Permutation Invariance of Deep Neural Networks with ReLUs

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Abstract. Consider a deep neural network (DNN) that is being used to suggest the direction in which an aircraft must turn to avoid a possible collision with an intruder aircraft. Informally, such a network is well-behaved if it asks the ownship to turn right (left) when an intruder approaches from the left (right). Consider another network that takes four inputs – the cards dealt to the players in a game of contract bridge – and decides which team can bid game. Loosely speaking, if you exchange the hands of partners (north and south, or east and west), the decision would not change. However, it will change if, say, you exchange north’s hand with east. This permutation invariance property, for certain permutations at input and output layers, is central to the correctness and robustness of these networks.

Permutation invariance of DNNs is really a two-safety property, i.e. it can be verified using existing techniques for safety verification of feed-forward neural networks (FFNNs), by composing two copies of the network. However, such methods do not scale as the worst-case complexity of FFNN verification is exponential in the size of the network.

This paper proposes a sound, abstraction-based technique to establish permutation invariance in DNNs with ReLU as the activation function. The technique computes an over-approximation of the reachable states, and an under-approximation of the safe states, and propagates this information across the layers, both forward and backward. The novelty of our approach lies in a useful tie-class analysis, that we introduce for forward propagation, and a scalable 2-polytope under-approximation method that escapes the exponential blow-up in the number of regions during backward propagation.

An experimental comparison shows the efficiency of our algorithm over that of verifying permutation invariance as a two-safety property (using FFNN verification over two copies of the network).

1 Introduction

Artificial neural networks are now ubiquitous. They are increasingly being allowed and used to handle increasingly more complex tasks, that used to be unimaginable for a machine to perform. This includes driving cars, playing games, maneuvering air traffic, recognizing speech, interpreting images and videos,
creating art, and numerous other things. While this is exciting, it is crucial to understand that neural networks are responsible for a lot of decision making, some of which can have disastrous consequences if gone wrong. Thus, it is important to understand and verify the trustworthiness of a network, especially as they react with an uncertain environment. Towards this goal, this paper addresses the problem of verifying permutation invariance of deep neural networks (DNNs).

Consider a DNN that is being used to suggest the direction in which an aircraft must turn to avoid a possible collision with an intruder aircraft. Informally, such a network is well-behaved if it asks the ownship to turn right (left) when an intruder approaches from the left (right). Consider another network that takes four inputs – the cards dealt to the players in a game of contract bridge – and decides which team can bid game. Loosely speaking, if you exchange the hands of partners (north and south, or east and west), the decision would not change. However, it will change if, say, you exchange north’s hand with east. Such permutation invariance properties, for certain permutations at input and output layers, are important to the correctness and robustness of these networks.

Formally, given a DNN $N$, permutations $\sigma_{in}$ and $\sigma_{out}$, two vectors $B_1$ and $B_2$ of dimension as large as the input size of the neural network and a positive real $M$, the permutation invariance is defined as: if the inputs of the network lie between $B_1$ and $B_2$ component-wise, then permuting the input of the network by $\sigma_{in}$ leads to the output being permuted by $\sigma_{out}$ up to a tolerance of $M$. That is,

$$B_1 \leq x \leq B_2 \Rightarrow |\sigma_{out}(N(x)) - N(\sigma_{in}(x))| \leq M$$

Permutation invariance of DNNs is really a two-safety property, i.e. it can be verified using existing techniques for safety verification of feed-forward neural networks (FFNNs), by composing two copies of the network. A straightforward way to do this would be encode the network and the property as SMT constraints, and solve it using Z3 [2]. It is invariably more efficient, however, to use specially designed solvers and frameworks such as Reluplex [10] and Marabou [11,12]. Still, these methods do not scale well, and are particularly inapplicable in this case (which requires doubling the network size), as the worst-case complexity of FFNN verification is exponential in the size of the input network.

This paper proposes a technique to verify the permutation invariance property in DNN.\footnote{We assume the activation function to be ReLU (Rectified Linear Unit); written simply as ‘Relu’ sometimes} Our technique computes, at each layer, an over-approximation of the reachable states (moving forward from the input layer), and also an under-approximation of the safe states (moving backward from the final layer at which the property is specified). If the reachable states fall entirely within the safe region in any of the layers, the property is established. Otherwise, we obtain a witness to exclusion at each layer and run spuriousness checks to see if we can get an actual counterexample.

The novelty of our approach lies in the way we propagate information across layers. For the forward propagation of reachable states, as affine regions, we have...
introduced the notion of tie classes. The purpose of tie classes is to group together the Relu nodes that will always get inputs of the same sign. This grouping cuts down on the branching required to account for active and inactive states of all the Relu nodes during forward propagation. Intuitively, tie classes let us exploit the underlying symmetry of the network, with respect to the inputs and the permutation. The backward propagation relies on convex polytope propagation. During the propagation one may have to account for multiple cases, based on the possible signs of the inputs to the Relu nodes (corresponding to each quadrant of the space in which the polytope resides), leading to an exponential blow-up in the worst case. We address this by proposing a 2-polytope under-approximation method that is efficient (does not depend on LP/SMT solving), scalable, as well as effective. Note that the forward propagation may also be done using convex polytope propagation (which is how it is usually done, e.g. [17]), but it requires computing the convex hull each time, which is an expensive operation. In contrast, tie-class analysis helps us propagate the affine regions efficiently.

The core contributions made in this paper are:

- an approach for verifying permutation invariance in DNNs, that is novel in its:
  - forward propagation, which is based on a useful tie-class analysis, and
  - backward propagation, that uses a scalable 2-polytope under-approximation method
- a proof of soundness of the proposed approach,
- a prototype tool that implements our approach, and an experimental evaluation of its efficiency.

The rest of this paper is organized as follows. After covering the necessary background in Sect. 2, we present an informal overview of our approach in Sect. 3. This is followed by the details of our forward and backward propagation techniques in Section 4 along with a running example that interleaves the two sections. We describe our implementation and experimental results in Sect. 5. The paper ends with a discussion of the related work (Sect. 6) and our concluding remarks (Sect. 7).

2 Preliminaries

We represent vectors in $n$-dimensional space as row matrices, i.e., with one row and $n$ columns. A linear transform $T$ from and $n$ dimensional space to an $m$ dimensional space can then be represented by a matrix $M$ with $n$ rows and $m$ columns, and we have: $T(\vec{x}) = \vec{x}M$.

Convex Polytopes A convex polytope is defined as a conjunction of a set of linear constraints indexed by $i$ of the form $\vec{x} . \vec{v}_i \leq c_i$, for fixed vectors $\vec{v}_i$ and constants $c_i$. Geometrically, it is a convex region in space enclosed within a set of planar boundaries. Symbolically, we can represent a convex polytope by arranging all the $\vec{v}_i$'s into the columns of a matrix $M$, and letting the components of a row vector $\vec{b}$ to be constants $b_i$: $\vec{x} M \leq \vec{b}$.
**Pullback** The pullback of a convex polytope $P$ (given by $\mathcal{F} M_p \leq b^\top_p$), over an affine transform $T$ (given by $\mathcal{F} \to \mathcal{F} M_T + t_T$), is defined as the set of all points $\mathcal{F}$ such that $T(\mathcal{F})$ lies inside $P$, i.e., $T(\mathcal{F}) \in P \iff \mathcal{F} M_T M_p \leq b^\top_T M_p$.

**Affine Region** An $n$-dimensional affine subspace is the set of all points generated by linear combinations of a set of basis vectors $\mathcal{V}_i$, $0 \leq i < k$, added to a center $\mathcal{C}$: $\{ \mathcal{F} \mid \mathcal{F} = (\Sigma_{i=0}^{k-1} \alpha_i \mathcal{V}_i) + \mathcal{C} \}$, for some real $\alpha_i$.

We define an affine region as a constrained affine subspace by bounding the values of $\alpha$ to be between $-1$ and $1$. Formally, an affine region $A[\mathcal{B}_A, \mathcal{C}]$ is defined by a set of basis vectors $\mathcal{V}_i$, $0 \leq i < k$, represented by a matrix $\mathcal{B}_A$, as the following set of points: $\mathcal{F} \in A \iff (\exists \alpha \mathcal{F} = \alpha \mathcal{B}_A + \mathcal{C} \land |\alpha| \leq 1)$.

**Pushforward** We define the pushforward ($A_T$) of an affine region $A$ (defined by $\mathcal{B}_A$ and $\mathcal{C}_A$), across an affine transform $T$, (given by $\mathcal{F} \to \mathcal{F} M_T + t_T$), as the set of points: $\mathcal{F} \in A_T \iff (\exists \alpha \mathcal{F} = \alpha \mathcal{B}_A M_T + \mathcal{C}_A M_T + t_T \land |\alpha| \leq 1)$. This is the image of $A$ under $T$. (In a DNN context, a separate $M_T$ and $t_T$ is associated with each layer that is constructed from the weights and bias used at that layer.)

**DNN Notation and Conventions** We number the layers of the neural network as $0$, $1$, $2$, and so on, up to $n-1$. A layer is said to consist of an affine transform followed by a Relu layer. The affine transform of layer $i$ is given by $\mathcal{F} \to \mathcal{F} W_i + b^\top_i$, where $W_i$ are the weights and $b^\top_i$ are biases. We denote the input vectors by $\mathcal{x}_0$ feeding into the affine transform of layer $0$, and in general for $i > 0$, the input of layer $i$’s affine transform (the output of the $(i-1)^{th}$ layer’s Relu) as $\mathcal{x}_i$. The output of layer $i$’s affine transform (the input to layer $i$’s Relu) is labeled as $\mathcal{y}_i$. Finally, the output is $\mathcal{x}_n$. Also, we maintain copies of each variable’s original and permuted value (using a primed notation). So, we have:

$$\mathcal{x}_0, \mathcal{x}_0 \to \mathcal{F} W_0 + b^\top_0 \to \mathcal{y}_0, \mathcal{y}_0 \to \text{Relu} \to \mathcal{x}_1, \mathcal{x}_1 \to \mathcal{F} W_1 + b^\top_1 \to \mathcal{y}_1, \mathcal{y}_1 \to \text{Relu} \to \cdots \mathcal{y}_{n-1}, \mathcal{y}_{n-1} \to \text{Relu} \to \mathcal{x}_n, \mathcal{x}_n$$

Here, $W_i$ and $b^\top_i$ represent the action of the layer on the input of the $i$th layer and $x_i$. Then, the invariance property we wish to verify has the following form:

$$B_1 \leq \mathcal{x}_0, \mathcal{x}_0 \leq B_2 \land \mathcal{x}_0 = \sigma_{in}(\mathcal{x}_0) \Rightarrow |\mathcal{x}_n - \sigma_{out}(\mathcal{x}_n)| \leq M$$

Note that the precondition here is an affine region and the postcondition is a conjunction of linear inequalities, involving permutations.
3 Informal Overview

Algorithm 1 presents a high-level pseudocode of our approach. The input to it is the network $N$ with $n$ layers, and the invariance property given as a $(\text{pre}, \text{post})$ pair of formulas. The algorithm begins by converting the pre-condition to an affine region by calling $\text{initPre}$ (line 3) and expressing the postcondition as a convex polytope by calling $\text{initPost}$ (line 4), without any loss of precision, as illustrated in the following example. Then it propagates the affine region forward, to obtain an over-approximation of the set of reachable values as an affine region at each subsequent layers (line 6). Similarly, an under-approximation of the safe region – as a union of two convex polytopes – is calculated at each layer, propagating the information backward from the output layer (line 8). If the reachable region at any layer is contained within the safe region, we have a proof that the property holds (lines 9-13).

Algorithm 1 Overview of our approach

```plaintext
1: inputs: $N$, $n$, $\text{pre}$, $\text{post}$
2: globals: $\text{reach}[n]$, $\text{safe}[n]$
3: $\text{reach}[0] \leftarrow \text{initPre}(\text{pre}, N)$
4: $\text{safe}[n-1] \leftarrow \text{initPost}(\text{post}, N)$
5: for $i \in [1 \ldots n]$ do
6:   $\text{reach}[i] \leftarrow \text{forwardPropagate}(\text{reach}[i-1], N)$
7: for $i \in [n-2 \ldots 0]$ do
8:   $\text{safe}[i] \leftarrow \text{backwardPropagate}(\text{safe}[i+1], N)$
9: for $i \in [1 \ldots n]$ do
10: if $(\text{reach}[i] \land \neg\text{safe}[i])$ is unsatisfiable then
11:   return property holds
12: else /* there must be a satisfying witness */
13:   spuriousnessCheck(witness, i)
```

If the inclusion check does not succeed, then our algorithm attempts to construct an actual counterexample from the witness to the inclusion check failure (see Alg. 2). In general, pulling back the witness to the first layer is as hard as pulling back the postcondition. So, we try to find several individual input points that lead to something close to the witness at the layer where the inclusion fails, allowing us to check a number of potential counterexamples. In lines 5-6 (Alg. 2) we repeatedly apply $\text{pullBackCex}$ and collect these approximate pull back points layer by layer backwards until the input layer. We now simulate these points forward to check if the output of the DNN lies within the safe region in lines 11-17. If for any point it does not, we have successfully constructed a counterexample. Otherwise, if we cannot find any potential counterexamples (line 10), or if all the potential counterexamples are safe (line 17), the witness represents a spurious counterexample and the algorithm returns inconclusive.

The details of $\text{forwardPropagate}$, $\text{backwardPropagate}$, $\text{pullBackCex}$ are discussed in the next section. In the remainder of this section, we present an example and describe the pre-processing part of our algorithm.

3.1 Running Example

Consider the neural network shown in Fig. 2. Here, we have separated the result of computing the weighted sum from that of the application of the $\text{Relu}$ into
Algorithm 2 Spuriousness checking algorithm

1: procedure spuriousnessCheck (counterexample, layer)
2: \[ cexes \leftarrow \text{counterexample} \] \quad \triangleright \text{list of potential counterexamples}
3: while \( cexes \neq \emptyset \lor \text{layer} > 0 \) do
4: \[ \text{prevCexes} \leftarrow \emptyset \] \quad \triangleright \text{collect (approximate) pullbacks in the previous layer, for every c’example}
5: for \( \text{cex} \in \text{cexes} \) do
6: \[ \text{prevCexes} \leftarrow \text{pullBackCex}(\text{cex}, \text{layer}, N) \]
7: \[ \text{cexes} \leftarrow \text{prevCexes} \]
8: \[ \text{layer} \leftarrow \text{layer} - 1 \]
9: if \( \text{cexes} = \emptyset \) then
10: \[ \text{return inconclusive} \] \quad \triangleright \text{pullback failed, no potential counterexamples}
11: for \( \text{cex} \in \text{cexes} \) do
12: for \( j \in [0 \ldots n] \) do
13: \[ \text{cex} \leftarrow \text{simulateLayer}(\text{cex}, j, N) \]
14: if \( \text{cex} \in \text{safe}[j] \) then
15: \[ \text{break} \]
16: \[ \text{return (property failed, cex)} \] \quad \triangleright \text{actual counterexample found}
17: \[ \text{return inconclusive} \] \quad \triangleright \text{all potential counterexamples are safe}

separate nodes, represented by dashed and solid circles respectively. Also, we show the weights as labels on the arrows coming into a combination point, and biases as labels of arrows emerging from the point. The arrows for weights that are 0 have been omitted. The values at (output of) each node in the network for the input in the range \([0.5 0]\) are shown in the diagram at that node.

This network has the following symmetry property: \(0 \leq x_{00}, x_{01}, x’_{00}, x’_{01} \leq 1 \land x_{00} = x’_{01} \land x_{01} = x’_{00} \Rightarrow |x_{40} x_{41} - [x’_{40} x’_{41}]| \leq 0.1\). This expresses the fact that flipping the inputs leads to the outputs being flipped.

Preprocessing: The \(W_i\) and \(\vec{b}_i\) are calculated as follows: If the weights and bias of layer \(i\) are \(W^o\) and \(\vec{b}^o\), then \(W_i = \begin{bmatrix} W^o & 0 \\ 0 & W^o \end{bmatrix}\) and \(\vec{b}_i = [\vec{b}^o, \vec{b}^o]\) as we need to track both the original and permuted values at each layer. For this example we have:

\[
W_0 = \begin{bmatrix}
1000 & -1000 & 1000 & -1000 & 0 & 0 & 0 & 0 \\
1000 & 1000 & -1000 & 1000 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1000 & -1000 & 1000 & -1000 \\
0 & 0 & 0 & 0 & -1000 & 1000 & -1000 & 1000
\end{bmatrix}
\]
\[
W_1 = \begin{bmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
-1 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & -1 & 0 \\
0 & 0 & 0 & -1
\end{bmatrix}
\]
\[
\vec{b}_0 = [0, 0, -1, -1, 0, 0, -1, -1]
\]
\[
\vec{b}_1 = [0, 0, 0, 0]
\]
Action of \textit{initPre} and \textit{initPost}: Now, \textit{initPre} calculates \textit{reach}[0] as the following affine region given by basis \( B_0 \) and center \( c_0' \), and \textit{initPost} expresses \textit{safe}[2] as a convex polytope:

\begin{align}
\text{reach}[0]:
&\exists \alpha: [\overrightarrow{x}_0, \overrightarrow{x}_4] = \alpha B_0 + \overrightarrow{c}_0, \quad |\alpha| \leq 1 \\
&\begin{bmatrix}
0.5 & 0 & 0 & 0.5 \\
0 & 0.5 & 0.5 & 0
end{bmatrix}
\begin{bmatrix}
\overrightarrow{x}_0 \\
\overrightarrow{x}_4
end{bmatrix}
\leq
\begin{bmatrix}
1 & 0 & -1 & 0 \\
0 & 1 & 0 & -1 \\
0 & -1 & 0 & 1 \\
-1 & 0 & 1 & 0
end{bmatrix}
\begin{bmatrix}
0.1 \\
0.1 \\
0.1 \\
0.1
end{bmatrix}
\end{align}

\textit{Forward Propagation:} \textit{ForwardPropagate} then propagates across the layers to get affine regions that are over-approximations for the reachable region for that layer. While propagation across the linear layer can be done easily via matrix multiplication, propagating across the \textit{Relu} layer is in general is hard, since we need to take into account all possible branching behaviors. We do this via a tie class analysis (section 4.2) that exploits the inherent symmetry of the network and precondition. For this network, propagating across the first linear layer gives us an affine region given by the basis and center:

\begin{align}
\text{reach}[1]:
&B_0' = 
\begin{bmatrix}
500 & -500 & 500 & -500 & 500 & -500 & 500 \\
-500 & 500 & -500 & 500 & 500 & -500 & 500
end{bmatrix} \\
&c_0' = [0, 0, -1, 0, 0, -1, 0, -1]
end{align}

Then, propagating across the \textit{Relu} using the tie class analysis (section 4.2) gives us the basis \( B_1 \) and center \( c_1' \) for \textit{reach}[1]. Similarly, the algorithm propagates across the second layer to get \( B_1', c_1', B_2 \) and \( c_2' \). In this case, the affine
region before and after the *Relu* turn out to be the same, and there is no loss in precision going from $B'_1$ to $B_2$. The matrices are:

$$
B_1 = \begin{bmatrix}
500 & 0 & 0 & 0 & 0 & 500 & 0 & 0 \\
-500 & 0 & 0 & 0 & 0 & -500 & 0 & 0 \\
0 & -500 & 0 & 0 & -500 & 0 & 0 & 0 \\
0 & 500 & 0 & 0 & 0 & 0 & 0 & 500 \\
0 & 0 & 500 & 0 & 0 & 0 & 0 & -500 \\
0 & 0 & 0 & -500 & 0 & 0 & 0 & -500 \\
0 & 0 & 0 & 500 & 0 & 0 & 0 & 500 \\
\end{bmatrix}
$$

$$
B'_1, B_2 = \begin{bmatrix}
500 & 0 & 0 & -500 \\
-500 & 0 & 0 & 500 \\
0 & -500 & -500 & 0 \\
0 & 500 & 500 & 0 \\
-500 & 0 & 0 & -500 \\
500 & 0 & 500 & 0 \\
0 & -500 & -500 & 0 \\
\end{bmatrix}
$$

$$
\vec{c}_1 = [0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0]
$$

$$
\vec{c}'_1, \vec{c}_2 = [0 \ 0 \ 0]
$$

*(2)*

**Inclusion check:** Now, we see that if we substitute $\vec{x}$ with the form given in reach[2] into safe[2] (which is the postcondition $||x_{40} \ x_{41}|| - ||x'_{40} \ x'_{41}|| \leq 0.1$), the right side of the inequality simplifies to 0. So, reach[2] is included in safe[2]. This is done by an algorithm (section 4.5) that checks this using an LP solver, and since it succeeds in this case, it returns *property holds.*

Note that for this example, it was unnecessary to perform any back propagation of the safe[i] to previous layers, as the inclusion check succeeded at the output layer. In general, back propagation (section 4.3) would be performed to compute under-approximations. Spuriousness check (section 4.5) will be needed if the inclusion check fails.

## 4 Forward and Backward Propagation

### 4.1 Preparation

**InitPre and construction of reach[0]:** An input precondition on an input layer of the form $\vec{B}_1 \leq \vec{x}_0, \vec{x}_0 \leq \vec{B}_2$ with $\vec{x}_0 = \sigma(\vec{x}_0)$ can always be converted into an equivalent affine region characterized by the formula:

$$
(\exists \vec{\alpha} : |\vec{x}_0, \vec{x}_0| = \vec{\alpha} V + \vec{\gamma}, |\vec{\alpha}| \leq 1),
$$

with the centre as $\vec{c} = \frac{\vec{B}_1 + \vec{B}_2}{2}$, and the matrix $V$ representing the set of basis vectors defined as follows.

For input size of $n$, $V$ is a concatenation of two $n \times n$ matrices $[V_1; V_2]$ with 2n columns. The elements of $V_1$ are all 0 except the main left to right diagonal being set to $1/2(B_2[i] - B_1[i])$. $V_2$ is constructed by applying $\sigma$ permutation for each of the columns of $V_1$.

Consider the precondition $[1, 3, 2, 2, 1, 3] \leq [x_0, x_1, x_2, x_2, x_0, x_1] \leq [2, 4, 3, 3, 4, 2]$ on an input vector of size 3 and a permutation of it. The matrix $V$ to express it as an affine region is

$$
\begin{bmatrix}
1/2 & 0 & 0 & 0 & 1/2 & 0 \\
0 & 1/2 & 0 & 0 & 0 & 1/2 \\
0 & 0 & 1/2 & 1/2 & 0 & 0 \\
\end{bmatrix}
$$
**InitPost and construction of safe**: A postcondition of the form $|x_n' - \sigma_{out}(x_n)| \leq M$ can be written as $||x_n' x_n||L| \leq M$ where each column of $L$ calculates one of the differences of corresponding components. This can be transformed into a conjunction of two sets of linear constraints given by $|x_n' x_n|L \leq M$ and $-|x_n' x_n|L \leq -M$, which represents a single convex polytope over $2n$ variables.

### 4.2 Forward Propagation using Tie Classes

Let $reach_j = \{(x_j' x_j) | \exists \bar{\alpha} : [x_j' x_j] = \bar{\alpha} B_j + \bar{c}_j, |\bar{\alpha}| \leq 1\}$, be the affine region representing an over-approximation of reachable points at the input to layer $j$; $forwardP rapporte$ constructs $reach_{j+1}$ as an affine region that is an over-approximation for the set of all points produced when $reach_j$ is propagated to the input of layer $j + 1$. $reach_{j+1}$, is constructed by forward propagating $reach_j$ first across the affine transform at $j$ to produce an affine region $A_j$, which is then further forward propagated across the Relu layer.

Forward propagation across the linear transform given by $\bar{x} \rightarrow \bar{x} W_j + \bar{b}_j$ is straightforward and precise as it can be computed as a simple linear pushforward across $W_j$, i.e., $A_j([y_j' y_j]) \Leftrightarrow (\exists \bar{\alpha} : [y_j' y_j] = \bar{\alpha} B_j' + \bar{c}_j', |\bar{\alpha}| \leq 1)$, where $B_j' = B_j W_j$ and $c_j'$ as $\bar{c}_j W_j + \bar{b}_j$.

Propagating $A_j$ across Relu is more complex and challenging as it requires, in general, a detailed case analysis of the polarity and strength of the components of the basis vectors and the scaling $\alpha$; rather than performing it precisely, $reach_{j+1}$ is constructed as an affine region over-approximates the Relu image. Several methods can be used to construct an over-approximation that make different tradeoffs between precision and efficiency. One can construct the smallest affine region (or polytope) that includes all the reachable values possible across the Relu [17]. Computing the smallest region can be inefficient as it is an optimization problem requiring several expensive LP or convex-hull calls. Our method efficiently constructs an over-approximate affine region that, while sub-optimal, is effective for checking permutation invariance properties.

Our method to construct the over-approximate affine region relies on looking for similarities in the polarity of the components of the vectors belonging to $reach_j$ that are preserved when a Relu is applied to the region. For this purpose we introduce a new concept called tie classes associated with an affine region which is described below.

### Propagating over Relu with Tie Classes

Given an affine region $A$ defined by a basis $\vec{v}_i$ and center $\vec{c}$ we define a binary relation, tied, over the set of indices denoting the components of any vector $\vec{x}$ in $A$ as follows.

---

5 We assume the indices range from 0 to $n - 1$ for vectors of size $n$. 
Definition 1 (Tied). Given an affine region $\mathcal{A}$ characterized by the condition $\exists \alpha : \mathcal{A} = \sum_i \alpha_i \vec{v}_i + \vec{c}$, $|\alpha_i| \leq 1$, and two indices $i_1$ and $i_2$ in the index set, we say $i_1$ and $i_2$ are tied iff for every vector $\vec{x}$ in $\mathcal{A}$ the components at $i_1$ and $i_2$ have the same sign.

It is easy to see that the binary relation being tied is an equivalence relation on the index set of vectors $\vec{x}$ that generates an equivalence class defined as follows.

Definition 2 (Tie Class). A tie class for an affine region $\mathcal{A}$ is the equivalence class (partitioning) of the index set for the vectors in $\mathcal{A}$ induced by the equivalence relation tied for $\mathcal{A}$.

Consider the affine region generated by the basis $\vec{v}_i$ and $\vec{c}$:

- $\vec{v}_0 = [1 \ 0 \ 0 \ 2]$
- $\vec{v}_1 = [0 \ 1 \ 0.5 \ 0]$
- $\vec{c} = [0.5 \ 2 \ 1 \ 1]$

For this region, the indices 0 and 3 are tied because every vector in the region the component 3 is always 2 times the component 0, since the component 3 of the $\vec{v}_i$ and the $\vec{c}$ are 2 times the component 0. Similarly, indices 1 and 2 are tied as well. For this region, the tie equivalence class is $\{0 : \{0, 3\}, 1 : \{1, 2\}\}$

Tie class based transformation of Basis Vectors

To help construct the basis vectors for the over-approximation of the output of Relu, we define a transformation of the set of basis vectors at the input to Relu. For each tie class $j$ in the equivalence class induced, and each vector $\vec{v}_i$ in the input basis set, we construct a vector $\vec{v}_i^j$ by setting all the components of $\vec{v}_i$ that are not in the tie class $j$ to 0. Similarly, we get a $\vec{c}_j$ from $\vec{c}$ for each tie class $j$. For the example above, we have:

- $\vec{v}_0^0 = [1 \ 0 \ 0 \ 2]$
- $\vec{v}_1^0 = [0 \ 0 \ 0 \ 0]$
- $\vec{c}_0 = [0.5 \ 0 \ 0 \ 1]$
- $\vec{c}_1 = [0 \ 2 \ 1 \ 0]$

We now state the following lemma:

Lemma 1. Given $\vec{x} = \sum_i \alpha_i \vec{v}_i + \vec{c}$, we can write $\text{Relu}(\vec{x}) = \sum_{i,j} \alpha_i^j \vec{v}_i^j + \sum_j \beta_j \vec{c}_j$ where each $\alpha_i^j$ is either $\alpha_i$ or is 0, and each $\beta_j$ is either 0 or 1. Moreover, the components of $\text{Relu}(\vec{x})$ with indices in a tie class $j$ are 0 if and only if $\alpha_i^j$ and $\beta_j$ are 0.

The proofs have been moved to Appendix A for lack of space.

This lemma states that there exists an oracle that, given an $\vec{x}$ in reach$_j$, can determine whether to set each $\alpha_i^j$ to $\alpha_i^j$ or 0 and each $\beta_j$ to 0 or 1 so that we can express $\text{Relu}(\vec{x})$ in the above form. Regardless of what the oracle chooses we can always replace the condition $\alpha_i^j = \alpha_i^j \lor \alpha_i^j = 0$ with $|\alpha_i^j| \leq 1$ as an over-approximation. Now, if we can somehow replace $\sum_j \beta_j \vec{c}_j$ with a single vector,
we will have found our output affine region. The following theorem proves that we can replace this sum with $\text{Relu}(\overrightarrow{c})$.

**Theorem 1.** Given $\overrightarrow{x} = \sum_i \alpha_i \overrightarrow{v}_i + \overrightarrow{c}, |\overrightarrow{c}| \leq 1$, in an affine region $A$, there are scalars $\alpha_i$ such that:

1. $\text{Relu}(\overrightarrow{x}) = \sum_{i,j} \alpha_{i,j} \overrightarrow{v}_{i,j} + \text{Relu}(\overrightarrow{c})$
2. $|\alpha_{i,j}| \leq 1$ for all $i$ and $j$.

The above theorem proves that the affine region given by the basis $\overrightarrow{v}_{i,j}$ and the center $\text{Relu}(\overrightarrow{c})$ is an over-approximation for the Relu image of $A$. Given $\overrightarrow{v}_i$ and $\overrightarrow{c}$, it is easy to compute $\overrightarrow{v}_{i,j}$ and $\text{Relu}(\overrightarrow{c})$ if we know what the tie classes are, since this only involves setting certain components to 0. All we need to do now is compute the tie classes for the given $\overrightarrow{v}_i$ and $\overrightarrow{c}$.

**Algorithm 3 Checking tiedness**

1. **inputs:** $A, \overrightarrow{v}_i, \overrightarrow{c}, i_1, i_2$
2. if $\forall j : \frac{v_{i,j}}{v_{i,j}^0} = \frac{v_{i,j}^0}{v_{i,j}^0}$ then return tied
3. else if $c_{i,j}^0 \geq 0$ and $c_{i,j}^0 \geq 0$ then
   4. if $i_1$ or $i_2$ component of some $\overrightarrow{x} \in A < 0$
      then return not tied
   5. else return tied
4. else if $c_{i,j}^0 < 0$ and $c_{i,j}^0 < 0$ then
5. if $i_1$ or $i_2$ component of some $\overrightarrow{x} \in A > 0$
   then return not tied
6. else return tied
7. else return not tied

**Computing Tie Classes**

To compute tie classes, for every pair of indices $i_1$ and $i_2$, we check whether $i_1$ and $i_2$ are tied, and then group them together. One way to check if two $i_1$ and $i_2$ are in the same tie class using two LP queries involving the $\alpha_i$: one which constrains the value of component $i_1$ of $x$ to positive and component $i_2$ to negative, and vice versa. If any of these are feasible, $i_1$ and $i_2$ cannot be in the same tie class. Else, they are in the same tie class. This needs to be repeated for each pair of $i_1$ and $i_2$, which amounts to $n \times (n-1)$ LP calls for $n$ Relu nodes, which is inefficient. Instead, we state another property of tie classes that will allow us to compute the tie classes more efficiently:

**Theorem 2.** Two indices $i_1$ and $i_2$ are in the same tie class if and only if one of the following is true:

1. The $i_1$ and $i_2$ components of $\overrightarrow{x}$ are always both positive.
2. The $i_1$ and $i_2$ components of $\overrightarrow{c}$ are always both negative.
3. The vector formed by the $i_1$ and $i_2$ components of the $\overrightarrow{v}_k$ and $\overrightarrow{c}$ are parallel.

In other words, if $v_{k,j}^0$ is the $l$-component of $\overrightarrow{v}_k$, and $c^l$ is the $l$-component of $\overrightarrow{c}$, then $[v_{1,j}^0, v_{2,j}^0, \ldots, v_{j,j}^0] = k[v_{1,j}^0, v_{2,j}^0, \ldots, v_{j,j}^0]$ for some real $k > 0$.

Algorithm 3 uses Theorem 2 to check if $i_1$ and $i_2$ are in the same tie class. The queries in lines 5, 7, 12 and 14 can be reduced to looking for $\alpha_j$ such that $\sum_j \alpha_{j,j} v_{j,j}^0 + c_j < 0$. Such queries can be solved via an LP call, but we use Lemma 2 to avoid LP calls and check these queries efficiently.
Lemma 2. The maximum and minimum values of $\sum \alpha_i v_i$, for real $\alpha_i$, fixed real $v_i$, constrained by $|\alpha_i| \leq 1$, are $\sum |v_i|$ and $-\sum |v_i|$ respectively.

If the network has a lot of inherent symmetry with respect to the input permutation, it is more likely for different neurons in the same layer to be tied together, leading to larger tie classes. This, in turn, reduces the number of basis vectors required to construct our over-approximation of the $\text{Relu}$ image, and improves the quality of the over-approximation. Thus, we can expect our over-approximation to perform well for checking permutation invariance.

4.3 Backward (Polytope) Propagation

The goal of backward propagation is, given a convex $P: \vec{x}^T L \leq \vec{u}$, to symbolically construct a region, that is a reasonable under-approximation of $\text{WeakestPrecond}(\text{Layer}, P)$. Back propagating $P$ across the linear part of a layer is easy as it can be done precisely by simply pulling back $P$ across a linear transform using matrix multiplication.

Back propagating it across $\text{Relu}$ is more challenging because the $\text{WeakestPrecond}($Relu, $P)$ may potentially involve many quadrants, the number of which are worst-case exponential in the dimension of the space. Keeping track of all of the quadrants is infeasible. A sound single polytope solution is to use $P \land \vec{x} \geq 0$ ignoring the entire “non-positive” region at the input, but this is too imprecise. Our compromise solution is to use a union of two polytopes: one that includes the positive region $P \land \vec{x} \geq 0$ and another that includes as much of the non-positive region as possible. Our goal then is to devise a solution that efficiently constructs a 2-polytope under-approximation by only inexpensive linear algebraic manipulations, i.e., without using an LP or an SMT solver. We describe two methods that differ only in the way it constructs the non-positive polytope at the input to $\text{Relu}$ - one that works when $P$ includes the 0 vector and another when it does not.

A note on cumulative back propagation: If we continue to back propagate a union of two polytopes produced by $\text{Relu}$ for each polytope across all layers, we will still end up with an exponential number of polytopes as we move backwards along the layers. To avoid this situation, we use the following simplification for performance. We keep the 2-polytope under-approximation only to perform inclusion check (line 10 in Algorithm 1). The polytope corresponding to the negative region is dropped before it is subsequently back propagated further into earlier layers. This simplification is sound because dropping one of the polytopes still represents an under-approximation.

$\text{Relu}$ Backpropagation around Zero The main intuition used to construct the negative region to be included in the under-approximation is as follows: if 0 is inside $P$, then the entire negative quadrant with all negative values will be in $\text{WeakestPrecond}($Relu, $P)$, since any negative vector gets mapped to 0 by $\text{Relu}$. Therefore, the region $\vec{x} \leq 0$ can be included in the under-approximation. We
try to do better by including a region of the form \( \vec{x} \leq \vec{\eta} \), where all components of \( \vec{\eta} \) are non-negative. A sufficient condition that such an \( \vec{\eta} \) should satisfy is:

\[
\forall \vec{y} \leq \vec{\eta} \Rightarrow \vec{y} L \leq \vec{u}.
\]

We construct the most liberal \( \vec{\eta} \) satisfying the necessary condition as per an optimality criterion described below.

The optimality measure we use is \( \prod \eta_i \), where \( \eta_i \) are the components of \( \vec{\eta} \). Intuitively, it covers the maximum “volume”. For each inequality \( \vec{x} . \vec{v} \leq \vec{u} \) in \( P \), we can maximise this measure by finding the \( \vec{\eta} \) at which the partial derivative of this product with respect to each \( \eta_i \) is 0, constrained by \( \vec{x} . \vec{v} = \vec{u}_k \). This can be done by solving a set of linear equations in \( \eta_i \). Thus we get one \( \vec{\eta} \) satisfying each inequality and maximising the product, and taking the component wise minimum of these gives us our final \( \vec{\eta} \). A detailed description of this process is given in Appendix B.

This computation only involves solving a set of linear equations for each inequality in \( P \), and then taking minimums. This can be done very efficiently by standard linear algebra algorithms.

**Relu Backpropagation along Quadrant with Center Point** When \( P : \vec{x} L \leq \vec{u} \) does not contain 0, we use the following method. We pick a non-positive quadrant, and add all the points in that quadrant that map to points in \( \vec{x} L \leq \vec{u} \) via the \( \text{Relu} \).

Say we have a non-positive quadrant, represented by a matrix \( Q \), so that \( \vec{x} Q \leq 0 \) describes the linear conditions stating that \( \vec{x} \) is in the chosen quadrant. Now, in the given quadrant, \( \text{Relu} \) behaves like a linear projection that sets the components chosen to be negative to zero. Let this projection be given by the matrix \( \Pi Q \). Then, if \( \vec{x} \) satisfies \( \vec{x} Q \leq 0 \) and \( \vec{x} \Pi Q L \leq \vec{u} \), \( \text{Relu}(\vec{x}) = \vec{x} \Pi Q \) satisfies \( \vec{x} L \leq \vec{u} \). So, it is sound to add the convex polytope \( \vec{x} Q \leq 0 \land \vec{x} \Pi Q L \leq \vec{u} \) to the under-approximation.

The above lets us capture the negative side behavior for any given non-positive quadrant, but leaves the question of choosing the quadrant open. The choice of the quadrant to use is made based on the following center point heuristic: If the center point of \( \text{reach}[i] \) is in a quadrant, we can have reasonably high confidence of the over-approximation being in that quadrant. Since we wish to find an under-approximation that has the best chance of containing \( \text{reach}[i] \), we pick the quadrant which contains the center point.

**4.4 Inclusion Checking**

Our goal is to check whether \( \text{reach}[i] \), given by basis \( B \) and center \( \vec{c} \), is included in \( \text{safe}[i] \), given as union of \( P_1 : \vec{x} L_1 \leq \vec{u}_1 \) and \( P_2 : \vec{x} L_2 \leq \vec{u}_2 \).

Inclusion check is challenging because the right hand side is a disjunction of two convex polytopes. The fact that \( \text{reach}[i] \) is represented as an affine region also makes the task complicated as an affine region cannot easily be converted into a convex polytope over \( \vec{x} \). We implement inclusion check by performing multiple LP calls each of which is designed to be simple. Depending on the method used for back propagation, we have two cases. For both the cases, we
reduce the problem to checking validity over all \((\vec{x})\) of a query of the following form:

\[(\exists \vec{a} : \vec{x} = \vec{a} B + \vec{c} \wedge |\vec{a}| \leq 1 \wedge \vec{x} . \vec{v} \geq k) \Rightarrow \vec{x} L \leq \vec{u}\]

**Backpropagation along quadrant:** In this case, each of the two polytopes \(P_1\) and \(P_2\) is entirely contained in separate quadrants. There is a hyperplane that separates these quadrants, let it be given by \(\vec{x} . \vec{v} = k\). Each polytope lies entirely on one side of this hyperplane. Let’s say that \(\vec{x} L_1 \leq \vec{u}_1\) lies on the side given by \(\vec{x} . \vec{v} \leq k\) and \(\vec{x} L_2 \leq \vec{u}_2\) lies on the side given by \(\vec{x} . (-\vec{v}) \leq k\). Then, it suffices to show that all points in \(\text{reach}[i]\) satisfying \(\vec{x} . \vec{v} \leq k\) are in \(\vec{x} L_1 \leq \vec{u}_1\), and all points satisfying \(\vec{x} . (-\vec{v}) \leq k\) are in \(\vec{x} L_2 \leq \vec{u}_2\). This gives us two queries of the above form.

**Backpropagation around 0:** In this case if \(\vec{x}\) does not satisfy any constraint in \(\vec{x} \leq \vec{f}\), it must be in the positive side polytope \(\vec{x} L_1 \leq \vec{u}_1\). Thus, for each constraint in \(\vec{x} \leq \vec{f}\), we check if all \(\vec{x}\) in \(\text{reach}[i]\) that do not satisfy the constraint are included the convex polytope. This gives us \(n\) checks of the above form for \(n\) dimensional \(\vec{x}\).

**Solving the above query:** To solve the earlier validity query, we negate it and then substitute \(\vec{x}\) from \(\vec{x} = \vec{a} B + \vec{c}\) to reduce the other constraints to one on \(\vec{a}\) to get the following UNSAT query:

\[|\vec{a}| \leq 1 \wedge \vec{a} B . \vec{v} \geq k - \vec{c} . \vec{v} \wedge \neg(\vec{a} B L \leq \vec{u} - \vec{c} L)\]

This check can be done by taking each constraint in the convex polytope \(\vec{a} B L \leq \vec{u} - \vec{c} L\) and checking if an \(\vec{a}\) within \(|\vec{a}| \leq 1 \wedge \vec{a} B\) violates it. Each such query is passed to an LP solver. This means that in the worst case there are as many LP calls as \(n\) times the number of basis vectors in \(B\). However, each LP call only has one linear constraint, the other constraints simply bound the value of \(\vec{a}\), and thus can be solved very efficiently.

### 4.5 Counterexample Checking

If the inclusion fails, we obtain a point that witnesses the violation of the inclusion (of the over-approximation in the under-approximation, at some layer). We wish to find several approximate pullbacks\(^6\) of this layer by layer until the input layer, giving us several potential counterexamples. This is what \(\text{pullBackCex}\) does, given a point \(\vec{z}_{j+1}\) at layer \(j + 1\) and an over-approximation \(A_j\) at layer \(j\), it returns a list of points in \(A_j\) which lead to points closer than \(D\) (in terms

\(^6\) When we use the term “pullback” in this section, it refers to the pullback of the *counterexample* to get a finite list of points, and should not be confused with pullback of *safe*[\(i\)]
of euclidean distance) to $\overrightarrow{z_{j+1}}$ under the action of layer $j$. Then, we can use this function repeatedly layer by layer to obtain the set of potential counterexamples at the input. Here, $D$ is a parameter that we tune.

Note that the pullback of $\overrightarrow{z_{j+1}}$ across the linear layer given by $W_j$ and $\overrightarrow{b_j}$ is the $\overrightarrow{x}$ satisfying $\overrightarrow{x}W_j + \overrightarrow{b_j} - \overrightarrow{z_{j+1}} = 0$. Pulling this region back over $\text{Relu}$ is in general hard, since there are potentially exponentially many quadrants to consider. However, if we pick a quadrant, the action of $\text{Relu}$ reduces to a linear transform setting the negative axes to 0. Then, if this linear transform is $\Pi$, the pullback within this quadrant are the $\overrightarrow{x}$ satisfying $\overrightarrow{x}\Pi W_j + \overrightarrow{b_j} - \overrightarrow{z_{j+1}} = 0$. Now, say $A_j$ is given by $\exists \overrightarrow{\alpha}: \overrightarrow{x} = \overrightarrow{\alpha} B_j + \overrightarrow{c_j}, |\overrightarrow{\alpha}| \leq \overrightarrow{b_j}$. Then, we generate several possible values of $|\overrightarrow{\alpha}| \leq 1$ randomly. Corresponding to these we get several $\overrightarrow{z_j} = \overrightarrow{\alpha} B_j + \overrightarrow{c_j}$ in $A_j$. For each such $\overrightarrow{z_j}$, we find the pullback of $\overrightarrow{z_{j+1}}$ in the quadrant to which $\overrightarrow{z_j}$ belongs using the method described above. This gives us a large list of points in $A_j$ from a variety of different quadrants.

The probability of any of the $\overrightarrow{z_j}$ generated being an approximate pullback is still quite low, as they have essentially been randomly generated. To improve this probability, we move the $\overrightarrow{\alpha}$ in the direction which causes $\overrightarrow{\alpha} B_j \Pi W_j + \overrightarrow{c_j} \Pi W_j + \overrightarrow{b_j} - \overrightarrow{z_{j+1}} = \overrightarrow{z_j} \Pi W_j + \overrightarrow{b_j} - \overrightarrow{z_{j+1}}$ to come closest to 0 as far as we can without the bounds on $\alpha$ being violated. This brings the $\text{Relu}$ image of $\overrightarrow{z_j}$ as close to $\overrightarrow{z_{j+1}}$ as possible. We now simulate the $\overrightarrow{z_j}$ for one layer, and discard those that lead to points farther than $D$ from $\overrightarrow{z_{j+1}}$ under the action of the layer, to get our required list of points. Note that this step can end up eliminating all the $\overrightarrow{z_j}$, in which case the approximate pullback of the counterexample fails.

As we repeat this process for previous layers, the distance of the approximate pullbacks from the original counterexample increases by a factor of $D$. To counteract this, we scale $D$ down by the number of layers at the beginning of the algorithm.

4.6 Example (continued from Sect. 3.1)

Consider the neural network shown in Fig. 2. Here, we have separated the result of computing the weighted sum from that of the application of the $\text{Relu}$ into separate nodes, represented by dashed and solid circles respectively. Also, we show the weights as labels on the arrows coming into a combination point, and biases as labels of arrows emerging from the point. The arrows for weights that are 0 have been omitted. The values at (output of) each node in the network for the input in the range $[0.5, 0]$ are shown in the diagram at that node.

This network has the following symmetry property: $0 \leq x_{00}, x_{01}, x'_{00}, x'_{01} \leq 1 \land x_{00} = x'_{01} \land x_{01} = x'_{00} \Rightarrow |[x_{40} x_{41}] - [x'_{40} x'_{41}]| \leq 0.1$. This expresses the fact that flipping the inputs leads to the outputs being flipped.

**Preprocessing:** The $W_i$ and $\overrightarrow{b_i}$ are calculated as follows: If the weights and bias of layer $i$ are $W^o$ and $\overrightarrow{b^o}$, then $W_i = [W_i^0 0\ W_i^o]$ and $\overrightarrow{b_i} = [\overrightarrow{b^o} \overrightarrow{b^o}]$ as we need...
to track both the original and permuted values at each layer. For this example we have:

\[
W_0 = \begin{bmatrix}
1000 & -1000 & 1000 & -1000 & 0 & 0 & 0 & 0 \\
-1000 & 1000 & -1000 & 1000 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1000 & -1000 & 1000 & -1000 \\
0 & 0 & 0 & 0 & -1000 & 1000 & -1000 & 1000
\end{bmatrix}
\]

\[
\vec{b}_0 = [0 0 -1 -1 0 0 -1 -1]
\]

\[
W_1 = \begin{bmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
-1 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & -1 & 0 \\
0 & 0 & 0 & -1
\end{bmatrix}
\]

\[
\vec{b}_1 = [0 0 0 0]
\]

**Action of initPre and initPost:** Now, initPre calculates reach[0] as the following affine region given by basis \(B_0\) and center \(\vec{c}_0\), and initPost expresses safe[2] as a convex polytope:

### reach[0]:

\[
\exists \vec{a} : \vec{x}_0 = \vec{c}_0 + \vec{a} \cdot B_0, \quad |\vec{a}| \leq 1
\]

\[
B_0 = \begin{bmatrix}
0.5 & 0 & 0 & 0.5 \\
0 & 0.5 & 0.5 & 0
\end{bmatrix}
\]

\[
\vec{c}_0 = [0.5 \ 0.5 \ 0.5 \ 0.5]
\]

### safe[2]:

\[
\begin{bmatrix}
1 & 0 & -1 & 0 \\
0 & 1 & 0 & -1 \\
0 & -1 & 0 & 1 \\
-1 & 0 & 1 & 0
\end{bmatrix} \begin{bmatrix}
\vec{x}_0 \\
\vec{x}_1 \\
\vec{x}_2 \\
\vec{x}_3
\end{bmatrix} \leq \begin{bmatrix}
0.1 & 0.1 & 0.1 & 0.1
\end{bmatrix}
\]

(3)

**Forward Propagation:** ForwardPropagate then propagates across the layers to get affine regions that are over-approximations for the reachable region.

Fig. 2. \(\sigma = (0\rightarrow 1, 1\rightarrow 0), \ g = 1000\)
for that layer. While propagation across the linear layer can be done easily via matrix multiplication, propagating across the \textit{Relu} layer is in general is hard, since we need to take into account all possible branching behaviors. We do this via a tie class analysis (section 4.2) that exploits the inherent symmetry of the network and precondition. For this network, propagating across the first linear layer gives us an affine region given by the basis and center:

\[
B'_0 = \begin{bmatrix} 500 & -500 & 500 & -500 & 500 & -500 & 500 & -500 \\ -500 & 500 & -500 & 500 & 500 & -500 & 500 & -500 \\ \end{bmatrix}, \quad \vec{c}'_0 = [0 0 -1 -1 0 0 -1 -1]
\]

Then, propagating across the \textit{Relu} using the tie class analysis (section 4.2) gives us the basis \(B_1\) and center \(\vec{c}_1\) for \textit{reach}[1]. Similarly, the algorithm propagates across the second layer to get \(B'_1, \vec{c}_1, B_2\) and \(\vec{c}_2\). In this case, the affine region before and after the \textit{Relu} turn out to be the same, and there is no loss in precision going from \(B'_1\) to \(B_2\). The matrices are:

\[
\begin{align*}
B_1 &= \begin{bmatrix} 500 & 0 & 0 & 0 & 0 & 500 & 0 & 0 \\ -500 & 0 & 0 & 0 & 0 & -500 & 0 & 0 \\ 0 & -500 & 0 & 0 & -500 & 0 & 0 & 0 \\ 0 & 500 & 0 & 0 & 500 & 0 & 0 & 0 \\ 0 & 0 & 500 & 0 & 0 & 0 & 0 & 500 \\ 0 & 0 & -500 & 0 & 0 & 0 & 0 & -500 \\ 0 & 0 & 0 & -500 & 0 & 0 & -500 & 0 \\ 0 & 0 & 0 & 500 & 0 & 0 & 500 & 0 \\ \end{bmatrix} \\
\vec{c}_1 &= [0 0 0 0 0 0 0 0] \\
\end{align*}
\]

\[
\begin{align*}
B'_1, B_2 &= \begin{bmatrix} 500 & 0 & 0 & -500 \\ -500 & 0 & 0 & 500 \\ 0 & -500 & -500 & 0 \\ 0 & 500 & 500 & 0 \\ -500 & 0 & 0 & -500 \\ 500 & 0 & 0 & 500 \\ 0 & 500 & 500 & 0 \\ 0 & -500 & -500 & 0 \\ \end{bmatrix} \\
\vec{c}_1', \vec{c}_2 &= [0 0 0 0] \\
\end{align*}
\]

\[
(4)
\]

Inclusion check: Now, we see that if we substitute \(\vec{r}'\) with the form given in \textit{reach}[2] into \textit{safe}[2] (which is the postcondition \(\|x_{40} x_{41} - [x'_{40} x'_{41}]\| \leq 0.1\)), the right side of the inequality simplifies to 0. So, \textit{reach}[2] is included in \textit{safe}[2]. This is done by an algorithm (section 4.4) that checks this using an LP solver, and since it succeeds in this case, it returns \textit{property holds}.

Note that for this example, it was unnecessary to perform any back propagation of the \textit{safe}[i] to previous layers, as the inclusion check succeeded at the output layer. In general, back propagation (section 4.3) would be performed to compute under-approximations. Spuriousness check (section 4.5) will be needed if the inclusion check fails.
5 Experiments

We have demonstrated our algorithm using a prototype implementation written in python\(^8\). As an additional step after tie-class analysis, we optimise the basis obtained by removing linearly dependent vectors using singular value decomposition. Numerical calculations including matrix multiplication and singular value decomposition were done using the *numpy* library. For the inclusion checks, the LP solver provided in the *scipy* library was used. All times are in reported here are in seconds. All the experiments were run on an Intel i7 9750H processor with 6 cores and 12 threads with 32 GB RAM.

We have compared our algorithm with the Marabou \cite{11,12} implementation of the Reluplex \cite{10} on a few DNNs of various sizes with the following target behavior: for \(n\) inputs, there should be \(n\) outputs so that if input \(i\) is the largest among all the inputs, output \(i\) should be 1. These networks have three layers excluding the input layer, with sizes \(2n(n-1), n(n-1)\) and \(n\) respectively. We check the following permutation invariance property:

\[
0 \leq \overrightarrow{x} \leq 1 \Rightarrow |\sigma(N(\overrightarrow{x})) - N(\sigma(\overrightarrow{x}))| \leq \epsilon
\]

Where \(\sigma\) represents the permutation sending \(1 \rightarrow 2, 2 \rightarrow 3, \ldots, n \rightarrow 1\) cyclically, and \(\epsilon\) varies across the experiments. Note that if the network follows the target behavior exactly, then this property should hold.

We first demonstrate our algorithm on a set of hand-crafted networks for which we have manually fixed the weights. The first layer has two neurons \(p_{i,j}\) and \(q_{i,j}\) for each pair \((i, j)\) of inputs. The input to the *Relu* for these neurons are \(1000(i-j)\) and \(1000(i-j) - 1\) respectively. The second layer has one neuron \(r_{i,j}\) for each pair \((i, j)\) of inputs, and the input to it’s *Relu* is \(p_{i,j} - q_{i,j}\). The output layer has one output \(s_i\) for each input \(i\), with \(2 \sum_j r_{i,j} - 2n + 3\) being fed into it’s *Relu*. Intuitively, \(r_{i,j}\)’s output is designed to be 1 whenever \(i\) is considerably bigger than \(j\), and 0 otherwise, and \(s_i\) calculates \(\land_j (i > j)\), achieving the desired behavior.

This hand-crafted DNN for this example is quite symmetric, in that the intermediate calculations being performed are symmetrically linked to the input. That is, permuting the inputs leads to a more complicated permutation of the intermediate layers. Thus, intuitively it should be easy to to prove the symmetry property we have described. However, as the input to the network varies within the precondition region, the input to the *Relu* nodes regularly switch between positive and negative. This can potentially lead to exponentially many case-splits unless an effective abstraction is used. Table 1 compares the time taken by our algorithm and by Marabou on these networks. Our algorithm converges very quickly in every case whereas Marabou times out (after 100 seconds) in all but the smallest case. The test result demonstrates that the over-approximation and under-approximation used in our algorithm form an effective abstraction for this example, and is likely to be so for similar, symmetric networks. Note that in the

\(^8\) We will be submitting an artifact containing all the benchmarks, our implementation, and the scripts to reproduce our experimental results.
table when a time is given as \( t \), it is denoting that a timeout was declared after \( t \) seconds.

### Table 1. Comparison of Marabou and Our Algorithm on Safe Synthetic Networks

| Number of Inputs | Size of Network | Our Algorithm Time | Splits |
|------------------|-----------------|---------------------|-------|
| 3                | 21              | 0.074               | 4.833 | 2046 |
| 4                | 40              | 0.112               | > 100.8 | > 11234 |
| 5                | 65              | 0.163               | > 101.9 | > 5186 |
| 6                | 96              | 0.269               | > 100.1 | > 2243 |
| 7                | 133             | 0.493               | > 106.8 | > 1533 |
| 8                | 176             | 0.911               | > 126.5 | > 475 |
| 9                | 225             | 1.477               | > 183.9 | > 467 |
| 10               | 280             | 2.276               | > 158.7 | > 394 |

We also test our algorithm on an unsafe problem using the same hand-crafted network from the previous example. To do so, we change the permutation on the output side to be the identity permutation. As permuting the inputs cyclically should not leave the outputs unchanged, we should always find a counterexample in these tests. The results are given in Table 2 and show that our counterexample search is able to find counterexamples in a way that is competitive with Marabou, especially for networks with 8 or more inputs.

### Table 2. Comparison of Marabou and Our Algorithm on Unsafe Synthetic Networks

| Number of Inputs | Size of Network | Our Algorithm | Marabou Time | Splits |
|------------------|-----------------|---------------|--------------|-------|
| 3                | 21              | 0.048         | 0.187        | 68    |
| 4                | 40              | 0.074         | 0.202        | 38    |
| 5                | 65              | 0.132         | 0.267        | 47    |
| 6                | 96              | 0.233         | 0.603        | 60    |
| 7                | 133             | 0.422         | 1.085        | 64    |
| 8                | 176             | 0.809         | 71.89        | 299   |
| 9                | 225             | 1.508         | 5.011        | 91    |
| 10               | 280             | 2.157         | 29.09        | 202   |

Finally, we compare the performance of our algorithm with Marabou on some DNNs for the same problem that have been trained using stochastic gradient descent to have the target behavior described above. A large number of randomly generated input points and the corresponding 1-hot output vectors were used as the training data. Note that unlike the hand-crafted networks, for the trained networks we have no guarantee that the property will hold. The accuracy column tracks the percentage of test inputs for which the property holds. We compare the algorithms on trained networks of various sizes, and with various values of
Table 3. Comparison of Marabou and Our Algorithm on Trained Networks (INCONS denotes that the algorithm returned inconclusive; TO denotes a timeout; SAFE denotes that the property was proved; CEX denotes that the property was refuted and a counterexample was returned)

| n | Size | \(\epsilon\) | Accuracy | Our Algorithm | Marabou |
|---|------|--------------|----------|---------------|---------|
|   |      |             |          | Time | Result | Time | Splits | Result |
| 3 | 21   | 0.1         | 94.0%    | 0.023 | CEX    | 0.023 | 10      | CEX    |
| 3 | 21   | 0.3         | 99.5%    | 0.109 | CEX    | 0.028 | 15      | CEX    |
| 3 | 21   | 0.5         | 100%     | 0.249 | INCONS | 0.034 | 16      | CEX    |
| 3 | 21   | 0.7         | 100%     | 0.158 | INCONS | 1.335 | 320     | SAFE   |
| 3 | 21   | 0.9         | 100%     | 0.204 | INCONS | 1.330 | 274     | SAFE   |
| 4 | 40   | 0.1         | 98.3%    | 0.057 | CEX    | 0.375 | 47      | CEX    |
| 4 | 40   | 0.3         | 99.1%    | 0.114 | CEX    | 0.495 | 51      | CEX    |
| 4 | 40   | 0.5         | 99.8%    | 0.112 | CEX    | 0.464 | 50      | CEX    |
| 4 | 40   | 0.7         | 99.9%    | 0.110 | CEX    | 0.426 | 48      | CEX    |
| 4 | 40   | 0.9         | 100%     | 0.119 | CEX    | 0.418 | 49      | CEX    |
| 5 | 65   | 0.1         | 97.1%    | 0.197 | CEX    | 0.684 | 35      | CEX    |
| 5 | 65   | 0.3         | 98.5%    | 0.209 | CEX    | 0.708 | 35      | CEX    |
| 5 | 65   | 0.5         | 99.5%    | 0.188 | CEX    | 0.682 | 35      | CEX    |
| 5 | 65   | 0.7         | 99.7%    | 0.202 | CEX    | 0.699 | 36      | CEX    |
| 5 | 65   | 0.9         | 99.9%    | 0.224 | CEX    | 21.26 | 563     | CEX    |
| 6 | 96   | 0.1         | 98.0%    | 0.012 | CEX    | 3.070 | 85      | CEX    |
| 6 | 96   | 0.3         | 98.6%    | 0.018 | CEX    | 3.138 | 85      | CEX    |
| 6 | 96   | 0.5         | 99.2%    | 0.014 | CEX    | 3.314 | 85      | CEX    |
| 6 | 96   | 0.7         | 99.4%    | 0.013 | CEX    | 3.327 | 85      | CEX    |
| 6 | 96   | 0.9         | 99.7%    | 0.012 | CEX    | 3.292 | 85      | CEX    |
| 7 | 133  | 0.1         | 87.5%    | 0.011 | CEX    | 5.651 | 84      | CEX    |
| 7 | 133  | 0.3         | 96.1%    | 0.012 | CEX    | 5.810 | 86      | CEX    |
| 7 | 133  | 0.5         | 98.1%    | 1.153 | CEX    | 5.991 | 84      | CEX    |
| 7 | 133  | 0.7         | 98.7%    | 1.081 | CEX    | 5.957 | 84      | CEX    |
| 7 | 133  | 0.9         | 99.5%    | 1.229 | CEX    | 113.6 | 531     | CEX    |
| 8 | 176  | 0.1         | 65.7%    | 0.012 | CEX    | 44.42 | 258     | CEX    |
| 8 | 176  | 0.3         | 68.5%    | 1.584 | CEX    | 42.80 | 258     | CEX    |
| 8 | 176  | 0.5         | 71.3%    | 1.586 | CEX    | 43.60 | 258     | CEX    |
| 8 | 176  | 0.7         | 73.1%    | 1.630 | CEX    | 43.23 | 258     | CEX    |
| 8 | 176  | 0.9         | 75.6%    | 1.550 | CEX    | 44.60 | 258     | CEX    |
| 9 | 255  | 0.1         | 58.4%    | 1.193 | CEX    | > 120.3 | > 228 | TO |
| 9 | 255  | 0.3         | 70.2%    | 1.310 | CEX    | > 127.9 | > 179 | TO |
| 9 | 255  | 0.5         | 83.3%    | 1.336 | CEX    | > 132.5 | > 225 | TO |
| 9 | 255  | 0.7         | 93.3%    | 1.350 | CEX    | > 131.6 | > 215 | TO |
| 9 | 255  | 0.9         | 98.4%    | 2.159 | CEX    | > 133.5 | > 217 | TO |
| 10 | 280 | 0.1         | 20.8%    | 4.040 | CEX    | > 130.4 | > 58 | TO |
| 10 | 280 | 0.3         | 31.0%    | 3.966 | CEX    | > 125.0 | > 58 | TO |
| 10 | 280 | 0.5         | 39.7%    | 4.100 | CEX    | > 124.3 | > 58 | TO |
| 10 | 280 | 0.5         | 50.5%    | 3.991 | CEX    | > 130.1 | > 58 | TO |
| 10 | 280 | 0.5         | 62.3%    | 4.063 | CEX    | > 125.4 | > 58 | TO |
The results (Table 3) show that our algorithm compares quite favorably with Marabou, especially as the network size increases. Though small in number, our benchmarks are challenging due to their size and complexity of verification. We attribute the efficiency of our approach to a number of design elements that are crucial in our approach—a layer by layer analysis, abstractions (that help reduce case-splits), under-approximations (that lead to good counterexamples), algebraic manipulations instead of LP/SMT calls, etc. A downside of our algorithm is that it may sometimes return inconclusive. A counterexample-guided refinement procedure can help tackle this issue.

6 Related Work

The field of DNN verification has gained significant attention in the last several years. DNNs are being used more and more in safety- and business-critical systems, and therefore it becomes crucial to formally argue that the presence of ML components do not compromise on the essential and desirable system-properties. Efforts in formal verification of neural networks have relied on abstraction-refinement [14,13], constraint-solving [11,18,3,1], abstract interpretation [7,15,16], layer-by-layer search [8,19], two-player games [20], and several other approaches [9,21].

The most closely related work to ours is using a DNN verification engine such as Reluplex [10] and Marabou [11,12] to verify permutation invariance properties by reasoning over two copies of the network. Reasoning over multiple copies also comes up in the context of verifying Deep Reinforcement Learning Systems [6]. However, verification of DNNs is worst-case exponential in the size of the network and therefore our proposal to handle permutation invariance directly (instead of multiplying the network-size) holds a lot of promise.

Polytope propagation has been quite useful in the context of neural network verification (e.g [17,22]). In the case of forward propagation, however, it requires computing the convex hull each time, which is an expensive operation. In contrast, our tie-class analysis helps us propagate the affine regions efficiently. In the backward direction, even though we rely on convex polytope propagation, we mitigate the worst-case exponential blow-up by using a 2-polytope underapproximation method that does not depend on LP or SMT solving, and is both scalable and effective.

In general, the complexity of a verification exercise can be mitigated by abstraction-refinement techniques; in particular, technique such as [5] for DNN verification. The essential idea is to let go of an exact computation, which is achieved by merging of neurons in [5]. In [13], the authors propose construction of a simpler neural network with fewer neurons, using interval weights such that the simplified network over-approximates the output range of the original neural network. Our work is similar in spirit, in that it avoids exact computation unless really necessary for establishing the property. In practice, these techniques can even be used complementary to one another.
7 Conclusion

We presented a technique to verify permutation invariance in DNNs. The novelty of our approach is a useful tie-class analysis, for forward propagation, and a scalable 2-polytope under-approximation method, for backward propagation. Our approach is sound (not just for permutation invariance properties, but for general safety properties too), efficient, and scalable. It is natural to wonder whether the approximately computed (reachable and safe) regions may be refined to eliminate spurious counterexamples, and continue the propagation till the property is proved or refuted. Our approach is definitely amenable to a counterexample-guided refinement. In particular, the spurious counterexamples can guide us to split \textit{ReLU} nodes (to refine over-approximations), and add additional safe regions (to refine under-approximations). This would require us to maintain sets of affine regions and convex polytopes at each layer, which is challenging but an interesting direction to pursue.

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A Proofs

In the following proofs, we refer to the input affine region over-approximating the points before the $\text{Relu}$ by $A$, given by basis $B$ and center $c$.

Lemma 1 Given $\mathbf{x} = \sum_i \alpha_i \mathbf{v}_i + c$, we can write $\text{Relu}(\mathbf{x}) = \sum_i \alpha_i \mathbf{v}_i^{\prime} + \sum_j \beta_j \mathbf{c}_j^{\prime}$ where each $\alpha_i^{\prime}$ is either $\alpha_i$ or is 0, and each $\beta_j$ is either 0 or 1. Moreover, the components of $\text{Relu}(\mathbf{x})$ with indices in a tie class $j$ are 0 if and only if $\alpha_i^{\prime}$ and $\beta_j$ are 0.

Note: Here $i$ is an index for the components of vectors, and varies between 0 and $n - 1$, where $n$ is the dimension of the underlying space. Say there are $t$ tie classes. Then, $j$ is an index for the tie class and varies between 0 and $t - 1$. Thus, there are a total $tn$ terms in $\sum_i \alpha_i^{\prime} \mathbf{v}_i$ and $t$ in $\sum_j \beta_j \mathbf{c}_j$.

Proof. We are given an $\mathbf{x} = \sum_i \alpha_i \mathbf{v}_i + c$. Since each pair of components of $\mathbf{x}$ in each tie class never have different signs, all the components of $\mathbf{x}$ in any given tie class will have the same sign.

Say the components whose indices are in the tie classes $j_1, j_2, \cdots, j_k$ have positive sign, the rest all have non-positive sign. Then, for any component of $\text{Relu}(\mathbf{x})$ whose index is in some $j_l$, $1 \leq l \leq k$, their value will be the same as that of $\mathbf{x}$, as their corresponding component of $\mathbf{x}$ is positive. On the other hand, if the component’s index is not in any $j_l$, it will be 0 since the corresponding component of $\mathbf{x}$ is negative.

Now consider the sum of vectors, $\sum_i \alpha_i \mathbf{v}_i^{\prime} + \mathbf{c}_j^{\prime}$ for some $j_l, 1 \leq l \leq k$. There are $n$ many $\mathbf{v}_i^{\prime}$s in this sum. For indices in $j_l$ the values of the components of $\mathbf{v}_i^{\prime}$ and $\mathbf{v}_i$ are the same for the same $i$, and the component of $\mathbf{c}_j^{\prime}$ is the same as that of $\mathbf{c}_j$. So, for these indices, the component of $\sum_i \alpha_i \mathbf{v}_i^{\prime} + \mathbf{c}_j^{\prime}$ is the same as that of $\mathbf{x}$. For any index outside $j_l$, the components of all the index $\mathbf{v}_i^{\prime}$ and that of $\mathbf{c}_j^{\prime}$ is 0. So, for these indices, the component of $\sum_i \alpha_i \mathbf{v}_i^{\prime} + \mathbf{c}_j^{\prime}$ is 0.

Now, consider the following sum of terms of the above form, with $k$ many terms. This is a sum that involves $nk$ many $\mathbf{v}_i^{\prime}$, while the rest of the $n(t - k)$ of these $\mathbf{v}_i^{\prime}$ may be considered to have a zero component here. Similarly, there are $k$ $\mathbf{c}_j^{\prime}$s, and $t - k$ $\mathbf{c}_j$ may be considered to have 0 components.

$$\sum_i \alpha_i \mathbf{v}_i^{\prime} \mathbf{v}_i + \sum_i \alpha_i \mathbf{v}_i^{\prime} \mathbf{v}_i + \sum_i \alpha_i \mathbf{v}_i^{\prime} \mathbf{v}_i + \cdots + \sum_i \alpha_i \mathbf{v}_i^{\prime} \mathbf{v}_i$$

For any index in some $j_l, 1 \leq l \leq k$, the component of $\sum_i \alpha_i \mathbf{v}_i^{\prime} + \mathbf{c}_j^{\prime}$ has the same value as $\mathbf{x}$, while the components of all the other terms are 0. Thus, the component of the sum is the same as that of $\mathbf{x}$. For any index not in any $j_l$, the components of all the terms are 0, so the component of the sum is 0. Hence, we have that the sum is $\text{Relu}(\mathbf{x})$. 

Thus, we can set $\alpha'_{il}$ to $\alpha_i$ for all $jl$, and for other tie classes, we can set $\alpha_i$ to 0. Similarly, we can set $\beta_{jl}$ to 1 for all $jl$, and other tie classes we set $\beta_j$ to 0. This gives us an expression for $\text{Relu}(x)$ of the required form. Also, we see that the components of $\text{Relu}(\vec{c})$ with indices in a tie class $j$ are 0 if and only if $\alpha'_{ij}$ and $\beta_j$ are 0.

To prove theorem 1, we prove two intermediate lemmas.

**Lemma 3.** For any given tie class $j$, the components of $\vec{c}$ in the tie class are either all positive, or all non-positive.

**Proof.** This comes directly from the definition of tie class. We notice that if we set all $\alpha_i$ to 0, we get that $\vec{c}$ is a vector in $A$. Then, by definition, it’s components that are in the same tie class will all be positive, or all be negative. $\square$

**Lemma 4.** Given two vectors $\vec{a}$ and $\vec{b}$ and a tie class $j_0$ so that:

1. $\vec{a}$ and $\vec{a} + \vec{b}$ are in $A$
2. the nonzero components of $\vec{a}$ all have indices in $j_0$
3. for any index $i$, if the $i$ component of $\vec{b}$, $b_i \neq 0$, then $i \in j_0$.
4. the components of $\vec{a}$ and $\vec{a} + \vec{b}$ with indices in $j_0$ have different signs

then there is a $0 \leq \gamma \leq 1$ so that $\vec{a} = -\gamma \vec{b}$.

**Proof.** Let $\vec{d} = \vec{a} + \vec{b}$. As $\vec{a}$ and $\vec{d}$ are in $A$, we have:

$$\vec{a} = \sum_i \alpha_i \vec{v}_i^a + \vec{c}$$

$$\vec{d} = \sum_i \alpha_i \vec{v}_i^d + \vec{c}$$

For some $-1 \leq \alpha_i^a, \alpha_i^d \leq 1$. Now, for any real $0 < \gamma < 1$

$$\vec{a} + \gamma \vec{b} = (1 - \gamma) \vec{a} + \gamma \vec{d}$$

$$= \sum_i ((1 - \gamma) \alpha_i^a + \gamma \alpha_i^d) \vec{v}_i + \vec{c}$$

As $-1 \leq (1 - \gamma) \alpha_i^a + \gamma \alpha_i^d \leq 1$, $\vec{a} + \gamma \vec{b}$ lies in $A$. All nonzero components of $\vec{a}$ and $\vec{b}$ have indices that lie in the same tie class $j_0$, and so all nonzero components of $\vec{a} + \gamma \vec{b}$ have indices in $j_0$ as well. By definition of tie class, for any $0 < \gamma < 1$, all these components must have the same sign. So, all components of $\vec{a} + \gamma \vec{b}$ with indices in $j_0$ have the same sign.
Now, consider the function that takes $\gamma$ to a component of $\vec{a} + \gamma \vec{b}$ with an index belonging to $j_0$. This is a real valued function on $(0, 1)$. At $\gamma = 0$, $\vec{a} + \gamma \vec{b} = \vec{a}$, and at $\gamma = 1$, $\vec{a} + \gamma \vec{b} = \vec{a} + \vec{b}$. So the value of the function at 0 and 1 must have opposite signs. Then, there is some $0 \leq \gamma_0 \leq 1$ for which the value of the function is 0. But, since all the components of $\vec{a} + \gamma \vec{b}$ with indices in $j_0$ have the same sign, all these components must be zero. All other components of $\vec{a} + \gamma \vec{b}$ is zero as well. So, we have:

$$\vec{a} + \gamma \vec{b} = 0 \Rightarrow \vec{a} = -\gamma \vec{b}$$

\[\square\]

**Theorem**

Given a $\vec{x} = \sum_i a_i \vec{v}_i + \vec{c}$, $|\alpha_i| \leq 1$ in $A$, there are scalars $\alpha_i^{ij}$ so that:

1. $\text{Relu}(\vec{x}) = \sum_{i,j} \alpha_i^{ij} \vec{v}_i^{ij} + \text{Relu}(\vec{c})$
2. $|\alpha_i^{ij}| \leq 1$ for all $i$ and $j$.

**Proof.** Given any $\vec{x}$ of the given form, we firstly apply lemma 1 to get the following expression for $\text{Relu}(\vec{x})$:

$$\text{Relu}(\vec{x}) = \sum_{i,j} \alpha_i^{ij} \vec{v}_i^{ij} + \sum_j \beta_j \vec{c}_j$$

Where each $\alpha_i^{ij}$ is either 0 or $\alpha_i$, and each $\beta_j$ is 0 or 1.

Now, we know from lemma 3 that for each tie class, the components of $\vec{c}$ are all positive, or all negative. So, each $\vec{c}_j$ is either all positive, or all negative. Thus, we have:

$$\text{Relu}(\vec{c}) = \sum_j \beta_j \vec{c}_j$$

Where $\beta_j$ is 1 if $\vec{c}_j$ has all positive components, and 0 otherwise.

For each tie class $j$, we wish to replace $\sum_j \beta_j \vec{c}_j$ in $\text{Relu}(\vec{x})$ with $\text{Relu}(\vec{c})$ by adjusting the values of $\alpha_i^{ij}$. So, it suffices to find $\alpha_i^{''ij}$ so that the following holds:

$$\sum_i \alpha_i^{''ij} \vec{v}_i^{ij} + \beta_j \vec{c}_j = \sum_i \alpha_i^{''ij} \vec{v}_i^{ij} + \beta_j^{'} \vec{c}_j = \sum_i \alpha_i^{''ij} \vec{v}_i^{ij} + \text{Relu}(\vec{c})$$

To do this adjustment, we look at four cases, depending on the sign of components of $\vec{x}$ in $j$, and the sign of components of $\vec{c}_j$:

**Case 1:** Components of $\vec{x}$ in $j$ and components of $\vec{c}_j$ are both positive. In this case, by lemma 1, $\beta_j$ is 1, and as components of $\vec{c}_j$ are positive $\beta_j^{'}$ is also 1.
So, we can set $\alpha_i^{''ij}$ to $\alpha_i^{ij}$. 
Case 2: Components of \( \vec{x} \) in \( j \) and components of \( \vec{c}_j \) are both negative or 0. In this case, since \( \text{Relu}(\vec{x}) = 0 \) we can simply set \( \alpha_i'' = 0 \).

Case 3: Components of \( \vec{x} \) in \( j \) are positive, but components of \( \vec{c}_j \) are negative or 0. In this case, \( \beta_j' \) is 0, and by lemma \[4\] \( \beta_j \) is 1, and the components of \( \vec{x} \) with indices in the tie class \( j \) are same as that of \( \sum_i \alpha_i v_i^{(j)} + c_j' \), with \( \alpha_i' = \alpha_i \).

Now, if we set \( \vec{d} = \vec{c}_j \) and \( \vec{b} = \sum_i \alpha_i v_i^{(j)} \), we can use lemma \[4\] to get a \( \gamma \) so that:

\[
\vec{d} = -\gamma \vec{b}
\]

\[
\Rightarrow \vec{c}_j = -\gamma \sum_i \alpha_i v_i^{(j)}
\]

\[
\Rightarrow \sum_i \alpha_i v_i^{(j)} + \beta_j c_j = \sum_i (1-\gamma)\alpha_i v_i^{(j)} + \beta_j c_j
\]

Now, as \( 0 \leq \gamma \leq 1 \), we have \( 0 \leq 1-\gamma \leq 1 \), and so if we set \( \alpha_i'' = (1-\gamma)\alpha_i \), we have \( |\alpha_i''| \leq |\alpha_i| \leq 1 \). Thus, we have found the required \( \alpha_i'' \).

Case 4: Components of \( \vec{x} \) in \( j \) are non-positive, but components of \( \vec{c}_j \) are positive. Similarly to case 3, \( \beta_j' \) is 1, and lemma \[4\] gives us \( \beta_j \) and \( \alpha_i' \) are all 0.

Again we set \( \vec{d} = \vec{c}_j \) and \( \vec{b} = \sum_i \alpha_i v_i^{(j)} \) and use lemma \[4\] to get a \( \gamma \) so that:

\[
\vec{d} = -\gamma \vec{b}
\]

\[
\Rightarrow \vec{c}_j = -\gamma \sum_i \alpha_i v_i^{(j)}
\]

\[
\Rightarrow \sum_i \alpha_i v_i^{(j)} + \beta_j c_j = \sum_i \gamma\alpha_i v_i^{(j)} + c_j
\]

Again, we can set \( \alpha_i'' = \gamma \alpha_i \), and as \( 0 \leq \gamma \leq 1 \), the bounds are satisfied.

Thus, given an \( \vec{x} \), for each tie class \( j \) we can always find the required \( \alpha_i'' \), and we are done.

\[\square\]

Theorem 2 Two indices \( i \) and \( j \) are in the same tie class if and only if one of the following is true:

1. The \( i \) and \( j \) components of \( \vec{x} \) are always both positive.
2. The \( i \) and \( j \) components of \( \vec{x} \) are always both negative.
3. The vector formed by the \( i \) and \( j \) components of the \( \vec{v}_k \) and \( \vec{c} \) are parallel.

In other words, if \( v_i^k \) is the \( i \)-component of \( \vec{v}_k \), and \( c_i^l \) is the \( i \)-component of \( \vec{c} \), then \( [v_i^1, v_i^2, \cdots v_i^l, \cdots v_i^s] = k[v_i^1, v_i^2, \cdots c_i^l, \cdots c_i^s] \) for some real \( k > 0 \).

Proof. Forward direction: Say \( i \) and \( j \) are in the same tie class and that 1 and 2 do not hold. We show that 3 must hold.

Since 1 and 2 does not hold, we can take a \( \vec{x}_1^2 \) in \( A \) where both \( i \) and \( j \) components are positive, and a \( \vec{x}_2^2 \) where both are negative. We use an argument similar to the proof of Lemma \[4\].
Consider the line segment joining the two points. The points on this line segment have the form \( \lambda \vec{x}_1 + (1 - \lambda)\vec{x}_2, 0 \leq \lambda \leq 1. \) Since \( A \) is linear, all the points on this line segment are in \( A. \) Consider the \( i \) coordinate of the points on this line. It is positive when \( \lambda = 0, \) and negative when \( \lambda = 1. \) So, for some value of \( \lambda_0, \) the \( i \) coordinate of \( \lambda_0 \vec{x}_1 + (1 - \lambda_0)\vec{x}_2 \) is 0. Since \( i \) and \( j \) are in the same tie class, \( j \) component of this point is also 0. So, if the \( i \) and \( j \) components of \( \vec{x}_1 \) is \( x_i^1 \) and \( x_j^1, \) and that of \( \vec{x}_2 \) be \( x_i^2 \) and \( x_j^2 \) respectively, we have:

\[
\begin{align*}
\lambda x_i^1 + (1 - \lambda)x_i^2 &= 0 \\
\Rightarrow \frac{x_i^1}{x_i^2} &= \frac{\lambda - 1}{\lambda} \\
\end{align*}
\]
and, \( \lambda x_j^1 + (1 - \lambda)x_j^2 = 0 \)

\[
\begin{align*}
\Rightarrow \frac{x_j^1}{x_j^2} &= \frac{\lambda - 1}{\lambda} = \frac{x_i^1}{x_i^2} \\
\Rightarrow \frac{x_i^1}{x_i^2} &= \frac{x_j^1}{x_j^2} = k
\end{align*}
\]

Now, if we pick any \( \vec{x} \neq 0 \) in \( A, \) if it’s \( i \)-component is positive, it’s \( j \) component must also be positive. Then, we can replace \( \vec{x}_1 \) with \( \vec{x} \) in the above argument to derive that the ratio of the \( i \) component to the \( j \) component of \( \vec{x} \) must be \( k. \) Similarly, if \( i \)-component of \( \vec{x} \) is negative, we can replace \( \vec{x}_2 \) with it. So, for any \( \vec{x} \) in \( A, \) the \( i \) component of \( \vec{x} \) is \( k \) times the \( j \) component. Since \( i \) and \( j \) are in the same tie class, \( k \) must be positive.

Let the vector formed by the \( i \) components of \( \vec{v}_i \) and \( \vec{w} \) be, \( \vec{u}_i \) and that from the \( j \) components be \( \vec{w}_j. \) For each \( \vec{x} = \sum \alpha_i \vec{v}_i + \vec{w}, \) we let \( \vec{\alpha} \) be a vector whose last component is 1, and the \( i \) component is \( \alpha_i, \) that is, \( \vec{\alpha} = [\alpha_1 \alpha_2 \cdot \cdot \cdot 1]. \) Then, \( x_i^i = \vec{\alpha} . \vec{u}_i, \) and \( x_i^j = \vec{\alpha} . \vec{w}_j, \) where \( x_i^i \) and \( x_i^j \) are the \( i \) and \( j \) components of \( \vec{x}. \) Quantifying over all \( \vec{x}, \) we have:

\[
\forall \vec{\alpha}, \vec{\alpha} . \vec{u}_i = k \vec{\alpha} . \vec{w}_j \\
\Rightarrow \vec{u}_i = k \vec{w}_j
\]

So, \( u_i \) and \( u_j \) are parallel and we are done with the proof of the forward direction.

**Backward direction:** It is clear that if 1 or 2 hold, \( i \) and \( j \) must be in the same tie class. If 3 holds, we have, borrowing the notation from the proof of the forward direction, some \( k > 0 \) for which:

\[
\vec{u}_i = k \vec{w}_j \\
\Rightarrow \forall \vec{\alpha}, \ vec{\alpha} . \vec{u}_i = k \vec{\alpha} . \vec{w}_j
\]
So, for all $x$ in $A$, $x^i = kx^j, k > 0$, so $x^i$ and $x^j$ have the same sign. Thus, $i$ and $j$ are in the same tie class. This completes the proof of the backward direction.

**Lemma** The maximum and minimum values of $\sum \alpha_i v_i$, for real $\alpha_i$, fixed real $v_i$, constrained by $|\alpha_i| \leq 1$, are $\sum_i |v_i|$ and $-\sum_i |v_i|$ respectively.

**Proof.** Say the maximum is achieved by some set of $\alpha_i$. Then, if for some $i \alpha_i$ and $v_i$ have opposite signs, then inverting the sign of $\alpha_i$ gives us a larger value. So, $\alpha_i$ must have the same sign as $v_i$, and $\alpha_i v_i = |\alpha_i| v_i = |\alpha_i||v_i|$. Now, if we can increase the absolute value of $\alpha_i$, the value of the sum must increase, so we must have $|\alpha_i| = 1$. Thus, the maximum value is given by $\sum_i |v_i|$. If the minimum is less than $-\sum_i |v_i|$, inverting it's sign will give a maximum greater than $\sum_i |v_i|$. The value of $-\sum_i |v_i|$ can be attained by reversing the signs of the $\alpha_i$ that gives us the maximum. So, the minimum must be $-\sum_i |v_i|$.

**B Details of Backpropagation around 0**

As stated in section 4.3, there are two steps for backpropagation around 0. The first step finds one optimal $\vec{n}_R$ satisfying inequality in the input convex polytope $P$. The second step takes the component wise minimum of the $\vec{n}_R$ to get the required $\vec{n}$. Splitting the process of finding the $\vec{n}$ into two steps allows us to reduce this to solving sets of linear equations.

**Optimizing for a single inequality:**

In this step, for each inequality $\vec{x} \cdot \vec{w} \leq u$ in $P$, we find an optimal $\vec{\eta}$ satisfying $\vec{\eta} \cdot \vec{w} \leq u$. If $P$ is given by $\vec{x} L \leq \vec{u}$, then $\vec{w}$ a row of $L$, and $u$ is the corresponding component of $\vec{u}$.

First, we show that we can assume without loss of generality that $w_0^0 = 1$, where $w_0^0$ is the 0 component of $\vec{w}$. We can do this since $\vec{w} \neq 0$, so at least one component is non-zero, and we can call it $w_0^0$. Then, we can scale all other components of $\vec{w}$ and $u$ by $w_0^0$ and set $w_0^0 = 1$ without changing the inequality.

If $\vec{\eta} \cdot \vec{w} < u$, we can increase at least one component of $\vec{\eta}$ keeping the others unchanged, and so we can increase the product. So, an optimal $\vec{\eta}$ must satisfy $\vec{\eta} \cdot \vec{w} = u$. Now, we can substitute $\eta_0$ from $\vec{\eta} \cdot \vec{w} = u$ into $\prod \eta_i$ to get:

$$\prod_{i=0}^{n-1} \eta_i = \left(u - \sum_{i=1}^{n-1} \eta_i v_i\right) \prod_{i=1}^{n-1} \eta_i$$

Now, we use the following standard fact: for any real valued function with $m$ real valued inputs $f(x_1, x_2, \ldots, x_n)$, at an input where $f$ is maximum the partial derivative of $f$ with respect to each $x_i$ must be 0. We define $f$ as:

$$f(\eta_1, \eta_2, \cdots \eta_{n-1}) = \left(u - \sum_{i=1}^{n-1} \eta_i v_i\right) \prod_{i=1}^{n-1} \eta_i$$
Then we can take the partial derivative of $f$ with respect to each $\eta_i$ and equate it to 0 to get conditions that an optimal $\eta_i$ must satisfy:

$$\Rightarrow \frac{\partial f}{\partial \eta_j} = v_j \prod_{i=1}^{n-1} \eta_i + \left( u - \sum_{i=1}^{n-1} \eta_i v_i \right) \prod_{i=j+1}^{n-1} \eta_i = 0$$

$$\Rightarrow v_j \eta_j + u - \sum_{i=1}^{n-1} \eta_i v_i = 0$$

Here we have assumed that no $\eta_i$ is never 0, which we can do since if any $\eta_i$ is 0, the product becomes 0.

Thus, we have reduced finding the optimal $\eta^*_i$ to solving a set of linear equations, one for each $j$. Since 0 lies in the interior of the polytope, and our equation is a constraint in the polytope, we have $u > 0$. So, we can always solve the above equations to get $\eta_i > 0$.

**Finding an $\eta^*$ satisfying all inequalities:** We note that if $\eta^* \cdot \overrightarrow{w} \leq u$ holds then $0 \leq \overrightarrow{x} \leq \eta^* \Rightarrow \overrightarrow{x} \cdot \overrightarrow{w} \leq u$ holds, since all involved vectors are positive. Then, if we find some $\eta^*$ so that $\eta^* \cdot \overrightarrow{w}_k \leq u_k$ holds for all inequalities $\eta^* \cdot \overrightarrow{w}_k \leq u_k$ in the input polytope, we have:

$$\forall k: 0 \leq \overrightarrow{x} \leq \eta^* \Rightarrow \overrightarrow{x} \cdot \overrightarrow{w}_k \leq u_k$$

$$\Rightarrow \quad 0 \leq \overrightarrow{x} \leq \eta^* \Rightarrow \overrightarrow{x} L \leq \overrightarrow{u}$$

To find such an $\eta^*$, we repeat the above process for each inequality in $\overrightarrow{x} \cdot \overrightarrow{w}_k \leq u_k$, and for each we get an set of $\eta^*_k$, one for each inequality. Then, if we take $\eta_i$ as the minimum of $\eta^*_k$ over all $k$, the obtained $\eta^*$ will satisfy all inequalities in $\overrightarrow{x} L \leq \overrightarrow{u}$. 