

# Verification of Recurrent Neural Networks for Cognitive Tasks via Reachability Analysis

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**Abstract.** Recurrent Neural Networks (RNNs) are one of the most successful neural network architectures that deals with temporal sequences, e.g. speech and text recognition. Recently, RNNs have been shown to be useful in cognitive neuroscience as a model of decision-making. RNNs can be trained to solve the same behavioral tasks performed by humans and other animals in decision-making experiments, allowing for a direct comparison between networks and experimental subjects. Analysis of RNNs is expected to be a simpler problem than the analysis of neural activity. However, in practice, reasoning about an RNN’s behaviour is a challenging problem. In this work, we take the formal verification approach to the analysis of RNNs. We make two main contributions. First, we analyse the cognitive domain and formally define a set of useful properties to analyse for a popular experimental task. Second, we employ and adapt well-known verification techniques to our focus domain, i.e. a polytope propagation, an invariant detection and a counter-example guided abstraction refinement, to perform verification efficiently. Our experiments show that our techniques can effectively solve classes of benchmarks that are challenging for the state-of-the-art verification tool.

## 1 Introduction

Deep neural networks are among the most successful artificial intelligence technologies making impact in a variety of practical applications, including computer vision and natural language processing. Recently, RNNs have been employed in cognitive neuroscience to help us to understand decision-making in humans and other animals [22, 25, 36, 28]. However, whether we use neural networks for a computer vision task or for a cognitive task, we would like to better understand the mechanistic process behind this technology.

One way to understand neural networks is to formally analyse their properties. Indeed, formal verification of neural networks is a rapidly growing research area [16, 43, 32]. The main question that verification tackles is: given a network structure and a set of properties, check whether a neural network fulfills these properties. For example, properties may include whether an image is susceptible to an adversarial perturbation in a computer vision classification task [32], or whether a controller avoids unnecessary turning action for an aircraft control problem [16].

Roughly speaking, there are two main approaches in verification: complete and incomplete methods. A complete verification framework guarantees that a method either proves that the property holds

or finds a counterexample to this property. So, if it terminates, then it gives an exact answer regarding satisfaction of a property to check [16, 20]. An incomplete verification framework guarantees that a method either proves a property or it remains unknown whether the property holds. Unlike complete verification methods, incomplete methods do not always provide definite answers to verification questions. However, they are more computationally efficient.

A lot of progress has been made in verifying neural networks over the last few years. The majority of work focuses on analyzing *feed-forward* neural networks [16, 17, 45, 30], while verification of *recurrent* neural networks has received significantly less attention [2, 41]. One reason for this is that, conceptually, verification of recurrent networks is no different from verification of feed-forward networks if we assume that the depth of unfolding is bounded. One can convert a recurrent network to a feed-forward network by unfolding the network’s transition relation for a fixed number of steps [2]. Unfortunately, in practice, the depth of the unfolding can be large since we might need to repeat the transition relation more than hundred times, leading to deep networks. Reasoning about such deep networks is very challenging for both complete methods, where the number of neurons is large, and incomplete methods, where approximation errors accumulate with network depth.

In this work, we propose a novel approach to analyse RNNs. The main idea is to identify and exploit special properties of recurrent networks that allow us to reason about them efficiently. Here we focus on an important special class of recurrent neural networks which are trained to solve cognitive behavioral tasks [34], analogous to the tasks given to human and animal subjects in decision-making studies. Subjects and trained networks exhibit similar task performance as measured by response times and the probability of a correct response across difficulty levels [22]. Additionally, linear projections of RELU unit activations correspond qualitatively and quantitatively to neural activity as measured through electrophysiological recordings [22, 25, 36, 28]. Cognitive tasks can be solved with recurrent networks which have a shallow transition relation, a deep unfolding depth, and, more importantly, have only few modes of operation. The domain specific properties of these networks make them amenable to formal analysis. Our proposed approach employs three building blocks for analysis of these networks: a polytope propagation, an invariant detection and a counter-example guided abstraction refinement (CEGAR). Polytope propagation is feasible (an exact propagation up to some depth and approximate afterward) because the transition relation of RNN is a shallow perception. An invariant detection is possible because we have only few modes of operation and each mode spans over a prolonged time interval. Finally, CEGAR is effective because computed approximate reachability regions are often

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sufficient to prove a property, so only few refinements are necessary.

We make the following contributions. First, we analyse the cognitive domain and define properties of the network that are important to verify in this domain. Second, we propose new methods to verify properties of RNNs. Our approach consists of two phases. We adapt the "easy-to-verify networks" paradigm for training recurrent networks. Then, we perform verification using a hybrid polytope propagation, invariant detection and counter-example guided refinement technique. Third, we perform a comparative analysis of our approach with several modern verification tools. Also, we provide insights why these networks are hard to reason about for existing tools, like SMT-based solvers. Our experimental results demonstrate that our proposed techniques effectively address the verification challenge of the exponential increase of polytopes in reachability analysis, but at the same time being sufficiently precise for the property to check. By our discussion, we also draw attention to the remaining challenge on dealing with the increasing number of facets.

## 2 Background

We give details of feed-forward NNs and Mixed Integer Linear Programming (MILP) in Appendix A of the full version of the paper [1]. **Recurrent Neural Networks.** A *Recurrent Neural Network* (RNN) is a neural network that operates over a sequence of inputs [13]. At each time-step  $k$ , a network consumes an input  $x^k$  and its hidden state  $s^k$ , produces the next hidden state  $s^{k+1}$  and an output  $o^k$ . A simple version of recurrent network can be described using the following transition function:

$$s^{k+1} = f(W_{s \rightarrow s}s^k + W_{x \rightarrow h}x^k + b_s), \quad (1)$$

$$o^k = g(W_{s \rightarrow o}s^k + b_o), \quad (2)$$

where  $f$  and  $g$  are non-linear functions,  $W_{s \rightarrow s}$ ,  $W_{x \rightarrow s}$ ,  $W_{s \rightarrow o}$ ,  $b_s$  and  $b_o$  are parameters to learn. In this work,  $f$  and  $g$  are RELU operators. We define the exact structure of the network in Section 4. If we assume that the length of input is bounded by  $n$ , we can transform an RNN to a feed-forward network by unrolling the transition relation of an RNN for  $n$  time steps, e.g. [13]. There are two main structural differences between feed-forward networks and recurrent neural networks that are relevant from the verification standpoint. The first difference is the depth of the networks. As RNNs operate over long input sequences, unrolling the transition relation leads to deep networks with a large number of layers. Therefore, the resulting unfolded network is very challenging to reason about for both complete and incomplete methods. The second difference is that feed-forward networks apply different linear transformations at each time step, while recurrent networks use the same transformation.

**Polytope and its representation.** We recall the definition of a closed convex polytope (or polytope for short) and its two representations:  $\mathcal{V}$ -polytope and  $\mathcal{H}$ -polytope [15]. A  $\mathcal{V}$ -polytope is a convex hull of a finite set  $Y = \{y^1, \dots, y^n\}$  of point in  $\mathbb{R}^d$ :

$$\mathcal{V}\text{-}\mathcal{P} = \text{conv}(Y) := \left\{ \sum_{i=1}^m \lambda_i y^i \mid \lambda_1, \dots, \lambda_n \geq 0, \sum_{i=1}^n \lambda_i = 1 \right\}$$

An  $\mathcal{H}$ -polytope is the solution of a finite system of linear inequalities:

$$\mathcal{H}\text{-}\mathcal{P} = \mathcal{H}\text{-}\mathcal{P}(A, b) := \{y \in \mathbb{R}^d \mid a_i^T y \leq b_i, i \in [1, m]\}$$

assuming that the set of solutions is bounded, where  $A \in \mathbb{R}^{m \times d}$  is a real matrix with rows  $a_i^T$  and  $b \in \mathbb{R}^m$  is a real vector with entries  $b_i$ .

A *polytope* is a convex closed subset  $P$  of  $\mathbb{R}^d$  that can be represented as a  $\mathcal{V}$ -polytope or an  $\mathcal{H}$ -polytope. We use both representations in our algorithms. There are existing libraries, for example CDD [9] and PPL [5], which provides the functionality for the conversion between the two representations.

**Safe Inductive Invariant of a State Transition System** An RNN can also be treated as state transition system. For a state transition system over state variables  $V$ , input variables  $Inp$  transition relation  $Tr$  and initial states  $Init: \langle V, Inp, Tr, Init \rangle$ , and a set of error states  $Bad$ , a safe inductive invariant is defined as a formula  $Inv$  such that the following formulas are valid:

$$Init(V) \implies Inv(V) \quad (3)$$

$$Inv(V) \wedge Tr(V, Inp, V') \implies Inv(V') \quad (4)$$

$$Inv(V) \wedge Bad(V) \implies \perp \quad (5)$$

The safe inductive invariant  $Inv$ , if it exists, guarantees that the error states are unreachable. Additionally, assumptions on  $Inp$  may be added to describe invariants under a certain input condition.  $Init$  in (3) can be replaced with a state predicate  $p(V)$ , which represents the safe inductive invariant for transitions starting from the particular set of state that satisfies predicate  $p(V)$ .

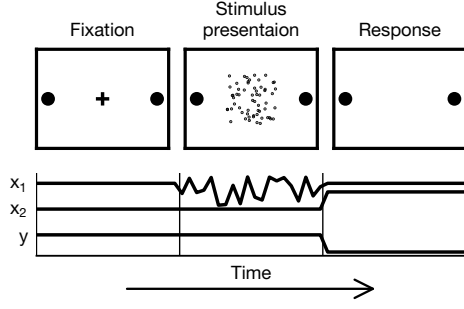
**Interval Arithmetic or Bound Propagation** Interval arithmetic computes the upper and lower bounds for a layer based on the bounds of the previous layer. It is a fast but relatively conservative bound estimation. Recently, Xiao et al. [44] proposed an improvement: to estimate the bound of a layer, it backtracks as much as possible rather than directly using the bounds of the previous layer. This gives a tighter bound without incurring much computational overhead.

## 3 Related work

A *complete verification framework* guarantees that a method either proves that the property holds or finds a counterexample to this property. For example, frameworks like Reluplex [16], Marabou [17], MIPVerify [38] provide complete verification algorithms. These frameworks are based on Satisfiability Modulo Theories (SMT) or/and MILP search engines. The main issue with this approach is scalability. For example, neural networks used for computer vision tasks contain millions of parameters. Theoretically, large networks allow us to generate their formal specifications. However, in practice, these formalizations are challenging to reason about for modern solvers. For example, SMT-based verification frameworks, like Reluplex [16] and Marabou [17], are able to deal with about thousand neurons networks [18]. Another complete verification approach is to perform forward polytope propagation [40, 39]. We start with a polytope that represents the initial space and track how this space changes as we progress through the network. In theory, we can obtain an exact representation of the output space. However, in practice, it faces the challenge of an increasing number of polytopes. Therefore it is usually combined with abstraction techniques [11, 31], which often results in an incomplete verification framework. Compared to the previous work [40] that uses the star set representation, our usage of the generic  $\mathcal{H}$ - and  $\mathcal{V}$ -polytope representation allows making advantage of existing polytope libraries, and it is also more friendly to the convex hull computation and the invariant construction.

An *incomplete verification framework* guarantees that it either proves a property or it remains unknown whether the property holds. Examples of such frameworks are FastLin [43], Crown [45], and DeepZ [30]. The main underlining idea is to perform safe approximate reasoning about behaviour of a NN. If the approximate reasoning is sufficient to prove a property then incomplete methods succeed otherwise they fail. However, if the number of layers is large, e.g. more than hundred layers, over-approximation methods tend to produce loose bounds and are not able to check the property.

Another relevant line of work is on invariant detection in feed forward networks. First, the term invariant has been previously used



**Figure 1.** The random dot motion task [27, 29] as shown to subjects (above), and as adapted for a recurrent neural network via two inputs  $x_1$  and  $x_2$  and one expected output  $y$  (below).

in the verification efforts of feed-forward networks to refer to a region in the input space that can imply a certain output property [21]. In [14], the authors propose to search for invariance properties of the network that are decision patterns of neurons activations in feed-forward networks. In our work, we focus on the region in the input space of a layer whose image (output region) does not fall outside under the same mode of operation. In other words, we are looking at an *inductive* invariant, so our invariants can be computed for a transition relation of an RNN.

#### 4 RNNs for cognitive domains

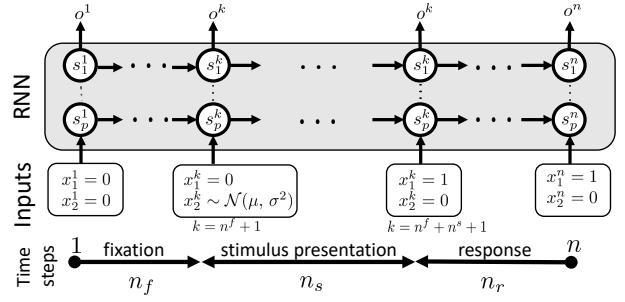
**Cognitive task.** The random dot motion task (Figure 1) [27, 29] is a cognitive task given to humans and other animals in order to study decision-making in the presence of noisy stimuli [12]. In this task, dots on a video screen move in random directions, but with a mean direction either to the left or right. After a fixed duration stimulus presentation, subjects must identify and report this mean direction of motion. Task difficulty varies trial to trial through increased or decreased total strength of motion in either direction, known as motion coherence. Subjects interact with the task using eye movements, as captured by a high-speed camera and real-time eye-tracking software. This task consists of three phases:

- *fixation*: the subject initiates a trial by directing their gaze to the fixation cross at the center of the screen,
- *stimulus presentation*: a moving dots stimulus (sensory evidence) is presented to the subject for a fixed duration of time,
- *response*: the subject responds to the stimulus by directing their gaze to the left or right target, indicating the perceived mean direction of motion.

Successful performance on this task is thought to rely on integrating the noisy sensory evidence across time [23, 24, 27, 12].

To adapt this task for a recurrent neural network (Figure 1), the task elements are encapsulated within two input streams  $x_1$  and  $x_2$ , and the expected output within a single stream  $y$ . The first input  $x_1$  represents the noisy stimulus (sensory evidence) via a Gaussian random variable with fixed variance and non-zero mean, where positive (negative) values indicate perceived rightward (leftward) direction of motion, and zero indicates the lack of the stimulus on the screen. The second input  $x_2$  changes from 0 to 1 to indicate the beginning of the response period, which in this study was fixed to the end of stimulus presentation. The expected output of the network  $y$  represents the horizontal position of an eye movement, which is zero during the fixation and stimulus presentation periods and +1 or -1 for the response period, matching the mean direction of motion in a given trial.

**Overview of the network.** The recurrent neural network is trained



**Figure 2.** An unfolded RNN for  $n$  time steps. At each step the network consumes two inputs and emits an output. The state space is represented by state neurons  $s_j^k$ ,  $j \in [1, p]$ ,  $k \in [1, n]$ . Each mode of operation, fixation, stimulus and response, run for  $n_f$ ,  $n_s$  and  $n_r$  time steps, respectively.

to simulate behavioral patterns of a subject during a cognitive task. Figure 2 shows a schematic representation of the recurrent network. The network operates over  $n$  times steps. As we mentioned above, we observe that the network has three modes of operation mimicking the three phases of the cognitive experiment. We split the interval  $[1, n]$  into three sub-intervals:  $\text{FX} \cup \text{SM} \cup \text{RS} = [1, n]$ . The fixation phase spans over the following interval  $\text{FX} = [1, n_f]$ , the stimulus presentation spans over the interval  $\text{SM} = [n_f + 1, n_f + n_s]$  and the response spans over the interval  $\text{RS} = [n_f + n_s + 1, n_f + n_s + n_r]$ . At each step, the network consumes an input signal  $x^k$  and produces an output signal  $o^k$ ,  $k = 1, \dots, n$ .

**Network specification.** Each input  $x^k$  consists of two input values:  $x_1^k$  and  $x_2^k$ . Figure 1 shows an example of input signal ( $x_1^k$  and  $x_2^k$ ,  $k \in [1, n]$ ). The first input,  $x_1^k$ , corresponds to the stimulus signal. Note that it is constant over the fixation and response phases:

$$\text{if } k \in \text{SM} \text{ then } x_1^k \sim \mathcal{N}(\mu, \sigma^2) \text{ otherwise } x_1^k = 0 \quad (6)$$

Note that during the stimulus presentation phase,  $x_1^k$  are samples from a Gaussian distribution with a task parameters  $\mu$  and  $\sigma$ , where  $\mu > 0$  represents the case when dots (noisy stimuli) move to the left, and  $\mu < 0$  to the right. The second input,  $x_2^k$ ,  $k = 1, \dots, n$ , is an indicator input that signals whether the network is in the response phase or not.

$$\text{if } k \in \text{FX} \cup \text{SM} \text{ then } x_2^k = 0 \text{ otherwise } x_2^k = 1 \quad (7)$$

At each step the network produced an output  $o^k$ ,  $k = 1, \dots, n$ . During the training, we encourage the output signal to stay 0 in  $\text{FX} \cup \text{SM}$  phases, and move toward  $-1/1$  during the response phase.

The transition relation of the network has the following structure,  $k = 1, \dots, n$ :

$$s^{k+1} := F(s^k, x^k) = W_{rec} \text{RELU}(s^k) + W_{in} x^k + b_{rec} \quad (8)$$

$$o^k := O(s^k) = W_{out} \text{RELU}(s^k) + b_{out}, \quad (9)$$

where  $\text{RELU}(z) = \max(z, 0)$ ,  $W_{rec}$  and  $b_{rec}$  are a recurrent connectivity matrix and a bias, respectively,  $W_{in}$  is an input connectivity matrix,  $W_{out}$  and  $b_{out}$  is an output connectivity matrix and a bias, respectively. We recall that the purpose of the network is to mimic the cognitive experiment. During an experiment, the subject makes a decision, e.g. left or right. Hence, the network also has to make a decision. Given a trained RNN  $\mathcal{R}$ , we define a decision function of the network,  $C_{\mathcal{R}}(o)$ , as follows:

$$C_{\mathcal{R}}(o) = \begin{cases} 1 & \text{if } o^k \geq 0.5, \forall k \in [n-r, n], \\ -1 & \text{if } o^k \leq -0.5, \forall k \in [n-r, n], \\ 0 & \text{otherwise,} \end{cases} \quad (10)$$

where  $r$  is a parameter specified by a user. In other words, given an

input  $x$ , we say that the network outputs 1 if the last  $r$  outputs are above 0.5, the network outputs  $-1$  if the last  $r$  outputs are below  $-0.5$  and no decision is made otherwise.

**Training the network.** In order to train the network with a similar reward structure to human and animal subjects, we wanted the network to make a choice of  $\pm 1$  during the response period, even when the stimulus is ambiguous. This reflects the fact that subjects are only rewarded for correct responses, so a random response will be rewarded on 50% of trials but a failure to respond is never rewarded. Under a mean squared error loss, an optimal network would not make a choice if the stimulus was unclear. To encourage the network to guess, we designed a loss function such that a random choice of  $\pm 1$  has a lower expected value than remaining at  $y = 0$ . This was accomplished using a slope proportional to the square root of the error for outputs ranging from  $-1$  to  $1$ , and squared error outside of this region. More concretely, the loss function is defined as

$$\mathcal{L} = \sum_{t \in \text{FX} \cup \text{SM}} (y^t - o^t)^2 + \sum_{t \in \text{RS}} h(y^t, o^t)$$

$$h(y, o) = \begin{cases} 1 + (o \times \text{sign}(y) + 1)^2, & o \times \text{sign}(y) < -1 \\ (|o \times \text{sign}(y) - 1|/2)^{1/2}, & -1 \leq o \times \text{sign}(y) \leq 1 \\ (o \times \text{sign}(y) - 1)^2, & 1 < o \times \text{sign}(y) \end{cases}$$

**Properties of the network.** We highlight several properties relevant to verification of the recurrent networks described above. First, as the network encodes a simple behavioral pattern, the transitions relation can be described with a small numbers of neurons. Second, the network dynamics mimic the three phases of the original experiment, so it has only three modes of operation. We can disregard the first phase during verification because all inputs are constants. Third, the input signal is well defined in the sense that points are sampled from a known distribution. This contrasts with computer vision tasks, where we cannot formally define all images of cars, for example. Finally, the depth of the recurrent network is large, namely hundred layers, as we simulated each trial for 110 time steps.

**Properties to verify.** We define a set of properties for networks that solve the random dot motion task.

**Property 1** checks whether the network always makes the correct choice for a given threshold value  $p > 0$  ( $p' < 0$ ):

$$\min_{k \in \text{SM}} (x_1^k) > p \Rightarrow C_{\mathcal{R}}(o) = 1, \quad (11)$$

$$\max_{k \in \text{SM}} (x_1^k) < p' \Rightarrow C_{\mathcal{R}}(o) = -1. \quad (12)$$

If all stimulus points are above a positive threshold then the network should output 1, otherwise  $-1$ . Here  $p, p'$  are parameters of the property. We can consider a weaker variant of this property:

$$\sum_{k \in \text{SM}} x_1^k > p \Rightarrow C_{\mathcal{R}}(o) = 1; \quad \sum_{k \in \text{SM}} x_1^k < p' \Rightarrow C_{\mathcal{R}}(o) = -1.$$

While classical theories of decision-making [23, 24] suggest that subjects integrate (in the mathematical sense) sensory evidence over time, recent approaches have questioned this perspective [35, 42, 46, 37]. The weaker version of this property tests whether sensory evidence is handled in a sensible way, i.e. when all sensory evidence is in a particular direction, the choice should always be in the specified direction. The stronger version tests whether there exists a stream of sensory evidence which indicates the network is not integrating all available information, i.e. that the mean is sufficiently large in one direction but the network chooses the other direction.

**Property 2** checks whether a single spike at the  $j$ th point triggers a

choice when all other stimulus points suggest the opposite.

$$(x_1^j < p') \wedge (x_1^k > p), k \in S \setminus \{j\} \Rightarrow C_{\mathcal{R}}(o) = 1, \quad (13)$$

$$(x_1^j > p) \wedge (x_1^k < p'), k \in S \setminus \{j\} \Rightarrow C_{\mathcal{R}}(o) = -1. \quad (14)$$

If subjects do not integrate sensory evidence, alternative hypotheses imply that an instantaneous spike in evidence may trigger a choice [42, 37, 35], even if it opposes the mean direction of evidence. This property tests if such a spike is capable of triggering a choice despite consistent sensory evidence in the opposite direction.

In our experiments, we focus on verification of Property 1 and Property 2. We also define the following property for future exploration.

**Property 3** checks whether there exists an input that leads to oscillating output state or a change in decision during the last steps:

$$\max_{k \in [n-r, n]} (|o^k - o^{k-1}|) > 1, \quad (15)$$

where  $r$  is a parameter specified by a user. Subjects experience changes of mind in the random-dot motion task [26]. These changes were not explicitly discouraged in the behavioral task, and likewise, are not explicitly penalized by objective function.

## 5 Overview of the proposed approach

Our approach consists of two phases. In the first phase we train an easier to verify network following ideas from [44]. While we had to adapt this approach to work for recurrent neural networks, we achieved a significant reduction of the network size without losing performance on the main cognitive task (Section 4). We discuss our result of the first phase in Appendix B in the full version [1].

In the second phase, we perform property verification on RNN via reachability analysis. Suppose the property is of the form  $C(s^0, x^0, x^1, \dots) \Rightarrow P(o^n)$ . In reachability analysis, we start from state  $s^0$  and compute the set of states  $\text{Reach}^{(i)} : \{s^i \mid s^i = F(s^{i-1}, x^{i-1}), s^{i-1} \in \text{Reach}^{(i-1)}\}$  for each layer until reaching layer  $n$ , where  $F$  is as defined in (8). Then, we compute the output range based on  $\text{Reach}^{(n)}$  and check if it satisfies  $P$ . To this end, we need to (1) have a representation of the set of reachable states (2) compute the reachable set for each layer till the final output.

We use a finite union of convex polytopes as the representation of the reachable set on a layer. We compute the reachable set layer by layer, which we call *propagating polytopes*. The details are given in Section 6.1. As the number of polytopes usually increases along with the number of layers, we discuss two techniques in Section 6.2 and Section 6.3 to keep the representation tractable.

## 6 Verification of RNNs

In this paper, we use a union of convex polytopes to represent the set of reachable states. This is more precise than other similar representations, such as Zonotope [10]. In particular, our representation captures precisely (i.e., without any over-approximation) the output region of an RNN with ReLU activation functions applied to an input that is a finite union of polytopes.

The core of reachability analysis is to efficiently propagate the reachable set throughout the network. We first introduce the general method of polytope propagation and then present our approaches to tackle the exponential increase of the number of polytopes.

### 6.1 Polytope propagation

The general method of propagating a polytope over a layer is presented in Algorithm 1. The inputs are the parameters of a layer, the linear inequality constraints ( $\mathcal{H}$ -polytope or  $\mathcal{H}$ -representation) of a polytope, and the input constraint.

**Algorithm 1:** PROPAGATEPOLYTOPEONELAYER( $W_{rec}$ ,  $W_{in}$ ,  $b_{rec}$ ,  $H$ ,  $I$ ): Propagate one polytope for one layer.

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**Input:**  $W_{rec}, W_{in}, b_{rec}$ : weights and bias of a layer,  $H$ :  $\mathcal{H}$ -representation of the polytope to propagate,  $I$ : input constraints.  
**Output:**  $P_{out}$ : set of polytopes.

```

1  $P_{out} \leftarrow \emptyset$ ;
2  $F \leftarrow \text{ENCODEMILP}(W_{rec}, W_{in}, b_{rec})$ ;
3  $C \leftarrow H \wedge I \wedge F$ ;
4  $A \leftarrow \text{GETFEASIBLEASSIGNMENTS}(C)$ ;
5 for each  $a \in A$  do
6    $RS \leftarrow \text{RELUSTATUSCONSTR}(a)$ ;
7    $P_{sub} \leftarrow H \wedge I \wedge RS$ ;
8    $V_{sub} \leftarrow \text{GETVERTICES}(P_{sub})$ ;
9    $T \leftarrow \text{GETTRANSFORMMATRIX}(W_{rec}, W_{in}, b_{rec}, a)$ ;
10   $V'_{sub} \leftarrow \text{MATRIXMUL}(T, V_{sub})$ ;
11   $H'_{sub} \leftarrow \text{GETHRESP}(V'_{sub})$ ;
12   $P_{out} \leftarrow P_{out} \cup \{\text{POLYTOPE}(V'_{sub}, H'_{sub})\}$ 
13 return  $P_{out}$ ;
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**The MILP encoding** We follow the MILP encoding from [8] that uses a binary indicator variable for each ReLU activation function. Value 1 of the indicator variable implies the corresponding ReLU is inactive (its output stays 0), and value 0 indicates the ReLU is active (the output is equal to the input). We use the IBM ILOG CPLEX solver to solve the MILP problem. CPLEX computes all feasible assignments of the indicator variables. This is represented by the function GETFEASIBLEASSIGNMENTS in Algorithm 1.

**Example 6.1.** Consider an RNN with two neurons ( $n = 2$ ) and one input, and the following weight matrices:

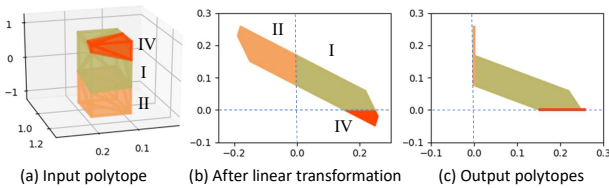
$$W_{rec} = \begin{bmatrix} 0.1 & 0.2 \\ 0.3 & -0.4 \end{bmatrix}, W_{in} = \begin{bmatrix} 0.2 \\ -0.1 \end{bmatrix}, b_{rec} = \begin{pmatrix} -0.2 \\ 0.5 \end{pmatrix}$$

Suppose for a layer  $k$ , a polytope to propagate  $P$  is given as a box  $P : (\hat{s}_0^k, \hat{s}_1^k, x_0^k)^T \in [0.1, 0.2] \times [1.0, 1.2] \times [-1.0, 1.0]$  (where  $\hat{s}^k$  represents  $\max(s^k, 0)$ ). The polytope  $P$  is shown in Figure 3(a). The linearly mapped polytope (before ReLU) is shown in Figure 3(b). By solving the MILP problem, the set of feasible indicator variable assignments is  $\{(0, 0), (1, 0), (0, 1)\}$  for the three pieces I, II and IV, respectively. Each of the three is itself a polytope, which we call a sub-polytope (of  $F(P)$ ).

**Get the representation of each sub-polytope** As shown previously, each indicator variable assignment corresponds to a sub-polytope and a different ReLU mapping. Therefore, we'd like to get the representation of these sub-polytopes, and apply the corresponding mapping separately. The  $\mathcal{H}$ -representation of such polytope can be constructed by adding the corresponding ReLU status constraints, which are generated by the function RELUSTATUSCONSTR in the algorithm. For instance, for sub-polytope II in Example 6.1, its corresponding ReLU status constraints are:

$$\begin{cases} W_{rec}[0, :](\hat{s}_0^k, \hat{s}_1^k)^T + W_{in}[0, :]x_0^k + b_{rec}[0] \leq 0 \\ -W_{rec}[1, :](\hat{s}_0^k, \hat{s}_1^k)^T - W_{in}[1, :]x_0^k - b_{rec}[1] \leq 0 \end{cases}$$

**Apply transformation for each sub-polytope** For each sub-polytope obtained in the previous step, we can construct a linear transformation matrix that captures its unique ReLU mapping, as



**Figure 3.** Polytope propagation on Example 6.1.

**Algorithm 2:** CEGAR( $F, P_{init}, I, T, N, S, U$ ): Polytope propagation using the CEGAR method.

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**Input:**  $F$ : RNN's input-output relation of one layer,  $P_{init}$ : initial polytopes,  $I$ : input constraints,  $T$ : abstraction threshold,  $N$ : number of layers,  $S$ , and  $U$ : safe and unsafe regions, respectively.  
**Output:** SAFE or UNSAFE.

```

1  $PolytopeSet \leftarrow P_{init}$ ;
2 while  $PolytopeSet \neq \emptyset$  do
3    $OutputPolytopes \leftarrow \text{PROPAGATEPOLYTOPE}(F, S, I, T, N)$ ;
4    $PolytopeSet \leftarrow \emptyset$ ;
5   for each  $p \in OutputPolytopes$  do
6     if  $p \subseteq U$  then return UNSAFE;
7     if  $p \subseteq S$  then continue;
8      $layer, P_{precise} \leftarrow \text{GETPRECISE}(p)$ ;
9     if  $layer = N$  then return UNSAFE;
10     $PolytopeSet \leftarrow PolytopeSet \cup P_{precise}$ 
11 return SAFE;
```

---

well as the same linear mapping related to the weights and bias. Such matrix operates on the vertex representation (which can be obtained from  $\mathcal{H}$ -representation using conversion functions in libraries like PPL or CDD, as represented by GETVERTICES in Algorithm 1). After the transformation, we reconstruct the  $\mathcal{H}$ -representation of the new polytope using existing libraries (function GETHRESP). In Example 6.1, the three sub-polytopes mapped differently, and the resulted polytopes are shown in Figure 6.1 (c).

An additional note on the implementation: when constructing the  $\mathcal{H}$ -representation we take special care for the degenerate polytopes (low-dimensional polytopes in a high-dimensional space). They are projected into the appropriate low-dimensional space where we construct a low-dimensional  $\mathcal{H}$ -polytope. We use singular value decomposition (SVD) for dimensionality reduction and its results provide the projection matrix to and from the low-dimensional space. This allows us to interchangeably use the QuickHull method and the double description method in computing  $\mathcal{H}$ -representation, as on certain cases one outperforms the other. On the other hand, ELINA [33] and PPL [5] uses only double description method in the conversion as QuickHull suffers from degenerate cases.

The above description provides a summary of applying linear and ReLU transformation on polytopes in  $\mathcal{H}$ - and  $\mathcal{V}$ -representation to compute the reachable set. It uses generic polytope libraries QuickHull and CDD and existing algorithms. In the worse case, the size of  $\mathcal{H}$ - and  $\mathcal{V}$ -representation grow exponentially that hinders significantly the scalability of naive polytope propagation.

**Bound estimation with polytope propagation** Recall that a big challenge in polytope propagation is coping with an increasing number of polytopes. Our solution is to integrate interval arithmetic from Section 2 with polytope propagation. For each polytope  $P$ , we estimate the interval bound on the output layers  $F(P)$ , which gives us a bounding box  $B$  around  $F(P)$ . If  $B$  is sufficient to conclude that  $F(P)$  is safe, we skip the computation of  $F(P)$  and use  $B$  instead.

## 6.2 The CEGAR Approach

Abstraction, a.k.a. over-approximation, is another common approach to cope with an increasing number of polytopes. One abstraction is to group the polytopes that are close to each other and use their convex hull as the abstraction of the reachable regions. Testing the closeness of polytopes is expensive. Instead, we use a simple heuristic: we group the sub-polytopes that come from the same polytope in the previous layer. This heuristic is based on the fact that these sub-polytopes are connected, and thus would not be too far from each other. This grouping is an over-approximation — it can turn unreachable states reachable, but not the other way around. In the implementation, we start this abstraction when the number of polytopes exceed



a user-controlled threshold. We keep a record of the layer where abstraction is started. For each abstracted polytope in this layer, we keep a reference to the corresponding precise polytopes. Once abstraction is started on in one layer, it is applied in all subsequent layers.

Sometimes, our abstraction is too coarse to prove the desired properties. In such a case, we apply the counter-example-guided abstraction refinement (CEGAR) principle [6]. For a polytope  $P$  that lies partially inside the unsafe region where some property fails (in other words, the polytope is ambiguous), we backtrack to a polytope  $P_0$  in a previous layer where we are about to apply abstraction. From  $P_0$ , we again start propagation, first using the exact propagation method, until the threshold is reached again. This refinement may lead to success in proving the property (all output polytopes are in the safe region) or disproving the property (there exists at least one output polytope that is completely inside the unsafe region). In either case, the CEGAR procedure terminates. Otherwise, for the ambiguous polytopes, we again backtrack to the previous layer to refine the abstractions. Our detailed CEGAR procedure presented in Algorithm 2. The CEGAR loop is guaranteed to terminate — in the worst case it will degenerate to propagating exact polytopes.

We note that our abstraction function (the convex hull of transformed polytopes) and our refinement function (replace the convex hull with union of convex polytopes) are an application of the standard finite-power-set domain from abstract interpretation on the convex polytopes [3].

### 6.3 Learning Invariants

Another approach we used to avoid the explosion of the number of polytopes is to find polytopes that represent a safe inductive invariant. For a given RNN with a fixed constraint on the inputs for each layer, we can define an *inductive invariant polytope* similar to a safe inductive invariant in a state transition system. We use  $Q = F(P)$  to denote the image of  $P$  under transformation  $F$ . If  $Q$  is completely inside  $P$ , then  $P$  is an inductive invariant polytope. Unlike in FNN, in RNN  $P$  and  $Q$  are comparable as RNN uses the same hidden neurons for all iterations. Additionally, if such  $P$  is safe (does not fall out of the safe region), we can conclude  $P$  and all states reachable from  $P$  are safe. Thus, there is no need to propagate  $P$  further.

We construct an inductive invariant polytope from a given polytope. Given polytope  $P_0$ , let  $Q_0$  be its image (a union of convex polytopes).  $P_0$  is an inductive invariant if  $Q_0$  is contained in  $P_0$ . If this is not the case, let  $P_1$  be the “join” of  $P_0$  and  $Q_0$ . It is guaranteed that  $P_1 \supseteq Q_0$  and  $P_1 \supseteq P_0$ . If  $P_1$  contains its image  $Q_1$ , then  $P_1$  is inductive. If not, let  $P_2$  be the “join” of  $P_1$  and  $Q_1$ , and we continue to check on  $P_2$ . This process continues until either  $P_i$  becomes inductive or unsafe. If  $P_i$  becomes inductive, we successfully find a safe inductive invariant polytope  $P_i$  which contains the given polytope  $P_0$ . If  $P_i$  grows out of the safe region, the construction fails as our relaxation creates too abstract a polytope. We will go with the exact image of  $P_0$ , namely  $Q_0$  and try in the next layer if we can construct a safe inductive invariant polytope from any polytope in  $Q_0$ . This procedure is illustrated in Figure 4.

In the above procedure, we use a “join” operation that produces a convex polytope containing the given polytopes. There are different choices on its implementation. Theoretically, to guarantee the termination of the above iterative procedure, the standard widening operator from the finite powerset of convex polytopes [4] can be used. However, it could be too abstract as each of its application either results in an increase of the dimension of the polytope or in a decrease of the number of constraints. On the other hand, the tight

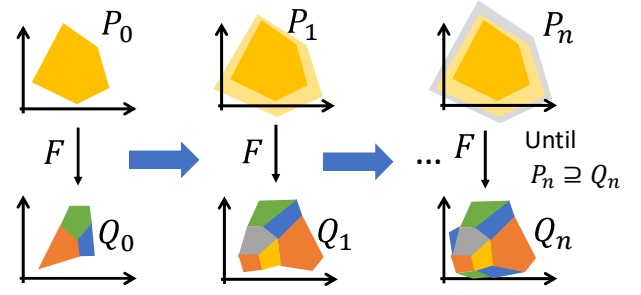


Figure 4. Illustration of constructing safe inductive invariant polytopes.

join achieved using the convex hull of polytopes could incur a higher computation cost, and it might take more iterations (or never) get to a fixed point. Here, we propose a light-weight join operator called *constraint relaxation*. For an  $\mathcal{H}$ -polytope  $P : \{y \in \mathbb{R}^d \mid a_i^T y \leq b_i, i \in [1, m]\}$ , joined with a  $\mathcal{V}$ -polytope  $Q : \text{conv}(\{y^1, \dots, y^n\})$ , we relax the constraints  $a_i^T y \leq b_i, i \in [1, m]$  for each vertex of  $Q$ . If for a vertex  $y^k$ , the left-hand-side of the  $i$ -th inequality constraint  $a_i^T y$  is greater than the right-hand-side  $b_i$ , we increase  $b_i$  to match with  $a_i^T y$ . Geometrically, this is equivalent to translating the hyperplanes that form  $P$  to include  $Q$ . Additionally, to ensure the resulted polytope is still closed, we intersect it with the smallest box that contains all vertices of  $P$  and  $Q$ .

The invariants are relative to the input constraints. As our RNN operates in three modes with different input constraints, the invariants we construct is only for one mode of operation. As the states at the end of fixation period can be pre-computed, we only construct invariants in the stimulus period and response period. In order to estimate whether an invariant in the stimulus period is safe or not, we again use the interval arithmetic to estimate the bounds in the response period for a candidate invariant polytope, and terminate the iteration if such conservative estimation already concludes it is unsafe.

## 7 Experimental Evaluation

**Network specification.** The network specification is as described by transitions (8)–(9), where  $s^k \in \mathbb{R}^7, k \in [1, n]$ . We unfold the network for 110 steps, so  $n_f = 10, n_s = 50$  and  $n_r = 50$ . Inputs of the network are specified in Section 4. The parameters of the stimulus noise are as follows:  $\mu$  is from a given set  $M = \cup_{h \in [0, 10]} \{-2^h/1000, 2^h/1000\}$  and  $\sigma = 0.3$ . We use TensorFlow to train RNNs. For the choice function (10), we used  $r = 10$ . We used a machine with i5-8300H CPU and 32GB of memory.

**Properties specification** We consider Property 1 and Property 2. For Property 1, we selected 30 ranges for the stimulus input, chosen around the mean values  $M$  (see above), which are used to generate the training data. The sizes of the ranges are relative to the absolute value of signal mean. Specifically, the ranges are in the form of  $[m \cdot 2^{-\delta}, m \cdot 2^{\delta}]$  (if  $m > 0$ ) or  $[m \cdot 2^{-\delta}, m \cdot 2^{\delta}]$  (if  $m < 0$ ), where  $m \in M, M = \cup_{h \in \{0.5, 7.9, 10\}} \{-2^h/1000, 2^h/1000\}, \delta \in \{0.2, 0.5, 0.7\}$ .

For Property 2, we enumerate a few positions of the pulses at the  $i$ -th input, ( $i \in \{1, \dots, 4\}$ ), while keeping the rest in a fixed range in the opposite direction (in similar ranges as Property 1).

We set 100 minutes as the time out limit for each stimulus range. For simplicity, we name our methods as PP (polytope propagation with interval arithmetic), CEGAR (PP plus counter-example-guided abstraction refinement) and Inv. (PP plus invariant construction). For CEGAR, the polytope bound to start approximation is set to be as small as 50 to favor a more abstract representation. There is no theoretical obstacle to integrate CEGAR and invariant, however, through

experiments, we found that this often worsens the overall performance as the invariant construction will be using a more abstract polytope as the starting point, which will more likely result in a failure of reaching a safe invariant.

**NNV framework** NNV is a direct comparison to the polytope propagation method we used. It is a MATLAB toolbox for neural network verification and performs reachability analysis using the star set representation [39]. Polytopes can be precisely captured by this representation. As the number of star set increases, NNV can also over-approximate the reachable region on a layer using an interval hull. We refer to the exact and interval hull approximation method as NNV-ex. and NNV-app. respectively in the following texts.

The computation in polytope propagation can be relatively easy to scale with the number of threads as the polytopes on the same layer are independent. Therefore, in this experiment, we focus on single-thread performance and limit all methods to using a single thread.

**SPACER model checker** We have also attempted to apply SPACER [19] – a state-of-the-art model checker included in Z3 [7]. SPACER has been successfully applied for verification of a variety of recurrent models from the domain of software verification, smart-contract analysis, and verification of control systems. Conceptually, SPACER is also based on polytope propagation. However, it propagates the *under-approximation* of bad states *backwards* from a property violation towards the initial condition. Throughout, it generalizes the polytopes based on symbolic reasoning about the transition relation. Unlike other techniques in this paper, SPACER is based on symbolic (as opposed to numeric) computation, using infinite precision arithmetic and symbolic quantifier elimination. While it is able to solve variants of Property 1, the running time is not competitive (over 20 hours). The main bottleneck is the blow up due to infinite precision arithmetic. It is interesting to explore whether similar techniques or ideas can be lifted to the numerical setting.

**Metrics** The number of solved instances under the time and resource limit is one of the metrics we can use to compare the performance. As for the solving time, it is hard to make a good comparison by just using the average time of solved instances, because the difficulty for solving different stimulus ranges varies greatly and the solving time ranges from around 0.1 second to greater than 5000 seconds. Therefore, for each stimulus range, we compute the relative time based on the fastest method on the that range, namely  $t_{rel} = t_{real}/t_{min}$ . An average of such relative time can be used to reflect the overall ranking of a method. A small average relative time indicates that the method ranks better in time on the instances it solves. We also report the number of ranges that one method gives the fastest answer.

**Table 1.** Summary of Experiments Results on Property 1

Regions		PP	CEGAR	Inv.	NNV-ex.	NNV-app.
Simple (19)	#. solved	19	19	19	16	19
	Ave. $t_{rel}$	1.04	1.05	1.04	1.62	135.82
Positive (8)	#. solved	4	7	8	0	3
	Ave. $t_{rel}$	1.80	3.44	3.90	-	1.00
Negative (3)	#. solved	0	0	0	3	3
	Ave. $t_{rel}$	-	-	-	1.00	1.00
All (30)	#. solved	23	25	27	19	25
	Ave. $t_{rel}$	1.17	1.62	1.89	1.49	98.7
	#. fastest	16	0	4	7	3

**Evaluation results** For Property 1, among the 30 stimulus ranges, 3 violates the property:  $[m \cdot 2^{-\delta}, m \cdot 2^{\delta}]$ , where  $m = 2^0/1000$ ,  $\delta \in \{0.2, 0.5, 0.7\}$ . For the remaining cases, the property is checked to be valid. According to the difficulty and the location of the checked

stimulus ranges, we categorized them into three types:

- simple region (I): solvable by interval arithmetic.
- challenging regions: positive (II) and negative (III), both unsolvable by interval arithmetic.

A summary of the results on all types of ranges is listed in Table 1. The detailed results can be found in the appendix.

In general, our techniques perform well for the simple regions and positive challenging regions, and NNV-ex. and NNV-app. work well on the negative challenging regions. The invariant method solves the most instances, although in average it does not always rank the fastest on the instances it can solve. The hybrid polytope propagation method (PP) ranks the fastest for the instances it can solve.

Property 2 is shown to be harder than Property 1 as the pulse on the opposite direction usually adds a significant disturbance on the states and drives the reachable region. For this property, we only experimented with the Inv and the NNV-ex. method. The experiment results are summarized in Table 2 (detailed results can be found in the appendix). The NNV-ex. is capable of solving 6 more ranges, with a relatively lower average solving time. However, the two have the same number of uniquely solved instances. Although not tested here, we expect the NNV-app. method will be able to solve more instances than NNV-ex. within the time-limit.

**Table 2.** Summary of Experiments Results on Property 2

Regions	Inv.	NNV-ex.
#. solved	23	<b>29</b>
Ave. time (solved)	804.3	<b>29.58</b>
Uniquely solved	4	4

**Discussion and Lessons Learned** For Property 1, the difference of performance pattern on the positive and negative categories leads us to a further investigation on the underlying causes. It turned out that the challenges in the positive regions are mainly the explosion on the number of polytopes. Among them, the “invariant” method solves the most regions in the time limit, as its invariants save the efforts of propagating safe polytopes. The challenges in the negative regions are mainly the increasing number of facets. The  $\mathcal{H}$ - and  $\mathcal{V}$ -polytope representation are known to have issues to scale with the exponentially increasing number of facets, as is also the reason for our methods to fail on the negative regions (in the experiments, we observed the number of facets quickly increased to the scale of  $10^5$  within the first 15 timesteps). On the other hand, the star set representation handles better with a large number of facets as it uses a higher dimension space for coefficients and does not keep the representation of facets in the original space. This trade-off delays the blow-up. When it is the time for containment check (required by invariant method), one still needs to convert the star-set representation to projected  $\mathcal{H}$ - and  $\mathcal{V}$ -polytopes, as is implemented by NNV. And as the previous work admitted, obtaining convex hull (required by the CEGAR method) on the star set representation becomes more expensive [44].

For Property 2, in the case of having a pulse stimulus in the opposite direction, there is no clear separation on where the number of polytope dominates vs. where the number of facets dominates. The two challenges are now mixed up. To successfully verify this property, the analysis method must be able to handle both the exponential increase of the number of polytopes and the exponential increase of the number of facets. Exploring solutions to both challenges is left for future work.

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## A Background

**Feed-forward neural networks.** A *feed-forward neural network* (FNN) is a function that takes an input  $x \in \mathbb{R}^d$ , applies a sequence of transformations and produces an output vector  $o$ ,  $o \in \mathbb{R}^p$ . Transformations are usually grouped in blocks called layers. Each layer is a composition of a linear and a non-linear transformations. Each layer produces an intermediate representation  $a^{(k)} \in \mathbb{R}^{p_k}$ ,  $k \in [1, m]$ . The first layer takes the input  $x$  and produces an intermediate state  $a^{(1)}$  that is passed to the next layer. The final layer takes  $a^{(m-1)}$  as an input and produces an output  $o$ . A network can be described as a composition of functions, assuming  $a^{(1)} = x$ , as follows:

$$a^{(k+1)} = f_j(W^{(k)}a^{(k)} + b^{(k)}), k \in [1, m-1] \quad (16)$$

$$o = f_m(W^{(m)}a^{(m)} + b^{(m)}), \quad (17)$$

where  $f_j$  is a non-linear function,  $W^{(k)}$  is a linear transformation matrix and  $b^{(k)}$  is a bias vector at the  $k$ th layer,  $k \in [1, m]$ .

**Mixed Integer Linear Programming (MILP).** We briefly overview MILP technology as we use it for the polytopes propagation. MILP solves linear problems over a set of integer and real valued variables. MILP contains a set of decision variables, a set of linear constraints over these variables and an objective function to be optimized (minimized or maximized) that is linear in decision variables. Without loss of generality we consider a minimization formulation of a MILP. Let  $x_1, \dots, x_n$  be a set of decision variables, a mixed integer linear program can be written as

$$\min \sum_i c_i x_i \quad (18)$$

$$\text{subject to } \sum_i a_{ij} x_i \geq b_j, j \in [1, m] \quad (19)$$

$$x_i \in \mathbb{Z}, i \in \mathcal{I}_1,$$

$$x_i \in \mathbb{R}, i \in \mathcal{I}_2,$$

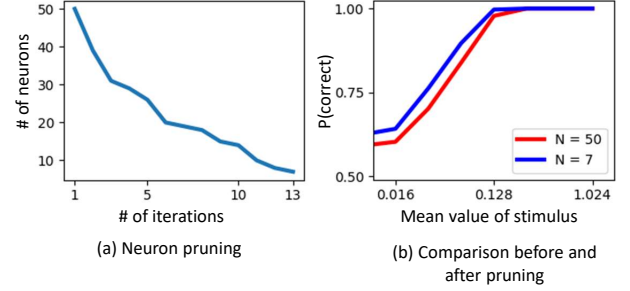
where  $\mathcal{I}_1$  is a set of indices of integer variables and  $\mathcal{I}_2$  is a set of indices of real variables,  $\mathcal{I}_1 \cup \mathcal{I}_2 = [1, n]$ .

## B Train an easier-to-verify RNN

In the first phase of our approach, we train a recurrent network that is simpler to verify for decision procedures, like MILP or SMT solvers [44]. There are two main bottlenecks for decision procedures to reason about neural networks. The first issue is that there is a large number of variables in linear constraints, like a typical linear constraint (18) used in a MILP formulation of a network [8]. For example, if we have a fully-connected layer then the number of variables in (18) equals to the number of neurons in the previous layer. The second issue is the presence of  $\text{RELU} = \max(x, 0)$  operators in a MILP or SMT formulation as these are piecewise linear functions. Each piecewise linear transformation introduces a binary branching factor for the solver. Note that the number of max operations equals to the number of neurons in the network. In [44], Xiao *et al.* initiated research on training easier to verify networks and introduced two techniques, weights sparsification and RELUS stabilization, that are very effective for feed-forward networks.

The main idea of RELUS stabilization is to train a network in such a way that piecewise linear functions, RELUS, are linearized. We say that a neuron  $s_i^k$  is *stable* if for all possible inputs of the network  $\text{sign}(\text{lb}(s_i^k)) = \text{sign}(\text{ub}(s_i^k))$ , where  $\text{lb}(s_i^k)$  is the smallest value that a neuron can take and  $\text{ub}(s_i^k)$  is the largest value that a neuron can take for all possible inputs. We encourage stabilization of

RELUS during the training by using bounds propagation techniques and adding an extra term to the loss function. Note that if lower and upper bounds of  $s_i^k$  have the same sign then we know that RELU degenerates to a linear function from a piece-wise linear function. We applied stabilization of neurons in our training procedure. Interestingly, we found that there are state neurons  $s_j^k$  such that  $\text{ub}(s_j^k) < 0$ ,  $k \in [1, n]$ . In other words, there is  $s_j^k$  that is stable for all  $k$ . This means that  $\text{RELU}(s_j^k) = 0$  at all time steps signaling that a state space can be reduced. Hence, we reduce the number of state neurons and retrained the smaller network from scratch. Surprisingly, our re-training procedure was extremely effective in reducing the network size. For example, we have successfully reduced the size of the state vector from 50 to 7.



**Figure 5.** Reducing RNN for easier verification

We also experimented with weights sparsification idea from [44]. This idea is based on: (a) use the L1 regularization during the training to encourage small weights and (b) set small weights, i.e. weights that are smaller than a given threshold, to zero as a post-processing step. However, we noted that the quality of the network is very sensitive to weights sparsification. We were *not* able to achieve significant reductions in the number of non-zero parameters compare to results reported in [44]. However, it is not surprising. Note that if we zero one element of a transformation matrix in (8)–(9), we zero this weight at each timestamp as the same matrix is used at each step. Hence, an RNN’s structure seems to be less favorable to weights sparsification compared to feed-forward networks.

## C Experiments (additional tables)

Here we report the detailed experiment results for Property 1 and 2. For Property 1, we listed both the relative time (in Table 3) and the time in seconds (in Table 4). For region category I, the solving time is usually less than a second, except in some cases NNV-app. will take slightly more time to deal with the increasing number of polytopes. In this regions, after rounding of the measured time, CEGAR and inv. report the same number in time as PP in the table, but in general PP has lowest overhead in region I. For NNV-app., it always terminates under the time limit, however, in some cases, it is not precise enough to check the validity of the property.

For Property 2, the results are reported in Table 5. Among the 48 stimulus regions, 3 are checked to guarantee the correct prediction even in presence of the spike on the opposite direction, 30 are shown to be vulnerable to the spike and the remaining 15 regions are still in unknown status. For Property 1, there is no remaining stimulus regions left unchecked, although not all methods work on a given region. As is not the case for Property 2. The difficulty comes from the mixing challenges of both the number of polytopes and the number of facets in a polytope, which points out a direction of future work.

**Table 3.** Results of Experiments on Property 1 (relative timing)

$\delta$	M	lower bound	upper bound	Category	PP	CEGAR	invariant	NNV-ex.	NNV-app.	Fastest
0.2	0.001	0.000871	0.001149	I	1.00	1.01	1.03	1.05	1.05	PP
	0.032	0.027858	0.036758	I	1.00	1.02	1.01	1.10	1.10	PP
	0.128	0.111430	0.147033	I	1.00	1.02	1.01	T.O.	881.10	PP
	0.512	0.445722	0.588134	I	1.00	1.01	1.01	T.O.	367.58	PP
	1.024	0.891444	1.176267	I	1.00	1.02	1.01	T.O.	1171.75	PP
0.5	0.001	0.000708	0.001415	I	1.00	1.01	1.02	1.07	1.07	PP
	0.032	0.022627	0.045255	II	1.84	4.28	1.00	T.O.	(16.01)*	inv
	0.128	0.090510	0.181019	II	1.00	2.59	3.25	T.O.	(4.70)*	PP
	0.512	0.362039	0.724077	II	T.O.	2.15	1.00	T.O.	(0.11)*	inv
	1.024	0.724077	1.448155	II	T.O.	T.O.	3.01	T.O.	1.00	NNV-app.
0.7	0.001	0.000616	0.001626	I	1.00	1.03	1.01	1.12	1.12	PP
	0.032	0.019698	0.051984	II	3.21	4.34	1.00	T.O.	(18.90)*	inv
	0.128	0.078793	0.207937	II	1.15	1.15	1.00	T.O.	(1.72)*	inv
	0.512	0.315173	0.831746	II	T.O.	T.O.	19.13	T.O.	1.00	NNV-app.
	1.024	0.630346	1.663493	II	T.O.	6.15	1.78	T.O.	1.00	NNV-app.
0.2	-0.001	-0.001149	-0.000871	I	1.14	1.15	1.14	1.00	1.00	NNV-ex.
	-0.032	-0.036758	-0.027858	I	1.00	1.01	1.00	1.48	1.48	PP
	-0.128	-0.147033	-0.111430	I	1.00	1.00	1.01	2.35	2.35	PP
	-0.512	-0.588134	-0.445722	I	1.00	1.01	1.00	1.31	1.32	PP
	-1.024	-1.176267	-0.891444	I	1.00	1.01	1.00	1.43	1.43	PP
0.5	-0.001	-0.001415	-0.000708	I	1.50	1.52	1.51	1.00	1.00	NNV-ex.
	-0.032	-0.045255	-0.022627	I	1.00	1.01	1.01	1.62	1.62	PP
	-0.128	-0.181019	-0.090510	I	1.00	1.00	1.00	4.23	4.23	PP
	-0.512	-0.724077	-0.362039	I	1.03	1.03	1.02	1.00	1.00	NNV-ex.
	-1.024	-1.448155	-0.724077	III	T.O.	T.O.	T.O.	1.00	1.00	NNV-ex.
0.7	-0.001	-0.001626	-0.000616	I	1.00	1.01	1.00	1.00	1.00	NNV-ex.
	-0.032	-0.051984	-0.019698	I	1.00	1.01	1.01	1.25	1.25	PP
	-0.128	-0.207937	-0.078793	I	1.00	1.03	1.02	3.32	3.32	PP
	-0.512	-0.831746	-0.315173	III	T.O.	T.O.	T.O.	1.00	1.00	NNV-ex.
	-1.024	-1.663493	-0.630346	III	T.O.	T.O.	T.O.	1.00	1.00	NNV-ex.

\* The abstraction is too coarse to determine the validity of the property.

**Table 4.** Results of Experiments on Property 1 (time in seconds)

$\delta$	M	lower bound	upper bound	Category	PP	CEGAR	inv.	NNV-ex.	NNV-app.	Fastest
0.2	0.001	0.000871	0.001149	I	0.17	0.17	0.18	0.18	0.18	PP
	0.032	0.027858	0.036758	I	0.17	0.17	0.17	0.19	0.19	PP
	0.128	0.111430	0.147033	I	0.17	0.17	0.17	T.O.	145.48	PP
	0.512	0.445722	0.588134	I	0.17	0.17	0.17	T.O.	61.31	PP
	1.024	0.891444	1.176267	I	0.17	0.18	0.17	T.O.	202.50	PP
0.5	0.001	0.000708	0.001415	I	0.17	0.17	0.17	0.18	0.18	PP
	0.032	0.022627	0.045255	II	42.80	99.70	23.28	T.O.	(372.70)*	inv
	0.128	0.090510	0.181019	II	150.50	390.10	489.27	T.O.	(707.00)*	PP
	0.512	0.362039	0.724077	II	T.O.	2026.70	942.63	T.O.	(104.10)*	inv
	1.024	0.724077	1.448155	II	T.O.	T.O.	824.06	T.O.	273.60	NNV-app.
0.7	0.001	0.000616	0.001626	I	0.17	0.18	0.17	0.19	0.19	PP
	0.032	0.019698	0.051984	II	106.80	144.30	33.22	T.O.	(627.80)*	inv
	0.128	0.078793	0.207937	II	540.00	537.20	468.29	T.O.	(807.90)*	inv
	0.512	0.315173	0.831746	II	T.O.	T.O.	5556.55	T.O.	290.50	NNV-app.
	1.024	0.630346	1.663493	II	T.O.	2534.50	733.53	T.O.	411.80	NNV-app.
0.2	-0.001	-0.001149	-0.000871	I	0.16	0.16	0.16	0.14	0.14	NNV-ex.
	-0.032	-0.036758	-0.027858	I	0.16	0.16	0.16	0.24	0.24	PP
	-0.128	-0.147033	-0.111430	I	0.16	0.16	0.16	0.38	0.38	PP
	-0.512	-0.588134	-0.445722	I	0.17	0.17	0.17	0.22	0.22	PP
	-1.024	-1.176267	-0.891444	I	0.16	0.16	0.16	0.23	0.23	PP
0.5	-0.001	-0.001415	-0.000708	I	0.16	0.16	0.16	0.11	0.11	NNV-ex.
	-0.032	-0.045255	-0.022627	I	0.16	0.16	0.16	0.26	0.26	PP
	-0.128	-0.181019	-0.090510	I	0.16	0.16	0.16	0.68	0.68	PP
	-0.512	-0.724077	-0.362039	I	0.33	0.33	0.33	0.32	0.32	NNV-ex.
	-1.024	-1.448155	-0.724077	III	T.O.	T.O.	T.O.	0.32	0.32	NNV-ex.
0.7	-0.001	-0.001626	-0.000616	I	0.35	0.36	0.35	0.35	0.35	NNV-ex.
	-0.032	-0.051984	-0.019698	I	0.28	0.28	0.28	0.35	0.35	PP
	-0.128	-0.207937	-0.078793	I	0.30	0.31	0.30	0.99	0.99	PP
	-0.512	-0.831746	-0.315173	III	T.O.	T.O.	T.O.	0.55	0.55	NNV-ex.
	-1.024	-1.663493	-0.630346	III	T.O.	T.O.	T.O.	0.53	0.53	NNV-ex.

\* The abstraction is too coarse to determine the validity of the property.

**Table 5.** Results of Experiments on Property 2 (time in seconds)

$\delta$	M	lower bound	upper bound	pulse position	Invariant	NNV-exact	Safe
0.2	0.001	0.000871	0.001149	1	18.75	0.70	✗
				2	3.5	0.43	✗
				3	4.5	0.35	✗
				4	5.3	0.37	✗
	0.032	0.027858	0.036758	1	3145.8	3.57	✗
				2	4546.6	1.25	✗
				3	23.8	0.41	✗
				4	24.8	0.35	✗
	0.128	0.111430	0.147033	1	724.4	T.O.	✓
				2	T.O.	T.O.	?
				3	1802.2	T.O.	✓
				4	12.9	T.O.	✓
0.7	0.032	0.019698	0.051984	1	T.O.	T.O.	?
				2	883.0	T.O.	✗
				3	T.O.	T.O.	?
				4	T.O.	T.O.	?
	0.128	0.078793	0.207937	1	T.O.	T.O.	?
				2	T.O.	T.O.	?
				3	T.O.	T.O.	?
				4	T.O.	T.O.	?
	0.512	0.315173	0.831746	1	T.O.	T.O.	?
				2	T.O.	T.O.	?
				3	T.O.	T.O.	?
				4	T.O.	T.O.	?
0.2	-0.001	-0.001149	-0.000871	1	511	46.12	✗
				2	304.6	43.74	✗
				3	504.6	41.37	✗
				4	470.6	39.82	✗
	-0.032	-0.036758	-0.027858	1	133.1	45.93	✗
				2	390.2	43.14	✗
				3	223.6	40.85	✗
				4	3291.5	38.78	✗
	-0.128	-0.147033	-0.111430	1	T.O.	46.23	✗
				2	T.O.	39.87	✗
				3	T.O.	35.52	✗
				4	21.9	32.54	✗
0.7	-0.032	-0.051984	-0.019698	1	207.3	45.92	✗
				2	1245.5	43.29	✗
				3	T.O.	40.11	✗
				4	T.O.	38.14	✗
	-0.128	-0.207937	-0.078793	1	T.O.	47.21	✗
				2	T.O.	37.89	✗
				3	T.O.	32.46	✗
				4	T.O.	26.16	✗
	-0.512	-0.831746	-0.315173	1	T.O.	45.21	✗
				2	T.O.	T.O.	?
				3	T.O.	T.O.	?
				4	T.O.	T.O.	?