmatrix} \) ReLU \( (0.5 \ [x_1]) \), which is a valid instantiation of the weights in \( g \). Otherwise, if \( x_1 \leq 0 \), we find \( f(x_1) = \begin{bmatrix} 2 \\ 0 \end{bmatrix} \) ReLU \( (-0.5 \ [x_1]) \), which is again a valid instantiation. Hence in all cases, the true output \( f(x_1) \) can be made by some valid instantiation of the weights in \( g \). Therefore, \( f(x_1) \in g(x_1) \) for all \( x_1 \) and so \( g \) over-approximates \( f \).
Abstract Neural Networks

Sufficiency Condition The soundness of this particular instantiation can be generalized to a sufficiency theorem, Theorem 2, for soundness of the layer-wise abstraction algorithm. Its statement relies on the activation function satisfying the weakened intermediate value property, which is defined below:

Definition 20. A function \( f : \mathbb{R} \rightarrow \mathbb{R} \) satisfies the Weakened Intermediate Value Property (WIVP) if, for every \( a_1 \leq a_2 \leq \cdots \leq a_n \in \mathbb{R} \), there exists some \( b \in [a_1, a_n] \) such that \( f(b) = \sum_{i} f(a_i) \).

Every continuous function satisfies the IVP and hence the WIVP. Almost all commonly-used activation functions, except for thresh, are continuous and, therefore, satisfy the WIVP. However, the WIVP is not equivalent to the IVP, as the below proof shows by constructing a function \( f \) such that \( f((a, b)) = \mathbb{Q} \) for any non-empty open interval \((a, b)\).

Proof. Please see Appendix B for the proof of this theorem. \qed

We now state the soundness theorem below, which is proved in Section 7.

Theorem 2. Let \( \mathfrak{A} \) be a set of weight set abstract domains and \( \Sigma \) a set of activation functions. Suppose (i) each \( \sigma \in \Sigma \) has entirely non-negative outputs, and (ii) each \( \sigma \in \Sigma \) satisfies the Weakened Intermediate Value Property (Definition 20). Then \( T = \text{AbstractLayerWise}(\mathfrak{A}, \Sigma)(N, P, A) \) (Algorithm 3) soundly over-approximates the DNN \( N \).

6.2 Interval Hull Domain with Leaky ReLUs

Something different happens if we slightly modify \( f \) in Example 7 to use an activation function producing negative values in the intermediate dimensions. This is quite common of activation functions like Leaky ReLU and tanh, and was not mentioned by Prabhakar et al. \[30\]. For example, we will take the Leaky ReLU function (Definition 4) with \( c = 0.5 \) and consider the DNN \( f(x_1) = \begin{bmatrix} 1 & 1 \\ 1 & 0 \\ 0 & 1 \end{bmatrix} \text{LReLU} \left( \begin{bmatrix} 1 \\ -1 \end{bmatrix} [x_1]; 0.5 \right) \). Using the same partitioning gives us the INN \( g(x_1) = \begin{bmatrix} 2 \\ 0 \end{bmatrix} \text{LReLU} \left( \begin{bmatrix} -1 \\ 1 \end{bmatrix} [x_1]; 0.5 \right) \).

Surprisingly, this small change to the activation function in fact makes the constructed ANN no longer over-approximate the original DNN. For example, note that \( f(1) = \begin{bmatrix} 0.5 \\ 1 \end{bmatrix} \) and consider \( g(1) \). In \( g \), the output of the LReLU is one-dimensional, hence, it will have either positive, negative, or zero sign. But no matter how the weights in the final matrix are instantiated, every component of \( g(1) \) will have the same (or zero) sign, and so \( f(1) \notin g(1) \), because \( f(1) \) has mixed signs.
**Necessary Condition: Non-Negative Values** We can generalize this counterexample to the following necessary condition on soundness:

**Theorem 3.** Suppose some $\sigma \in \Sigma$ is an activation function with neither entirely non-negative nor entirely non-positive outputs, and every $A \in \mathbf{A}$ is at least as precise as the interval hull abstraction. Then there exists a neural network $N$ that uses $\sigma$ and a partitioning $P$ such that $T = \text{AbstractLayerWise}(\mathbf{A}, \Sigma)(N, P, A)$ does not over-approximate $N$.

*Proof.* Please see Appendix C for the proof of this theorem.

**Handling Negative Values** Thankfully, there is a workaround to support sometimes-negative activation functions. The constructive theorem below implies that a given DNN can be modified into a *shifted* version of itself such that the input-output behavior on any arbitrary bounded region is retained, but the intermediate activations are all non-negative.

**Theorem 4.** Let $N$ be a DNN and suppose that, on some input region $R$, the output of the activation functions are lower-bounded by a constant $C$. Then, there exists another DNN $N'$, with at most one extra dimension per layer, which satisfies (i) $N'(x) = N(x)$ for any $x \in R$, (ii) $N'$ has all non-negative activation functions, and (iii) the new activation functions $\sigma'$ are of the form $\sigma'(x) = \max(\sigma(x) + |C|, 0)$.

Notably, the proof of this theorem is constructive with a straightforward construction. The one requirement is that a lower-bound $C$ be provided for the output of the nodes in the network. This lower-bound need not be tight, and can be computed quickly using the same procedure discussed for upper bounds immediately following Equation 1 in Prabhakar et al. [30]. For tanh in particular, its output is always lower-bounded by $-1$ so we can immediately take $C = -1$ for a network using only tanh activations.

*Proof.* Please see Appendix D for the proof of this theorem.

### 6.3 Interval Hull Abstraction with Non-Continuous Functions

Another way that the constructed ANN may not over-approximate the DNN is if the activation function does not satisfy the Weakened Intermediate Value Property (WIVP) (Definition 20). For example, consider the threshold activation function (Definition 1) with parameters $t = 1$, $v = 0$ and the same overall network, i.e. $f(x_1) = \begin{bmatrix} 1 \\ 1 \\ 0 \\ 0 \\ 1 \end{bmatrix} \text{thresh} \left( \begin{bmatrix} -1 \\ 1 \\ |x_1| \\ 1, 0 \right)$ and the same partitioning. We get the INN $g(x_1) = \begin{bmatrix} 0.2 \\ 0.2 \end{bmatrix} \text{thresh} \left( [0, 1] |x_1|; 1, 0 \right)$. We have $f(1) = \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}^T$, however, in $g(1)$, no matter how we instantiate the $[-1, 1]$ weight, the output of the thresh unit will either be 0 or 1. But then the output of the first output component must be either 0 or 2, neither of which is 1, and so $g$ does not over-approximate $f$. 


Necessary Condition: WIVP  We can generalize this example to the following necessary condition:

**Theorem 5.** Suppose some $\sigma \in \Sigma$ is an activation function which does not satisfy the WIVP, and every $A \in \mathfrak{A}$ is at least as precise as the interval hull abstraction. Then there exists a neural network $N$ using only the identity and $\sigma$ activation functions and partitioning $P$ such that $T = \text{AbstractLayerWise}(\mathfrak{A}, \Sigma)(N, P, A)$ does not over-approximate $N$.

*Proof.* Please see Appendix E for the proof of this theorem.

While this is of some theoretical curiosity, in practice almost all commonly-used activation functions do satisfy the WIVP. Nevertheless, if one does wish to use such a function, one way to soundly over-approximate it with an ANN is to replace the scalar activation function with a set-valued one. The ANN semantics can be extended to allow picking any output value from the activation function in addition to any weight from the weight set.

For example, consider again the $\text{thresh}(x; 1, 0)$ activation function. It can be completed to a set-valued activation function which satisfies the WIVP such as

$$\text{thresh}'(x; 1, 0) := \begin{cases} \{x\} & \text{if } x > 1 \\ \{a \mid a \in [0, 1]\} & \text{if } x = 1 \\ \{0\} & \text{otherwise} \end{cases}.$$  

The idea is that we “fill the gap” in the graph. Whereas in the original threshold function we had an issue because there was no $x \in [0, 1]$ which satisfied $\text{thresh}(x; 1, 0) = \frac{f(0) + f(1)}{2} = \frac{1}{2}$, on the set-valued function we can take $x = 1 \in [0, 1]$ to find $\frac{1}{2} \in \text{thresh}'(1; 1, 0)$.

### 6.4 Powerset Abstraction, ReLU, and $\alpha_{\text{bin}}$

Recall that $\alpha$ (Algorithm 11) requires abstracting the, usually-infinite, set of all merged matrices $D^T W^{(i)} C$. However, in Section 5.1 we showed that for convex abstract domains it suffices to only consider the finitely-many binary mergings. The reader may wonder if there are abstract domains for which it is not sufficient to consider only the binary PCMs. This section presents such an example.

Suppose we use the same ReLU DNN $f$ as in Section 6.1 for which we noted before the corresponding INN over-approximates it. However, suppose instead of intervals we used the powerset abstract domain, i.e., $\alpha(S) = S$ and $A \sqcup B = A \cup B$. If we (incorrectly) used $\alpha_{\text{bin}}$ instead of $\alpha$, we would get the powerset ANN $g(x_1) = \left\{ \left[ \begin{array}{c} 2 \\ 0 \\ 2 \end{array} \right], \left[ \begin{array}{c} 2 \\ 0 \\ 2 \end{array} \right] \right\} \text{ReLU} \left( \left\{ \left[ \begin{array}{c} 1 \\ -1 \end{array} \right] \right\} \left[ x_1 \right] \right)$. Recall that $f(1) = [1 \ 1 \ 0]^T$.

However, with $g(1)$, the first output will always be either 0 or 2, so $g$ does not over-approximate $f$. The basic issue is that to get the correct output, we need to instantiate the inner weight to 0.5, which is in the convex hull of the original weights, but is not either one of the original weights itself.

Note that, in this particular example, it is possible to find an ANN that over-approximates the DNN using only finite sets for the abstract weights. However, this is only because ReLU is piecewise-linear, and the size of the sets needed
will grow exponentially with the number of dimensions. For other activation functions, e.g., tanh infinite sets are required in general.

In general, non-convex abstract domains will need to use some other method of computing an over-approximation of $\hat{u}$. One general-purpose option is to use techniques such as those developed for symbolic abstraction [32] to iteratively compute an over-approximation of the true $A^{(i)}$ and use that instead.

7 Proof of Sufficient Conditions

We now prove Theorem 2 which provides sufficient conditions on the activation functions for which Algorithm 3 produces an ANN that soundly over-approximates the given DNN.

The structure of the proof is illustrated in Figure 3 To show that ANN $T$ over-approximates DNN $N$, we must show that $N(v) \in T(v)$ for every $v$. This occurs, by definition, only if there exists some instantiation $T_v \in \gamma(T)$ of $T$ for which $N(v) = T_v(v)$. Recall that an instantiation of an ANN is a DNN formed by replacing each abstract weight $A^{(i)}$ with a concrete weight matrix $H^{(i)} \in \gamma(A^{(i)})$.

In particular, our proof will proceed layer-by-layer. On an input $v = v^{(0)}$, the $i$th layer of DNN $N$ maps $v^{(i-1)}$ to $v^{(i)}$ until the output $v^{(n)}$ is computed. We will prove that, for each abstract layer $(A^{(i)}, \sigma^{(i)}, A^{(i)})$, there is a matrix $H^{(i)} = \nabla(A^{(i)}, v^{(i-1)}) \in \gamma(A^{(i)})$ for which the instantiated layer $(H^{(i)}, \sigma^{(i)})$, roughly speaking, also maps $v^{(i-1)}$ to $v^{(i)}$. However, by design the abstract layer will have fewer dimensions, hence the higher-dimensional $v^{(i-1)}$ and $v^{(i)}$ may not belong to its domain and range (respectively). We resolve this by associating with each vector $v^{(i)}$ in the intermediate spaces of $N$ a mean representative vector $v^{(i)}_{/P^{(i)}}$ in the intermediate spaces of $T_v$. Then we can rigorously prove that the instantiated layer $(H^{(i)}, \sigma^{(i)})$ maps $v^{(i-1)}_{/P^{(i-1)}}$ to $v^{(i)}_{/P^{(i)}}$. Applying this fact inductively gives us $T_v(v^{(0)}) = (N(v))_{/P^{(n)}}$. Because $P^{(0)}$ and $P^{(n)}$ are the singleton partitionings, this gives us exactly the desired relationship $T_v(v) = N(v)$.

7.1 Vector Representatives

Our proof relies heavily on the concept of representatives.

Definition 21. Given a vector $v = (v_1, v_2, \ldots, v_n)$ and a partitioning $P$ of $\{1, 2, \ldots, n\}$ with $|P| = k$, we define the convex representative set of $v$ under $P$ to be

$$R(v, P) = \{(z_1, z_2, \ldots, z_k) \mid \forall j, \min_{v_j \in P_j} v_j \leq z_j \leq \max_{v_j \in P_j} v_j\}.$$  

$R(v, P)$ is referred to as $AV(v)$ in Prabhakar et al. [30], and is always a box in $\mathbb{R}^k$.

One representative will be particularly useful, so we give it a specific notation:

Definition 22. Given a vector $(v_1, v_2, \ldots, v_n)$ and a partitioning $P$ of $\{1, 2, \ldots, n\}$ with $|P| = k$, we define the mean representative of $v$ under $P$ to be

$$v_{/P} = \left(\frac{\sum_{j \in P_1} v_j}{|P_1|}, \ldots, \frac{\sum_{j \in P_k} v_j}{|P_k|}\right).$$
satisfies the equality \( H = H_R \cdot \Gamma \), where \( H_R \) represents the ANN such that the instantiation has the same output as the original DNN on \( v(0) \).

Example 8. Consider the vector \( v := (5, 6, 11, 2, 1) \) and the partitioning \( P = \{(1, 3), (2, 4, 5)\} \). Then we have \( |P| = (5 + 11)/2, (6 + 2 + 1)/3 \) = (8, 3) and \( R(v, P) = \{(z_1, z_2) \mid z_1 \in [5, 11], z_2 \in [1, 6]\} \).

7.2 Proof of Soundness Theorem

The operation \( \triangledown \) presented in Algorithm 4 shows how to instantiate an abstract weight matrix such that it has input/output behavior corresponding to that of the original DNN layer. We now prove the correctness of Algorithm 4.

**Lemma 1.** Given any \( w' \in R(Mv, P^{in}) \), a vector \( v \) with non-negative entries, and \( H = \triangledown(M, P^{in}, P^{out}, v, w') \), then \( H \in \Gamma(\hat{a}(M, P^{in}, P^{out})) \) and \( H(v_{/P^{in}}) = w' \).

**Proof.** To prove correctness of Algorithm 4, it suffices to show that (i) \( C \) and \( D \) are PCMs, and (ii) the returned matrix \( H \) satisfies the equality \( H(v_{/P^{in}}) = w' \).

\( C \) is a PCM by construction: The \( \ell \)th column only has non-zero entries for rows that are in the \( \ell \)th partition. The sum of all entries in a column is \( \sum_{j \in P_i^{in}} v_j / (\sum_{k \in P_i^{in}} v_k) = 1 \). All entries are non-negative by assumption on \( v \).

\( D \) is also a PCM: The \( \ell \)th column only has two entries. It suffices to show that \( D_{a,i} \) is in \([0, 1]\), which follows because \( w' \in R(Mv, P^{out}) \) implies \( w'_i \) is in between the minimum \( b \) and maximum \( a \).

By associativity, line 11 is equivalent to returning \( H = D^T ME \) where \( E = \text{ScaleCols}(C, s) \). Thus, to show that \( H(v_{/P^{in}}) = w' \), it suffices to show (i) that \( E(v_{/P^{in}}) = v \), and (ii) that \( D^T M v = w' \).

Note that here \( E_{j,i} = C_{j,i} |P_i^{in}| \). Then to show (i), consider any index \( j \in P_i^{in} \). Then we find that the \( j \)th output component of \( E(v_{/P^{in}}) \) is \( v_j / (\sum_{k \in P_i^{in}} v_k) |P_i^{in}| / (|P_i^{in}|) = v_j \). Hence, the entire output vector is \( v \).

To show (ii), note that each column of \( D \) is exactly the convex combination that produces the output \( w'_i \) from the maximum/minimum indices of \( M v \).
Algorithm 4: $\gamma(M, P^{\text{in}}, P^{\text{out}}, v, w')$

**Input:** An $n \times m$ matrix $M$. Partitionings $P^{\text{in}}, P^{\text{out}}$. A vector $v$ with non-negative entries. A vector $w' \in R(Mv, P^{\text{out}})$.

**Output:** A matrix $H \in \gamma(\hat{\alpha}(M, P^{\text{in}}, P^{\text{out}}))$ such that $H(v/P^{\text{in}}) = w'$.

1. $C, D \leftarrow 0_{|P^{\text{in}}| \times n}, 0_{|P^{\text{out}}| \times m}$
2. for $i = 1, 2, \ldots, |P^{\text{in}}|$ do
   3. for $j \in P^{\text{in}}_i$ do
      4. $C_{j,i} \leftarrow v_j / (\sum_{k \in P^{\text{in}}_i} v_k)$
   5. $w \leftarrow Mv$
6. for $i = 1, 2, \ldots, |P^{\text{out}}|$ do
   7. $a, b \leftarrow \text{argmax}_{p \in P^{\text{out}}_i} w_p, \text{argmin}_{p \in P^{\text{out}}_i} w_p$
   8. $D_{a,i} \leftarrow (w'_i - w_b) / (w_a - w_b)$
   9. $D_{b,i} \leftarrow 1 - D_{a,i}$
10. $s \leftarrow (|P^{\text{in}}_1|, \ldots, |P^{\text{in}}_m|)$
11. return $\text{ScaleCols}(D^TMC, s)$

In total then, the returned matrix is in $\gamma(\hat{\alpha}(M, P^{\text{in}}, P^{\text{out}}))$ and satisfies $H(v/P^{\text{in}}) = w'$.

The next lemma implies that we can always find such a $w' \in R(Mv, P^{\text{in}})$ satisfying the relations in Figure 3.

**Lemma 2.** Let $\sigma$ be an activation function satisfying the WIVP, $w$ any vector, and $P$ a partitioning the dimensions of $w$. Then there exists a vector $w' \in R(w, P)$ such that $\sigma(w') = (\sigma(w))/P$.

**Proof.** Because $\sigma^{(i)}$ is defined to be a component-wise activation function, we can assume WLOG that $P^{(i)}$ has only a single partition, i.e., $P^{(i)} = \{\{1, 2, \ldots, s^{(i)}\}\}$.

In that case, label the components of $w^{(i)}$ such that $w_1^{(i)} \leq w_2^{(i)} \leq \ldots \leq w_n^{(i)}$. Then the statement of the lemma is equivalent to the assertion that there exists some $b \in [w_1^{(i)}, w_n^{(i)}]$ such that $\sigma^{(i)}(b) = (\sum_j w_j^{(i)})/n$. But this is exactly the definition of the WIVP. Hence, by assumption that $\sigma^{(i)}$ satisfies the WIVP, we complete the proof.

We are finally prepared to prove the soundness theorem. It is restated here for clarity.

**Theorem 2.** Let $\mathfrak{A}$ be a set of weight set abstract domains and $\Sigma$ a set of activation functions. Suppose (i) each $\sigma \in \Sigma$ has entirely non-negative outputs, and (ii) each $\sigma \in \Sigma$ satisfies the Weakened Intermediate Value Property (Definition 20). Then $T =\text{AbstractLayerWise}(\mathfrak{A}, \Sigma)(N, P, A)$ (Algorithm 3) soundly over-approximates the DNN $N$. 
Proof. A diagram of the proof is provided in Figure 3. Consider the $i$th layer. By Lemma 2, there exists some vector $\mathbf{w}'(i) \in R(\mathbf{u}(i), \mathcal{P}(i))$ such that $\sigma(i)(\mathbf{w}'(i)) = \mathbf{v}/\mathcal{P}(i)$. Furthermore, by Lemma 1 there exists some $H(i) \in \gamma(A(i))$ such that $H(i)(\mathbf{v}(i-1)/\mathcal{P}(i-1)) = \mathbf{w}'(i)$. Therefore, in total we can instantiate the $i$th abstract layer to $(H(i), \sigma(i))$, which maps $\mathbf{v}(i-1)/\mathcal{P}(i-1)$ to $\mathbf{v}(i)/\mathcal{P}(i)$.

By applying this construction to each layer, we find an instantiation of the ANN that maps $\mathbf{v}(0)/\mathcal{P}(0)$ to $\mathbf{v}(n)/\mathcal{P}(n)$. Assuming $\mathcal{P}(0)$ and $\mathcal{P}(n)$ are the singleton partitionings, then, we have that the instantiation maps $\mathbf{v}(0) = \mathbf{v}$ to $\mathbf{v}(n) = N(\mathbf{v})$, as hoped for. Hence, $N(\mathbf{v}) \in T(\mathbf{v})$ for any such vector $\mathbf{v}$, and so the ANN overapproximates the original DNN.

8 Related Work

The recent results by Prabhakar et al. [30] are the closest to this paper. Prabhakar et al. introduce the notion of Interval Neural Networks and a sound quotienting (abstraction) procedure when the ReLU activation function is used. Prabhakar et al. also proposed a technique for verification of DNNs using ReLU activation functions by analyzing the corresponding INN using a MILP encoding. Prabhakar et al. leaves open the question of determining the appropriate partitioning of the nodes, and their results assume the use of the ReLU activation function and interval domain. We have generalized their results to address the subtleties of other abstract domains and activation functions as highlighted in Section 6.

There exists prior work [2, 28, 8] on models using interval-weighted neural networks. The goal of such approaches is generally to represent uncertainty, instead of improve analysis time of a corresponding DNN. Furthermore, their semantics are defined using interval arithmetic instead of the more-precise semantics we give in Section 4. Nevertheless, we believe that future work may consider applications of our more general ANN formulation and novel abstraction algorithm to the problem of representing uncertainty.

There have been many recent approaches exploring formal verification of DNNs using abstractions. ReLuVal [38] computes interval bounds on the outputs of a DNN for a given input range. Neurify [37] extends ReLuVal by using symbolic interval analysis. Approaches such as DeepPoly [34] and $\mathcal{AI}^2$ [9] perform abstract interpretation of DNNs using more expressive numerical domains such as polyhedra and zonotopes. In contrast, Abstract Neural Networks introduced in this paper use abstract values to represent the weight matrices of a DNN, and are a different way of applying abstraction to DNN analysis.

This paper builds upon extensive literature on numerical abstract domains [5, 24, 12, 23], including libraries such as APRON [16] and PPL [1]. Of particular relevance are techniques for verification of floating-point computation [1, 29, 20].

Techniques for compression of DNNs reduce their size using heuristics [15, 7, 14]. They can degrade accuracy of the network, and do not provide theoretical guarantees. Gokulanathan et al. [12] use the Marabou Verification Engine [19] to
simplify neural networks so that the simplified network is equivalent to the given network. Shriver et al. [33] refactor the given DNN to aid verification, though the refactored DNN is not guaranteed to be an overapproximation.

9 Conclusion and Future Directions

We introduced the notion of an Abstract Neural Network (ANN). The weight matrices in an ANN are represented using numerical abstract domains, such as intervals, octagons, and polyhedra. We presented a framework, parameterized by abstract domain and DNN activation function, that performs layer-wise abstraction to compute an ANN given a DNN. We identified necessary and sufficient conditions on the abstract domain and the activation function that ensure that the computed ANN is a sound over-approximation of the given DNN. Furthermore, we showed how the input DNN can be modified in order to soundly abstract DNNs using rare activation functions that do not satisfy the sufficiency conditions are used. Our framework is applicable to DNNs that use activation functions such as ReLU, Leaky ReLU, and Hyperbolic Tangent. Our framework can use convex abstract domains such as intervals, octagons, and polyhedra. Code implementing our framework can be found at

https://github.com/95616ARG/abstract_neural_networks.

The results in this paper provide a strong theoretical foundation for further research on abstraction of DNNs. One interesting direction worth exploring is the notion of completeness of abstract domains [11] in the context of Abstract Neural Networks. Our framework is restricted to convex abstract domains; the use of non-convex abstract domains, such as modulo intervals [25] or donut domains [10], would require a different abstraction algorithm. Algorithms for computing symbolic abstraction might show promise [31,21,35,36,32].

This paper focused on feed-forward neural networks. Because convolutional neural networks (CNNs) are special cases of feed-forward neural networks, future work can directly extend the theory in this paper to CNN models as well. Such future work would need to consider problems posed by non-componentwise activation functions such as MaxPool, which do not fit nicely into the framework presented here. Furthermore, extensions for recursive neural networks (RNNs) and other more general neural-network architectures seems feasible.

On the practical side of things, it would be worth investigating the impact of abstracting DNNs on the verification times. Prabhakar et al. [30] demonstrated that their abstraction technique improved verification of DNNs. The results in this paper are a significant generalization of the results of Prabhakar et al., which were restricted to interval abstractions and ReLU activation functions. We believe that our approach would similarly help scale up verification of DNNs.

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A Proof of Theorem 1

In Section 5.1 we argued that, when the abstract domain used is convex, $\hat{\alpha}$ and $\hat{\alpha}_{bin}$ produce the same result. Hence the latter (which is computable) can be
used in place of the former when executing Algorithm\footnote{We now prove this fact. To do so, we use the following Lemma, which implies a similar claim for the PCMs:}

**Lemma 3.** Let $\mathcal{P}$ be a partitioning of $\{1, 2, \ldots, n\}$. Then every PCM $C \in \text{PCMs}(\mathcal{P})$ is a convex combination of the binary PCMs $\text{BinPCMs}(\mathcal{P})$.

**Proof.** Let $C \in \text{PCMs}(\mathcal{P})$. It suffices to construct $C$ as a convex combination of the binary PCMs $B_i \in \text{BinPCMs}(\mathcal{P})$.

We first note that the columns in the binary PCMs are independent — given two binary PCMs $B_1$ and $B_2$ the PCM $B_3$ formed by setting the $i$th column of $B_3$ to be either the $i$th column of $B_1$ or that of $B_2$ arbitrarily is always a valid binary PCM. Because of this, we can consider each column separately, i.e., assume that $C$ and the $B_i$s have only a single column.

In that case, the binary PCMs can be thought of as length-$n$ vectors each with all zero entries except for a single 1 entry. Similarly, $C$ must have zeros in the entries where the binary PCMs all have zeros, and the non-zero entries must be positive and sum to one. But this is equivalent to stating that $C$ lies in the convex span of the binary PCMs $B_i$, as claimed.

Then we can prove

**Theorem 1.** If $A$ is convex, then $\hat{\alpha}(M, \mathcal{P}^{\text{in}}, \mathcal{P}^{\text{out}}, A) = \hat{\alpha}_{\text{bin}}(M, \mathcal{P}^{\text{in}}, \mathcal{P}^{\text{out}}, A)$.

**Proof.** By convexity, it suffices to show that every $D^TMC$ with $C$ and $D$ being PCMs can be written as a convex combination of the $F^TME$ matrices, with $E$ and $F$ being binary PCMs of $\mathcal{P}^{\text{in}}$ and $\mathcal{P}^{\text{out}}$ respectively. Note that the scaling is uniform, so we may ignore the ScaleCols.

By Lemma\footnote{we can write $C$ as a convex combination of the binary PCMs $E_j$, i.e., $C = \sum_j \alpha_j E_j$. We can similarly write $D$ as a convex combination of the binary PCMs $F_k$, i.e., $D = \sum_k \beta_k F_k$. By distributivity, then, we have}

$$D^TMC = \sum_j \sum_k \alpha_j \beta_k F_k^T M E_j.$$  

The $F_k^T M E_j$ matrices are exactly the binary mergings used by $\hat{\alpha}_{\text{bin}}$, hence it suffices now to show that the $\alpha_j \beta_k$ coefficients are non-negative and sum to one. They are non-negative by construction, and sum to one because

$$\sum_j \sum_k \alpha_j \beta_k = \sum_j \left( \sum_k \beta_k \right) = \sum_j \alpha_j \cdot 1 = \sum_j \alpha_j = 1.$$  

Therefore, any such $D^TMC$ is a convex combination of the binary mergings, as claimed, and hence $\hat{\alpha}(M, \mathcal{P}^{\text{in}}, \mathcal{P}^{\text{out}}, A) = \hat{\alpha}_{\text{bin}}(M, \mathcal{P}^{\text{in}}, \mathcal{P}^{\text{out}}, A)$.\qed
B The WIVP is Strictly Weaker Than the IVP

In Section 6.1 we stated that the WIVP was strictly weaker than the IVP, i.e., there exists a function $f$ which satisfies the WIVP but not the IVP. The below proof constructs such a function.

**Proof.** Let $g$ be any strongly Darboux function, e.g., Conway’s Base 13 function [26]. The strongly Darboux property implies that the postimage of any non-empty open interval under $g$ is all of $\mathbb{R}$.

Then, let $h$ be any surjective map from $\mathbb{R} \rightarrow \mathbb{Q}$. For example, we can take

$$h(x) = \begin{cases} x & x \in \mathbb{Q} \\ 0 & x \notin \mathbb{Q}. \end{cases}$$

Finally, define

$$f(x) := h(g(x))$$

and note that (i) $f(x) \in \mathbb{Q}$ for every $x$ while (ii) the postimage of any non-empty open interval under $f$ is exactly $\mathbb{Q}$.

First, $f$ does not satisfy the IVP because, for instance, 1 and 2 are in the image of $f$ but not $\sqrt{2}$.

On the other hand, $f$ does satisfy the WIVP. To see this, consider any $a_1 \leq a_2 \leq \cdots \leq a_n$. If they are all the same, then $f(a_i)$ is equal to the average. Otherwise, note that each $f(a_i) \in \mathbb{Q}$ hence

$$\frac{\sum_i f(a_i)}{n} \in \mathbb{Q} = f([a_1, a_n])$$

and so there exists a $b \in (a_1, a_n) \subseteq [a_1, a_n]$ with $f(b) = \frac{\sum_i f(a_i)}{n}$ as desired.

Therefore, the WIVP is strictly weaker than the IVP. \qed

C Proof of Theorem 3

In Section 6.2 we stated a necessary condition for sound abstraction via Algorithm 3 namely that the activation functions have non-negative outputs. We now proceed to prove this theorem, restated below.

**Theorem 3.** Suppose some $\sigma \in \Sigma$ is an activation function with neither entirely non-negative nor entirely non-positive outputs, and every $A \in \mathcal{A}$ is at least as precise as the interval hull abstraction. Then there exists a neural network $N$ that uses $\sigma$ and a partitioning $\mathcal{P}$ such that $T = \text{AbstractLayerWise}(\mathcal{A}, \Sigma)(N, \mathcal{P}, A)$ does not over-approximate $N$.

**Proof.** Label $x, y \in \mathbb{R}$ such that $\sigma(x) < 0$ but $\sigma(y) > 0$. We will then take the DNN defined by the function

$$N(v) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \sigma \begin{pmatrix} x \\ y \end{pmatrix} v$$
and the partitioning

\[ P = (\{{1}\}, \{{1, 2}\}, \{{1}\}, \{2\}) \]

which collapses all of the hidden dimensions. Then the corresponding interval ANN is given by

\[ T_{\text{Int}}(v) = \begin{bmatrix} [0, 2] \\ [0, 2] \end{bmatrix} \sigma(\begin{bmatrix} [x, y] \end{bmatrix} v). \]

But then the components of \( N(1) \) have opposite signs, which can never happen for an instantiation of \( T_{\text{Int}}(1) \), hence \( N(1) \not\in T_{\text{Int}}(1) \). If we used any more-precise abstraction than intervals to get an ANN \( T \) we would have \( T(1) \subseteq T_{\text{Int}}(1) \), hence still \( N(1) \not\in T(1) \). Therefore, \( T \) does not over-approximate \( N \), completing the proof.

**D Proof of Theorem 4**

**Theorem 4.** Let \( N \) be a DNN and suppose that, on some input region \( R \), the output of the activation functions are lower-bounded by a constant \( C \). Then, there exists another DNN \( N' \), with at most one extra dimension per layer, which satisfies (i) \( N'(x) = N(x) \) for any \( x \in R \), (ii) \( N' \) has all non-negative activation functions, and (iii) the new activation functions \( \sigma' \) are of the form \( \sigma'(x) = \max(\sigma(x) + |C|, 0) \).

**Proof.** We will construct \( N' \) with layers \((W(i)', \sigma(i)')\).

We will first define the activation functions \( \sigma(i)' \) used by \( N' \). For every \( i < n \) set \( \sigma(i)'(x) := \max(\sigma(i)(x) + |C|, 0) \). For \( i = n \) set \( \sigma(n)' := \sigma(n) \). Note that, by assumption for any input in \( R \) we will have \( \sigma(i)(x) + |C| > 0 \), so the max is just needed to ensure that the activation function is formally non-negative on the entirety of \( \mathbb{R} \).

We now define the weight matrices \( W(i)' \) used by \( N \). For \( i = 1 \), set \( W(1)' = W(1) \). For every \( i > 1 \), define \( W(i)' \) such that

\[ W(i)'v := W(i)(v - |C|) = W(i)v - W(i)|C|, \]

where we have abused notation to let \( C \) here refer to the vector with every component fixed to the constant \( C \). Note that adding constant terms such as this can be done by adding a single additional dimension to each layer according to a standard transformation.

We now argue that \( N \) and \( N' \) have the same output on any vector \( v \). Let \( v^{(1)}, v^{(2)}, \ldots, v^{(n)} \) be the post-activation vector after each layer in the original DNN as defined in Definition 3 and \( v^{(1)'}, \ldots, v^{(n)'} \) be the same for the constructed DNN on an input \( v \).
Finally, for the last layer we have
\[
\mathbf{v}^{(i)'} = \sigma^{(i)}(W^{(i)}v^{(i-1)'}) = \max(\sigma^{(i)}(W^{(i)}(v^{(i-1)'}) - |C|)) + |C|, 0)
\]
\[
= \max(\sigma^{(i)}(W^{(i)}((v^{(i-1)} + |C|) - |C|)) + |C|, 0)
\]
\[
= \max(\sigma^{(i)}(W^{(i)}v^{(i-1)})) + |C|, 0)
\]
\[
= \max(\mathbf{v}^{(i)} + |C|, 0) = \mathbf{v}^{(i)} + |C|.
\]

If \( \mathbf{v} \in R \), then we have by assumption that \( C \) is a lower-bound for the value of \( \mathbf{v}^{(i)} \) and hence this gives simply
\[
\mathbf{v}^{(i)'} = \max(\mathbf{v}^{(i)} + |C|, 0) = \mathbf{v}^{(i)} + |C|.
\]

Finally, for the last layer we have
\[
\mathbf{v}^{(n)'} = \sigma^{(n)'}(W^{(n)}v^{(n-1)'}) = \sigma^{(n)}(W^{(n)}(v^{(n-1)'}) - |C|))
\]
\[
= \sigma^{(n)}(W^{(n)}((v^{(n-1)} + |C|) - |C|))
\]
\[
= \sigma^{(n)}(W^{(n)}v^{(n-1)})
\]
\[
= \mathbf{v}^{(n)}
\]
as desired.

We now provide an example of this construction.

Example 9. In the LeakyReLU example from Section 6.2, suppose we are only interested in the behavior of \( f \) for \( x_1 \in [-1, 1] \). On that domain, the output of the LReLU is at least \(-0.5\), hence we can take \( C = -0.5 \). Applying the construction from the theorem, we have
\[
f'(x_1) = \begin{bmatrix} 1 & 1 \\ 1 & 0 \end{bmatrix} \text{LReLU}' \begin{bmatrix} 1 \\ 0 \end{bmatrix} \begin{bmatrix} 1 \\ -1 \end{bmatrix} \begin{bmatrix} 0.5 \end{bmatrix}
\]
where \( \text{LReLU}'(x; 0.5) := \max(\text{LReLU}(x; 0.5) + 0.5, 0) \).

Now consider, for example, \( x_1 = -1 \). In the original network we had
\[
f(-1) = \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} \text{LReLU} \begin{bmatrix} -1 \\ 0 \end{bmatrix} \begin{bmatrix} 0.5 \end{bmatrix} = \begin{bmatrix} -0.5 \\ 0.5 \end{bmatrix}
\]
noticing that the output of the LReLU had a negative component. In the new network, on the other hand, we have
\[
f'(x_1) = \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} \text{LReLU}' \begin{bmatrix} 1 \\ 0 \end{bmatrix} \begin{bmatrix} 0.5 \end{bmatrix} = \begin{bmatrix} -0.5 \\ 0.5 \end{bmatrix}
\]
where we can see that indeed the output of the new activation function \( \text{LReLU}' \) is non-negative.
E Proof of Theorem 5

In Section 6.3 we claimed that activation functions satisfying the WIVP is a necessary condition for soundness of Algorithm 3. This is formalized by the theorem below, which we now prove.

**Theorem 5.** Suppose some $\sigma \in \Sigma$ is an activation function which does not satisfy the WIVP, and every $A \in \mathfrak{A}$ is at least as precise as the interval hull abstraction. Then there exists a neural network $N$ using only the identity and $\sigma$ activation functions and partitioning $P$ such that $T = \text{AbstractLayerWise}(\mathfrak{A}, \Sigma)(N, P, A)$ does not over-approximate $N$.

**Proof.** Let $a_1 \leq a_2 \leq \cdots \leq a_n$ be the points violating the WIVP for $\sigma$, i.e. there does not exist any $b \in [a_1, a_n]$ such that

$$\sigma(b) = \frac{\sum_i a_i}{n}.$$ 

We can then take the DNN given by

$$N(v) = \begin{bmatrix} 1 & 1 & \cdots & 1 \end{bmatrix} \sigma \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix} v$$

and the partitioning

$$P = (\{\{1\}\}, \{\{1, \ldots, n\}\}, \{\{1\}\})$$

which collapses all of the hidden dimensions. Then in the interval abstraction we get the ANN

$$T(v) = [[n, n]] \sigma ([[a_1, a_n]] v).$$

Now, consider $N(1)$ and $T(1)$. We have by definition that

$$N(1) = \sigma(a_1) + \cdots + \sigma(a_n).$$

Suppose for sake of contradiction that $T$ over-approximates $N$. Then we must have $N(1) \in T(1)$. Then there must be an assignment to the weights in $T$ which matches $N$, i.e., then there must be a $b \in [a_1, a_n]$ and $m \in [n, n]$ such that

$$m \sigma(b) = f(1) = \sum_i \sigma(a_i).$$

But $m \in [n, n]$ implies $m = n$, hence in that case we have

$$\sigma(b) = \frac{\sum_i \sigma(a_i)}{n}.$$ 

But $b \in [a_1, a_n]$, contradicting the assumption that $\sigma$ violates the WIVP at $a_1, \ldots, a_n$ and so completing the proof. \qed