

Algorithms for Verifying Deep Neural Networks

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Deep neural networks are widely used for nonlinear function approximation with applications ranging from computer vision to control. Although these networks involve the composition of simple arithmetic operations, it can be very challenging to verify whether a particular network satisfies certain input-output properties. This article surveys methods that have emerged recently for soundly verifying such properties. These methods borrow insights from reachability analysis, optimization, and search. We discuss fundamental differences and connections between existing algorithms. In addition, we provide pedagogical implementations of existing methods and compare them on a set of benchmark problems.

1 Introduction

Neural networks [15] have been widely used in many applications, such as image classification and understanding [17], language processing [24], and control of autonomous systems [26]. These networks represent functions that map inputs to outputs through a sequence of layers. At each layer, the input to that layer undergoes an affine transformation followed by a simple nonlinear transformation before being passed to the next layer. These nonlinear transformations are often called *activation functions*, and a common example is the *rectified linear unit* (ReLU), which transforms the input by setting any negative values to zero. Although the computation involved in a neural network is quite simple, these networks can represent complex nonlinear functions by appropriately choosing the matrices that define the affine transformations. The matrices are often learned from data using a form of stochastic gradient descent.

Neural networks are being used for increasingly important tasks, and in some cases, incorrect outputs can lead to costly consequences. **Traditionally, validation of neural networks has largely focused on evaluating the network on a large collection of points in the input space and determining whether the outputs are as desired. However, since the input space is effectively infinite in cardinality, it is not feasible to check all possible inputs.** Even networks that perform well on a large sample of inputs may not correctly generalize to new situations and may be vulnerable to adversarial attacks [29].

This article surveys a class of methods that are capable of formally verifying properties of deep neural networks over the full input space. A property can be formulated as a statement that if the input belongs to some set \mathcal{X} , then the output will belong to some set \mathcal{Y} . To illustrate, in classification problems, it can be useful to verify that points near a training example belong to the same class as that example. In the control of physical problems, it can be useful to verify that the outputs from a network satisfy hard safety constraints.

The verification algorithms that we survey are *sound*, meaning that they will only report that a property holds if the property actually holds. Some of the algorithms that we discuss are also *complete*, meaning that whenever the property holds, the algorithm will correctly



神经网络被用于越来越重要的任务，在某些情况下，错误的输出会导致代价高昂的后果。传统上，神经网络的验证主要集中在对输入空间中大量点的网络进行评估并确定输出是否符合要求。但是，由于输入空间的基数实际上是无限的，因此检查所有可能的输入是不可行的。即使在大量输入样本上表现良好的网络也可能无法正确地推广到新情况，并且可能容易受到对抗性攻击[29]。

本文概述了一类能够在整个输入空间上正式验证深度神经网络属性的方法。可将一个属性表示为以下语句：如果输入属于某个集合 \mathcal{X} ，则输出将属于某个集合 \mathcal{Y} 。为了说明这一点，在分类问题中，验证训练示例附近的点是否属于该集合可能很有用。与该示例相同的类。在控制物理问题时，验证网络输出满足严格的安全约束可能很有用。

我们调查的验证算法是可靠的，这意味着只有该属性实际存在时，它们才会报告该属性是否拥有。我们讨论的某些算法也是完整的，这意味着只要该属性成立，该算法便会正确声明其持有。但是，某些算法在使用近似值时会损害完整性，以提高计算效率。

state that it holds. However, some of the algorithms compromise completeness in their use of approximations to improve computational efficiency.

The algorithms may be classified based on whether they draw insights from these **three categories** of analysis:

1. **Reachability.** These methods use layer-by-layer reachability analysis of the network. Representative methods are ExactReach [46], MaxSens [44], and Ai2 [14]. **Some other approaches also use reachability methods (such as interval arithmetic)** to compute the bounds on the values of the nodes.
2. **Optimization.** These methods use optimization to falsify the assertion. The function represented by the neural network is a constraint to be considered in the optimization. As a result, the optimization problem is not convex. In *primal optimization*, different methods are developed to encode the nonlinear activation functions as linear constraints. Examples include NSVerify [23], MIPVerify [38], and ILP [4]. The constraints can also be simplified through *dual optimization*. Representative methods for dual optimization are Duality [12], ConvDual [43], and Certify [31].
3. **Search.** These methods search for a case to falsify the assertion. Search is usually combined with either reachability or optimization, as the latter two methods provide possible search directions. Representative methods for *search and reachability* are ReluVal [40], DLV [18], FastLin [41], and Fast-Lip [41]. Representative methods for *search and optimization* are Reluplex [20], Planet [13], BaB [7], and Sherlock [10]. Some of these methods call Boolean satisfiability (SAT) or satisfiability modulo theories (SMT) solvers [3] to verify networks with only ReLU activations.

利用可达性。这些方法使用网络的逐层可达性分析。代表性方法是ExactReach [46], MaxSens [44]和Ai2 [14]。其他一些方法也使用可达性方法（例如区间算法）来计算节点值的界限。

优化。这些方法使用优化来伪造断言。神经网络代表的功能是优化中要考虑的约束。结果，优化问题不是凸面的。在原始优化中，开发了不同的方法将非线性激活函数编码为线性约束。示例包括NSVerify [23], MIPVerify [38]和ILP [4]。约束也可以通过双重优化来简化。双重优化的代表性方法是Duality [12], ConvDual [43]和Certify [31]。

搜索。这些方法搜索案例以伪造断言。Search通常与Reachability或Optimization相结合，因为后两种方法提供了可能的搜索方向。Search和Reachability结合的代表性方法是ReluVal [40], DLV [18], FastLin [41]和Fast-Lip [41]。Search和Optimization结合的代表性方法是Reluplex [20], Planet [13], BaB [7]和Sherlock [10]。其中一些方法称为布尔可满足性(SAT)或可满足性模理论(SMT)求解器[3]，以仅通过ReLU激活来验证网络。

Scope of this article. This article introduces a unified mathematical framework for verifying neural networks, classifies existing methods under this framework, provides pedagogical implementations of existing methods,¹ and compares those methods on a set of benchmark problems.²

The following topics are not included in the discussion:

下列话题不在讨论的范围内

neural network testing methods that generate better test cases [16], [30], [36], [37];
white box approaches that build meaningful mappings from network parameters to some functional description [28];

- verification of binarized neural networks [8], [9], [27];
- closed-loop safety, stability and robustness by executing control policies defined by neural networks [11], [45], or verification of recurrent neural networks [2];
- training or retraining methods to make a network satisfy a property [25], [31], [43];
- robustness of the verification algorithm under floating point arithmetic [33].

Section 2 discusses the mathematical problem for verification. Section 3 gives an overview of the categories of methods that we will consider. Section 4 introduces preliminary and background mathematics. Section 5 discusses reachability methods. Section 6 discusses methods for primal optimization. Section 7 discusses methods for dual optimization. Section 8 discusses methods for search and reachability. Section 9 discusses methods for search and optimization. Section 10 compares those methods. Section 11 concludes the article.

第2节讨论了验证数学问题。第3节概述了我们将考虑的方法类别。第4节介绍了基础数学和背景数学。第5节讨论了可达性方法。第6节讨论了原始优化的方法。第7节讨论了双重优化的方法。第8节讨论了搜索和可达性的方法。第9节讨论了搜索和优化方法。第10节比较了这些方法。第11节总结了这篇文章。

我们的实现以Julia编程语言提供。我们发现该语言非常适合以人类可读的形式进行指定[5]。完整的实现请参见以下网址。

¹ Our implementation is provided in the **Julia programming** language. We have found the language to be ideal for specifying in human readable form [5]. The full implementation may be found at <https://github.com/sisl/NeuralVerification.jl>.

² There have been other reviews of methods for verifying neural networks. Leofante et al. review primal optimization methods that encode ReLU networks as mixed integer programming problems together with search and optimization under the framework of Boolean satisfiability and SMT [22]. Xiang et al. review a broader range of verification techniques in addition to safe control and learning [48]. Salman et al. review and compare methods that use convex relaxations to compute robustness bounds of ReLU networks [32].

2 Problem Formulation

We first review feedforward neural networks and introduce the mathematical formulation of the verification problem. We will then discuss the results provided by various algorithms along with the properties of soundness and completeness. In our discussion, we will use lowercase letters in italics for scalars and scalar functions (x), lowercase letters in upright bold for vectors and vector functions (\mathbf{x}), uppercase letters in upright bold for matrices and matrix functions (\mathbf{X}), and calligraphic uppercase letters for sets and set functions (\mathcal{X}).

我们首先回顾一下前馈神经网络，并介绍验证问题的数学公式。然后，我们将讨论各种算法提供的结果以及健全性和完整性。在我们的讨论中，我们将对标量和标量函数(x)使用斜体小写字母，对向量和矢量函数(\mathbf{x})使用直角粗体的小写字母，对于矩阵和矩阵函数(\mathbf{X})使用直角粗体的大写字母，以及用书法体表示集合和集合函数(\mathcal{X})。

2.1 Feedforward Neural Network

Consider an n -layer *feedforward neural network* that represents a function \mathbf{f} with input $\mathbf{x} \in \mathcal{D}_{\mathbf{x}} \subseteq \mathbb{R}^{k_0}$ and output $\mathbf{y} \in \mathcal{D}_{\mathbf{y}} \subseteq \mathbb{R}^{k_n}$, i.e., $\mathbf{y} = \mathbf{f}(\mathbf{x})$, where k_0 is the input dimension and k_n is the output dimension. All non-vector inputs or outputs are reshaped to vectors. Each layer in \mathbf{f} corresponds to a function $\mathbf{f}_i : \mathbb{R}^{k_{i-1}} \rightarrow \mathbb{R}^{k_i}$, where k_i is the dimension of the hidden variable \mathbf{z}_i in layer i . Moreover, we set $\mathbf{z}_0 = \mathbf{x}$ and $\mathbf{z}_n = \mathbf{y}$. Hence, the network can be represented by

$$\mathbf{f} = \mathbf{f}_n \circ \mathbf{f}_{n-1} \circ \cdots \circ \mathbf{f}_1, \quad (1)$$

where \circ means function ^{函数组合}composition. The function at layer i is

$$\mathbf{z}_i = \mathbf{f}_i(\mathbf{z}_{i-1}) = \sigma_i(\mathbf{W}_i \mathbf{z}_{i-1} + \mathbf{b}_i), \quad (2)$$

which consists of a linear transformation defined by a weight matrix $\mathbf{W}_i \in \mathbb{R}^{k_i \times k_{i-1}}$ and a bias vector $\mathbf{b}_i \in \mathbb{R}^{k_i}$, and an activation function $\sigma_i : \mathbb{R}^{k_i} \rightarrow \mathbb{R}^{k_i}$. All activation functions are assumed to be monotone and non-decreasing. For simplicity, let $\hat{\mathbf{z}}_i := \mathbf{W}_i \mathbf{z}_{i-1} + \mathbf{b}_i$ denote the node value before activation. Let $z_{i,j}$ be the value of the j th node in the i th layer, $\mathbf{w}_{i,j} \in \mathbb{R}^{1 \times k_{i-1}}$ be the j th row in \mathbf{W}_i , $w_{i,j,k}$ be the k th entry in $\mathbf{w}_{i,j}$, $b_{i,j}$ be the j th entry in \mathbf{b}_i . In the case that the activation function is node-wise, we denote the activation for the j th node as $\sigma_{i,j}$. Then

$$z_{i,j} = \sigma_{i,j}(\mathbf{w}_{i,j} \mathbf{z}_{i-1} + b_{i,j}) = \sigma_{i,j} \left(\sum_k w_{i,j,k} z_{i-1,k} + b_{i,j} \right) = \sigma_{i,j}(\hat{z}_{i,j}). \quad (3)$$

Figure 1 shows the structure of a feedforward neural network.

A network is defined in algorithm 2.1. The definitions of different activation functions are listed in algorithm 2.2.

2.2 Verification Problem

Verification involves checking whether input-output relationships of a function hold. The input constraint is imposed ^{强加}by a set $\mathcal{X} \subseteq \mathcal{D}_{\mathbf{x}}$. The corresponding output constraint is imposed by a set $\mathcal{Y} \subseteq \mathcal{D}_{\mathbf{y}}$. In the following discussion, **we call the sets \mathcal{X} and \mathcal{Y} constraints**. Solving the *verification problem* requires showing that the following assertion holds: **解决验证问题需要证明以下断言成立**

$$\mathbf{x} \in \mathcal{X} \Rightarrow \mathbf{y} = \mathbf{f}(\mathbf{x}) \in \mathcal{Y}. \quad (4)$$

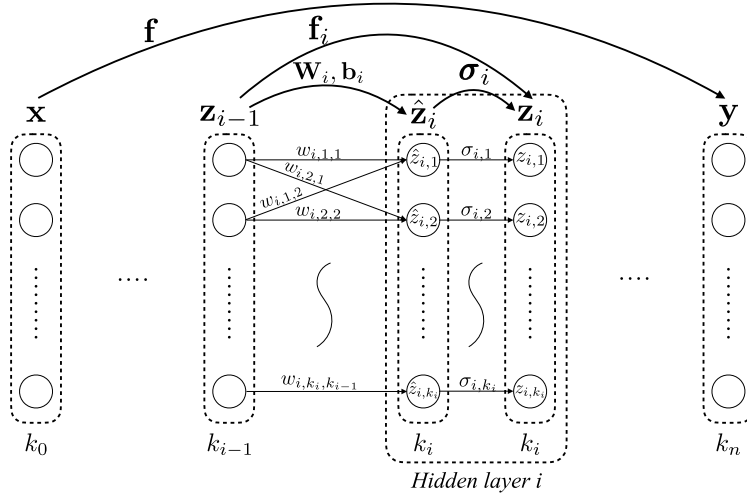


Figure 1. Illustration of a feedforward neural network and the notations used in this article.

```

abstract type ActivationFunction end

struct Layer{F<:ActivationFunction, N<:Number}
  weights::Matrix{N}
  bias::Vector{N}
  activation::F
end

struct Network
  layers::Vector{Layer}
end

```

Algorithm 2.1. Network structure. A network is a list of layers. Each layer consists of weights \mathbf{W} , bias \mathbf{b} , and activation σ .

```

struct GeneralAct <: ActivationFunction end
struct ReLU <: ActivationFunction end
struct Id <: ActivationFunction end
(f::GeneralAct)(x) = f(x)
(f::ReLU)(x) = max.(x, 0)
(f::Id)(x) = x

```

Algorithm 2.2. Activation functions. This paper mostly focuses on networks with ReLU activations. Other piece-wise linear activations can be encoded by multiple ReLU activations. For example, the Max activation function can be encoded using the following relationship: $\text{Max}(x, y) = \text{ReLU}(x - y) + y$. Composing multiple Max functions can enable the encoding of the Max pooling operator.

For example, to verify robustness in a classification network,³ we need to ensure that all samples in the neighborhood of a given input \mathbf{x}_0 are classified with the same label. Suppose the desired label is $i^* \in \{1, \dots, k_n\}$. We need to ensure that $y_{i^*} > y_j$ for all $j \neq i^*$. The input and output constraints are

$$\mathcal{X} = \{\mathbf{x} : \|\mathbf{x} - \mathbf{x}_0\|_p \leq \epsilon\}, \quad (5a)$$

$$\mathcal{Y} = \{\mathbf{y} : y_{i^*} > y_j, \forall j \neq i^*\}, \quad (5b)$$

where ϵ is the maximum allowable disturbance in the input space. The metric to measure disturbance can be any ℓ_p norm, though the ℓ_∞ or the ℓ_1 norms are common because they lead to linear constraints.

Our formulation is broader than classification problems. In general, the input set \mathcal{X} and the output set \mathcal{Y} can have any geometry. For simplicity, we assume that \mathcal{X} is a polytope, and \mathcal{Y} is either a polytope or the complement of a polytope. A *polytope* is a generalization of the three-dimensional polyhedron and is defined as the intersection of a set of half-spaces.⁴ Since any compact domain can be approximated by a finite set of polytopes for any required accuracy, this formulation can be easily extended to arbitrary geometries. Moreover, the complement of a polytope allows the encoding of unbounded sets. By default, a polytope is a closed set, while its complement is an open set.

³ Given an input, a classification network outputs weights over several labels. The input is assigned the label with the highest weight.

⁴ This is the definition of a *convex polytope*; alternative definitions exist, but this is the one we will use here.

⁵ In our implementations, we use the definitions in `LazySets.jl`, which is a Julia package for calculus with convex sets [6]. The implementation can be found at <https://github.com/JuliaReach/LazySets.jl>.

Our discussion will focus on the following four subclasses of polytopes:⁵

- *Halfspace-polytope* (or *H-polytope*), which represents polytopes using a set of linear inequality constraints

$$\mathbf{C}\mathbf{x} \leq \mathbf{d}, \quad (6)$$

where $\mathbf{C} \in \mathbb{R}^{k \times k_0}$, $\mathbf{d} \in \mathbb{R}^k$, and k is the number of inequality constraints that are defining the polytope. A point \mathbf{x} is in the polytope if and only if $\mathbf{C}\mathbf{x} \leq \mathbf{d}$ is satisfied.

- *Vertex-polytope* (or *V-polytope*), which represents polytopes using a set of vertices. Mathematically, it is described by a concatenation of all vertices \mathbf{v}_i for $i \in \{1, \dots, k\}$,

$$[\mathbf{v}_1 \quad \mathbf{v}_2 \quad \dots \quad \mathbf{v}_k], \quad (7)$$

where k is the number of vertices. A point \mathbf{x} is in the polytope if and only if \mathbf{x} is in the convex hull of the vertices.

- *Hyperrectangle*, which corresponds to a high-dimensional rectangle, defined by

$$|\mathbf{x} - \mathbf{c}| \leq \mathbf{r}, \quad (8)$$

where $\mathbf{c} \in \mathbb{R}^{k_0}$ is the center of the hyperrectangle and $\mathbf{r} \in \mathbb{R}^{k_0}$ is the radius of the hyperrectangle.

- *Halfspace*, which is represented by a single linear inequality constraint

$$\mathbf{c}^\top \mathbf{x} \leq d, \quad (9)$$

where $\mathbf{c} \in \mathbb{R}^{k_0}$ and $d \in \mathbb{R}$.

In our discussion, we may refer to hyperrectangles as *intervals*. A hyperrectangle that has uniform side lengths is called a *hypercube*. The set in (5b) corresponds to a halfspace-polytope. When $p = \infty$, the set in (5a) corresponds to a hyperrectangle centered at \mathbf{x}_0 with uniform radius ϵ .

The verification problem is defined in algorithm 2.3.

```

struct Problem{P, Q}
  network::Network
  input::P
  output::Q
end

```

Algorithm 2.3. Problem definition. It consists of a network to be verified, an input set constraint, and an output set constraint. The types P and Q can be any sets that match the requirements of the algorithm.

2.3 Results

Verification algorithms attempt to identify whether (4) holds. In some cases, algorithms may return *unknown* if no conclusion can be drawn. Different algorithms output different types of results as listed below and illustrated in figure 2.

- *Counter example result*, which is a counter example $x^* \in \mathcal{X}$ with

$$f(x^*) \notin \mathcal{Y}. \quad (10)$$

The property (4) is violated if such a counter example is found.

- *Adversarial result*, which is the maximum allowable disturbance with respect to an ℓ_p norm while maintaining $f(x) \in \mathcal{Y}$:

$$\epsilon(x_0, f, \mathcal{Y}, p) := \min_{x, \text{ s.t. } f(x) \in \mathcal{Y}} \|x - x_0\|_p. \quad (11)$$

The property (4) is violated if the input set \mathcal{X} exceeds the maximum allowable disturbance,

$$\epsilon(x_0, f, \mathcal{Y}, p) < \max_{x \in \mathcal{X}} \|x - x_0\|_p. \quad (12)$$

- *Reachability result*, which is the output reachable set:

$$\mathcal{R}(\mathcal{X}, f) := \{y : y = f(x), \forall x \in \mathcal{X}\}. \quad (13)$$

The property (4) is violated if the reachable set does not belong to the output set \mathcal{Y} ,

$$\mathcal{R}(\mathcal{X}, f) \not\subseteq \mathcal{Y}. \quad (14)$$

Algorithm 2.4 provides definitions of these result types used in our implementation. The status may be `:holds`, `:violated`, or `:Unknown`.

2.4 Soundness and Completeness 正确性和完备性

The result returned by a particular solver may not always be correct. A specific instance of (4) can either *hold* or be *violated*. The status from a solver can be holds, violated, or unknown. Ideally, a solver only outputs holds or violated to match the actual status of a given problem. However, some algorithms make approximations that can result in a mismatch. For example, the computed reachable set (denoted $\tilde{\mathcal{R}}$) may be an over-approximation of \mathcal{R} in (13). Then, even if $\tilde{\mathcal{R}} \not\subseteq \mathcal{Y}$, i.e., the solver returns violated, it is possible that $\mathcal{R} \subset \mathcal{Y}$, i.e., the property actually holds.

过度近似

某些求解器返回的结果并不一定是正确的，公式4可能被满足或不满足。求解器返回的结果应该处于满足、不满足、未知三个状态。因为虽然在理想状态下，我们希望求解器仅返回满足或不满足，但许多算法在计算时，为了性能做了过度近似，计算出来的可达集仅为公式(13)中R的过度近似 \tilde{R} 。所以当 \tilde{R} 不为Y的子集时，求解器返回不满足，但是如果真实的R如果还是Y的子集的话，其实还是满足的。

We use the following definitions to categorize solvers: 因此，我们可以对求解器做如下的分类：

- *Soundness*, which requires that when the solver returns holds, the property actually holds.

1. 健全性：满足就返回满足，不满足就返回不满足

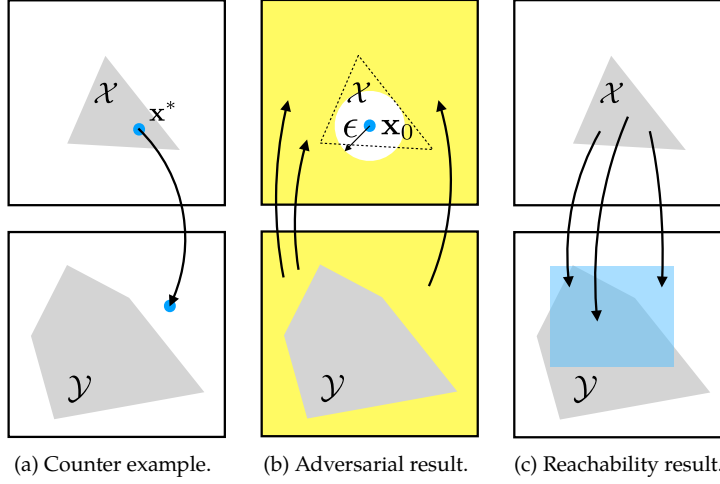


Figure 2. Illustration of different results. The upper square represents the input domain. The lower square represents the output domain. The input set \mathcal{X} and the output set \mathcal{Y} are shown as gray polygons. In (a), a counter example is found. In (b), the input set exceeds the maximum allowable disturbance (white circle in the input domain). In (c), the output reachable set (blue set in the output domain) does not belong to the output set.

```

abstract type Result end

struct BasicResult <: Result
  status::Symbol
end

struct CounterExampleResult <: Result
  status::Symbol
  counter_example::Vector{Float64}
end

struct AdversarialResult <: Result
  status::Symbol
  max_disturbance::Float64
end

struct ReachabilityResult <: Result
  status::Symbol
  reachable::Vector{<:AbstractPolytope}
end

```

Algorithm 2.4. Result types. `BasicResult` is for satisfiability only. `CounterExampleResult` also outputs a counter example if the problem is not satisfied. `AdversarialResult` outputs the maximum allowable disturbance. `ReachabilityResult` outputs the reachable set.

2. 完整性：要求，首先求解器不能返回unknown。其次，如果求解器返回违例，那么该属性确实违例
- *Completeness*, which requires that (i) the solver never returns unknown; and (ii) if the solver returns violated, the property is actually violated.
3. 可终止：要求求解器总是能在有限步后停止
- *Termination*, which requires that the solver always finishes after a finite number of steps.

A method that is sound, complete, and terminating always outputs the correct result with no unknowns. All methods discussed in this survey are sound and terminating, but not all of them are complete. Some methods use over-approximations to speed up computation and result in incompleteness. Our implementation may be slightly different from the original implementation of some methods. For example, the original implementation of DLV is always complete and is sound under the minimality assumption of the search tree. Our implementation is sound but not complete. The differences will not affect the key concepts of the methods. And we point out the differences in the detailed discussion of the methods.

Table 1 summarizes the characteristics of all methods considered in this survey. The input and output sets may include hyperrectangles (HR), halfspaces (HS), halfspace-polytopes (HP), vertex-polytopes (VP), and polytope complements (PC). Additionally, the superscripts in the table indicate the following constraints on the output sets:

1. The polytope has to be bounded, this restriction is not due to a theoretical limitation, but rather to our implementation and will eventually be relaxed.
2. Polytope complements encode unbounded sets. They are used in optimization-based methods, to be explained in section 6. These methods usually encode the complement of the output set as a constraint and require the constraint to be convex. The complement of a polytope complement is a convex polytope, hence satisfies the requirement.
3. The output set must be 1-dimensional.

sound, complete且terminating的方法始终会输出正确的结果，而不会产生unknown。本调查中讨论的所有方法都是sound且terminating的方法，但并非所有方法都是complete的。一些方法使用over-approximations来加快计算速度并导致incomplete。我们的实现可能与某些方法的原始实现略有不同。例如，DLV的原始实现总是complete的，并且在搜索树的最小假设下是合理的。我们的实现是sound的，但是incomplete的。差异不会影响方法的关键概念。并且我们指出了在方法详细讨论中的差异。

表1总结了本次调查中考虑的所有方法的特点。输入和输出集可以包括超矩形（HR），半空间（HS），半空间多面体（HP），顶点多面体（VP）和多面体补体（PC）。此外，表中的上标指示对输出集的以下约束：

1. 多面体必须是有界的，这种限制不是由于理论上的限制，而是由于我们的实现，最终将被放宽。
2. 多面体补体编码无界集合。它们在基于优化的方法中使用，将在第6节中进行说明。这些方法通常将输出集的补码编码为约束，并且要求约束是凸的。多面体补体的补体是凸多面体，因此满足要求。
3. 输出集必须是一维的。

| Method Name | Activation | Approach | Input/Output | Completeness |
|-----------------|------------------|-------------------------|-----------------------------|--------------|
| ExactReach [46] | ReLU | Exact Reachability | HP/HP(bounded) ¹ | ✓ |
| AI2 [14] | Piecewise Linear | Split and Join | HP/HP(bounded) ¹ | × |
| MaxSens [44] | Any | Interval Arithmetic | HP/HP(bounded) ¹ | × |
| NSVerify [23] | ReLU | Naive MILP | HR/PC ² | ✓ |
| MIPVerify [38] | ReLU and Max | MILP with bounds | HR/PC ² | ✓ |
| ILP [4] | ReLU | Iterative LP | HR/PC ² | × |
| Duality [12] | Any | Lagrangian Relaxation | HR(uniform)/HS | × |
| ConvDual [43] | ReLU | Convex Relaxation | HR(uniform)/HS | × |
| Certify [31] | Differentiable | Semidefinite Relaxation | HR/HS | × |
| Fast-Lin [41] | ReLU | Network Relaxation | HR/HS | × |
| Fast-Lip [41] | ReLU | Lipschitz Estimation | HR/HS | × |
| ReluVal [40] | ReLU | Symbolic Interval | HR/HR | ✓ |
| DLV [18] | Any | Search in Hidden Layers | HR/HR(1-D) ³ | ✓* |
| Sherlock [10] | ReLU | Local and Global Search | HR/HR(1-D) ³ | × |
| BaB [7] | Piecewise Linear | Branch and Bound | HR/HR(1-D) ³ | × |
| Planet [13] | Piecewise Linear | Satisfiability (SAT) | HR/PC ² | ✓ |
| Reluplex [20] | ReLU | Simplex | HR/PC ² | ✓ |

Table 1. List of existing methods. We name the method if it does not have a name. The entries under “activation” show the type of activations supported in the methods. The entries under “approach” summarize the key ideas of the methods. All the methods presented in this paper are sound and the methods that are complete as defined in section 2.4 are marked in the “completeness” column. For DLV, the original implementation is complete but may not be sound, while our implementation is sound but not complete.

3 Overview of Methods 各种方法的概述

This section overviews existing methods that are studied in this survey. Their common components will be outlined. As mentioned earlier, there are three basic verification methods, *i.e.*, reachability, optimization, and search. Regarding the three basic methods, we categorize those methods into the following five categories as shown in figure 3. The methods are also summarized in table 1.

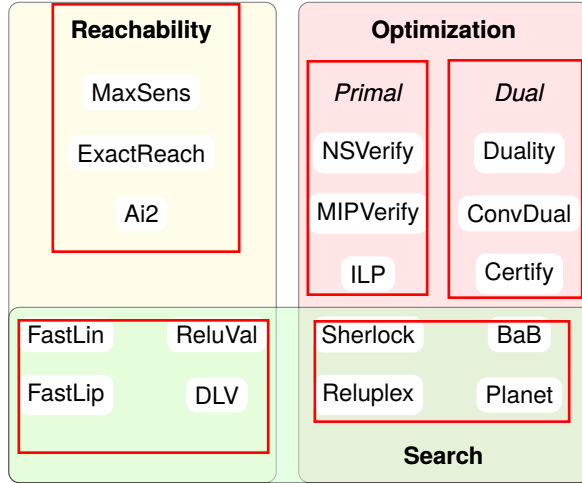


Figure 3. Overview of all methods in the survey. Given the three basic methods: reachability, optimization, and search, existing methods are divided into five categories: reachability, primal optimization, dual optimization, search and reachability, and search and optimization. Relationships among different methods are shown in the figure.

图3. 调查中所有方法的概述。给定三种基本方法：可达性，优化和搜索，现有方法分为五类：可达性，原始优化，双重优化，搜索和可达性以及搜索和优化。图中显示了不同方法之间的关系。

3.1 Reachability

These methods perform layer-by-layer reachability analysis to compute the reachable set $\mathcal{R}(\mathcal{X}, f)$. They usually generate `ReachabilityResult`.

ExactReach [46] computes the exact reachable set for networks with only ReLU activations. The key insight is that if the input set to a ReLU function is a union of polytopes, then the output reachable set is also a union of polytopes. As there is no over-approximation, this method is sound and complete. However, because the number of polytopes grows exponentially with each layer, this method does not scale.

Ai2 [14] uses representations that over-approximate the reachable set. It trades precision of the reachable set for scalability of the algorithm. It works for any piecewise linear activation functions, such as ReLU and max pooling. Due to its approximation, the number of geometric objects to be traced during layer-by-layer analysis is greatly reduced. Though Ai2 is not complete, it scales well.

MaxSens [44] partitions the input domain into small grid cells, and loosely approximates the reachable set for each grid cell considering the maximum sensitivity of the network at each grid cell. Sensitivity of a function is equivalent to the Lipschitz constant of the function. The union of those reachable sets is the output reachable set. The finer the partition, the tighter the output reachable set. MaxSens is not complete. It works for any activation function and scales well.

这些方法执行逐层可达性分析以计算可达集 $\mathcal{R}(\mathcal{X}, f)$ 。它们通常生成`ReachabilityResult`。

ExactReach [46] 计算仅通过ReLU激活的网络的精确可达集。关键的见解是，如果ReLU函数的输入集是多面体的并集，那么输出可达集也是多面体的并集。由于没有过度逼近，因此该方法是合理且完整的。但是，由于多拓扑的数目随每一层呈指数增长，因此该方法无法扩展。

Ai2 [14] 使用的表示过于接近可达到的集合。它用可达集的精度换取算法的可伸缩性。它适用于任何分段线性激活函数，例如ReLU和max pooling。由于其近似值，可以大大减少在逐层分析过程中要跟踪的几何对象的数量。尽管Ai2不完备，但可以很好地扩展。

MaxSens [44] 将输入域划分为小网格单元，并考虑到每个网格单元的网络最大灵敏度，大致估计每个网格单元的可达集。函数的灵敏度等于函数的Lipschitz常数。这些可达集的并集就是输出可达集。分区越精细，输出可达设置越紧密。MaxSens是不完备的。它适用于任何激活函数并可以很好地扩展。

原始优化

3.2 Primal Optimization

Primal optimization methods try to falsify assertion (4). The network structure is a constraint to be considered in the optimization. Existing methods only work for ReLU activations. Different methods are developed to encode the network as a set of linear constraints or mixed integer linear constraints by exploiting the piecewise linearity in the ReLU. **The encoding methods will be discussed in section 6.1.** The return type can be either `CounterExampleResult` or `AdversarialResult`, depending on the objective of the optimization.

NSVerify [1], [23] encodes the network as a set of mixed integer linear constraints. It solves a feasibility problem without an objective function. It tries to find a counter example for the verification problem.⁶ This method is sound and complete.

MIPVerify [38] also encodes the network as a set of mixed integer linear constraints. There are two differences between MIPVerify and NSVerify. First, MIPVerify determines the bounds on the nodes to tighten the constraints. Second, MIPVerify solves an adversarial problem that tries to estimate the maximum allowable disturbance on the input side. This method is also complete.

ILP (iterative linear programming) [4] encodes the network as a set of linear constraints by linearizing the network at a reference point. The optimization problem in ILP is an adversarial problem that tries to estimate the maximum allowable disturbance on the input side. It iteratively solves the optimization. This method is not complete as it only considers one linear segment of the network.

双重优化

3.3 Dual Optimization

In primal optimization methods, different methods are developed to encode the constraints imposed by the network. We can also use dual optimization to simplify the constraints. In dual optimization, the constraints are much simpler than those in primal optimization. On the other hand, objectives in dual optimization, which correspond to the constraints in primal optimization, are much more complicated than those in the primal problem. Relaxations are usually involved during the construction of the dual problem. Due to relaxation, these approaches are incomplete. The return type is `BasicResult`.

Duality [12] solves a Lagrangian relaxation of the optimization problem to obtain bounds on the output. The dual problem is formulated as an unconstrained convex optimization problem, which can be computed efficiently. Duality works for any activation function.

ConvDual [43] also uses a dual approach to estimate the bounds on the output. It obtains a simplified dual problem by first making a convex relaxation of the network in the primal optimization. The bounds are heuristically computed by choosing a fixed, dual feasible solution, without any explicit optimization. In this way, ConvDual is more computationally efficient than Duality. In the original ConvDual approach, the bounds are then used to robustly train the network. This survey focuses on the method to compute the bounds.

Certify [31] uses a semidefinite relaxation to compute over approximated certificates (*i.e.*, bounds). It only works for neural networks with only one hidden layer. It works for any activation function that is differentiable almost everywhere.⁷ In the original Certify approach, the certificates are then optimized jointly with network parameters to provide an adaptive regularizer that improves robustness of the network. This survey focuses on the method to obtain the certificates.

原始优化方法试图伪造断言(4)。网络结构是优化中要考虑的约束。现有方法仅适用于ReLU激活。通过利用ReLU中的分段线性,开发了多种方法来将网络编码为一组线性约束或混合整数线性约束。编码方法将在第6.1节中讨论。返回类型可以是CounterExampleResult或AdversarialResult,具体取决于优化的目标。

(1). NSVerify[1][23]将网络编码为一组混合整数线性约束。它解决了没有目标函数的可行性问题。它试图找到一个针对验证问题的反例。这种方法是不完备的。

(2). MIPVerify[38]也将网络编码为一组混合整数线性约束。MIPVerify和NSVerify之间有两个区别。首先,MIPVerify确定节点上的边界以收紧约束。其次,MIPVerify解决了一个对抗性问题,该问题试图估计输入侧的最大允许干扰。此方法也是不完备的。

(3). ILP(迭代线性规划)[4]通过在参考点处线性化网络将网络编码为一组线性约束。ILP中的优化问题是一个对抗性问题,试图估计输入侧的最大允许干扰。迭代地解决优化问题。该方法不完备,因为它仅考虑网络的一个线性段。

⁶ NSVerify [1] is developed for verification of a closed-loop system that has neural network components. It has been extended to verify recurrent neural networks [2]. We only review the method used to verify non-recurrent neural networks, which was first discussed in [23].

NSVerify [1]是为验证具有神经网络组件的闭环系统而开发的。它已被扩展以验证递归神经网络[2]。我们仅回顾用于验证非递归神经网络的方法,该方法在[23]中首次讨论。

在原始优化方法中,开发了不同的方法来对网络施加的约束进行编码。我们还可以使用双重优化来简化约束。在双重优化中,约束要比原始优化中的约束简单得多。另一方面,与原始优化中的约束相对应的对偶优化中的目标要比原始问题中的目标复杂得多。对偶问题的构造通常涉及松弛。由于松弛,这些方法是不完备的。返回类型为BasicResult。

Duality[12]解决了优化问题的拉格朗日松弛,以获得输出的边界。对偶问题被公式化为无约束凸优化问题,可以有效地对其进行计算。对偶适用于任何激活功能。

ConvDual [43]还使用对偶方法来估计输出范围。通过首先在原始优化中使网络凸松弛来获得简化的对偶问题。通过选择固定的对偶可行解进行启发式计算,而无需任何显式优化。这样,ConvDual在计算上比对偶性更高。在原始的ConvDual方法中,边界随后用于稳健地训练网络。本调查着重于计算边界的方法。

Certify [31]使用半定松弛来计算近似证书(即边界)。它仅适用于只有一层隐藏层的神经网络。它适用于几乎在任何地方都可以区分的任何激活功能。7在原始的Certify方法中,然后将证书与网络参数一起进行优化,以提高网络健壮性的自适应正则化器。本调查着重于获取证书的方法。

⁷ Differentiable a.e. means that the function is differentiable everywhere except for countably many points. Piecewise linear activation functions are all differentiable a.e.

可区分的a.e.意味着该功能在除许多点之外的任何地方都是可微的。分段线性激活函数都是可微的。

3.4 Search and Reachability

Reachability methods need to balance computational efficiency and precision of the approximation. When reachability is combined with search, it is possible to improve both efficiency and accuracy. These methods usually search in the input or the hidden spaces for a counter example. However, due to over-approximation in reachability analysis, these methods are sound but incomplete.

ReluVal [39], [40] uses symbolic interval analysis along with search to minimize over-approximations of the output sets. During the search process, ReluVal iteratively bisects its input range. This process is called iterative interval refinement, which is also used in BaB [7].

Fast-Lin [41] computes a certified lower bound on the allowable input disturbance for ReLU networks using a layer-by-layer approach and binary search in the input domain.

Fast-Lip [41] depends on Fast-Lin to compute the bounds on the activation functions, and further estimates the local Lipchitz constant of the network. In general, Fast-Lin is more scalable than Fast-Lip, while Fast-Lip provides better solutions for ℓ_1 bounds.

DLV [18] searches for adversarial inputs layer by layer in the hidden layers. This is the only approach that searches in the hidden spaces we have seen so far. DLV supports any activation function.

可达性方法需要在计算效率和近似精度之间取得平衡。将可达性与搜索结合在一起时，可以同时提高效率和准确性。这些方法通常在输入或隐藏空间中搜索反例。但是，由于在可达性分析中过于逼近，因此这些方法是合理的，但并不完整。

ReluVal [39], [40]使用符号区间分析和搜索来最大程度地减少输出集的过度逼近。在搜索过程中，ReluVal迭代将其输入区间一分为二。此过程称为迭代区间细化，BaB [7]中也使用了这种方法。

Fast-Lin [41]使用逐层方法和输入域中的二进制搜索来计算ReLU网络的允许输入干扰的认证下界。

Fast-Lip [41]依赖于Fast-Lin计算激活函数的界限，并进一步估计网络的局部Lipchitz常数。通常，Fast-Lin比Fast-Lip具有更好的可伸缩性，而Fast-Lip为 ℓ_1 界提供了更好的解决方案。

DLV [18]在隐藏层中逐层搜索对抗性输入。这是到目前为止我们所看到的隐藏空间中搜索的唯一方法。DLV支持任何激活功能。

3.5 Search and Optimization

Search can also be combined with optimization. We can either search in the input space, or search in the function space. Searching in the function space is done by exploring possible activation patterns. An activation pattern is an assignment (e.g., on or off for ReLU) to each activation function in the network. These methods may use SAT or SMT.

Sherlock [10] estimates the output range using a combination of local search and global search. Local search solves a linear program to find local optima. Global search solves a mixed integer linear program to escape local optima, which is similar to the method in NSVerify and MIPVerify. Sherlock is incomplete.

BaB [7] uses branch and bound to compute the output bounds of a network. It has a modularized design that can serve as a unified framework that can support other methods such as Reluplex and Planet.

Planet [13] integrates with a SAT solver for tree search in the function space. The objective of the search is to find an activation pattern of ReLU networks that maps an input in \mathcal{X} to an output not in \mathcal{Y} . It combines optimization-based filtering and pruning in the search process. Planet is complete.

Reluplex [20] performs tree search in the function space. It extends the simplex algorithm, a standard algorithm for solving linear programming (LP) instances, to support ReLU networks. The algorithm is called Reluplex, for ReLU with the simplex method. Reluplex is complete.

搜索也可以与优化相结合。我们可以在输入空间中搜索，也可以在函数空间中搜索。搜索函数空间是通过探索可能的激活函数来完成。激活模式是对网络中每个激活函数的分配(例如，对ReLU开启或关闭)。这些方法可以使用SAT或SMT。

Sherlock [10]使用局部搜索和全局搜索的组合来估计输出范围。局部搜索求解线性程序以找到局部最优值。全局搜索解决了一个混合整数线性规划以逃避局部最优的情况，这类似于NSVerify和MIPVerify中的方法。Sherlock是不完备的。

BaB [7]使用分支定界法来计算网络的输出界限。它具有模块化设计，可以用作支持其他方法(例如Reluplex和Planet)的统一框架。

Planet [13]与SAT求解器集成在一起，用于在函数空间中进行树搜索。搜索的目的是找到ReLU网络的激活模式，该模式将 \mathcal{X} 中的输入映射到非 \mathcal{Y} 的部分。在搜索过程中，它结合了基于优化的过滤和修剪。Planet也是不完备的。

Reluplex [20]在函数空间中执行树搜索。它扩展了单纯形算法(一种用于解决线性规划(LP)实例的标准算法)，以支持ReLU网络。对于单纯形法的ReLU，该算法称为Reluplex。Reluplex是完备的。

4 Preliminaries 预备知识

This section introduces additional notation and operations that will be used in different verification algorithms to be discussed in the following sections.⁸ Section 4.1 discusses interval arithmetic to compute node-wise bounds given an input set. Such node-wise bounds are needed in many methods, such as MIPVerify, Duality, ConvDual, Planet, and Reluplex. Section 4.2 discusses interval refinement, which is used in ReluVal and BaB. Section 4.3 discusses methods

⁸ First-time readers may skip this section and refer back when going into the details of the algorithms.

to compute network gradient and bounds on the gradient given a non-trivial input set. The bounds on the gradient are used in ReluVal and FastLin. Section 4.4 introduces specific notation for ReLU activations.

We use $[a]_+ := \max\{a, 0\}$ and $[a]_- = \min\{a, 0\}$ to represent the positive and negative parts of a scalar variable a . For a vector \mathbf{a} or a matrix \mathbf{A} , $[\cdot]_+$ and $[\cdot]_-$ take element-wise max and min, respectively.

4.1 Bounds

The lower and upper bounds on $z_{i,j}$, i.e., the value of node j at layer i after activation, are denoted $\ell_{i,j}$ and $u_{i,j}$. The lower and upper bounds on $\hat{z}_{i,j}$, i.e., the value of node j at layer i before activation, are denoted $\hat{\ell}_{i,j}$ and $\hat{u}_{i,j}$. The after-activation bounds for the whole layer i are denoted ℓ_i and \mathbf{u}_i . The before-activation bounds for the whole layer i are denoted $\hat{\ell}_i$ and $\hat{\mathbf{u}}_i$. The bounds can be computed using different methods. For example, MaxSens uses interval arithmetic, which will be discussed in section 5.4. Planet uses optimization to compute tight bounds, which will be discussed in section 9.3. Because the optimization is difficult to solve, ConvDual and FastLin relax the network constraints and analytically compute the bounds using dynamic programming, which will be discussed in section 7.3 and section 8.2. Here we introduce interval arithmetic.

Interval arithmetic By interval arithmetic, given the bounds at layer $i - 1$, the bounds at layer i satisfy

$$\hat{\ell}_{i,j} = \min_{\mathbf{z}_{i-1} \in [\ell_{i-1}, \mathbf{u}_{i-1}]} \mathbf{w}_{i,j} \mathbf{z}_{i-1} + b_{i,j} = [\mathbf{w}_{i,j}]_+ \ell_{i-1} + [\mathbf{w}_{i,j}]_- \mathbf{u}_{i-1} + b_{i,j}, \quad (15a)$$

$$\hat{u}_{i,j} = \max_{\mathbf{z}_{i-1} \in [\ell_{i-1}, \mathbf{u}_{i-1}]} \mathbf{w}_{i,j} \mathbf{z}_{i-1} + b_{i,j} = [\mathbf{w}_{i,j}]_+ \mathbf{u}_{i-1} + [\mathbf{w}_{i,j}]_- \ell_{i-1} + b_{i,j}, \quad (15b)$$

$$\ell_{i,j} = \min_{\hat{z}_{i,j} \in [\hat{\ell}_{i,j}, \hat{u}_{i,j}]} \sigma_{i,j}(\hat{z}_{i,j}) = \sigma_{i,j}(\hat{\ell}_{i,j}), \quad (15c)$$

$$u_{i,j} = \max_{\hat{z}_{i,j} \in [\hat{\ell}_{i,j}, \hat{u}_{i,j}]} \sigma_{i,j}(\hat{z}_{i,j}) = \sigma_{i,j}(\hat{u}_{i,j}), \quad (15d)$$

where the implicit assumption for the last two equalities is that the activation $\sigma_{i,j}$ is non-decreasing. In the implementation, the bounds are usually stored as a list of hyperrectangles. The bounds with respect to the input constraint \mathcal{X} can be computed layer-by-layer using interval arithmetic (15), to be discussed in algorithm 5.5. In the following discussion, we write interval arithmetic with respect to linear mappings compactly as \otimes where

$$\mathbf{W} \otimes [\ell, \mathbf{u}] := [[\mathbf{W}]_+ \ell + [\mathbf{W}]_- \mathbf{u}, [\mathbf{W}]_+ \mathbf{u} + [\mathbf{W}]_- \ell], \quad (16)$$

where ℓ and \mathbf{u} can also be replaced with matrices. The function (16) is implemented in algorithm 4.1. Hence, $[\ell_i, \mathbf{u}_i] = \mathbf{W}_i \otimes [\ell_{i-1}, \mathbf{u}_{i-1}] + [\mathbf{b}_i, \mathbf{b}_i]$.

最后两个等式的潜在的假设是激活函数是非减少的。在实现中，边界通常存储为超矩形列表。可以使用区间算法（15）逐层计算相对于输入约束 \mathcal{X} 的边界，这将在算法5.5中进行讨论。在下面的讨论中，我们将关于线性映射的区间算法紧凑地写成 \otimes ，如下所示

区间传播朴素的julia实现

Algorithm 4.1. Function to compute linear mapping on intervals which corresponds to equation (16).

```
function interval_map(W, l, u)
    l_new = max.(W, 0) * l + min.(W, 0) * u
    u_new = max.(W, 0) * u + min.(W, 0) * l
    return (l_new, u_new)
end
```

4.2 Interval Refinement

Interval refinement is used in many methods including ReluVal and BaB. In those cases, a high dimensional interval $[\ell, \mathbf{u}]$ is split in two at index i^* :

$$[\ell, \mathbf{u}^*] \text{ and } [\ell^*, \mathbf{u}], \quad (17)$$

where $\mathbf{u}^* = \mathbf{u} - r_{i^*} \mathbf{e}_{i^*}$, $\ell^* = \ell + r_{i^*} \mathbf{e}_{i^*}$, $r_{i^*} = \frac{1}{2}(u_{i^*} - \ell_{i^*})$, and \mathbf{e}_i is a unit vector whose entries are all zero except at the i th entry. The index i^* is determined using different methods. For example, in BaB, the index i^* is chosen to be the longest dimension, *i.e.*, $i^* = \arg \max_i (u_i - \ell_i)$. The function to perform the split is implemented in algorithm 4.2. Figure 4 illustrates the split of a two dimensional interval.

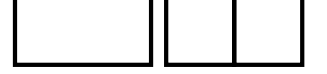


Figure 4. Illustration of interval split. The high dimensional interval on the left is split into two high dimensional intervals on the right, with respect to the horizontal axis.

```

function split_interval(dom::Hyperrectangle, i::Int64)
    input_lower, input_upper = low(dom), high(dom)
    input_upper[i] = dom.center[i]
    input_split_left = Hyperrectangle(low = input_lower, high = input_upper)
    input_lower[i] = dom.center[i]
    input_upper[i] = dom.center[i] + dom.radius[i]
    input_split_right = Hyperrectangle(low = input_lower, high = input_upper)
    return (input_split_left, input_split_right)
end

```

Algorithm 4.2. Function to split interval at a specified index. The argument `dom` is the interval to be split. The argument `index` is the index i^* where the interval should be split at. The function returns the two hyperrectangles after the split, which correspond to equation (17).

4.3 Gradient

The gradient of a neural network (of the output with respect to the input) satisfies the chain rule,

$$\nabla \mathbf{f} := \frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \frac{\partial \mathbf{y}}{\partial \hat{\mathbf{z}}_n} \frac{\partial \hat{\mathbf{z}}_n}{\partial \mathbf{z}_{n-1}} \cdots \frac{\partial \mathbf{z}_1}{\partial \hat{\mathbf{z}}_1} \frac{\partial \hat{\mathbf{z}}_1}{\partial \mathbf{x}} = \nabla \sigma_n \mathbf{W}_n \cdots \nabla \sigma_1 \mathbf{W}_1, \quad (18)$$

where $\nabla \sigma_i := \frac{\partial \mathbf{z}_i}{\partial \hat{\mathbf{z}}_i} \in \mathbb{R}^{k_i \times k_i}$.

In some cases, we evaluate the point-wise gradient $\nabla \mathbf{f}(\mathbf{x}_0)$ for some \mathbf{x}_0 . The point-wise gradient is easy to compute by following the chain rule as shown in the first function in algorithm 4.3. In other cases, *e.g.*, in ReluVal and FastLip, we need to compute the maximum gradient given an input set \mathcal{X} , *i.e.*, $\max_{\mathbf{x} \in \mathcal{X}} \nabla \mathbf{f}(\mathbf{x})$. The maximum over a vector is taken point-wise. The maximum gradient can be computed using interval arithmetic.

Denote the lower and upper bounds of $\nabla \sigma_i$ with respect to the input set \mathcal{X} as $\underline{\Lambda}_i \in \mathbb{R}^{k_i \times k_i}$ and $\overline{\Lambda}_i \in \mathbb{R}^{k_i \times k_i}$. The matrices $\underline{\Lambda}_i$ and $\overline{\Lambda}_i$ are diagonal. Due to the monotonicity assumption on σ_i ,
对角线
对角矩阵?
单调性假设

$$\overline{\Lambda}_i \geq \underline{\Lambda}_i \geq \mathbf{0}, \quad (19)$$

where the inequalities are interpreted point-wise.

Define $\mathbf{G}_i := \frac{\partial \mathbf{z}_i}{\partial \mathbf{x}}$ and $\hat{\mathbf{G}}_i := \mathbf{W}_i \mathbf{G}_{i-1}$. Denote the lower and upper bounds of \mathbf{G}_i as $\underline{\mathbf{G}}_i, \overline{\mathbf{G}}_i \in \mathbb{R}^{k_i \times k_0}$, and the lower and upper bounds of $\hat{\mathbf{G}}_i$ as $\underline{\hat{\mathbf{G}}}_i, \overline{\hat{\mathbf{G}}}_i \in \mathbb{R}^{k_i \times k_0}$. The bounds on the gradients are initialized as $\underline{\mathbf{G}}_0 = \overline{\mathbf{G}}_0 = \mathbf{I}$, and can be updated inductively using interval arithmetic by forward propagation,⁹

$$\mathbf{G}_i = \nabla \sigma_i \hat{\mathbf{G}}_i = \nabla \sigma_i \mathbf{W}_i \mathbf{G}_{i-1}. \quad (20)$$

Given $\underline{\mathbf{G}}_{i-1}$ and $\overline{\mathbf{G}}_{i-1}$,

$$[\underline{\hat{\mathbf{G}}}_i, \overline{\hat{\mathbf{G}}}_i] = \mathbf{W}_i \otimes [\underline{\mathbf{G}}_{i-1}, \overline{\mathbf{G}}_{i-1}]. \quad (21)$$

⁹ We can also use backward propagation in the chain rule to compute $\nabla \mathbf{f}$. Then the update equation becomes $\frac{\partial \mathbf{y}}{\partial \mathbf{z}_i} = \frac{\partial \mathbf{y}}{\partial \mathbf{z}_{i+1}} \nabla \sigma_{i+1} \mathbf{W}_{i+1}$.

The lower bound $\underline{\mathbf{G}}_i$ on the gradient \mathbf{G}_i is the minimum of $\nabla \sigma_i \hat{\mathbf{G}}_i$, where $\nabla \sigma_i \in [\underline{\Lambda}_i, \bar{\Lambda}_i]$ and $\hat{\mathbf{G}}_i \in [\hat{\underline{\mathbf{G}}}_i, \hat{\bar{\mathbf{G}}}_i]$. Since $\nabla \sigma_i \geq \mathbf{0}$ according to (19), the minimum of $\nabla \sigma_i \hat{\mathbf{G}}_i$ is achieved on the lower bound of $\hat{\mathbf{G}}_i$. Hence,

$$\underline{\mathbf{G}}_i = \min\{\underline{\Lambda}_i \hat{\underline{\mathbf{G}}}_i, \bar{\Lambda}_i \hat{\underline{\mathbf{G}}}_i\} = \underline{\Lambda}_i [\hat{\underline{\mathbf{G}}}_i]_+ + \bar{\Lambda}_i [\hat{\underline{\mathbf{G}}}_i]_-.$$
 (22)

Similarly, the upper bound on the gradient $\frac{\partial z_i}{\partial \mathbf{x}}$ satisfies

$$\bar{\mathbf{G}}_i = \underline{\Lambda}_i [\hat{\bar{\mathbf{G}}}_i]_- + \bar{\Lambda}_i [\hat{\bar{\mathbf{G}}}_i]_+.$$
 (23)

The function to compute the bounds on the gradient given a non-trivial input set is implemented in algorithm 4.3. There is a solver, called RecurJac [50], that can efficiently compute the maximum gradient in a recursive manner.¹⁰

计算最大梯度以递归的方式

¹⁰ <https://github.com/huanzhang12/RecurJac-Jacobian-Bounds>

```
function get_gradient(nnet::Network, x::Vector) 计算pointwise梯度
    z = x
    gradient = Matrix{Float64}(length(x), length(x))
    for (i, layer) in enumerate(nnet.layers)
        z_hat = affine_map(layer, z)
        o_gradient = act_gradient(layer.activation, z_hat) 计算激活函数的梯度
        gradient = Diagonal(o_gradient) * layer.weights * gradient
        z = layer.activation(z_hat)
    end
    return gradient
end

function get_gradient(nnet::Network, input::AbstractPolytope)
    LA, UA = act_gradient_bounds(nnet, input) 计算L, U
    return get_gradient(nnet, LA, UA)
end

function get_gradient(nnet::Network, LA::Vector{Matrix}, UA::Vector{Matrix})
    n_input = size(nnet.layers[1].weights, 2)
    LG = Matrix{Float64}(n_input, n_input)
    UG = Matrix{Float64}(n_input, n_input)
    for (i, layer) in enumerate(nnet.layers)
        LG_hat, UG_hat = interval_map(layer.weights, LG, UG)
        LG = LA[i] * max.(LG_hat, 0) + UA[i] * min.(LG_hat, 0)
        UG = LA[i] * min.(UG_hat, 0) + UA[i] * max.(UG_hat, 0)
    end
    return (LG, UG)
end
```

Algorithm 4.3. Functions to compute gradient. The first function computes point-wise gradient, where `act_gradient` (not shown) computes the gradient of the activation function. The second and third functions compute the bounds on the gradient given a non-trivial input set. The input to the second function is the input set. It calls `act_gradient_bounds` (not shown) to compute $\underline{\Lambda}_i$ and $\bar{\Lambda}_i$. The third function directly takes the bounds on the gradient of activation functions.

第二第三个函数计算给定非平凡输入集合的梯度边界。

第三个函数直接获得取激活函数的梯度的边界。

4.4 ReLU Activation

如果 σ_i 是ReLU激活函数，我们把一个二元向量的k次幂集和节点的激活状态进行关联。在第i层，给出节点的值的边界，我们定义节点所属的集合如下所示

If σ_i is a ReLU activation function, i.e., $\sigma_i(\hat{\mathbf{z}}_i) = [\mathbf{z}_i]_+$, we associate a binary vector $\delta_i \in \{0, 1\}^{k_i}$ for $i \in \{1, \dots, n\}$ to specify activation status (off or on) of the nodes. At layer i , given the bounds on the values of the nodes, we define the set of nodes that are activated Γ_i^+ , not activated Γ_i^- , and undetermined Γ_i as

$$\Gamma_i^+ = \{j : \hat{\ell}_{i,j} \geq 0\},$$
 (24a)

$$\Gamma_i^- = \{j : \hat{u}_{i,j} \leq 0\},$$
 (24b)

$$\Gamma_i = \{j : \hat{\ell}_{i,j} < 0 < \hat{u}_{i,j}\}.$$
 (24c)

下界大于零

上界小于零

不确定

The diagonal entries $\underline{\lambda}_{i,j}$ and $\bar{\lambda}_{i,j}$ of the bounds $\underline{\Lambda}_i, \bar{\Lambda}_i \in \mathbb{R}^{k_i \times k_i}$ on the gradient $\nabla \sigma_i$ satisfy that

$$\bar{\lambda}_{i,j} = \begin{cases} 1 & j \in \Gamma_i^+ \\ 0 & j \in \Gamma_i^- \\ 1 & j \in \Gamma_i \end{cases}, \quad \underline{\lambda}_{i,j} = \begin{cases} 1 & j \in \Gamma_i^+ \\ 0 & j \in \Gamma_i^- \\ 0 & j \in \Gamma_i \end{cases}. \quad (25)$$

5 Reachability

Reachability methods compute the output reachable set $\mathcal{R}(\mathcal{X}, \mathbf{f})$ to verify the problem through layer-by-layer analysis. This section first reviews the general methodology, and then discusses the specific methods. 本节首先回顾一般方法，然后讨论特定方法。

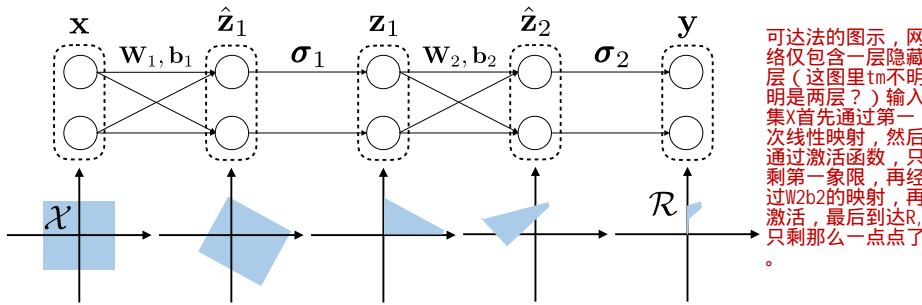


Figure 5. Illustration of reachability methods. The network in the illustration only contains one hidden layer. The input set \mathcal{X} is first passed through the linear mapping defined by \mathbf{W}_1 and \mathbf{b}_1 . Then it goes through the nonlinear mapping defined by σ_1 (ReLU is considered). The corresponding reachable sets are illustrated in the shaded area. The process is repeated for the next layer. And the output reachable set is then obtained.

5.1 Overview

The layer-by-layer propagation in reachability methods is illustrated in figure 5 and implemented in algorithm 5.1. The function `forward_network` computes \mathcal{R} . It calls `forward_layer` to perform layer-by-layer forward propagation. Once it computes the reachable set, `check_inclusion` verifies whether $\mathcal{R}(\mathcal{X}, \mathbf{f}) \subset \mathcal{Y}$. 检查是否包含

```
function solve(solver, problem::Problem)
    reach = forward_network(solver, problem.network, problem.input)
    return check_inclusion(reach, problem.output)
end

function forward_network(solver, nnet::Network, input::AbstractPolytope)
    reach = input
    for layer in nnet.layers
        reach = forward_layer(solver, layer, reach)
    end
    return reach
end

function check_inclusion(reach::Vector{<:AbstractPolytope}, output)
    for poly in reach
        issubset(poly, output) || return ReachabilityResult(:violated, reach)
    end
    return ReachabilityResult(:holds, similar(reach, 0))
end
```

Algorithm 5.1. General structure of reachability methods. The problem is solved by first performing layer-by-layer reachability analysis as specified in `forward_network`, then checking if the output reachable set belongs to the output constraint using `check_inclusion`. Different methods have different implementations of `forward_layer`. The outer loop `solve` can also vary between methods.

左边算法5.1介绍了通用可达性方法。问题被求解是在检查如果输出可达集是输出约束的集合的子集时判定为真。在不同的方法中，`forward_layer`的实现也有所不同。外层循环中的`solve`也可以在不同的方法中变化。

函数 `forward_layer` 关系到复杂映射。

其中线性映射的部分很简单

The function `forward_layer` involves the mapping $\mathbf{z}_{i-1} \mapsto \sigma_i(\mathbf{W}_i \mathbf{z}_{i-1} + \mathbf{b}_i)$. The linear mapping defined by $\mathbf{z}_{i-1} \mapsto \mathbf{W}_i \mathbf{z}_{i-1} + \mathbf{b}_i$ is relatively easy to handle. The nonlinear mapping $\hat{\mathbf{z}}_i \mapsto \sigma_i(\hat{\mathbf{z}}_i)$ is non-trivial. Different methods introduce different ways to handle nonlinear mappings. 因此, `forward_layer` 的实现随着不同的方法在变化。不同的方法中介绍了不同的方式去处理非线性映射。但是非线性映射是很难处理的。这篇文章中至少介绍了五种方法。Hence, the implementation of `forward_layer` varies across different methods. There are at least five different approaches in the literature:

- **精确可达性**, 适用于线性分段网络, 它计算了每一个线性分段的可达集, 并保留了所有集合的追踪路径。
Exact reachability (for piecewise linear networks), which computes the reachable set for every linear segment of the network and keeps track of all sets. This is done by **ExactReach** [46].
- **分割-合并**, 适用于无分段线性网络, 它计算了每一个线性分段的可达集, 并通过过度近似连接这些集合。
Split-and-join (for piecewise linear networks), which computes the reachable set for every linear segment of the network and joins those sets by over-approximation. This is done by **Ai2** [14].
- **区间算术**, 适用于单调的激活函数, 通过间隔算术分别计算每个节点的边界。
Interval arithmetic (for networks with monotone activation functions), which computes the bounds for each node separately by interval arithmetic. This is done by **MaxSens** [44].
- **符号传播**, 适用于分段线性网络, 它也使用区间算法计算节点的边界, 但使用符号表示来跟踪节点之间的依赖关系。
Symbolic propagation (for piecewise linear networks), which also computes the node-wise bounds using interval arithmetic but keeps track of dependencies among nodes using symbolic representations. This is done by **ReluVal** [40].
- **网络松弛**, 适用于分段线性网络。它根据网络的线性近似计算符号的下界和上界。
Network relaxation (for piecewise linear networks), which computes symbolic lower and upper bounds based on a linear approximation of the network. This is done by **FastLin** [41].

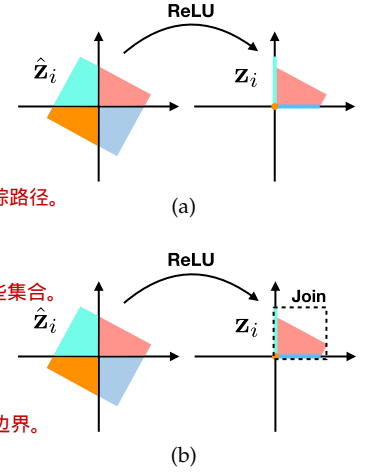


Figure 6. Illustration of different approaches to handle the nonlinear mapping $\hat{\mathbf{z}}_i \mapsto \sigma_i(\hat{\mathbf{z}}_i)$. (a) Exact reachability. (b) Split-and-join.

第一个方法是精确地, 没有近似。接下来的三种方法仅对通过不同层的几何对象进行近似。最后的方法对网络使用了近似。边界可以使用动态规划求解。The first method is exact without approximation. The next three methods only approximate the geometric objects passed through different layers. The last method approximates the network. The bounds can be computed using dynamic programming.

Figure 6 illustrates the difference between exact reachability and split-and-join in the case that the activation function is ReLU. Two nodes are considered, i.e., $\mathbf{z}_i \in \mathbb{R}^2$. Hence, there are four piecewise linear components in the nonlinear mapping $\hat{\mathbf{z}}_i \mapsto \sigma_i(\hat{\mathbf{z}}_i)$, which correspond to the four quadrants shown in the left plots of figure 6. Under ReLU, the set in the first quadrant (i.e., both values are greater than zero) is kept the same after the mapping. The sets in the second and the fourth quadrants (i.e., only one value is greater than zero) are mapped to line segments. The set in the third quadrant (i.e., both values are smaller than zero) is mapped to the origin. Exact reachability keeps track of all geometric objects after the mapping. In figure 6a, 四个象限, 一个输入集生成四个几何对象来表示可达到的集。在图6a中, 一个输入集生成四个几何对象来表示可达到的集。The number of geometric objects grows exponentially with the number of nodes at each layer. On the other hand, to improve scalability of the method, split-and-join methods merge all geometric objects together as shown in figure 6b. Mathematical derivations will be introduced in section 5.2 for exact reachability and in section 5.3 for split-and-join. 5.2节证明精确可达性, 5.3证明saj

Exact reachability and split-and-join methods do not distinguish individual nodes, but consider all nodes at a layer as a whole. Though these methods make it easy to track dependencies between nodes, the resulting high dimensional geometric objects (usually polytopes) can be inefficient to manipulate. Interval arithmetic considers node-wise reachability by computing reachable intervals for all nodes separately as shown in figure 7a. Consequently, the reachable set is a hyperrectangle, which is easy to manipulate. However, as the dependencies among nodes are removed, interval arithmetic may result in significant over-approximation. Symbolic propagation then introduces symbolic intervals to track those dependencies as shown in figure 7b. As illustrated in figure 7, symbolic propagation can generate much tighter bounds.¹¹

因此, 可达集是一个易于操作的超矩形集。然而, 由于去除节点之间的依赖关系, 区间算法可能会导致严重的过近似。符号传播然后引入符号间隔来跟踪这些依赖关系, 如图7b所示。像图7b中所说的那样, 引入符号传播可以收紧边界。区间算法通过计算所有节点的可达间隔来考虑节点的可达性, 如图7a所示。操纵

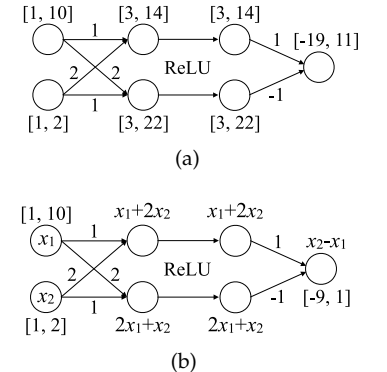


Figure 7. Illustration of the difference between interval arithmetic and symbolic propagation. (a) Interval arithmetic. (b) Symbolic propagation.

¹¹ To tighten the bounds in interval arithmetic, in addition to do symbolic propagation, we can also divide the input space into smaller intervals, and compute the reachable output intervals for those small intervals. This approach is used in **MaxSens** and **ReluVal**.

为了收紧区间算法的边界, 除了进行符号传播外, 我们还可以将输入空间划分为更小的区间, 并计算这些小区间的可达输出区间。该方法在**MaxSens**和**ReluVal**中得到了应用。

严格的数学推导将在第5.4节介绍区间算术，第8.1节介绍符号传播。

Rigorous mathematical derivations will be introduced in section 5.4 for interval arithmetic and section 8.1 for symbolic propagation.

For different methods, their outer loops, *e.g.*, the `solve` function, can also be different. The simplest outer loop is shown in algorithm 5.1, which works for ExactReach and Ai2. In some methods, the inputs are split into smaller segments to minimize over-approximation as illustrated in figure 8.¹² The reachable set for each segment is computed and then joined together. MaxSens uses this approach. However, blindly splitting the input set may not be efficient. By combining with search, we can look for the most influential inputs to split. ReluVal uses this approach. We may also use binary search to adjust the radius of the segment, which is adopted in FastLin.

This section discusses ExactReach, Ai2, and MaxSens. ReluVal and FastLin will be discussed in section 8.

5.2 ExactReach

ExactReach[46]对具有线性或ReLU激活函数的网络进行精确可达性分析。对于任何ReLU函数，如果输入集是多面体的并集，那么输出可达集也是多面体并集，如图6a所示。在实现中，输入集和输出集都被设置为超多面体。计算单个层的可达集的函数如算法5.2所示，这是算法5.1的主循环调用的函数。

ExactReach [46] performs exact reachability analysis for networks with linear or ReLU activations. For any ReLU function, if the input set is a union of polytopes, then the output reachable set is also a union of polytopes as shown in figure 6a. In the implementation, the input set and output set are both set to HPolytope. The function to compute the reachable set for a single layer is shown in algorithm 5.2, which is called in the main loop of algorithm 5.1.

The input set to layer i consists of a list of H-polytopes. One input H-polytope parameterized by $\mathbf{C} \in \mathbb{R}^{k \times k_{i-1}}$ and $\mathbf{d} \in \mathbb{R}^k$ defines a set

$$\mathcal{I} = \{\mathbf{z}_{i-1} : \mathbf{C}\mathbf{z}_{i-1} \leq \mathbf{d}\}, \quad (26)$$

where k is the number of constraints. After the linear mapping $\mathbf{z}_{i-1} \mapsto \mathbf{W}_i\mathbf{z}_{i-1} + \mathbf{b}_i$, the set before activation is denoted

$$\hat{\mathcal{I}} = \{\hat{\mathbf{z}}_i : \hat{\mathbf{C}}\hat{\mathbf{z}}_i \leq \hat{\mathbf{d}}\}, \quad (27)$$

where $\hat{\mathbf{C}} \in \mathbb{R}^{k \times k_i}$ and $\hat{\mathbf{d}} \in \mathbb{R}^k$. The number of inequality constraints k in (27) may be different from that in (26). The set $\hat{\mathcal{I}}$ can be computed by calling `linear_transform`, which converts \mathcal{I} into a V-polytope, applies the linear map to all vertices, then converts it back to an H-polytope.

The set $\hat{\mathcal{I}}$ can be partitioned into several non-intersecting subsets according to different activation patterns. The activation status for \mathbf{z}_i is denoted $\delta_i \in \{0, 1\}^{k_i}$. Since the entries in δ_i are binary, there is a bijection between δ_i and an integer $h \in \{0, 1, \dots, 2^{k_i} - 1\}$.¹³ Define a diagonal matrix $\mathbf{P}_h \in \mathbb{R}^{k_i \times k_i}$, whose diagonal entries are the entries in the binary vector δ_i . Hence, there is a correspondence between \mathbf{P}_h and the integer h . For a given activation δ_i , the before activation node $\hat{\mathbf{z}}_i$ needs to satisfy that if $\delta_{i,j} = 1$, then $\hat{z}_{i,j} \geq 0$; and if $\delta_{i,j} = 0$, then $\hat{z}_{i,j} \leq 0$. The subset of $\hat{\mathcal{I}}$ that corresponds to the h th activation pattern is

$$\hat{\mathcal{I}}_h = \{\hat{\mathbf{z}}_i : \mathbf{P}_h\hat{\mathbf{z}}_i \geq \mathbf{0}, (\mathbf{I} - \mathbf{P}_h)\hat{\mathbf{z}}_i \leq \mathbf{0}, \hat{\mathbf{C}}\hat{\mathbf{z}}_i \leq \hat{\mathbf{d}}\}. \quad (28)$$

In a compact form, the constraint on $\hat{\mathbf{z}}_i$ is

$$\begin{bmatrix} \hat{\mathbf{C}} \\ \mathbf{I} - 2\mathbf{P}_h \end{bmatrix} \hat{\mathbf{z}}_i \leq \begin{bmatrix} \hat{\mathbf{d}} \\ \mathbf{0} \end{bmatrix}. \quad (29)$$

The expression $\mathbf{I} - 2\mathbf{P}_h$ is a diagonal matrix whose entries are either 1 (for inactive nodes) or -1 (for active nodes). The constraint $(\mathbf{I} - 2\mathbf{P}_h)\hat{\mathbf{z}}_i \leq \mathbf{0}$ is a combination of the two constraints $\mathbf{P}_h\hat{\mathbf{z}}_i \geq \mathbf{0}$ and $(\mathbf{I} - \mathbf{P}_h)\hat{\mathbf{z}}_i \leq \mathbf{0}$.

对于不同的方法，它们的外部循环，例如solve函数，也可以是不同的。最简单的外循环如算法5.1所示，该算法适用于ExactReach和Ai2。在一些方法中，输入被分割成更小的片段，以减少近似，如图8所示，每个片段的可达集被计算，然后合并在一起。MaxSens使用了这种方法。然而，盲目分割输入集可能不是有效的。通过与搜索相结合，我们可以寻找最有影响的输入进行拆分。ReluVal使用了这种方法。我们也可以使用二分搜索来调整线段的半径，在FastLin中运用了这一点。

Recall `split_interval`, first introduced in section 4.

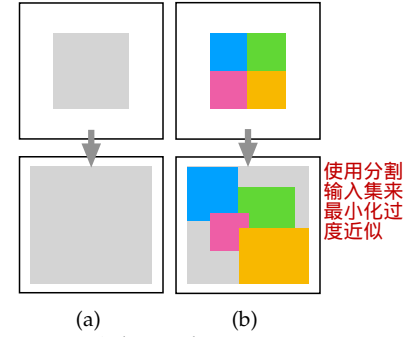


Figure 8. Splitting the input set to minimize over-approximation. The upper square is the input domain and the lower square is the output domain. (a) Over-approximated reachable set (gray square in the output domain) without partition. (b) Over-approximated reachable sets for different segments of the input set. Colors show correspondence.

¹³ When $h = 0$, all nodes are inactive. When $h = 2^{k_i} - 1$, all nodes are active.

For $\hat{\mathbf{z}}_i \in \hat{\mathcal{I}}_h$, the after activation nodes satisfy that $\mathbf{z}_i = \mathbf{P}_h \hat{\mathbf{z}}_i$. Hence, the reachable set \mathcal{O}_h for $\hat{\mathcal{I}}_h$ is a linear transform $\hat{\mathbf{z}}_i \rightarrow \mathbf{P}_h \hat{\mathbf{z}}_i$ of $\hat{\mathcal{I}}_h$ defined by (29). We write the linear transformation as

$$\mathcal{O}_h = \mathbf{P}_h \circ \hat{\mathcal{I}}_h. \quad (30)$$

The above process is implemented in `forward_partition`.

Finally, the output reachable set for \mathcal{I} is the union of all \mathcal{O}_h ,

$$\mathcal{O} = \bigcup_{h=0}^{2^{k_i}-1} \mathcal{O}_h. \quad (31)$$

It has been shown that the output set \mathcal{O} is *tight* [46], meaning that it is not an over-approximation in the sense that for any point \mathbf{z}_i in \mathcal{O} , there is a point \mathbf{z}_{i-1} in \mathcal{I} satisfying $\mathbf{z}_i = \mathbf{f}_i(\mathbf{z}_{i-1})$.

For one input polytope, the output for one layer generates 2^{k_i} polytopes. Hence, the number of polytopes grows exponentially with the depth. Though the empty sets can be pruned out in the process, it is still inefficient to keep track of the exact reachable set for large neural networks. Xiang, Tran, and Johnson developed a toolbox, called NNV,¹⁴ for efficient reachability analysis using parallel computation.

¹⁴ <https://github.com/verivital/nnv>.

```

struct ExactReach end

function forward_layer(solver::ExactReach, layer::Layer, input::HPolytope)
    input = affine_map(layer, input)
    return forward_partition(layer.activation, input)
end

function forward_partition(act::ReLU, input::HPolytope)
    n = dim(input)
    output = Vector{HPolytope}(undef, 0)
    C, d = tosimplehrep(input)
    dh = [d; zeros(n)]
    for h in 0:(2^n)-1
        P = getP(h, n)
        Ch = [C; I - 2P]
        input_h = HPolytope(Ch, dh)
        if !isempty(input_h)
            push!(output, linear_map(Matrix{Float64}(P), input_h))
        end
    end
    return output
end

```

Algorithm 5.2. ExactReach. The main process follows from algorithm 5.1. In the `forward_layer` function, each input set \mathcal{I} first goes through an affine map to $\hat{\mathcal{I}}$. Then the function `forward_partition` partitions $\hat{\mathcal{I}}$ into $\hat{\mathcal{I}}_h$ for the h th activation pattern. The output set \mathcal{O}_h for each $\hat{\mathcal{I}}_h$ is computed using linear transformation and the reachable set is a union of all these \mathcal{O}_h .

5.3 Ai2

In many cases, the exact reachable set is intractable. In Ai2 [14], an estimate $\tilde{\mathcal{R}}(\mathcal{X}, \mathbf{f})$ of the reachable set is obtained such that $\mathcal{R}(\mathcal{X}, \mathbf{f}) \subseteq \tilde{\mathcal{R}}(\mathcal{X}, \mathbf{f})$.

Ai2 uses an *abstract domain* to approximate the reachable set at each layer, which is represented by a set of logical formulas that capture certain geometric shapes, such as the geometries and their formulas introduced in section 2.2.¹⁵ The choice of abstract domain needs to balance between precision and scalability. For example, the polytopes used in ExactReach are precise but not scalable, while the hyperrectangles used in MaxSens are scalable but too loose. The original implementation of Ai2 uses zonotopes, center-symmetric convex closed polytopes, which are more scalable than polytopes and tighter than hyperrectangles. Due to lack of tools to manipulate geometries defined by zonotopes, we use polytopes in our implementation.

Ai2 works for piecewise linear activation functions, *e.g.*, ReLU and max pooling. Any piecewise linear activation function can be described as one conditional affine transformation (CAT), which consists of a set of linear conditions and a set of affine mappings corresponding to the linear conditions. For example, for a ReLU activation,

$$\sigma_i(\hat{\mathbf{z}}_i) = \begin{cases} \mathbf{P}_0 \hat{\mathbf{z}}_i & \text{if } (\mathbf{I} - 2\mathbf{P}_0) \hat{\mathbf{z}}_i \leq \mathbf{0} \\ \mathbf{P}_1 \hat{\mathbf{z}}_i & \text{if } (\mathbf{I} - 2\mathbf{P}_1) \hat{\mathbf{z}}_i \leq \mathbf{0} \\ \vdots & \\ \mathbf{P}_{2^{k_i}-1} \hat{\mathbf{z}}_i & \text{if } (\mathbf{I} - 2\mathbf{P}_{2^{k_i}-1}) \hat{\mathbf{z}}_i \leq \mathbf{0} \end{cases}, \quad (32)$$

where \mathbf{P}_h for different h is defined in section 5.2. Each condition corresponds to one specific activation pattern.

To propagate an abstract domain through a CAT, Ai2 introduces two basic operations: *meet* (\sqcap) and *join* (\sqcup). The meet operation splits an abstract domain into different subdomains that correspond to different conditions of the CAT. Due to the restriction of the abstract domain, those subdomains may be over-approximated and overlap with each other. For example, if the abstract domain is chosen to be hyperrectangles, then a subdomain corresponding to the condition $(\mathbf{I} - 2\mathbf{P}_h) \hat{\mathbf{z}}_i \leq \mathbf{0}$ is the smallest hyperrectangle that includes all points that satisfy the condition. After the meet operation, the reachable sets of those subdomains are computed with respect to the linear maps under the corresponding conditions. The join operation then uses one instance of the abstract domain to cover and approximate all the reachable sets. The implementation of the meet and join operations is deeply related to the chosen abstract domain. If the abstract domain is the polytope domain, ExactReach also splits the input set according to different cases and computes \mathcal{O}_h in different cases. However, ExactReach does not have a join operation. Instead, it keeps track of all sets in (31).

Our implementation is shown in algorithm 5.3. For simplicity, we only consider ReLU activations. The input and output sets are both polytopes.

An input set \mathcal{I} at layer i goes through the linear map defined by \mathbf{W}_i and \mathbf{b}_i . The matrix \mathbf{W}_i rotates the set \mathcal{I} and \mathbf{b}_i shifts the center of the set. The set after those linear maps is denoted $\hat{\mathcal{I}}$. Then the output set is

$$\hat{\mathcal{I}}_h = \hat{\mathcal{I}} \sqcap \{\hat{\mathbf{z}}_i : (\mathbf{I} - 2\mathbf{P}_h) \hat{\mathbf{z}}_i \leq \mathbf{0}\}, \quad (33a)$$

$$\mathcal{O}_h = \mathbf{P}_h \circ \hat{\mathcal{I}}_h, \quad (33b)$$

$$\mathcal{O} = \sqcup_{h=0}^{2^{k_i}-1} \mathcal{O}_h. \quad (33c)$$

where (33a) is the meet step, (33b) the linear mapping, and (33c) the join step. (33a) is the same as in (30). The meet function adds more constraints to the set. Since the mapping in (33b) is linear, we can efficiently compute the output set by simply mapping all vertices. Then all those sets are joined using a convex hull.¹⁶

¹⁵ A detailed discussion of an abstract domain for certifying neural networks can be found in [34]. An extended version of Ai2, called ERAN, which is robust to floating point arithmetic [34], can be found in <https://github.com/eth-sri/eran>. An approach that combines Ai2 with mixed integer optimization is discussed in Singh et al. [35].

¹⁶ The original implementation of Ai2 uses a zonotope to represent the abstract domain. The meet and join operations are implemented differently and are customized for zonotopes.

For one input polytope, the output reachable set is still one polytope. Hence, Ai2 is much more scalable than ExactReach, though the over-approximation results in incompleteness. Following Ai2, the authors introduced DeepZ [33], which can scale to other activation functions, and is robust to floating point operations. Recently, Yang et al. introduce a method combining abstract domain with symbolic propagation to further improve scalability and precision of the verification algorithm [49].

```

struct Ai2 end

function forward_layer(solver::Ai2, layer::Layer, input::AbstractPolytope)
    outlinear = affine_map(layer, input)
    relued_subsets = forward_partition(layer.activation, outlinear)
    return convex_hull(relued_subsets)
end

```

5.4 MaxSens

MaxSens [44] is also a reachability method that uses over-approximation. It works for networks with monotone activation functions and low-dimensional input and output spaces. The key idea of MaxSens is to grid the input space and compute the reachable set for each grid cell. The finer the grid cells, the smaller the over-approximation. Computing the reachable sets for different cells can be done in parallel.

Algorithm 5.4 provides an implementation of MaxSens. The input set is a hyperrectangle. The output set can be any abstract polytope. There is one more step in the main loop than in the general `solve` function in algorithm 5.1, which is to partition the input set into several grid cells. The `forward_layer` function takes a hyperrectangle input set and outputs the reachable hyperrectangle.

Suppose the input set at layer i is

$$\mathcal{I} = \{\mathbf{z}_{i-1} : |\mathbf{z}_{i-1} - \mathbf{c}_{i-1}| \leq \mathbf{r}_{i-1}\}, \quad (34)$$

where $\mathbf{c}_{i-1} \in \mathbb{R}^{k_{i-1}}$ is the center of the hyperrectangle and $\mathbf{r}_{i-1} \in \mathbb{R}^{k_{i-1}}$ is the radius of the hyperrectangle. The output reachable set is over-approximated by a hyperrectangle

$$\mathcal{O} = \{\mathbf{z}_i : |\mathbf{z}_i - \mathbf{c}_i| \leq \mathbf{r}_i\}, \quad (35)$$

where $\mathbf{c}_i, \mathbf{r}_i \in \mathbb{R}^{k_i}$.

For simplicity, define the following node-wise values for layer i ,

$$\beta_j = \sigma_{i,j}(\mathbf{w}_{i,j}\mathbf{c}_{i-1} + b_{i,j}), \quad (36a)$$

$$\beta_j^{max} = \sigma_{i,j}(\mathbf{w}_{i,j}\mathbf{c}_{i-1} + |\mathbf{w}_{i,j}|\mathbf{r}_{i-1} + b_{i,j}), \quad (36b)$$

$$\beta_j^{min} = \sigma_{i,j}(\mathbf{w}_{i,j}\mathbf{c}_{i-1} - |\mathbf{w}_{i,j}|\mathbf{r}_{i-1} + b_{i,j}), \quad (36c)$$

where $\sigma_{i,j}$ is the activation function for the j th node, and $\mathbf{w}_{i,j}$ is the j th row of \mathbf{W}_i . Due to monotonicity of $\sigma_{i,j}$, we have

$$z_{i,j} = \sigma_{i,j}(\mathbf{w}_{i,j}\mathbf{z}_{i-1} + b_{i,j}) \in [\beta_j^{min}, \beta_j^{max}], \forall \mathbf{z}_{i-1} \in \mathcal{I}. \quad (37)$$

There are three different ways to define the over-approximated set \mathcal{O} as illustrated in figure 9.

Algorithm 5.3. Ai2. Every set goes through meet and join as defined in equation (33). Note that in the case of H-polytope input sets, meet and join are equivalently replaced with `forward_partition` (defined in algorithm 5.2) and `convex_hull`, respectively. The meet operation computes the part of input that satisfies a given activation pattern by adding more linear constraints to the input `HPolytope` according to equation (33a).

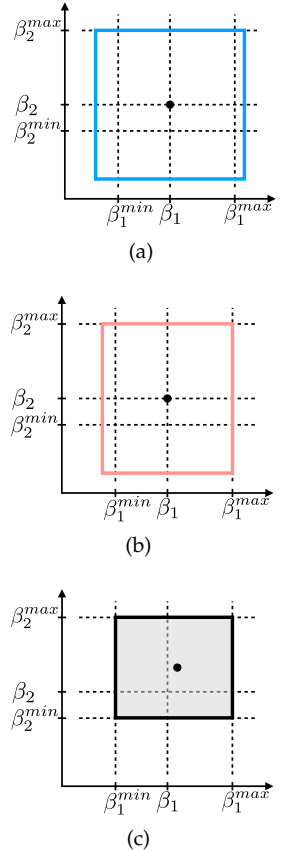


Figure 9. Illustration of different approximations of output reachable sets. (a) Center-aligned set with uniform radius. (b) Center-aligned set with non uniform radius. (c) Tight set.

- Center-aligned set with uniform radius.

As illustrated in figure 9a, the output set \mathcal{O} is constructed to be a hypercube by setting all entries of \mathbf{r}_i to be equal to its maximum element. Though the reachable set becomes looser, this method requires less memory to store intermediate results because we only need to store a scalar bound instead of a vector of bounds. The uniform bound indeed represents the “maximum sensitivity” of the network given the input set. However, since we use `Hyperrectangle` objects to store intermediate results anyway, a uniform bound does not significantly enhance efficiency. Hence, our implementation uses a non-uniform bound for both \mathcal{I} and \mathcal{O} .

- Center-aligned set with non-uniform radius.

As illustrated in figure 9b, the output set \mathcal{O} is no longer required to have uniform radius. By requiring that the center of the input hyperrectangle \mathcal{I} maps to the center of the output hyperrectangle \mathcal{O} , the center and radius of the \mathcal{O} can be obtained, for all $j \in \{1, \dots, k_i\}$,

$$c_{i,j} = \beta_j, \quad (38a)$$

$$r_{i,j} = \max_{\mathbf{z}_{i-1} \in \mathcal{I}} |\sigma_{i,j}(\mathbf{w}_{i,j}\mathbf{z}_{i-1} + b_{i,j}) - c_{i,j}| \quad (38b)$$

$$= \max\{\beta_j^{max} - \beta_j, \beta_j - \beta_j^{min}\}. \quad (38c)$$

where $r_{i,j}$ and $c_{i,j}$ are the j th entry in \mathbf{r}_i and \mathbf{c}_i . The last equality is due to the monotonicity of $\sigma_{i,j}$.

- Tight set.

A even tighter result can be obtained by directly using β_j^{min} and β_j^{max} as bounds and not aligning the centers of \mathcal{I} and \mathcal{O} . As illustrated in figure 9c, the center and radius of the tight set can be defined as

$$c_{i,j} = \frac{\beta_j^{min} + \beta_j^{max}}{2}, \quad (39a)$$

$$r_{i,j} = \frac{\beta_j^{max} - \beta_j^{min}}{2}. \quad (39b)$$

Equivalently, the output set can be represented as

$$\mathcal{O}^* = \{\mathbf{z}_i : \beta_j^{min} \leq z_{i,j} \leq \beta_j^{max}, \forall j\}. \quad (40)$$

It is easy to show that the resulting node-wise bounds are the same as the bounds computed in (15) by interval arithmetic.

The last two cases are implemented in `forward_node`. In algorithm 5.4, the solver has a boolean field `tight`. When `tight` is set to be true, it computes the set in (39). Otherwise, it computes the center-aligned set in (38). The center-aligned set is desired if we want to estimate the maximum sensitivity (or maximum gradient) of the network \mathbf{f} at the center of the input set.

The advantage of MaxSens over other reachability methods is that the number of geometric objects does not grow during the layer-by-layer propagation. The total number of hyperrectangles only depends on the the initial partition. Though the number of hyperrectangles will not grow during the layer-by-layer propagation, the error of over-approximation will accumulate quickly with respect to the number of layers. For networks with many input nodes, the number of hyperrectangles on the initial partition can be prohibitively large for a tight estimation. Otherwise, the computation with a sparse partition will be overly conservative [47]. To improve the initial partition, the authors developed a specification-guided method [47] that can adaptively choose the partition resolution according to the problem specification.

Some of the methods discussed later need to compute the bounds of each node. We implement the `get_bounds` function in algorithm 5.5 based on MaxSens, but with the tighter output reachable set (39), which is equivalent to the interval arithmetic introduced in (15) in section 4.

```

struct MaxSens
    resolution::Float64 = 1.0
    tight::Bool         = false
end

function solve(solver::MaxSens, problem::Problem)
    inputs = partition(problem.input, solver.resolution)
    f_n(x) = forward_network(solver, problem.network, x)
    outputs = map(f_n, inputs)
    return check_inclusion(outputs, problem.output)
end

function forward_layer(solver::MaxSens, L::Layer, input::Hyperrectangle)
    (W, b, act) = (L.weights, L.bias, L.activation)
    center = zeros(size(W, 1))
    gamma = zeros(size(W, 1))
    for j in 1:size(W, 1)
        node = Node(W[j,:], b[j], act)
        center[j], gamma[j] = forward_node(solver, node, input)
    end
    return Hyperrectangle(center, gamma)
end

function forward_node(solver::MaxSens, node::Node, input::Hyperrectangle)
    output = node.w' * input.center + node.b
    deviation = sum(abs.(node.w) .* input.radius)
     $\beta$  = node.act(output)
     $\beta_{\max}$  = node.act(output + deviation)
     $\beta_{\min}$  = node.act(output - deviation)
    if solver.tight
        return (( $\beta_{\max}$  +  $\beta_{\min}$ )/2, ( $\beta_{\max}$  -  $\beta_{\min}$ )/2)
    else
        return ( $\beta$ , max(abs( $\beta_{\max}$  -  $\beta$ ), abs( $\beta_{\min}$  -  $\beta$ )))
    end
end

```

Algorithm 5.4. MaxSens. The main `solve` function is slightly different from the general reachability method in algorithm 5.1 by adding a partition step. In `forward_layer`, the bounds are computed for each node using a method similar to interval arithmetic.


```

function get_bounds(problem::Problem)
    solver = MaxSens(1.0, true)
    bounds = Vector{Hyperrectangle}(length(nnet.layers) + 1)
    bounds[1] = input
    for (i, layer) in enumerate(nnet.layers)
        bounds[i+1] = forward_layer(solver, layer, bounds[i])
    end
    return bounds
end

```

Algorithm 5.5. Function to compute node-wise bounds. It outputs the tight bounds in MaxSens.

6 Primal Optimization

There can be many different designs of the optimization problem to verify (4). A common structure is

$$\min_{\mathbf{x}, \mathbf{y}} o(\mathbf{x}, \mathbf{y}, \mathcal{X}, \mathcal{Y}), \quad (41a)$$

$$\text{s.t. } \mathbf{x} \in \mathcal{X}, \mathbf{y} \notin \mathcal{Y}, \mathbf{y} = \mathbf{f}(\mathbf{x}), \quad (41b)$$

where $o(\mathbf{x}, \mathbf{y}, \mathcal{X}, \mathcal{Y})$ is an objective function, which may depend on the input \mathbf{x} , the output \mathbf{y} and their domains \mathcal{X} and \mathcal{Y} . We can either minimize or maximize the objective function. The major difficulty in solving (41) is the nonlinear and non-convex constraint imposed by the network \mathbf{f} .

NSVerify [23] and MIPVerify [38] reformulate the problem (41) into a mixed integer linear programming (MILP). Iterative LP (ILP) [4] approximates the problem (41) as a linear programming and solves it by iteratively adding the constraints.

This section first provides an overview of common methods to simplify the primal optimization problem, then discusses the three methods (*i.e.*, NSVerify, MIPVerify, ILP) in detail. For simplicity, we only consider ReLU activations. There are different ways to encode ReLU networks as linear constraints. The following two types of variables are usually used as decision variables in the optimization.¹⁷

- Variables for all nodes, *i.e.*, $\mathbf{z}_i \in \mathbb{R}^{k_i}$ for $i \in \{0, 1, \dots, n\}$.
- Variables for all activations, *i.e.*, $\delta_i \in \{0, 1\}^{k_i}$ for $i \in \{1, \dots, n\}$.

Our implementation uses JuMP.jl¹⁸ to model and solve the optimizations. In the following discussion, `Model` refers to a jump model and `solve(:Model)` calls the JuMP solver to solve the optimization problem encoded in the model.

6.1 Encoding Network as Constraints

Primal optimization needs to deal with the constraint imposed by the network. The constraint $\mathbf{y} = \mathbf{f}(\mathbf{x})$ is equivalent to

$$z_{i,j} = [\mathbf{w}_{i,j}\mathbf{z}_{i-1} + b_{i,j}]_+, \forall i \in \{1, \dots, n\}, \forall j \in \{1, \dots, k_i\}. \quad (42)$$

There are different ways to encode (42). For given activations δ_i , equation (42) can be encoded as linear constraints as shown in algorithms 6.1 to 6.3. For given bounds ℓ_i and \mathbf{u}_i , equation (42) can be encoded as linear constraints via triangle relaxation as shown in algorithm 6.4. Or (42) can be encoded as mixed integer linear constraints as shown in algorithms 6.5 and 6.6. In the following discussion, we use $\hat{z}_{i,j}$ for $\mathbf{w}_{i,j}\mathbf{z}_{i-1} + b_{i,j}$, though $\hat{z}_{i,j}$ is not a variable to be considered in the optimization.

¹⁷ NSVerify, MIPVerify, and ILP use these two kinds of variables. Other methods may use different sets of variables. For example, Reluplex uses \mathbf{z}_i and $\hat{\mathbf{z}}_i$ as decision variables.

¹⁸ <https://github.com/jump.jl>

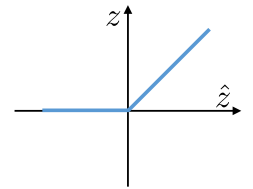


Figure 10. Illustration of ReLU activation function.

Linear constraints for given δ_i For a given activation δ_i for any i , the network can be encoded as a set of linear constraints for $j \in \{1, \dots, k_i\}$:

$$\delta_{i,j} = 1 \Rightarrow z_{i,j} = \hat{z}_{i,j} \geq 0, \quad (43a)$$

$$\delta_{i,j} = 0 \Rightarrow z_{i,j} = 0, \hat{z}_{i,j} \leq 0. \quad (43b)$$

The function is shown in algorithm 6.1. These constraints represent a subset of the original constraint (42), since the activation pattern is determined. This function is called in local search in Sherlock.

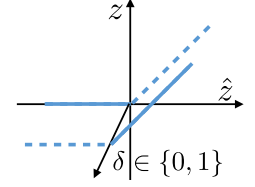


Figure 11. Illustration of linear encoding for given δ . If δ is unknown, it corresponds to mixed integer encoding. The δ axis is perpendicular to the $z - \hat{z}$ plane in 3D.

Algorithm 6.1. Encoding the network as linear constraints for given δ_i . The function `encode_newtork!` encodes the constraints layer by layer by calling `encode_layer!`. The encoding method is specified in the abstract type `AbstractLinearProgram`.

```

abstract type AbstractLinearProgram end
struct StandardLP <: AbstractLinearProgram end

function encode_network!(model::Model, network, z,  $\delta$ ,
                        encoding::AbstractLinearProgram)
    for (i, layer) in enumerate(network.layers)
        encode_layer!(encoding, model, layer, z[i], z[i+1],  $\delta[i]$ )
    end
    return encoding
end

function encode_layer! (::StandardLP, model, layer, zi, zi+1,  $\delta_{i+1}$ )
     $\hat{z}$  = affine_map(layer, zi)
    for j in 1:length(layer.bias)
        if  $\delta_{i+1}[j]$ 
            @constraint(model,  $\hat{z}[j] \geq 0.0$ )
            @constraint(model, zi+1[j] ==  $\hat{z}[j]$ )
        else
            @constraint(model,  $\hat{z}[j] \leq 0.0$ )
            @constraint(model, zi+1[j] == 0.0)
        end
    end
end

```

Relaxed linear constraints for given δ_i In some cases, we drop the inequalities in (43) to get a relaxed encoding to ensure that the optimization problem is still feasible for infeasible activation δ_i 's. The relaxed encoding is

$$\delta_{i,j} = 1 \Rightarrow z_{i,j} = \hat{z}_{i,j}, \quad (44a)$$

$$\delta_{i,j} = 0 \Rightarrow z_{i,j} = 0. \quad (44b)$$

The function is shown in algorithm 6.2 and illustrated in figure 12. This function is used in ILP.

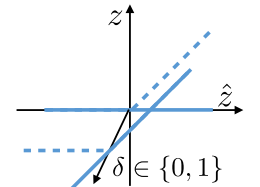


Figure 12. Illustration of relaxed linear encoding for given δ .

Slack linear constraints for given δ_i The previous relaxed linear encoding allows violation of the constraints imposed by ReLU's. We can use slack variables $s_{i,j}$'s to estimate the violations in the linear constraints (43):

$$\delta_{i,j} = 1 \Rightarrow \hat{z}_{i,j} + s_{i,j} \geq 0, \quad (45a)$$

$$\delta_{i,j} = 0 \Rightarrow \hat{z}_{i,j} - s_{i,j} \leq 0. \quad (45b)$$

The function is shown in algorithm 6.3. It is used in Planet in order to detect conflicts among different δ 's.

```

struct LinearRelaxedLP <: AbstractLinearProgram end

function encode_layer!(::LinearRelaxedLP, model, layer, zi, zi+1, δi+1)
     $\hat{z}$  = affine_map(layer, zi)
    for j in 1:length(layer.bias)
        if δi+1[j]
            @constraint(model, zi+1[j] ==  $\hat{z}$ [j])
        else
            @constraint(model, zi+1[j] == 0.0)
        end
    end
end

```

Algorithm 6.2. Encoding the network as relaxed linear constraints for given δ_i . Only the function `encode_layer!` is shown. The function `encode_network!` is the same as in algorithm 6.1.

```

struct SlackLP <: AbstractLinearProgram
    slack::Vector{Vector{VariableRef}}
end

function encode_layer!(SLP::SlackLP, model, layer, zi, zi+1, δi+1)
     $\hat{z}$  = affine_map(layer, zi)
    slack_vars = @variable(model, [1:length(layer.bias)])
    for j in 1:length(layer.bias)
        if δi+1[j]
            @constraint(model, zi+1[j] ==  $\hat{z}$ [j] + slack_vars[j])
            @constraint(model,  $\hat{z}$ [j] + slack_vars[j] >= 0.0)
        else
            @constraint(model, zi+1[j] == slack_vars[j])
            @constraint(model, 0.0 >=  $\hat{z}$ [j] - slack_vars[j])
        end
    end
    push!(SLP.slack, slack_vars)
end

```

Algorithm 6.3. Encoding the network as slack linear constraints for given δ_i . Only the function `encode_layer!` is shown. The function `encode_network!` is the same as in algorithm 6.1.

Triangle relaxation for given ℓ_i and \mathbf{u}_i When we can bound the value of the nodes, we can use Δ -relaxation to encode the constraint as

$$j \in \Gamma_i^+ \Rightarrow z_{i,j} = \hat{z}_{i,j}, \hat{z}_{i,j} \geq 0, \quad (46a)$$

$$j \in \Gamma_i^- \Rightarrow z_{i,j} = 0, \hat{z}_{i,j} \leq 0, \quad (46b)$$

$$j \in \Gamma_i \Rightarrow z_{i,j} \geq \hat{z}_{i,j}, z_{i,j} \geq 0, z_{i,j} \leq \frac{\hat{u}_{i,j}(\hat{z}_{i,j} - \hat{\ell}_{i,j})}{\hat{u}_{i,j} - \hat{\ell}_{i,j}}, \quad (46c)$$

where activated nodes Γ_i^+ , unactivated nodes Γ_i^- , and undetermined nodes Γ_i are introduced in (24). The function for Δ -relaxation is shown in algorithm 6.4. The function `linear_transform` corresponds to (15). Δ -relaxation is used in ConvDual and Planet.

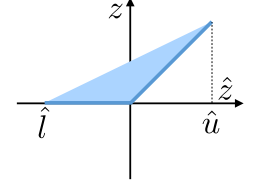


Figure 13. Illustration of triangle relaxation.

Algorithm 6.4. Encoding the network as linear constraints for given ℓ_i and \mathbf{u}_i via Δ -relaxation. Only the function `encode_layer!` is shown. The function `encode_network!` is the same as in algorithm 6.1.

```

struct TriangularRelaxedLP <: AbstractLinearProgram end

function encode_layer!(::TriangularRelaxedLP, model, layer, z_i, z_{i+1}, bounds)
     $\hat{z}$  = affine_map(layer, z_i)
     $\hat{z\_bound}$  = approximate_affine_map(layer, bounds)
     $\hat{\ell}$ ,  $\hat{u}$  = low( $\hat{z\_bound}$ ), high( $\hat{z\_bound}$ )
    for j in 1:length(layer.bias)
        if  $\hat{\ell}[j] > 0.0$ 
            @constraint(model, z_{i+1}[j] ==  $\hat{z}[j]$ )
        elseif  $\hat{u}[j] < 0.0$ 
            @constraint(model, z_{i+1}[j] == 0.0)
        else
            slope =  $\hat{u}[j] / (\hat{u}[j] - \hat{\ell}[j])$ 
            @constraints(model, begin
                z_{i+1}[j] >=  $\hat{z}[j]$ 
                z_{i+1}[j] <= slope * ( $\hat{z}[j] - \hat{\ell}[j]$ )
                z_{i+1}[j] >= 0.0
            end)
        end
    end
end

```

Parallel relaxation for given ℓ_i and \mathbf{u}_i Parallel relaxation is very similar to Δ -relaxation, except that (46c) becomes

$$j \in \Gamma_i \Rightarrow \frac{\hat{u}_{i,j}}{\hat{u}_{i,j} - \hat{\ell}_{i,j}} \hat{z}_{i,j} \leq z_{i,j} \leq \frac{\hat{u}_{i,j}}{\hat{u}_{i,j} - \hat{\ell}_{i,j}} (\hat{z}_{i,j} - \hat{\ell}_{i,j}). \quad (47)$$

Parallel relaxation is used in FastLin for network relaxation before applying reachability methods. To the best of our knowledge, it has not been used directly in any optimization method yet. The implementation of constraint encoding under parallel relaxation is not provided in the paper.

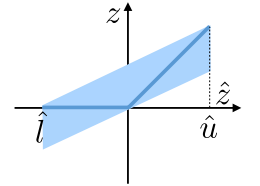


Figure 14. Illustration of parallel relaxation.

Naive mixed integer linear constraints The nonlinear constraint (42) can be formulated as a set of linear constraints:

$$z_{i,j} \geq \hat{z}_{i,j}, \quad (48a)$$

$$z_{i,j} \geq 0, \quad (48b)$$

$$z_{i,j} \leq \hat{z}_{i,j} + m\delta_{i,j}, \quad (48c)$$

$$z_{i,j} \leq m(1 - \delta_{i,j}), \quad (48d)$$

where m should be sufficiently large. If m is not large enough, the encoding may lead to error. The function is shown in algorithm 6.5. NSVerify calls this function.

```

struct MixedIntegerLP <: AbstractLinearProgram
  m::Float64
end

function encode_layer!(MIP::MixedIntegerLP, model, layer, z_i, z_{i+1}, \delta_{i+1})
  m = MIP.m
  \hat{z} = affine_map(layer, z_i)
  for j in 1:length(layer.bias)
    @constraints(model, begin
      z_{i+1}[j] >= \hat{z}[j]
      z_{i+1}[j] >= 0.0
      z_{i+1}[j] <= \hat{z}[j] + m * \delta_{i+1}[j]
      z_{i+1}[j] <= m - m * \delta_{i+1}[j]
    end)
  end
end

```

Algorithm 6.5. Encoding as mixed integer linear constraints using a sufficiently large number m . Only the function `encode_layer!` is shown. The function `encode_network!` is the same as in algorithm 6.1.

Mixed integer linear constraints for given ℓ_i and \mathbf{u}_i When we have the bounds, the constraints can be more tightly encoded:

$$z_{i,j} \geq \hat{z}_{i,j}, \quad (49a)$$

$$z_{i,j} \geq 0, \quad (49b)$$

$$z_{i,j} \leq \hat{u}_{i,j}\delta_{i,j}, \quad (49c)$$

$$z_{i,j} \leq \hat{z}_{i,j} - \hat{\ell}_{i,j}(1 - \delta_{i,j}). \quad (49d)$$

The function is shown in algorithm 6.6.

6.2 Objective Functions

In primal optimization, there are multiple ways to design the objective. Some of them are listed in algorithm 6.7.

Violation of linear constraints In many cases, the objective function is chosen to measure the violation of the constraints. For example, when \mathcal{Y} is represented by a half space (9), we maximize the following objective function

$$o := \mathbf{c}^\top \mathbf{y} - d. \quad (50)$$

Such design directly tells how much the output constraints can be violated in the problem (4). This objective is used in dual optimization methods, *e.g.*, Duality, ConvDual, and Certify.

```

struct BoundedMixedIntegerLP <: AbstractLinearProgram end

function encode_layer! (::BoundedMixedIntegerLP, model, layer,
                        zi, zi+1, δi+1, bounds)
     $\hat{z}$  = affine_map(layer, zi)
     $\hat{z}$ _bound = approximate_affine_map(layer, bounds)
     $\hat{l}$ ,  $\hat{u}$  = low( $\hat{z}$ _bound), high( $\hat{z}$ _bound)
    for j in 1:length(layer.bias)
        if  $\hat{l}[j] \geq 0.0$ 
            @constraint(model, zi+1[j] ==  $\hat{z}[j]$ )
        elseif  $\hat{u}[j] \leq 0.0$ 
            @constraint(model, zi+1[j] == 0.0)
        else
            @constraints(model, begin
                zi+1[j] >=  $\hat{z}[j]$ 
                zi+1[j] >= 0.0
                zi+1[j] <=  $\hat{u}[j] * \delta_{i+1}[j]$ 
                zi+1[j] <=  $\hat{z}[j] - \hat{l}[j] * (1 - \delta_{i+1}[j])$ 
            end)
        end
    end
end

```

Algorithm 6.6. Encoding as mixed integer linear constraints using the bounds on node values. Only the function `encode_layer!` is shown. The function `encode_network!` is the same as in algorithm 6.1.

Maximum disturbance The objective can also measure the maximum allowable disturbance. The disturbance with respect to a given input \mathbf{x}_0 is computed as

$$o := \|\mathbf{x} - \mathbf{x}_0\|_{\infty}. \quad (51)$$

The maximum allowable disturbance is computed by minimizing o with respect to the constraint that $\mathbf{f}(\mathbf{x}) \notin \mathcal{Y}$. This objective is used in MIPVerify and ILP.

Summation of variables The objective can also be

$$o := \sum_{i,j} z_{i,j} \text{ or } \sum_{i,j} s_{i,j}. \quad (52)$$

The summation of neurons is used to compute tighter bounds in Planet. The summation of slack variables is used in Planet.

6.3 NSVerify

NSVerify[23] takes any linear constraints \mathcal{X} and \mathcal{Y} , and considers networks with only ReLU activations. NSVerify encodes the ReLU activation functions as a set of mixed integer linear constraints. It does not need an objective. The method is sound and complete.

Our implementation is shown in algorithm 6.8. The solver needs to specify m in (48). The solver first initializes variables \mathbf{z}_i and δ_i for all i . Then the solver adds the input constraint $\mathbf{z}_0 \in \mathcal{X}$ as well as the complement of the output constraint $\mathbf{z}_n \notin \mathcal{Y}$. Then it encodes the network as a set of mixed integer linear constraints. If there is a solution for the optimization, then we get a counter example. If not, the property is satisfied. In the implementation, for simplicity, we require that \mathcal{X} is an `HPolytope` and \mathcal{Y} a `PolytopeComplement`.

```

function linear_objective!(model::Model, map::HPolytope, var)
    c, d = tosimplehrep(map)
    o = c * var - d
    @objective(model, Min, o)
    return o
end

function max_disturbance!(model::Model, var)
    o = symbolic_infty_norm(var)
    @objective(model, Min, o)
    return o
end

function min_sum!(model::Model, var)
    o = sum(sum.(var))
    @objective(model, Min, o)
    return o
end

function max_sum!(model::Model, var)
    o = sum(sum.(var))
    @objective(model, Max, o)
    return o
end

```

Algorithm 6.7. Objective functions: zero objective, linear objective, minimax disturbance, minimal summation, and maximal summation.

```

struct NSVerify
    optimizer
    m::Float64
end

function solve(solver::NSVerify, problem::Problem)
    network = problem.network
    model = Model(solver)
    neurons = init_neurons(model, network)
    deltas = init_deltas(model, network)
    add_set_constraint!(model, problem.input, first(neurons))
    add_complementary_set_constraint!(model, problem.output, last(neurons))
    encode_network!(model, network, neurons, deltas, MixedIntegerLP(solver.m))
    feasibility_problem!(model)
    optimize!(model)
    if termination_status(model) == OPTIMAL
        return CounterExampleResult(:violated, value.(first(neurons)))
    end
    if termination_status(model) == INFEASIBLE
        return CounterExampleResult(:holds)
    end
    return CounterExampleResult(:unknown)
end

```

Algorithm 6.8. NSVerify. The verification problem is encoded as a mixed integer linear program. The naive encoding discussed in algorithm 6.5 is used in NSVerify. The parameter m is specified by the solver.

6.4 MIPVerify

MIPVerify [38] can be viewed as a direct extension of NSVerify. It also encodes the network as mixed integer constraints. But the encoding is more efficient since MIPVerify pre-computes the bounds of the problem. In this way, the solver does not need to specify m as in NSVerify.¹⁹

Our implementation is shown in algorithm 6.9. Similar to NSVerify, the solver first initializes variables \mathbf{z}_i and δ_i for all i . Then the solver adds the complement of the output constraint $\mathbf{z}_n \notin \mathcal{Y}$. Then it computes the bounds for the neurons, and encodes the network as a set of mixed integer linear constraints. The objective is to compute the maximum allowable disturbance. The satisfiability is determined by comparing the allowable range of disturbance with the input set. In the implementation, for simplicity, we require that \mathcal{X} is a [Hyperrectangle](#) and \mathcal{Y} is a [PolytopeComplement](#). MIPVerify supports the max activation function and the ℓ_p norm in the objective, which have not been supported yet in our implementation.

¹⁹ The original code can be found at <https://github.com/vtjeng/MIPVerify.jl>.

Algorithm 6.9. MIPVerify. The verification problem is encoded as a mixed integer linear program. The bounds of node values are considered in the encoding. MIPVerify computes the maximum allowable disturbance.

```

struct MIPVerify
    optimizer
end

function solve(solver::MIPVerify, problem::Problem)
    model = Model(solver)
    neurons = init_neurons(model, problem.network)
    deltas = init_deltas(model, problem.network)
    add_complementary_set_constraint!(model, problem.output, last(neurons))
    bounds = get_bounds(problem)
    encode_network!(model, problem.network, neurons,
                    deltas, bounds, BoundedMixedIntegerLP())
    o = max_disturbance!(model, first(neurons) - problem.input.center)
    optimize!(model)
    if termination_status(model) == INFEASIBLE
        return AdversarialResult(:holds)
    end
    if value(o) >= maximum(problem.input.radius)
        return AdversarialResult(:holds)
    else
        return AdversarialResult(:violated, value(o))
    end
end

```

6.5 ILP

ILP [4] encodes ReLU networks as linear constraints. It only considers a linear portion of the network that has the same activation pattern as the reference input. In our implementation, the reference input is chosen as the center of the input constraint set. The resulting problem can be solved by simply encoding a linear program using (43), where $\delta_{i,j}$'s denote the activation status of the reference input. To speed up the computation, ILP introduces iterative constraint solving. It first drops all inequality constraints with respect to $\hat{z}_{i,j}$ in (43), *i.e.*, for all i and j , the following constraints are dropped

$$(2\delta_{i,j} - 1)\hat{z}_{i,j} \geq 0. \quad (53)$$

The above expression is a compact version of $\hat{z}_{i,j} \geq 0$ for $\delta_{i,j} = 1$ and $\hat{z}_{i,j} \leq 0$ for $\delta_{i,j} = 0$. Without (53), the linear encoding reduces to the relaxed linear encoding in (44). The inequality constraint with respect to $\hat{z}_{i,j}$ is iteratively added, if the solution at the current iteration violates (53) for any i and j .

Our implementation is shown in algorithm 6.10. For simplicity, we require that \mathcal{X} is a hyperrectangle and \mathcal{Y} the complement of a polytope, `PolytopeComplement`. The solver first computes the activation δ_i 's according to the reference input, *i.e.*, the center of \mathcal{X} . Then it initializes neuron variables \mathbf{z}_i 's, adds the complement of the output constraint $\mathbf{z}_n \notin \mathcal{Y}$, and adds an objective function for maximum allowable disturbance. We provide both the iterative implementation and the non-iterative implementation to solve the LP problem, where the iterative version corresponds to ILP.²⁰ In the non-iterative approach, the solver simply encodes the network using the linear constraints in (43). In the iterative approach, the solver first encodes the network using the relaxed linear constraints in (44) and solves the relaxed problem. If the resulting solution violates any inequality constraint (53), we add the constraint to the problem and solve the problem again. The process is repeated until all constraints (53) are satisfied. The process is guaranteed to converge in a finite number of steps since there are only finitely many constraints. The number of constraints equals the number of neurons.

²⁰ It is claimed in [4] that the iterative approach computes faster than the non-iterative approach.

7 Dual Optimization

Primal optimization needs to deal with complicated constraints. Another approach is to consider the dual problem of (41), which can be relaxed to many independent optimization problems [12], [43]. The objective considered in these methods is the violation of output constraints (50). The dual problem provides a valid bound on the violation. In particular, Duality [12] uses Lagrangian relaxation, which handles general activation functions such as ReLU, tanh, sigmoid, maxpool, and etc. ConvDual [43] solves the dual problem of convexified (41), which handles ReLU only. Certify [31] uses semidefinite relaxation, which handles networks with one hidden layer, whose activation functions are differentiable almost everywhere.

7.1 Dual Network

This section introduces the concept of *dual network*, which is deeply related to the dual problem of the optimization with respect to a neural network.²¹ The term “dual problem” refers to the Lagrangian dual problem, which is obtained by forming the Lagrangian of the optimization, using Lagrange multipliers to add the constraints to the objective function, and then solving for some primal variable values that optimize the Lagrangian. This process will be discussed in detail in section 7.2. The Lagrange multipliers are called dual variables. It will be shown that those dual variables form a dual network, whose structure is similar to the original network but which propagates in the opposite direction. Moreover, the dual variables encode the weights of corresponding nodes in a value function in the context of dynamic programming, if we regard the layer by layer propagation in a neural network as a dynamic system. In the following discussion, we first introduce the dual network in the context of dynamic programming, then point out its relationship with the Lagrangian dual problem.

²¹ The dual network discussed here is not the dual neural network (DNN) [52], which is a recurrent neural network (RNN) to solve quadratic programming.

Dynamic programming: General formulation Many algorithms optimize an objective function that depends on non-input variables in the neural network, but constrained on the input \mathbf{x} .

```

struct ILP
  optimizer
  iterative::Bool
end

function solve(solver::ILP, problem::Problem)
  nnet = problem.network
  x = problem.input.center
  model = Model(solver)
   $\delta$  = get_activation(nnet, x)
  neurons = init_neurons(model, nnet)
  add_complementary_set_constraint!(model, problem.output, last(neurons))
  o = max_disturbance!(model, first(neurons) - problem.input.center)
  if !solver.iterative
    encode_network!(model, nnet, neurons,  $\delta$ , StandardLP())
    optimize!(model)
    if (termination_status(model) != OPTIMAL)
      return AdversarialResult(:unknown)
    end
    return interpret_result(solver, value(o), problem.input)
  end
  encode_network!(model, nnet, neurons,  $\delta$ , LinearRelaxedLP())
  while true
    optimize!(model)
    if (termination_status(model) != OPTIMAL)
      return AdversarialResult(:unknown)
    end
    x = value.(first(neurons))
    matched, index = match_activation(nnet, x,  $\delta$ )
    if matched
      return interpret_result(solver, value(o), problem.input)
    end
    add_constraint!(model, nnet, neurons,  $\delta$ , index)
  end
end

function interpret_result(solver::ILP, o, input)
  if o >= maximum(input.radius)
    return AdversarialResult(:holds, o)
  else
    return AdversarialResult(:violated, o)
  end
end

function add_constraint!(model, network
  z::Vector{Vector{VariableRef}},
   $\delta$ ::Vector{Vector{Bool}},
  (i, j)::Tuple{Int64, Int64})
  layer = network.layers[i]
  val = layer.weights[j, :] * z[i] + layer.bias[j]
  if  $\delta$ [i][j]
    @constraint(model, val >= 0.0)
  else
    @constraint(model, val <= 0.0)
  end
end

```

Algorithm 6.10. ILP. ILP computes the maximum allowable disturbance and returns adversarial results. Both iterative and non-iterative approaches are provided. The iterative approach first relaxes inequality constraints in `encode_network!` using linear relaxation, and then iteratively adds those inequality constraints in `add_constraint!`. The function `match_activation` finds the node that is violating the inequality constraint equation (53). Its implementation is not shown.

There is a nonlinear relationship between the objective function and the input \mathbf{x} . As feedforward neural networks are considered, we can use dynamic programming to simplify the nonlinear optimization problem and obtain the dual problem. Suppose the problem under consideration is

$$\max_{\mathbf{x} \in \mathcal{X}} o := \sum_{i=0}^n o_i(\hat{\mathbf{z}}_i), \quad (54)$$

where o_i is the objective for different layers.²² Define the value function at layer i as

$$o_{i \rightarrow n}(\hat{\mathbf{z}}_i) := \max_{\hat{\mathbf{z}}_{i+1}, \dots, \hat{\mathbf{z}}_n} \sum_{k \geq i} o_k(\hat{\mathbf{z}}_k). \quad (55)$$

The value function represents the optimal value that can be achieved given certain initial state $\hat{\mathbf{z}}_i$. Hence, the value function o_i only has one variable $\hat{\mathbf{z}}_i$. The Bellman equation for dynamic programming can be written²³

$$o_{i \rightarrow n}(\hat{\mathbf{z}}_i) = \max_{\hat{\mathbf{z}}_{i+1} = \mathbf{W}_{i+1} \sigma_i(\hat{\mathbf{z}}_i) + \mathbf{b}_{i+1}} o_i(\hat{\mathbf{z}}_i) + o_{(i+1) \rightarrow n}(\hat{\mathbf{z}}_{i+1}). \quad (56)$$

The Bellman equation can be solved by backward dynamic programming. Then the original optimization (54) is reduced to the following problem,

$$\max_{\mathbf{x} \in \mathcal{X}} o_{0 \rightarrow n}(\mathbf{x}), \quad (57)$$

whose objective only depends on \mathbf{x} .

This approach is widely used in discrete-time optimal control for dynamic systems where $\hat{\mathbf{z}}_i$ are states at step i . In the following discussion, we derive the explicit solution for linear objectives.

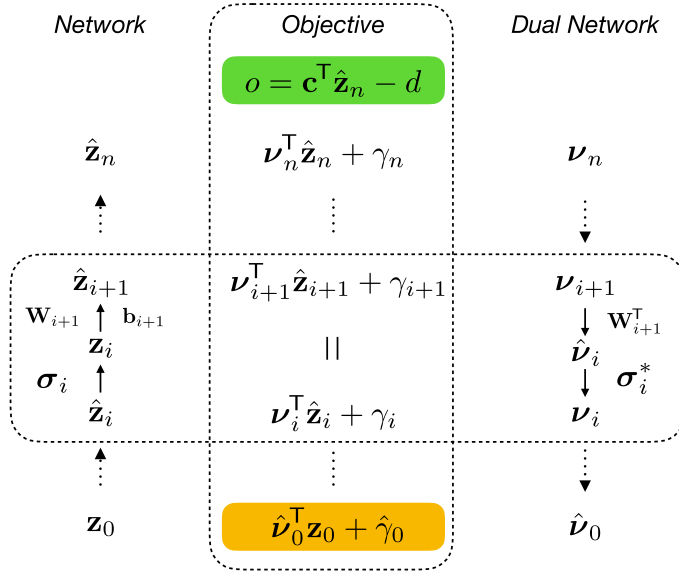


Figure 15. Illustration of dynamic programming and the dual network. Given an objective function o that depends on the network output, dynamic programming can transform o to a function that only depends on the network input. In the process, a dual network is constructed. The dual network propagates in the reverse order to the original network. All corresponding mappings are dual functions of the mappings in the original network. Moreover, the nodes \mathbf{v}_i in the dual network encode the weights of \mathbf{z}_i to the objective o . According to the stationary condition in dynamic programming, all expressions in the “objective” block are equivalent to one another. Then the objective function o that depends on the output (shaded in green) is transformed to a function that only depends on the input (shaded in yellow).

Dynamic programming: Linear objective Assume that $o_i(\hat{\mathbf{z}}_i) = \mathbf{c}_i^T \hat{\mathbf{z}}_i - d_i$ where $\mathbf{c}_i \in \mathbb{R}^{k_i}$ and $d_i \in \mathbb{R}$. Define $\mathbf{v}_i \in \mathbb{R}^{k_i}$ to be the dual variable for $\hat{\mathbf{z}}_i$, and $\hat{\mathbf{v}}_i \in \mathbb{R}^{k_i}$ to be the dual variable for \mathbf{z}_i . The dual variables encode the weights of the corresponding nodes in a value function, i.e.,

$$o_{i \rightarrow n}(\hat{\mathbf{z}}_i) = \mathbf{v}_i^T \hat{\mathbf{z}}_i + \gamma_i, \quad (58)$$

where $\gamma_i \in \mathbb{R}$ is a bias term. Consider o_n , we have the boundary constraint

$$\mathbf{v}_n = \mathbf{c}_n, \gamma_n = -d_i. \quad (59)$$

Plugging (58) into the Bellman equation (56), we have

$$\mathbf{v}_i^\top \hat{\mathbf{z}}_i + \gamma_i = \mathbf{c}_i^\top \hat{\mathbf{z}}_i - d_i + \mathbf{v}_{i+1}^\top \mathbf{W}_{i+1} \sigma_i(\hat{\mathbf{z}}_i) + \mathbf{v}_{i+1}^\top \mathbf{b}_{i+1} + \gamma_{i+1}. \quad (60)$$

Matching the coefficient of $\hat{\mathbf{z}}_i$ and the constant term on both sides, we obtain the backward relationship between \mathbf{v}_i, γ_i and $\mathbf{v}_{i+1}, \gamma_{i+1}$ as

$$\mathbf{v}_i = \mathbf{c}_i + \sigma_i^*(\hat{\mathbf{v}}_i), \quad (61a)$$

$$\hat{\mathbf{v}}_i = \mathbf{W}_{i+1}^\top \mathbf{v}_{i+1}, \quad (61b)$$

$$\gamma_i = \gamma_{i+1} + \mathbf{v}_{i+1}^\top \mathbf{b}_{i+1} - d_i, \quad (61c)$$

where σ_i^* is the dual function of σ_i , defined to satisfy²⁴

$$\sigma_i^*(\hat{\mathbf{v}}_i)^\top \hat{\mathbf{z}}_i \equiv \hat{\mathbf{v}}_i^\top \sigma_i(\hat{\mathbf{z}}_i). \quad (62)$$

In this way, the dual variables \mathbf{v}_i and $\hat{\mathbf{v}}_i$ indeed form a backward dual network. Figure 15 illustrates the original network, the value function, and the dual network in the case that $o_i = 0$ for $i < n$. Hence, the original optimization problem (54) can be solved by 1) backward computing the dual network from the boundary constraint at layer n to layer 0, 2) solving the reduced problem (57) that depends on the dual variables.

When σ_i is nonlinear, the dual function σ_i^* is difficult to handle, as it indeed depends on the value of $\hat{\mathbf{z}}_i$. In the case of ReLU activation, different approximations of σ_i are introduced to simplify the dual network. For example, ConvDual uses triangle relaxation and FastLin uses parallel relaxation. These approaches are to be introduced in section 7.3 and section 8.2.

Dual network and Lagrange multipliers The dual variables for dynamic programming are deeply related to Lagrange multipliers in Lagrangian dual problem. Let μ_i be the multiplier for the constraint $\hat{\mathbf{z}}_i = \mathbf{W}_i \mathbf{z}_{i-1} + \mathbf{b}_i$ and λ_i the multiplier for the constraint $\mathbf{z}_i = \sigma_i(\hat{\mathbf{z}}_i)$. Then the Bellman equation (56) can be rewritten as²⁵

$$o_{i \rightarrow n}(\hat{\mathbf{z}}_i) = \min_{\mu_{i+1}, \lambda_i} \max_{\hat{\mathbf{z}}_{i+1}, \mathbf{z}_i} o_i(\hat{\mathbf{z}}_i) + o_{(i+1) \rightarrow n}(\hat{\mathbf{z}}_{i+1}) + \mu_{i+1}^\top (\hat{\mathbf{z}}_{i+1} - \mathbf{W}_{i+1} \mathbf{z}_i - \mathbf{b}_{i+1}) + \lambda_i^\top (\mathbf{z}_i - \sigma_i(\hat{\mathbf{z}}_i)). \quad (63)$$

Using the linearity assumption $o_{(i+1) \rightarrow n}(\hat{\mathbf{z}}_{i+1}) = \mathbf{v}_{i+1}^\top \hat{\mathbf{z}}_{i+1} + \gamma_{i+1}$ in the above equation, we have

$$o_{i \rightarrow n}(\hat{\mathbf{z}}_i) = o_i^* + \min_{\mu_{i+1}, \lambda_i} \max_{\hat{\mathbf{z}}_{i+1}, \mathbf{z}_i} \mathbf{v}_{i+1}^\top \hat{\mathbf{z}}_{i+1} + \mu_{i+1}^\top (\hat{\mathbf{z}}_{i+1} - \mathbf{W}_{i+1} \mathbf{z}_i - \mathbf{b}_{i+1}) + \lambda_i^\top (\mathbf{z}_i - \sigma_i(\hat{\mathbf{z}}_i)), \quad (64)$$

where $o_i^* = \mathbf{c}_i^\top \hat{\mathbf{z}}_i - d_i + \gamma_{i+1}$. Rearrange the minimax problem,

$$\min_{\mu_{i+1}, \lambda_i} \max_{\hat{\mathbf{z}}_{i+1}, \mathbf{z}_i} (\mathbf{v}_{i+1} + \mu_{i+1})^\top \hat{\mathbf{z}}_{i+1} + (\lambda_i - \mathbf{W}_{i+1}^\top \mu_{i+1})^\top \mathbf{z}_i - \mu_{i+1}^\top \mathbf{b}_{i+1} - \lambda_i^\top \sigma_i(\hat{\mathbf{z}}_i). \quad (65)$$

By applying the result in footnote 25 to the first two terms in (65), we conclude that $\mathbf{v}_{i+1} + \mu_{i+1} = \mathbf{0}$ and $\lambda_i - \mathbf{W}_{i+1}^\top \mu_{i+1} = \mathbf{0}$. Hence, we have the following relationship

$$\mu_{i+1} = -\mathbf{v}_{i+1}, \lambda_i = -\hat{\mathbf{v}}_i. \quad (66)$$

The nodes in the dual network are indeed the Lagrange multipliers if we do not consider the bounds on \mathbf{z}_i 's. Duality in section 7.2 provides a formulation that considers the bounds. In this case, the conclusion from footnote 25 does not hold. As a result, the relationship between the dual network and the Lagrange multipliers in (66) breaks.

²⁴ To obtain an upper bound of the primal problem (54), the dual function only needs to satisfy $\sigma_i^*(\hat{\mathbf{v}}_i)^\top \hat{\mathbf{z}}_i \geq \hat{\mathbf{v}}_i^\top \sigma_i(\hat{\mathbf{z}}_i)$.

²⁵ The solution of the unconstrained problem $\min_{\mathbf{a}} \max_{\mathbf{b}} \mathbf{a}^\top \mathbf{b}$ is always $\mathbf{0}$ with $\mathbf{a} = \mathbf{b} = \mathbf{0}$. Hence, the optimal solution of the Bellman equation (63) is always $\mu_{i+1} = \hat{\mathbf{z}}_{i+1} - \mathbf{W}_{i+1} \mathbf{z}_i - \mathbf{b}_{i+1} = \mathbf{0}$ and $\lambda_i = \mathbf{z}_i - \sigma_i(\hat{\mathbf{z}}_i) = \mathbf{0}$.

Dual network and backpropagation When the objectives for hidden layers are all zero, *i.e.*, $o_i = 0$ for all $i < n$, the dual variable \mathbf{v}_i is indeed the gradient from the objective o to the hidden variable $\hat{\mathbf{z}}_i$. The gradients are usually computed in backpropagation to train deep neural networks [15].

7.2 Duality

Duality [12] takes a hyperrectangle as its input set and has a half space as its output set. The input hyperrectangle is denoted $|\mathbf{x} - \mathbf{x}_0| \leq \mathbf{r}$, where \mathbf{x}_0 and \mathbf{r} are the center and radius of the hyperrectangle. The output half space is denoted $\mathbf{c}^\top \mathbf{y} \leq d$. Then the optimization problem becomes

$$\max_{\mathbf{z}_0, \dots, \mathbf{z}_n, \hat{\mathbf{z}}_1, \dots, \hat{\mathbf{z}}_n} \mathbf{c}^\top \mathbf{z}_n - d, \quad (67a)$$

$$\text{s.t. } \mathbf{z}_i = \sigma_i(\hat{\mathbf{z}}_i), \forall i \in \{1, \dots, n\}, \quad (67b)$$

$$\hat{\mathbf{z}}_i = \mathbf{W}_i \mathbf{z}_{i-1} + \mathbf{b}_i, \forall i \in \{1, \dots, n\}, \quad (67c)$$

$$|\mathbf{z}_0 - \mathbf{x}_0| \leq \mathbf{r}. \quad (67d)$$

Given the bounds on \mathbf{z}_i and $\hat{\mathbf{z}}_i$, the optimal value of (67) is bounded by Lagrangian relaxation of the constraints

$$\max_{\mathbf{z}_0, \dots, \mathbf{z}_n, \hat{\mathbf{z}}_1, \dots, \hat{\mathbf{z}}_n} \mathbf{c}^\top \mathbf{z}_n - d + \sum_{i=1}^n \mu_i^\top (\hat{\mathbf{z}}_i - \mathbf{W}_i \mathbf{z}_{i-1} - \mathbf{b}_i) + \sum_{i=1}^n \lambda_i^\top (\mathbf{z}_i - \sigma_i(\hat{\mathbf{z}}_i)), \quad (68a)$$

$$\text{s.t. } \ell_i \leq \mathbf{z}_i \leq \mathbf{u}_i, \forall i \in \{1, \dots, n\}, \quad (68b)$$

$$\hat{\ell}_i \leq \hat{\mathbf{z}}_i \leq \hat{\mathbf{u}}_i, \forall i \in \{1, \dots, n\}, \quad (68c)$$

$$|\mathbf{z}_0 - \mathbf{x}_0| \leq \mathbf{r}, \quad (68d)$$

where $\lambda_i \in \mathbb{R}^{k_i}$ and $\mu \in \mathbb{R}^{k_i}$ are Lagrange multipliers. For any choice of λ and μ , (68) provides a valid upper bound on the optimal value of (67). This property is known as weak duality.

Since the objective and constraints are separable in the layers, the variables in each layer can be optimized independently. The boundary condition is $\lambda_n = -\mathbf{c}$. The objective function in (68) can be decomposed into the following three parts:

- Input layer value with respect to \mathbf{z}_0 .

$$f_0(\mu_1) = \max_{|\mathbf{z}_0 - \mathbf{x}_0| \leq \mathbf{r}} -\mu_1^\top (\mathbf{W}_1 \mathbf{z}_0 + \mathbf{b}_1), \quad (69a)$$

$$= -\mu_1^\top \mathbf{W}_1 \mathbf{x}_0 - \mu_1^\top \mathbf{b}_1 + \left| \mu_1^\top \mathbf{W}_1 \right| \mathbf{r}. \quad (69b)$$

- Layer value with respect to \mathbf{z}_i . For $i \in \{1, \dots, n-1\}$,

$$f_i(\lambda_i, \mu_{i+1}) = \max_{\ell_i \leq \mathbf{z}_i \leq \mathbf{u}_i} -\mu_{i+1}^\top (\mathbf{W}_{i+1} \mathbf{z}_i + \mathbf{b}_{i+1}) + \lambda_i^\top \mathbf{z}_i, \quad (70a)$$

$$= \left(\lambda_i - \mathbf{W}_{i+1}^\top \mu_{i+1} \right)^\top \frac{\ell_i + \mathbf{u}_i}{2} - \mu_{i+1}^\top \mathbf{b}_{i+1} + \left| \lambda_i - \mathbf{W}_{i+1}^\top \mu_{i+1} \right|^\top \frac{\mathbf{u}_i - \ell_i}{2}. \quad (70b)$$

- Activation value with respect to $\hat{\mathbf{z}}_i$. For $i \in \{1, \dots, n\}$,

$$\tilde{f}_i(\lambda_i, \mu_i) = \max_{\hat{\ell}_i \leq \hat{\mathbf{z}}_i \leq \hat{\mathbf{u}}_i} \mu_i^\top \hat{\mathbf{z}}_i - \lambda_i^\top \sigma_i(\hat{\mathbf{z}}_i), \quad (71a)$$

$$\leq \sum_j \max \{ \mu_{i,j} \hat{\ell}_{i,j}, \mu_{i,j} \hat{u}_{i,j} \} + \max \{ \lambda_{i,j} \sigma_{i,j}(\hat{\ell}_{i,j}), \lambda_{i,j} \sigma_{i,j}(\hat{u}_{i,j}) \}, \quad (71b)$$

where the inequality is taken by considering element-wise maximum.

Any choice of the dual variables λ_i, μ_i in (68) provides an upper bound of the primal problem (67). To obtain a tight bound, we need to minimize (68) with respect to the dual variables. Hence, the dual problem can be constructed as

$$\min_{\lambda_1, \dots, \lambda_n, \mu_1, \dots, \mu_n} f_0(\mu_1) + \sum_{i=1}^{n-1} f_i(\lambda_i, \mu_{i+1}) + \sum_{i=1}^n \tilde{f}_i(\lambda_i, \mu_i) - d, \quad (72a)$$

$$\text{s.t. } \lambda_n = -\mathbf{c}. \quad (72b)$$

The problem is satisfied if the optimal solution of (72) is negative; otherwise, it is not satisfied. Algorithm 7.1 provides an implementation.

7.3 ConvDual

ConvDual [43] takes a hypercube input set and a half space output set. The input hypercube is denoted $\|\mathbf{x} - \mathbf{x}_0\|_\infty \leq \epsilon$, where \mathbf{x}_0 and ϵ are the center and radius of the hypercube. The output half space is denoted $\mathbf{c}^\top \mathbf{y} \leq d$. ConvDual only considers ReLU networks. It first relaxes the constraint using Δ -relaxation. The primal optimization becomes a convex problem:²⁶

$$\max_{\mathbf{z}_0, \dots, \mathbf{z}_n, \hat{\mathbf{z}}_1, \dots, \hat{\mathbf{z}}_n} \mathbf{c}^\top \hat{\mathbf{z}}_n - d, \quad (73a)$$

$$\text{s.t. } z_{i,j} = \hat{z}_{i,j}, \forall i \in \{1, \dots, n-1\}, j \in \Gamma_i^+, \quad (73b)$$

$$z_{i,j} = 0, \forall i \in \{1, \dots, n-1\}, j \in \Gamma_i^-, \quad (73c)$$

$$z_{i,j} \geq \hat{z}_{i,j}, z_{i,j} \geq 0, z_{i,j} \leq \frac{\hat{u}_{i,j}(\hat{z}_{i,j} - \hat{\ell}_{i,j})}{\hat{u}_{i,j} - \hat{\ell}_{i,j}}, \forall i \in \{1, \dots, n-1\}, j \in \Gamma_i, \quad (73d)$$

$$\hat{\mathbf{z}}_i = \mathbf{W}_i \mathbf{z}_{i-1} + \mathbf{b}_i, \forall i \in \{1, \dots, n\}, \quad (73e)$$

$$\|\mathbf{z}_0 - \mathbf{x}_0\|_\infty \leq \epsilon. \quad (73f)$$

²⁶ ConvDual considers the pre-activation bounds of the last layer, which is equivalent to the case that the activation in the last layer is identity.

The optimization (73) can be regarded as an n -step dynamic program. We derive the dual problem and the dual network following the procedure of dynamic programming discussed in section 7.1. The original paper [43] directly applies the dual problem formulation.

Recall that \mathbf{v}_i and $\hat{\mathbf{v}}_i$ are the dual variables for $\hat{\mathbf{z}}_i$ and \mathbf{z}_i . The boundary condition is $\mathbf{v}_n = \mathbf{c}$ and $\gamma_n = -d$. The Bellman equation (60) is reduced to

$$\mathbf{v}_i^\top \hat{\mathbf{z}}_i + \gamma_i = \hat{\mathbf{v}}_i^\top \mathbf{z}_i + \mathbf{v}_{i+1}^\top \mathbf{b}_{i+1} + \gamma_{i+1}. \quad (74)$$

To obtain the backward relationship between \mathbf{v}_i, γ_i and $\mathbf{v}_{i+1}, \gamma_{i+1}$ similar to (61), we consider the following three cases. The sets Γ_i^+, Γ_i^- , and Γ_i encode activation conditions as defined in (24).

- For active node $j \in \Gamma_i^+$.
 $z_{i,j} = \hat{z}_{i,j}$. Hence, $v_{i,j} = \hat{v}_{i,j}$.
- For inactive node $j \in \Gamma_i^-$.
 $z_{i,j} = 0$. Hence, $v_{i,j} = 0$.
- For undetermined node $j \in \Gamma_i$. Consider the Δ -relaxation in (73d), the following conditions are satisfied,

$$\hat{v}_{i,j} z_{i,j} \leq \frac{\hat{v}_{i,j} \hat{u}_{i,j}}{\hat{u}_{i,j} - \hat{\ell}_{i,j}} \hat{z}_{i,j} - \frac{\hat{v}_{i,j} \hat{u}_{i,j} \hat{\ell}_{i,j}}{\hat{u}_{i,j} - \hat{\ell}_{i,j}} \quad \text{for } \hat{v}_{i,j} \geq 0, \quad (75a)$$

$$\hat{v}_{i,j} z_{i,j} \leq \alpha_{i,j} \hat{v}_{i,j} \hat{z}_{i,j} \quad \text{for } \hat{v}_{i,j} < 0, \quad (75b)$$


```

struct Duality
    optimizer
end

function solve(solver::Duality, problem::Problem)
    model = Model(solver)
    c, d = tosimplehrep(problem.output)
     $\lambda$  = init_multipliers(model, problem.network)
     $\mu$  = init_multipliers(model, problem.network)
    o = dual_value(solver, problem, model,  $\lambda$ ,  $\mu$ )
    @constraint(model, last( $\lambda$ ) .== -c)
    optimize!(model)
    return interpret_result(solver, termination_status(model), o - d[1])
end

function dual_value(solver::Duality, problem, model,  $\lambda$ ,  $\mu$ )
    bounds, layers = get_bounds(problem), problem.network.layers
    o = input_layer_value(layers[1],  $\mu$ [1], bounds[1])
    o += activation_value(layers[1],  $\mu$ [1],  $\lambda$ [1], bounds[1])
    for i in 2:length(layers)
        o += layer_value(layers[i],  $\mu$ [i],  $\lambda$ [i-1], bounds[i])
        o += activation_value(layers[i],  $\mu$ [i],  $\lambda$ [i], bounds[i])
    end
    @objective(model, Min, o)
    return o
end

function activation_value(layer::Layer,  $\mu_i$ ,  $\lambda_i$ , bound)
    o = zero(eltype( $\mu_i$ ))
    b_hat = approximate_affine_map(layer, bound)
    l_hat, u_hat = low(b_hat), high(b_hat)
    l, u = layer.activation(l_hat), layer.activation(u_hat)
    o += sum(symbolic_max( $\mu_i$  .* l_hat,  $\mu_i$  .* u_hat))
    o += sum(symbolic_max( $\lambda_i$  .* l,  $\lambda_i$  .* u))
    return o
end

function layer_value(layer::Layer,  $\mu_i$ ,  $\lambda_i$ , bound)
    c, r = bound.center, bound.radius
    o =  $\lambda_i$  * c -  $\mu_i$  * affine_map(layer, c)
    o += sum(symbolic_abs( $\lambda_i$  .- layer.weights *  $\mu_i$ ) .* r)
    return o
end

function input_layer_value(layer::Layer,  $\mu_i$ , input)
    W = layer.weights
    c, r = input.center, input.radius
    o = - $\mu_i$  * affine_map(layer, c)
    o += sum(symbolic_abs( $\mu_i$  * W) .* r)
    return o
end

```

Algorithm 7.1. Duality. Lagrangian relaxation is considered in Duality. The variables to be optimized are the Lagrange multipliers. The dual value is computed layer-wise. The function `input_layer_value` corresponds to equation (69). The function `layer_value` corresponds to equation (70). The function `activation_value` corresponds to equation (71). Duality returns basic satisfiability results.

where $\alpha_{i,j} \in [0, 1]$. (75) implies the following condition:

$$\hat{v}_{i,j} z_{i,j} \leq \frac{\hat{u}_{i,j}}{\hat{u}_{i,j} - \hat{\ell}_{i,j}} [\hat{v}_{i,j}]_+ \hat{z}_{i,j} + \alpha_{i,j} [\hat{v}_{i,j}]_- \hat{z}_{i,j} - \frac{\hat{u}_{i,j} \hat{\ell}_{i,j}}{\hat{u}_{i,j} - \hat{\ell}_{i,j}} [\hat{v}_{i,j}]_+. \quad (76)$$

Hence, the relationship among the dual variables that maximizes the value is

$$\gamma_i = \mathbf{v}_{i+1}^\top \mathbf{b}_{i+1} + \gamma_{i+1} - \sum_{j \in \Gamma_i} \frac{\hat{u}_{i,j} \hat{\ell}_{i,j}}{\hat{u}_{i,j} - \hat{\ell}_{i,j}} [\hat{v}_{i,j}]_+, \quad (77a)$$

$$v_{i,j} = \begin{cases} \hat{v}_{i,j} & j \in \Gamma_i^+ \\ 0 & j \in \Gamma_i^- \\ \frac{\hat{u}_{i,j}}{\hat{u}_{i,j} - \hat{\ell}_{i,j}} [\hat{v}_{i,j}]_+ + \alpha_{i,j} [\hat{v}_{i,j}]_- & j \in \Gamma_i \end{cases}, \quad (77b)$$

for $i \in \{1, \dots, n-1\}$. Note that when $j \in \Gamma_i$ and $v_{i,j} > 0$, $v_{i,j} = \frac{\hat{u}_{i,j}}{\hat{u}_{i,j} - \hat{\ell}_{i,j}} [\hat{v}_{i,j}]_+$. Then the term $\frac{\hat{u}_{i,j} \hat{\ell}_{i,j}}{\hat{u}_{i,j} - \hat{\ell}_{i,j}} [\hat{v}_{i,j}]_+$ can be simplified as $\hat{\ell}_{i,j} [v_{i,j}]_+$.

Then optimizing $\mathbf{v}_n^\top \hat{\mathbf{z}}_n + \gamma_n$ is equivalent to optimizing $\mathbf{v}_1^\top \hat{\mathbf{z}}_1 + \gamma_1 = \hat{\mathbf{v}}_0^\top \mathbf{z}_0 + \mathbf{v}_1^\top \mathbf{b}_1 + \gamma_1$. Hence,

$$\max_{\|\mathbf{z}_0 - \mathbf{x}_0\|_\infty \leq \epsilon} \hat{\mathbf{v}}_0^\top \mathbf{z}_0 + \mathbf{v}_1^\top \mathbf{b}_1 + \gamma_1, \quad (78a)$$

$$= \hat{\mathbf{v}}_0^\top \mathbf{x}_0 + \epsilon \|\hat{\mathbf{v}}_0\|_1 + \underbrace{\sum_{i=1}^n \mathbf{v}_i^\top \mathbf{b}_i - \sum_{i=1}^{n-1} \sum_{j \in \Gamma_i} \hat{\ell}_{i,j} [v_{i,j}]_+}_{\mathbf{v}_1^\top \mathbf{b}_1 + \gamma_1} - d, \quad (78b)$$

where γ_1 is computed according to (77a).

Then the dual problem of (73) is

$$\min_{\alpha_{i,j} \in [0,1]} \hat{\mathbf{v}}_0^\top \mathbf{x}_0 + \epsilon \|\hat{\mathbf{v}}_0\|_1 + \sum_{i=1}^n \mathbf{v}_i^\top \mathbf{b}_i - \sum_{i=1}^{n-1} \sum_{j \in \Gamma_i} \hat{\ell}_{i,j} [v_{i,j}]_+ - d, \quad (79a)$$

$$\text{s.t. } \mathbf{v}_n = \mathbf{c}, \quad (79b)$$

$$\hat{\mathbf{v}}_i = \mathbf{W}_{i+1}^\top \mathbf{v}_{i+1}, \forall i \in \{0, \dots, n-1\}, \quad (79c)$$

$$v_{i,j} = \begin{cases} 0 & j \in \Gamma_i^- \\ \hat{v}_{i,j} & j \in \Gamma_i^+ \\ \frac{\hat{u}_{i,j}}{\hat{u}_{i,j} - \hat{\ell}_{i,j}} [\hat{v}_{i,j}]_+ + \alpha_{i,j} [\hat{v}_{i,j}]_- & j \in \Gamma_i \end{cases} \quad \forall i \in \{1, \dots, n-1\}. \quad (79d)$$

The optimal solution of (79) provides an upper bound of the primal problem (73). If the dual value is smaller than 0, then the problem is satisfiable. The dual network consists of \mathbf{v}_i 's and is almost identical to the back-propagation network. The difference is that for nodes $j \in \mathcal{I}_i$, there is the additional free variable $\alpha_{i,j}$ that we can optimize over. One fixed and dual feasible solution of (79) is

$$\alpha_{i,j} = \frac{\hat{u}_{i,j}}{\hat{u}_{i,j} - \hat{\ell}_{i,j}}. \quad (80)$$

Under the condition, the dual network is linear. We will show in section 8.2 that the resulting dual network is identical to the case where we use parallel relaxation instead of Δ relaxation.

Our implementation is in algorithm 7.2. The value is computed in `dual_value`. The dual network is computed in `backprop!` layer by layer. For simplicity, we directly use (80) in the implementation. The bounds $\hat{\ell}_{i,j}$ and $\hat{u}_{i,j}$ and the sets Γ_i , Γ_i^- , and Γ_i^+ can be computed using different methods, *e.g.*, interval arithmetic introduced in section 4.1 and section 5.4. The original paper computes the bounds by formulating the bounding problem as several optimization problems similar to (73). The objectives are $\min z_{i,j}$ and $\max z_{i,j}$ for all i and j . Those problems can also be solved by dynamic programming. Moreover, the bounds can be computed inductively layer by layer. The details of the computation will be discussed in FastLin in section 8.2.

7.4 Certify

Certify [31] computes over-approximated certificates for a neural network with only one hidden layer. Similar to ConvDual, Certify also takes a hypercube input set $\|\mathbf{x} - \mathbf{x}_0\|_\infty \leq \epsilon$ and a half space output set $\mathbf{c}^\top \mathbf{y} \leq d$. It works for any activation function as long as the function is differentiable almost everywhere and its gradient is bounded. For simplicity, we assume that the derivative of the activation function is bounded by 0 and 1, *i.e.*, $\sigma'(\hat{z}) \in [0, 1]$ for any \hat{z} . If not, we can always scale it by a factor $\max_{\hat{z}} \sigma'(\hat{z})$ and add the factor in the following derivation. The primal optimization problem considered in Certify is

$$\max_{\|\mathbf{x} - \mathbf{x}_0\|_\infty \leq \epsilon} o(\mathbf{x}) = \mathbf{c}^\top \mathbf{f}(\mathbf{x}) - d. \quad (81)$$

Since o is differentiable almost-everywhere, then

$$o(\mathbf{x}) \leq o(\mathbf{x}_0) + \epsilon \max_{\|\mathbf{x} - \mathbf{x}_0\|_\infty \leq \epsilon} \|\nabla o(\mathbf{x})\|_1. \quad (82)$$

For a neural network with only one hidden layer, $o(\mathbf{x}) = \sum_j c_j \sigma_{1,j}(\mathbf{w}_{1,j} \mathbf{x} + b_{1,j})$. For simplicity, we omit the first index (index for layer 1) in σ , \mathbf{w} and b . Then

$$\nabla o(\mathbf{x}) = \sum_j c_j \sigma'_j(\mathbf{w}_j \mathbf{x} + b_j) \mathbf{w}_j^\top = \mathbf{W}^\top \text{diag}(\mathbf{c}) \nabla \sigma(\mathbf{W} \mathbf{x} + \mathbf{b}), \quad (83)$$

where $\nabla \sigma \in [0, 1]^{k_1}$ is the vertical stack of σ'_j . Let $\mathbf{s} = \sigma'(\mathbf{W} \mathbf{x} + \mathbf{b})$. Then

$$\|\nabla o(\mathbf{x})\|_1 \leq \max_{\mathbf{s} \in [0, 1]^{k_1}, \mathbf{t} \in [-1, 1]^{k_0}} \mathbf{t}^\top \mathbf{W}^\top \text{diag}(\mathbf{c}) \mathbf{s}, \quad (84a)$$

$$= \max_{\mathbf{s} \in [-1, 1]^{k_1}, \mathbf{t} \in [-1, 1]^{k_0}} \frac{1}{2} \mathbf{t}^\top \mathbf{W}^\top \text{diag}(\mathbf{c}) (\mathbf{1} + \mathbf{s}), \quad (84b)$$

$$= \max_{\mathbf{p} \in [-1, 1]^{1+k_1+k_0}} \frac{1}{4} \mathbf{p}^\top \underbrace{\begin{bmatrix} 0 & 0 & \mathbf{1}^\top \mathbf{W}^\top \text{diag}(\mathbf{c}) \\ 0 & 0 & \mathbf{W}^\top \text{diag}(\mathbf{c}) \\ \text{diag}(\mathbf{c}) \mathbf{W} \mathbf{1} & \text{diag}(\mathbf{c}) \mathbf{W} & 0 \end{bmatrix}}_{\mathbf{M}(\mathbf{c}, \mathbf{W})} \mathbf{p}, \quad (84c)$$

$$= \max_{\mathbf{p} \in [-1, 1]^{1+k_1+k_0}} \frac{1}{4} \langle \mathbf{M}(\mathbf{c}, \mathbf{W}), \mathbf{p} \mathbf{p}^\top \rangle, \quad (84d)$$

$$\leq \max_{\mathbf{p} \geq 0, p_{jj} \leq 1} \frac{1}{4} \langle \mathbf{M}(\mathbf{c}, \mathbf{W}), \mathbf{P} \rangle. \quad (84e)$$

```

struct ConvDual end

function solve(solver::ConvDual, problem::Problem)
    o = dual_value(solver, problem.network, problem.input, problem.output)
    if o >= 0.0
        return BasicResult(:holds)
    end
    return BasicResult(:unknown)
end

function dual_value(solver::ConvDual, network, input, output)
    layers = network.layers
    L, U = get_bounds(network, input.center, input.radius[1])
    v0, d = tosimplehrep(output)
    v = vec(v0)
    o = d[1]
    for i in reverse(1:length(layers))
        o -= v'*layers[i].bias
        v = layers[i].weights'*v
        if i>1
            o += backprop!(v, U[i-1], L[i-1])
        end
    end
    o -= input.center'*v + input.radius[1] * sum(abs.(v))
    return o
end

function backprop!(v::Vector{Float64}, u::Vector{Float64}, l::Vector{Float64})
    o = 0.0
    for j in 1:length(v)
        val = relaxed_ReLU(l[j], u[j])
        if val < 1.0
            v[j] = v[j] * val
            o += v[j] * l[j]
        end
    end
    return o
end

function relaxed_ReLU(l::Float64, u::Float64)
    u <= 0.0 && return 0.0
    l >= 0.0 && return 1.0
    return u / (u - l)
end

```

Algorithm 7.2. ConvDual. The dual problem of the verification problem is considered. Δ relaxation is applied. The dual problem is formulated by backward dynamic programming. The function `dual_value` explicitly computes the dual value equation (79) under the relaxation equation (80).

The inequality in (84a) is due to $\|\mathbf{q}\|_1 \leq \max_{\|\mathbf{p}\|_\infty \leq 1} \mathbf{p}^\top \mathbf{q}$. (84b) changes the range of \mathbf{s} . (84c) packs all variables into one vector $\mathbf{p} := [1, \mathbf{t}, \mathbf{s}]$ and packs all parameters into the matrix $\mathbf{M}(\mathbf{c}, \mathbf{W})$. (84d) exploits the equivalence between matrix trace and quadratic form. The inner product between two matrices is defined as $\langle \mathbf{M}, \mathbf{P} \rangle := \text{tr}(\mathbf{M}^\top \mathbf{P})$. (84e) is obtained by taking $\mathbf{P} := \mathbf{p}\mathbf{p}$. The matrix \mathbf{P} is positive semidefinite, *i.e.*, $\mathbf{P}^\top \succeq 0$. Moreover, the diagonal term $P_{jj} = p_j^2 \leq 1$ for $j \in \{1, \dots, 1 + k_0 + k_1\}$. Hence, the convex semidefinite relaxation of the value $o(\mathbf{x})$ is

$$\max_{\|\mathbf{x} - \mathbf{x}_0\|_\infty \leq \epsilon} o(\mathbf{x}) \leq o(\mathbf{x}_0) + \frac{\epsilon}{4} \max_{\mathbf{P} \succeq 0, P_{jj} \leq 1} \langle \mathbf{M}(\mathbf{c}, \mathbf{W}), \mathbf{P} \rangle. \quad (85)$$

The right-hand side of (85) provides an upper bound of (81). If the bound is smaller than zero, then the problem is satisfiable. It is worth noting that the semidefinite program (the max function) only depends on \mathbf{c} and \mathbf{W} . As it does not depend on the input \mathbf{x} , it only needs to be computed once for a problem.

Our implementation is shown in algorithm 7.3, which directly constructs and solves the semidefinite program in (85).

```

struct Certify
    optimizer
end

function solve(solver::Certify, problem::Problem)
    model = Model(solver)
    c, d = tosimplehrep(problem.output)
    v = c * problem.network.layers[2].weights
    W = problem.network.layers[1].weights
    M = getM(v[1, :], W)
    n = size(M, 1)
    P = @variable(model, [1:n, 1:n], PSD)
    output = c * compute_output(problem.network, problem.input.center) .- d[1]
    epsilon = problem.input.radius[1]
    o = output .+ epsilon/4 * tr(M*P)
    @constraint(model, diag(P) .<= ones(n))
    @objective(model, Max, first(o))
    optimize!(model)
    return interpret_result(solver, termination_status(model), first(o))
end

```

Algorithm 7.3. Certify. It solves the semidefinite program equation (85).

8 Search and Reachability

This section discusses methods that combine layer-by-layer reachability analysis with search. ReluVal [40] uses symbolic intervals for reachability analysis and then searches the input domain for potential violations using iterative interval refinement. FastLin [41] uses network approximation for reachability analysis and then uses binary search to estimate a certified lower bound of maximum allowable disturbance. FastLip [41] is built upon FastLin, which further estimates the local Lipschitz constant. DLV [18] performs layer-by-layer search in hidden layers for potential counter examples. Note that the return types of these methods are not necessarily reachability results.

8.1 ReluVal

ReluVal [40] takes a hyperrectangle input set $|\mathbf{x} - \mathbf{x}_0| \leq \mathbf{r}$ and any output set that implements the abstract polytope type. The reachability analysis is done symbolically, while the search is done through iterative interval refinement. Our implementation is shown in algorithms 8.1 to 8.3.

```

struct SymbolicInterval
  Low::Matrix{Float64}
  Up::Matrix{Float64}
  interval::Hyperrectangle
end

struct SymbolicIntervalMask
  sym::SymbolicInterval
  LA::Vector{Vector{Int64}}
  UA::Vector{Vector{Int64}}
end

```

Algorithm 8.1. The data structure in ReluVal. `SymbolicInterval` represents the symbolic interval defined in equation (86). `SymbolicIntervalMask` further includes the lower and upper bounds of $\nabla \sigma_i$, i.e., diagonal entries of the gradient bounds $\underline{\mathbf{A}}_i$ and $\overline{\mathbf{A}}_i$ introduced in section 4.3.

Symbolic interval propagation Reachability methods that use interval arithmetic usually provide very loose bounds, as they do not keep track of dependencies among the hidden nodes. Symbolic interval propagation can provide tighter bounds by keeping track of those dependencies layer by layer. Define the extended input as $\mathbf{x}^e := [\mathbf{x}, 1]$. Then a symbolic interval at layer i is defined as

$$\mathbf{z}_i \in [\mathbf{L}_i \mathbf{x}^e, \mathbf{U}_i \mathbf{x}^e], \text{ for } \mathbf{x} \in [\mathbf{x}_0 - \mathbf{r}, \mathbf{x}_0 + \mathbf{r}], \quad (86)$$

where $\mathbf{L}_i, \mathbf{U}_i \in \mathbb{R}^{k_i \times (k_0+1)}$ are coefficients in the symbolic interval. For example, the j th node at layer i is bounded by

$$\ell_{i,j} \mathbf{x}^e \leq z_{i,j} \leq \mathbf{u}_{i,j} \mathbf{x}^e, \quad (87)$$

where $\ell_{i,j}$ and $\mathbf{u}_{i,j}$ are the j th row in \mathbf{L}_i and \mathbf{U}_i respectively.

The data structure `SymbolicInterval` in algorithm 8.1 is introduced to keep track of symbolic intervals, where the field `Low` corresponds to \mathbf{L}_i^e , `Up` to \mathbf{U}_i^e , and `interval` to the hyperrectangle $[\mathbf{x}_0 - \mathbf{r}, \mathbf{x}_0 + \mathbf{r}]$.

Given the symbolic interval, $\mathbf{L}_i \mathbf{x}^e$ belongs to a hyperrectangle that centers at $\mathbf{L}_i [\mathbf{x}_0, 1]$ with radius $|\mathbf{L}_i| [\mathbf{r}, 0]$, where $|\mathbf{L}_i|$ is a matrix containing the element-wise absolute values of \mathbf{L}_i . Similarly, $\mathbf{U}_i \mathbf{x}^e$ belongs to a hyperrectangle that centers at $\mathbf{U}_i [\mathbf{x}_0, 1]$ with radius $|\mathbf{U}_i| [\mathbf{r}, 0]$. Let $\mathbf{a} \mathbf{x}^e$ be a symbolic representation for a scalar variable, where $\mathbf{a} \in \mathbb{R}^{k_0+1}$. Let $\underline{h}, \bar{h} : \mathbb{R}^{k_0+1} \rightarrow \mathbb{R}$ be functions that map the symbolic representation $\mathbf{a} \mathbf{x}^e$ to its concrete lower bound and upper bound respectively, such that

$$\underline{h}(\mathbf{a}) := \mathbf{a} [\mathbf{x}_0, 1] - |\mathbf{a}| [\mathbf{r}, 0], \quad (88a)$$

$$\bar{h}(\mathbf{a}) := \mathbf{a} [\mathbf{x}_0, 1] + |\mathbf{a}| [\mathbf{r}, 0]. \quad (88b)$$

The symbolic intervals are computed layer by layer by calling `forward_network` in algorithm 5.1. The function `forward_layer` is shown in algorithm 8.2, which consists of the following two steps:

- Symbolic interval propagation through the linear map $\hat{\mathbf{z}}_i = \mathbf{W}_i \mathbf{z}_{i-1} + \mathbf{b}_i$ for $i \in \{2, \dots, n\}$.

$$\hat{\mathbf{L}}_i = [\mathbf{W}_i]_+ \mathbf{L}_{i-1} + [\mathbf{W}_i]_- \mathbf{U}_{i-1} + [\mathbf{0} \ \mathbf{b}_i], \quad (89a)$$

$$\hat{\mathbf{U}}_i = [\mathbf{W}_i]_+ \mathbf{U}_{i-1} + [\mathbf{W}_i]_- \mathbf{L}_{i-1} + [\mathbf{0} \ \mathbf{b}_i]. \quad (89b)$$

For the first layer, the symbolic bounds are defined as horizontal concatenation of \mathbf{W}_1 and \mathbf{b}_1 ,

$$\hat{\mathbf{L}}_1 = \hat{\mathbf{U}}_1 = [\mathbf{W}_1 \ \mathbf{b}_1]. \quad (90)$$

This corresponds to `forward_linear` in algorithm 8.2.

- Symbolic interval propagation through ReLU activation function $\mathbf{z}_i = [\hat{\mathbf{z}}_i]_+$. For each node j , there are three possibilities: always active ($j \in \Gamma_i^+$), never active ($j \in \Gamma_i^-$), undetermined ($j \in \Gamma_i$). Similar to (24), we have

$$\Gamma_i^+ = \{j : \underline{h}(\hat{\ell}_{i,j}) \geq 0\}, \quad (91a)$$

$$\Gamma_i^- = \{j : \bar{h}(\hat{\mathbf{u}}_{i,j}) \leq 0\}, \quad (91b)$$

$$\Gamma_i = \{j : j \notin \Gamma_i^+ \cup \Gamma_i^-\}. \quad (91c)$$

Then the symbolic interval for node j is computed as

$$j \in \Gamma_i^+ \Rightarrow \ell_{i,j} = \hat{\ell}_{i,j}, \mathbf{u}_{i,j} = \hat{\mathbf{u}}_{i,j}, \quad (92a)$$

$$j \in \Gamma_i^- \Rightarrow \ell_{i,j} = \mathbf{u}_{i,j} = \mathbf{0}, \quad (92b)$$

$$j \in \Gamma_i \Rightarrow \ell_{i,j} = \mathbf{0}, \mathbf{u}_{i,j} = \begin{cases} \hat{\mathbf{u}}_{i,j} & \underline{h}(\hat{\mathbf{u}}_{i,j}) \geq 0 \\ [\mathbf{0} \ \bar{h}(\hat{\mathbf{u}}_{i,j})] & \underline{h}(\hat{\mathbf{u}}_{i,j}) < 0 \end{cases}. \quad (92c)$$

When the node is always active in (92a), we keep the symbolic dependency on the input variables. When the node is never active in (92b), all outputs should be 0. When the activation is undetermined in (92c), the lower bound is set to 0. If it is possible for the symbolic upper bound to be smaller than 0, the input dependencies will be thrown away. The upper bound is set to be its concrete maximum, *i.e.*, the first k_0 entries in $\mathbf{u}_{i,j}$ are set to zero. Otherwise, we keep the symbolic dependency of the upper bound on input variables.

This corresponds to `forward_act` in algorithm 8.2.

Given the symbolic interval propagation, the output reachable set is a hyper-rectangle such that

$$\tilde{\mathcal{R}} = \{\mathbf{y} : y_j \in [\underline{h}(\ell_{n,j}), \bar{h}(\mathbf{u}_{n,j})], \forall j = 1, \dots, k_n\}. \quad (93)$$

The output reachable set computed by symbolic interval propagation is tighter than simple interval arithmetic as illustrated in figure 7.

Given the reachable set $\tilde{\mathcal{R}}$, its relationship with respect to the output set \mathcal{Y} is examined in the function `check_inclusion` in algorithm 8.3, which may return the following four different results:

- The return status is `:holds` if $\tilde{\mathcal{R}} \subset \mathcal{Y}$.
- The return status is `:violated` if $\tilde{\mathcal{R}} \cap \mathcal{Y} = \emptyset$.
- In addition, we sample the input interval to check for counter examples.²⁷ If the output with respect to any sample point does not belong to \mathcal{Y} , the sample point is returned as an unsatisfied `CounterExampleResult`.

²⁷ Heuristically, only the middle point of the input interval is checked in both the original implementation and our implementation.

- Otherwise, the return status is :`Undetermined`.

If the status is undetermined, ReluVal performs iterative interval refinement to minimize over-approximation in $\tilde{\mathcal{R}}$.

Iterative interval refinement Although symbolic interval propagation can provide us with tighter bounds than simple interval arithmetic, it may still have significant over-approximation, especially when the input intervals are comparably large. Recall that MaxSens partitions the input intervals into smaller sets to minimize over approximations. ReluVal performs iterative interval refinement instead, which splits the intervals of input nodes according to their influence on the output.²⁸

We evaluate the influence by considering the bounds on gradients $\underline{\mathbf{G}}_n$ and $\overline{\mathbf{G}}_n$ defined in section 4, which essentially measure the sensitivity of the output with respect to each input feature. The bounds $\underline{\mathbf{G}}_n$ and $\overline{\mathbf{G}}_n$ can be obtained by calling the third `get_gradient` in algorithm 4.3. The bounds $\underline{\Lambda}_i$ and $\overline{\Lambda}_i$ on $\nabla \sigma_i$ are computed in the forward propagation, and recorded in the data structure `SymbolicIntervalMask` in algorithm 8.1.

For each refinement step, ReluVal bisects the interval for input node j that has the highest smear value

$$S_j := \sum_k \max\{|UG_{n,j,k}|, |LG_{n,j,k}|\} r_k, \quad (94)$$

where $UG_{n,j,k}$ and $LG_{n,j,k}$ are the j th row and k th column entries in $\overline{\mathbf{G}}_n$ and $\underline{\mathbf{G}}_n$, respectively. Let $j^* = \arg \max_j S_j$. The smear values are computed in `get_smear_index` in algorithm 8.3, which returns the index to split. The split is performed by `interval_split` in algorithm 4.2.

The main procedure is shown in algorithm 8.3 and illustrated in figure 16. We first compute the reachable set without splitting the interval. If the status of the reachability analysis is undetermined, iterative interval refinement will be performed. A list of reachable sets is maintained. The reachable sets correspond to different input intervals. At each iteration, a set in the list is picked out according to the tree search strategy specified by the solver (default depth first search). For the picked set, the bounds of its gradient are computed. Then it is split into two intervals according to the smear values. The reachable sets for the two smaller intervals are then computed. If a reachable set belongs to the output constraint, we drop the corresponding interval. If a counter example is found in an interval, we conclude that the problem is violated. Otherwise, we need to further split the interval whose reachable set is then pushed back to the list. If the list becomes empty, the property is verified to be hold.

8.2 FastLin

FastLin [41] computes the certified lower bound of the maximum allowable disturbance.²⁹ The method combines reachability analysis with binary search to estimate the bound, and returns an adversarial result. FastLin only works for ReLU activation functions. A general method that works for any activation function, called CROWN, is discussed in [51], but is not reviewed here.

The binary search procedure shown in the main function in algorithm 8.5 can be combined with any reachability method. In particular, FastLin computes the bounds based on linear approximation of the neurons. The method takes a hyperrectangle as input set and a polytope or the complement of a polytope as output set.

²⁸ The ReluVal paper discusses two approaches: baseline iterative refinement and optimizing iterative refinement. We consider optimizing iterative refinement.

²⁹ An earlier work [42] called CLEVER also estimates the lower bound. However, CLEVER is not sound, hence, is not reviewed here.

```

function forward_layer(solver::ReluVal, layer::Layer, input)
    return forward_act(forward_linear(input, layer))
end

function forward_linear(input::Hyperrectangle, layer::Layer)
    (W, b) = (layer.weights, layer.bias)
    sym = SymbolicInterval(hcat(W, b), hcat(W, b), input)
    LA = Vector{Vector{Int64}}(undef, 0)
    UA = Vector{Vector{Int64}}(undef, 0)
    return SymbolicIntervalMask(sym, LA, UA)
end

function forward_linear(input::SymbolicIntervalMask, layer::Layer)
    (W, b) = (layer.weights, layer.bias)
    output_Up = max.(W, 0) * input.sym.Up + min.(W, 0) * input.sym.Low
    output_Low = max.(W, 0) * input.sym.Low + min.(W, 0) * input.sym.Up
    output_Up[:, end] += b
    output_Low[:, end] += b
    sym = SymbolicInterval(output_Low, output_Up, input.sym.interval)
    return SymbolicIntervalMask(sym, input.LA, input.UA)
end

function forward_act(input::SymbolicIntervalMask, layer::Layer{ReLU})
    n_node, n_input = size(input.sym.Up)
    output_Low, output_Up = input.sym.Low[:, :], input.sym.Up[:, :]
    mask_lower, mask_upper = zeros(Int, n_node), ones(Int, n_node)
    interval = input.sym.interval
    for i in 1:n_node
        if upper_bound(input.sym.Up[i, :], interval) <= 0.0
            mask_lower[i], mask_upper[i] = 0, 0
            output_Up[i, :] = zeros(n_input)
            output_Low[i, :] = zeros(n_input)
        elseif lower_bound(input.sym.Low[i, :], interval) >= 0
            mask_lower[i], mask_upper[i] = 1, 1
        else
            mask_lower[i], mask_upper[i] = 0, 1
            output_Low[i, :] = zeros(n_input)
            if lower_bound(input.sym.Up[i, :], interval) < 0
                output_Up[i, :] = zeros(n_input)
                output_Up[i, end] = upper_bound(input.sym.Up[i, :], interval)
            end
        end
    end
    sym = SymbolicInterval(output_Low, output_Up, interval)
    LA = push!(input.LA, mask_lower)
    UA = push!(input.UA, mask_upper)
    return SymbolicIntervalMask(sym, LA, UA)
end

```

Algorithm 8.2. Symbolic interval propagation in ReluVal. The function `forward_layer` is called by `forward_network` in the layer-by-layer propagation. The function `forward_layer` consists of `forward_linear` for the linear mapping and `forward_act` for the nonlinear activation. The first `forward_linear` function is for the input layer, while the second `forward_linear` function is for the following layers. Except for the first layer, the data structure being passed through layers is `SymbolicIntervalMask`.

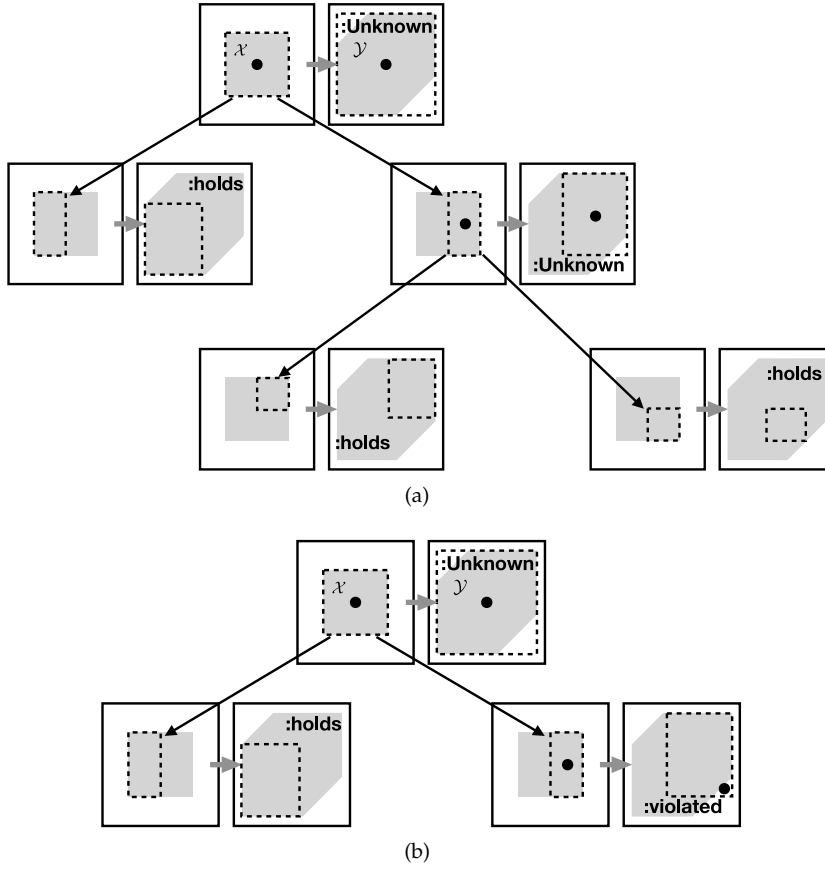


Figure 16. Illustration of iterative interval refinement. The two sub-figures illustrate two search trees in two different scenarios. Each node in the search tree consists of two boxes connected by an arrow. The left box corresponds to the input space and the right box corresponds to the output space. The input constraint and the output constraint are shaded in corresponding spaces. The dashed box in the input space represents the refined interval, while the dashed box in the output space represents the reachable set for that interval. If the reachable set belongs to \mathcal{Y} , then the status is holds. If the reachable set overlaps with \mathcal{Y} but is not a subset of \mathcal{Y} , the status is unknown. In this case, a point is sampled in the input space (black dot). If the output of that sample point does not belong to \mathcal{Y} , the status is violated. Otherwise, the interval is split into two. (a) Scenario 1: property holds as the reachable sets all belong to \mathcal{Y} . (b) Scenario 2: property violated as a counter example is found.

```

struct ReluVal
  tree_search::Symbol
end

function solve(solver::ReluVal, problem::Problem)
  reach = forward_network(solver, problem.network, problem.input)
  result = check_inclusion(reach.sym, problem.output, problem.network)
  result.status == :Unknown || return result
  reach_list = SymbolicIntervalMask[reach]
  while true
    length(reach_list) > 0 || return BasicResult(:holds)
    reach = pick_out!(reach_list, solver.tree_search)
    LG, UG = get_gradient(problem.network, reach.LA, reach.UA)
    feature = get_smear_index(problem.network, reach.sym.interval, LG, UG)
    intervals = split_interval(reach.sym.interval, feature)
    for interval in intervals
      reach = forward_network(solver, problem.network, interval)
      result = check_inclusion(reach.sym, problem.output, problem.network)
      result.status == :violated && return result
      result.status == :holds || (push!(reach_list, reach))
    end
  end
end

function check_inclusion(reach::SymbolicInterval, output, network)
  reachable = symbol_to_concrete(reach)
  issubset(reachable, output) && return BasicResult(:holds)
  middle_point = (high(reach.interval) + low(reach.interval))./2
  y = compute_output(network, middle_point)
  ∈(y, output) || return CounterExampleResult(:violated, middle_point)
  return BasicResult(:Unknown)
end

```

Algorithm 8.3. The main function in ReluVal. The reachable set for a given input interval is computed by calling `forward_network`, which then calls `forward_layer`. In order to perform iterative interval refinement, the `solve` function keeps track of a list of reachable sets that correspond to different input intervals. At each iteration, a set in the list is picked out according to the tree search strategy specified by the solver by `pick_out!`. For the picked set, the bounds of its gradient are computed by `get_gradient`. Then the index to be split is determined by `get_smear_index`. The interval is split into two by `split_interval`. The reachable sets for the two smaller intervals are then computed. The `check_inclusion` checks the status of each reachable set. If a counter example is found, the result is directly returned. If the status is unknown, we need to further split the input interval. The corresponding reachable set is pushed back to the list. If the list becomes empty, the problem is verified.

Reachability via network relaxation Given the bounds from interval arithmetic, a ReLU node that has an undetermined activation can be approximated using parallel relaxation.³⁰ Given the bounds ℓ_i and \mathbf{u}_i for $i \leq k$, the bounds $\hat{\ell}_{k+1}$ and $\hat{\mathbf{u}}_{k+1}$ can be computed by directly optimizing the node values. Similar to the derivation in ConvDual, we derive the lower and upper bounds using backward dynamic programming.³¹ The optimization and dynamic programming approach will provide tighter bounds than interval arithmetic discussed in section 4.1, since the correlation among nodes in the hidden layers is considered in the optimization problem, but not in interval arithmetic algorithms.

³⁰ Parallel relaxation is looser than Δ -relaxation.

³¹ The FastLin paper provides a different derivation.

The bounds are initiated as $\ell_0 = \mathbf{x}_0 - \epsilon \mathbf{1}$ and $\mathbf{u}_0 = \mathbf{x}_0 + \epsilon \mathbf{1}$. Given the bounds ℓ_i and \mathbf{u}_i for $i \leq k$, we show the derivation for ℓ_{k+1} and \mathbf{u}_{k+1} . For simplicity and without loss of generality, we assume that the $k+1$ th layer only contains one node. The derivation below can be easily extended to the case with multiple nodes. The lower and upper bounds of node \hat{z}_{k+1} are given by

$$\hat{\ell}_{k+1} = \min_{\|\mathbf{x}-\mathbf{x}_0\| \leq \epsilon} \hat{z}_{k+1}, \hat{\mathbf{u}}_{k+1} = \max_{\|\mathbf{x}-\mathbf{x}_0\| \leq \epsilon} \hat{z}_{k+1}. \quad (95)$$

For simplicity, we only show the detailed derivation of $\hat{\mathbf{u}}_{k+1}$. Recall that \mathbf{v}_i and $\hat{\mathbf{v}}_i = \mathbf{W}_{i+1} \mathbf{v}_{i+1}$ are the dual variables for $\hat{\mathbf{z}}_i$ and \mathbf{z}_i , and γ_i is the bias in the value function. The boundary conditions are $v_{k+1} = 1$ and $\gamma_{k+1} = 0$. Then the equation in (74) follows. The sets Γ_i^+ , Γ_i^- , and Γ_i for $i \leq k$ can be constructed using the known bounds according to (24). For $j \in \Gamma_i^+$, $v_{i,j} = \hat{v}_{i,j}$. For Γ_i^- , $v_{i,j} = 0$. These two cases are identical to the cases in ConvDual in section 7.3. For $j \in \Gamma_i$, consider the parallel relaxation (47) instead of Δ -relaxation, we have

$$\hat{v}_{i,j} z_{i,j} \leq \frac{\hat{v}_{i,j} \hat{\mathbf{u}}_{i,j}}{\hat{\mathbf{u}}_{i,j} - \hat{\ell}_{i,j}} \hat{z}_{i,j} - \frac{\hat{v}_{i,j} \hat{\mathbf{u}}_{i,j} \hat{\ell}_{i,j}}{\hat{\mathbf{u}}_{i,j} - \hat{\ell}_{i,j}} \quad \text{for } \hat{v}_{i,j} \geq 0, \quad (96a)$$

$$\hat{v}_{i,j} z_{i,j} \leq \frac{\hat{v}_{i,j} \hat{\mathbf{u}}_{i,j}}{\hat{\mathbf{u}}_{i,j} - \hat{\ell}_{i,j}} \hat{z}_{i,j} \quad \text{for } \hat{v}_{i,j} < 0, \quad (96b)$$

which is different from (75) in that there is no degree of freedom for a slack variable α . In this way, the relationship among the dual variables that maximizes the value is that for $i \in \{1, \dots, k\}$,

$$\gamma_i = \mathbf{v}_{i+1}^\top \mathbf{b}_{i+1} + \gamma_{i+1} - \sum_{j \in \Gamma_i} \hat{\ell}_{i,j} [v_{i,j}]_+, \quad (97a)$$

$$v_{i,j} = \begin{cases} \hat{v}_{i,j} & j \in \Gamma_i^+ \\ 0 & j \in \Gamma_i^- \\ \frac{\hat{\mathbf{u}}_{i,j}}{\hat{\mathbf{u}}_{i,j} - \hat{\ell}_{i,j}} \hat{v}_{i,j} & j \in \Gamma_i \end{cases}. \quad (97b)$$

The resulting dual network defined by $v_{i,j}$'s is identical to the dual network in ConvDual when $\alpha_{i,j}$ is chosen according to (80). For simplification, define a diagonal matrix $\mathbf{D}_i \in \mathbb{R}^{k_i \times k_i}$ whose diagonal entries $d_{i,j,j}$ for all j satisfy

$$d_{i,j,j} = \begin{cases} 1 & j \in \Gamma_i^+ \\ 0 & j \in \Gamma_i^- \\ \frac{\hat{\mathbf{u}}_{i,j}}{\hat{\mathbf{u}}_{i,j} - \hat{\ell}_{i,j}} & j \in \Gamma_i \end{cases}. \quad (98)$$

Then the dual network satisfies

$$\mathbf{v}_i = \mathbf{D}_i \mathbf{W}_{i+1}^\top \mathbf{v}_{i+1}, \forall i \leq k. \quad (99)$$

The dual variables provide an upper bound of \hat{z}_{k+1} such that $\hat{z}_{k+1} \leq \mathbf{v}_1^T \hat{\mathbf{z}}_1 + \gamma_1 = \hat{\mathbf{v}}_0^T \mathbf{x} + \mathbf{v}_1^T \mathbf{b}_1 + \gamma_1$ where \mathbf{x} satisfies the ℓ_p bounds $\|\mathbf{x} - \mathbf{x}_0\|_p \leq \epsilon$. According to (97a) and the boundary condition $\gamma_{k+1} = 0$,

$$\mathbf{v}_1^T \mathbf{b}_1 + \gamma_1 = \sum_{i=1}^n \mathbf{v}_i^T \mathbf{b}_i - \sum_{i=1}^{n-1} \sum_{j \in \Gamma_i} \hat{\ell}_{i,j}[v_{i,j}]_+ =: \mu^+. \quad (100)$$

Hence, the upper bound of \hat{z}_{k+1} is

$$\hat{u}_{k+1} := \max_{\|\mathbf{x} - \mathbf{x}_0\|_p \leq \epsilon} \hat{\mathbf{v}}_0^T \mathbf{x} + \mu^+ = \hat{\mathbf{v}}_0^T \mathbf{x}_0 + \epsilon \|\hat{\mathbf{v}}_0\|_q + \mu^+, \quad (101)$$

where q is the dual variable for p , i.e., $p^{-1} + q^{-1} = 1$. Our implementation only considers the case where $p = \infty$ and $q = 1$.

Similarly, the lower bound of \hat{z}_{k+1} can be computed as

$$\hat{\ell}_{k+1} := \min_{\|\mathbf{x} - \mathbf{x}_0\|_p \leq \epsilon} \hat{\mathbf{v}}_0^T \mathbf{x} + \mu^- = \hat{\mathbf{v}}_0^T \mathbf{x}_0 - \epsilon \|\hat{\mathbf{v}}_0\|_q + \mu^-, \quad (102)$$

where

$$\mu^- = \sum_{i=1}^n \mathbf{v}_i^T \mathbf{b}_i - \sum_{i=1}^{n-1} \sum_{j \in \Gamma_i} \hat{\ell}_{i,j}[v_{i,j}]_-. \quad (103)$$

We are using the same dual network for both the upper bound and the lower bound.

The above process should be performed iteratively from $k = 0$ to $k = n - 1$. If there are multiple nodes in layer $k + 1$, we need to combine all dual variables together. Denote the variables in the dual network and the value function for the j th node in layer $k + 1$ as $\mathbf{v}_i^{k+1,j}$ and $\gamma_i^{k+1,j}$ for $i \leq k + 1$. The derivation of $\mathbf{v}_i^{k+1,j}$ and $\gamma_i^{k+1,j}$ follows the discussion above, except for the boundary conditions. The boundary condition for the dual network is now $\mathbf{v}_{k+1}^{k+1,j} = [0, \dots, 0, 1, 0, \dots, 0]$ where the value is 1 for the j th entry and 0 otherwise. When we optimize the value for the j th node, the objective is $(\mathbf{v}_{k+1}^{k+1,j})^T \mathbf{z}_{k+1}$. The boundary condition for the bias is kept unchanged $\gamma_{k+1}^{k+1,j} = 0$. Define a vector $\gamma_i^{k+1} := [\gamma_i^{k+1,1}, \dots, \gamma_i^{k+1,k_{k+1}}] \in \mathbb{R}^{k_{k+1}}$. Define a matrix $\mathbf{V}_i^{k+1} \in \mathbb{R}^{k_i \times k_{k+1}}$ to be the horizontal concatenation of $\mathbf{v}_i^{k+1,j}$ for all $j \in \{1, \dots, k_{k+1}\}$, i.e.,

$$\mathbf{V}_i^{k+1} = [\mathbf{v}_i^{k+1,1} \quad \mathbf{v}_i^{k+1,2} \quad \dots \quad \mathbf{v}_i^{k+1,k_{k+1}}]. \quad (104)$$

The matrices \mathbf{V}_i^{k+1} for all $i \leq k + 1$ also have a network structure. According to (99), the network structure can be described by

$$\mathbf{V}_i^{k+1} = \mathbf{D}_i \mathbf{W}_{i+1}^T \mathbf{V}_{i+1}^{k+1}, \forall i \leq k, \quad (105)$$

with boundary condition

$$\mathbf{V}_{k+1}^{k+1} = \mathbf{I}. \quad (106)$$

Following (101) and (102), the upper and lower bounds for \hat{z}_{k+1} can be computed as

$$\hat{\mathbf{u}}_{k+1} = (\mathbf{V}_1^{k+1})^T \mathbf{W}_1 \mathbf{x}_0 + \epsilon \|(\mathbf{V}_1^{k+1})^T \mathbf{W}_1\|_q + \sum_{i=1}^n (\mathbf{V}_i^{k+1})^T \mathbf{b}_i - \sum_{i=1}^{n-1} [(\mathbf{V}_i^{k+1})]_+^T \mathbf{D}_i^* \hat{\ell}_i, \quad (107a)$$

$$\hat{\ell}_{k+1} = (\mathbf{V}_1^{k+1})^T \mathbf{W}_1 \mathbf{x}_0 - \epsilon \|(\mathbf{V}_1^{k+1})^T \mathbf{W}_1\|_q + \sum_{i=1}^n (\mathbf{V}_i^{k+1})^T \mathbf{b}_i - \sum_{i=1}^{n-1} [(\mathbf{V}_i^{k+1})]_-^T \mathbf{D}_i^* \hat{\ell}_i, \quad (107b)$$

where \mathbf{D}_i^* is a diagonal matrix whose j th diagonal entry is 1 for $j \in \Gamma_i$ and 0 otherwise. The q norm is taken row-wise, i.e., $\|(\mathbf{V}_1^{k+1})^T \mathbf{W}_1\|_q := [\|(\mathbf{v}_1^{k+1,1})^T \mathbf{W}_1\|_q, \dots, \|(\mathbf{v}_1^{k+1,k_{k+1}})^T \mathbf{W}_1\|_q]$.

Relationships among dual networks For every k , we indeed have a dual network of k hidden layers. The dual variables in the dual network are related. The correlations are derived below. Note that $\mathbf{V}_i^{k+1} = \mathbf{D}_i \mathbf{W}_{i+1}^\top \mathbf{V}_{i+1}^{k+1} = \mathbf{D}_i \mathbf{W}_{i+1}^\top \mathbf{D}_{i+1} \mathbf{W}_{i+2}^\top \cdots \mathbf{D}_k \mathbf{W}_{k+1}^\top$. And $\mathbf{V}_i^k = \mathbf{D}_i \mathbf{W}_{i+1}^\top \mathbf{V}_{i+1}^k = \mathbf{D}_i \mathbf{W}_{i+1}^\top \mathbf{D}_{i+1} \mathbf{W}_{i+2}^\top \cdots \mathbf{D}_{k-1} \mathbf{W}_k^\top$. Hence,

$$\mathbf{V}_i^{k+1} = \mathbf{V}_i^k \mathbf{D}_k \mathbf{W}_{k+1}^\top. \quad (108)$$

The relationships among all $\mathbf{V}_i^{k'}$ s are shown below.

$$\begin{array}{ccccccc} & & & & & & \mathbf{V}_n^n \\ & & & & & & \downarrow \mathbf{D}_{n-1} \mathbf{W}_n^\top \\ & & & & \mathbf{V}_{n-1}^{n-1} & \xrightarrow{\cdot \mathbf{D}_{n-1} \mathbf{W}_n^\top} & \mathbf{V}_{n-1}^n \\ & & & & \vdots & & \vdots \\ & & & & \vdots & & \vdots \\ & & & & \mathbf{V}_3^{n-1} & \xrightarrow{\cdot \mathbf{D}_{n-1} \mathbf{W}_n^\top} & \mathbf{V}_3^n \\ & & & & \downarrow \mathbf{D}_2 \mathbf{W}_3^\top & & \downarrow \mathbf{D}_2 \mathbf{W}_3^\top \\ & & & & \mathbf{V}_2^{n-1} & \xrightarrow{\cdot \mathbf{D}_{n-1} \mathbf{W}_n^\top} & \mathbf{V}_2^n \\ & & & & \downarrow \mathbf{D}_1 \mathbf{W}_2^\top & & \downarrow \mathbf{D}_1 \mathbf{W}_2^\top \\ & & & & \mathbf{V}_1^{n-1} & \xrightarrow{\cdot \mathbf{D}_{n-1} \mathbf{W}_n^\top} & \mathbf{V}_1^n \\ & & & & \vdots & & \vdots \\ & & & & \mathbf{V}_1^1 & \xrightarrow{\cdot \mathbf{D}_1 \mathbf{W}_2^\top} & \mathbf{V}_1^2 \\ & & & & \downarrow \mathbf{D}_1 \mathbf{W}_2^\top & & \downarrow \mathbf{D}_1 \mathbf{W}_2^\top \\ & & & & \mathbf{V}_1^2 & \xrightarrow{\cdot \mathbf{D}_2 \mathbf{W}_3^\top} & \mathbf{V}_1^3 \\ & & & & \downarrow \mathbf{D}_2 \mathbf{W}_3^\top & & \downarrow \mathbf{D}_2 \mathbf{W}_3^\top \\ & & & & \mathbf{V}_1^3 & \xrightarrow{\cdot \mathbf{D}_3 \mathbf{W}_4^\top} & \mathbf{V}_1^4 \\ & & & & \vdots & & \vdots \end{array} \quad (109)$$

There are two approaches to compute \mathbf{V}_i^k for different i and k .

1. To compute the dual network from scratch for every k .
2. To compute the dual network for $k+1$ by reusing the dual network from the last k following (108).

The first approach is used in the original implementation in FastLin. The second approach is used in the original implementation in ConvDual. The second approach is more computationally efficient, and is shown in algorithm 8.4.

Binary search The binary search process of the allowable disturbance ϵ is illustrated in figure 17. We keep track of lower and upper bounds of ϵ , denoted $\underline{\epsilon}$ and $\bar{\epsilon}$. The output reachable set for input set with radius ϵ is denoted $\mathcal{R}(\epsilon)$, which satisfies the bounds computed in (107). The variables $\underline{\epsilon}$ and $\bar{\epsilon}$ need to satisfy that

$$\mathcal{R}(\underline{\epsilon}) \subseteq \mathcal{Y}, \mathcal{R}(\bar{\epsilon}) \not\subseteq \mathcal{Y}. \quad (110)$$

At every search step, the reachable set $\mathcal{R}(\epsilon)$ for $\epsilon := \frac{\underline{\epsilon} + \bar{\epsilon}}{2}$ is computed. There are two possibilities.

- If $\mathcal{R}(\epsilon) \subseteq \mathcal{Y}$, then $\underline{\epsilon}$ is updated to be ϵ .
- If $\mathcal{R}(\epsilon) \not\subseteq \mathcal{Y}$, then $\bar{\epsilon}$ is updated to be ϵ .

The search process can be terminated if either the maximum iteration is reached or the bounds are close enough to each other, i.e., $\bar{\epsilon} - \underline{\epsilon}$ is small. The binary search is implemented in the main loop in algorithm 8.5.

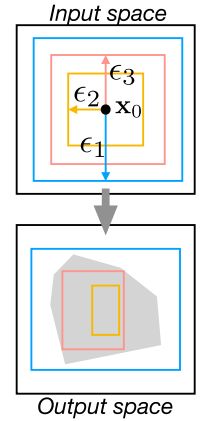


Figure 17. Illustration of the binary search in FastLin. The upper plot shows three different input sets with radius ϵ_1 , ϵ_2 , and ϵ_3 . The lower plot shows the output constraint \mathcal{Y} (gray area), and the output reachable sets that correspond to the three input sets. The first reachable set $\mathcal{R}(\epsilon_1)$ does not belong to \mathcal{Y} . Then a smaller radius ϵ_2 is chosen. The resulting reachable set $\mathcal{R}(\epsilon_2)$ is a subset of \mathcal{Y} . Then a larger radius $\epsilon_3 \in (\epsilon_2, \epsilon_1)$ is chosen. This process is repeated.

```

function get_bounds(nnet::Network, input::Vector{Float64}, ε::Float64)
    layers = nnet.layers
    n_layer = length(layers)
    l = Vector{Vector{Float64}}()
    u = Vector{Vector{Float64}}()
    γ = Vector{Vector{Float64}}()
    μ = Vector{Vector{Vector{Float64}}}()
    v1 = layers[1].weights'
    push!(γ, layers[1].bias)
    l1, u1 = input_layer_bounds(layers[1], input, ε)
    push!(l, l1)
    push!(u, u1)
    for i in 2:n_layer
        n_input = length(layers[i-1].bias)
        n_output = length(layers[i].bias)
        input_ReLU = relaxed_ReLU.(last(l), last(u))
        D = Diagonal(input_ReLU)
        WD = layers[i].weights*D
        v1 = v1 * WD'
        map!(g -> WD*g, γ, γ)
        for M in μ
            map!(m -> WD*m, M, M)
        end
        push!(γ, layers[i].bias)
        push!(μ, new_μ(n_input, n_output, input_ReLU, WD))
        ψ = v1' * input + sum(γ)
        eps_v1_sum = ε * vec(sum(abs, v1, dims = 1))
        neg, pos = all_neg_pos_sums(input_ReLU, l, μ, n_output)
        push!(l, ψ - eps_v1_sum + neg)
        push!(u, ψ + eps_v1_sum - pos)
    end
    return l, u
end

```

Algorithm 8.4. Reachability analysis in FastLin via network relaxation. The variables in the $(k + 1)$ th dual network is computed by reusing the variables in the k th dual network.


```

struct FastLin
    maxIter::Int64
     $\epsilon_0$ ::Float64
    accuracy::Float64
end

function solve(solver::FastLin, problem::Problem)
     $\epsilon_{\text{upper}}$  = 2 * max(solver. $\epsilon_0$ , maximum(problem.input.radius))
     $\epsilon$  = fill(maximum(problem.input.radius), solver.maxIter+1)
     $\epsilon_{\text{lower}}$  = 0.0
    n_input = dim(problem.input)
    for i = 1:solver.maxIter
        input_bounds = Hyperrectangle(problem.input.center, fill( $\epsilon[i]$ , n_input))
        output_bounds = forward_network(solver, problem.network, input_bounds)
        if issubset(output_bounds, problem.output)
             $\epsilon_{\text{lower}}$  =  $\epsilon[i]$ 
             $\epsilon[i+1]$  = ( $\epsilon[i]$  +  $\epsilon_{\text{upper}}$ ) / 2
            abs( $\epsilon[i]$  -  $\epsilon[i+1]$ ) > solver.accuracy || break
        else
             $\epsilon_{\text{upper}}$  =  $\epsilon[i]$ 
             $\epsilon[i+1]$  = ( $\epsilon[i]$  +  $\epsilon_{\text{lower}}$ ) / 2
        end
    end
    if  $\epsilon_{\text{lower}}$  > maximum(problem.input.radius)
        return AdversarialResult(:holds,  $\epsilon_{\text{lower}}$ )
    else
        return AdversarialResult(:violated,  $\epsilon_{\text{lower}}$ )
    end
end

```

Algorithm 8.5. FastLin. This main function shows the binary search process to determine the maximum allowable disturbance in the input space.

8.3 FastLip

FastLip [41] estimates the local Lipschitz constant, which is equivalent to what Certify computes in (84). Certify considers only networks with one hidden layer, while FastLip deals with networks with multiple layers. Same as in FastLin, FastLip takes in a hyperrectangle input set and a polytope output set. For simplicity, we assume the output set is only a half space defined by $\mathbf{c}^\top \mathbf{y} \leq d$. FastLip optimizes the following problem,

$$\min_{\mathbf{x}} \epsilon, \quad (111a)$$

$$\text{s.t. } \|\mathbf{x} - \mathbf{x}_0\|_q \geq \epsilon, \mathbf{y} = \mathbf{f}(\mathbf{x}), \mathbf{c}^\top \mathbf{y} \geq d. \quad (111b)$$

Let $o(\mathbf{x}) = \mathbf{c}^\top \mathbf{y} - d = \mathbf{c}^\top \mathbf{f}(\mathbf{x}) - d$. Assume ϵ satisfies the above optimization, then $o(\mathbf{x}) \geq 0$ for some \mathbf{x} with $\|\mathbf{x} - \mathbf{x}_0\|_q = \epsilon$. Similar to (81), we have the following relationship

$$0 \leq o(\mathbf{x}) \leq o(\mathbf{x}_0) + \epsilon \max_{\|\mathbf{x} - \mathbf{x}_0\|_q \leq \epsilon} \|\nabla o\|_p. \quad (112)$$

Hence, the solution of the problem (111) is bounded by

$$\min_{\|\mathbf{x} - \mathbf{x}_0\|_q \geq \epsilon, o(\mathbf{x}) \geq 0} \epsilon \geq -\frac{o(\mathbf{x}_0)}{\max_{\|\mathbf{x} - \mathbf{x}_0\|_q \leq \epsilon} \|\nabla o\|_p}. \quad (113)$$

The max over $\|\nabla o\|_p$ is hard to compute without knowing the optimal solution ϵ on the left hand side. In practice, the max over $\|\nabla o\|_p$ is taken over $\mathcal{X} = \{\mathbf{x} = \|\mathbf{x} - \mathbf{x}_0\|_q \leq \epsilon^{FastLin}\}$ where $\epsilon^{FastLin}$ is the solution obtained from FastLin. The adversarial bound is chosen as the minimum of $\epsilon^{FastLin}$ and the right hand side of (113). For simplicity, we only consider the norm with $p = 1$ and $q = \infty$.

As shown in (113), to compute the adversarial bound ϵ , we need to compute the gradient ∇o . Recall that Certify uses semidefinite relaxation to compute $\|\nabla o\|_1$. FastLip uses a different approach to estimate element-wise derivative $\nabla_{x_j} o = \frac{\partial o}{\partial x_j}$ for $j \in \{1, \dots, k_0\}$, then

$$\max_{\mathbf{x} \in \mathcal{X}} \|\nabla_{\mathbf{x}} o\|_1 \leq \sum_j \max_{\mathbf{x} \in \mathcal{X}} |\nabla_{x_j} o|. \quad (114)$$

The computation of the gradient follows from the method discussed in section 4.3, which uses interval arithmetic and considers the chain rule. Given the bounds computed in FastLin, the activation pattern can be determined. Hence, the lower and upper bounds of the gradients of the activation functions can be determined. Then the bounds on gradients $\underline{\mathbf{G}}_i$ and $\overline{\mathbf{G}}_i$ can be computed following (22) and (23).³² Given the bounds on the gradients, the gradient of o satisfies that

$$\underbrace{[\mathbf{c}]_+^\top \underline{\mathbf{G}}_n + [\mathbf{c}]_-^\top \overline{\mathbf{G}}_n}_{\mathbf{a}} \leq \nabla o \leq \underbrace{[\mathbf{c}]_+^\top \overline{\mathbf{G}}_n + [\mathbf{c}]_-^\top \underline{\mathbf{G}}_n}_{\mathbf{b}}. \quad (115)$$

³² The original paper uses a different set of equations. The two derivations are indeed equivalent.

Then the maximum 1-norm gradient is

$$\max_{\mathbf{x} \in \mathcal{X}} \|\nabla_{\mathbf{x}} o\|_1 \leq \sum_j \max_{\mathbf{x} \in \mathcal{X}} |\nabla_{x_j} o| = \sum_j \max\{|a_j|, |b_j|\}. \quad (116)$$

Then

$$\epsilon^{FastLip} := \min \left\{ \frac{-o(\mathbf{x}_0)}{\sum_j \max\{|a_j|, |b_j|\}}, \epsilon^{FastLin} \right\}. \quad (117)$$

Our implementation is shown in algorithm 8.6.

```

struct FastLip
    maxIter::Int64
     $\epsilon_0$ ::Float64
    accuracy::Float64
end

function solve(solver::FastLip, problem::Problem)
    c, d = tosimplehrep(convert(HPolytope, problem.output))
    y = compute_output(problem.network, problem.input.center)
    o = (c * y - d)[1]
    if o > 0
        return AdversarialResult(:violated, -o)
    end
    result = solve(FastLin(solver), problem)
    result.status == :violated && return result
     $\epsilon_{\text{fastLin}}$  = result.max_disturbance
    LG, UG = get_gradient(problem.network, problem.input)
    a, b = interval_map(c, LG, UG)
    v = max.(abs.(a), abs.(b))
     $\epsilon$  = min(-o/sum(v),  $\epsilon_{\text{fastLin}}$ )
    if  $\epsilon$  > maximum(problem.input.radius)
        return AdversarialResult(:holds,  $\epsilon$ )
    else
        return AdversarialResult(:violated,  $\epsilon$ )
    end
end

```

Algorithm 8.6. FastLip. FastLip depends on FastLin and further estimates the allowable input range by computing a local Lipschitz constant of the network.

8.4 DLV

DLV [18] searches not only the input space but also the hidden layers for a possible counter example. It uses a layer-by-layer approach. At layer i , it tries to find an assignment of the hidden nodes \mathbf{z}_i that satisfies the following two constraints:

1. Under the forward mapping $\mathbf{f}_{i+1 \rightarrow n} := \mathbf{f}_n \circ \dots \circ \mathbf{f}_{i+1}$, the output $\mathbf{f}_{i+1 \rightarrow n}(\mathbf{z}_i)$ does not belong to the desired constraint \mathcal{Y} .
2. Under the backward mapping $\mathbf{f}_{1 \rightarrow i} := \mathbf{f}_i \circ \dots \circ \mathbf{f}_1$, there is a valid input $\mathbf{x} \in \mathcal{X}$ such that $\mathbf{f}_{1 \rightarrow i}(\mathbf{x}) = \mathbf{z}_i$.

The conditions can be written concisely as

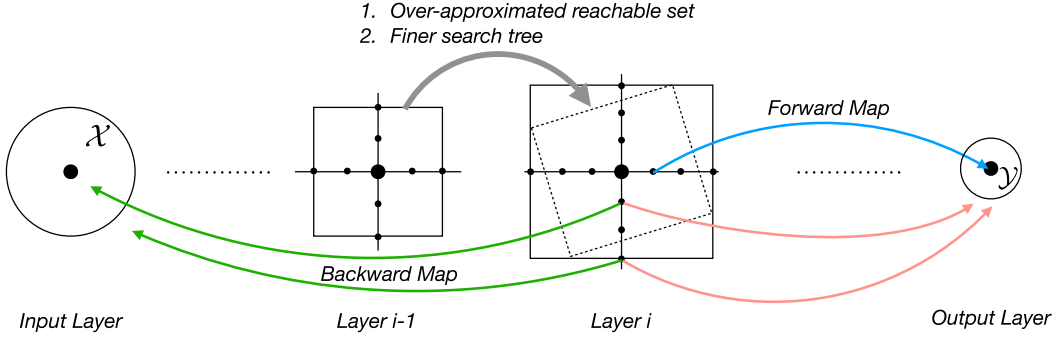
$$(\mathbf{f}_{1 \rightarrow i})^{-1}(\mathbf{z}_i) \cap \mathcal{X} \neq \emptyset, \quad (118a)$$

$$\mathbf{f}_{i+1 \rightarrow n}(\mathbf{z}_i) \notin \mathcal{Y}. \quad (118b)$$

Overall procedure To search for \mathbf{z}_i that satisfies (118), DLV does the following steps layer by layer.

1. Find a reachable set \mathcal{R}_i at layer i given the reachable set \mathcal{R}_{i-1} at layer $i-1$. The reachable set at the input layer is $\mathcal{R}_0 := \mathcal{X}$.
2. Build a search tree inside \mathcal{R}_i , denoted \mathcal{T}_i . The search tree \mathcal{T}_i should be a refinement of the search tree \mathcal{T}_{i-1} in the previous layer.³³

³³ The branches in the search tree are called ladders in the original paper [18].



3. Search for a counter example in the search tree \mathcal{T}_i that satisfies (118). If such an example is found, the property is violated. If not, we continue to the next layer.

The procedure is illustrated in figure 18. The key insight is that we can refine the search tree layer by layer. When it is closer to the output layer, it is easier to sample for counter examples. The original DLV implementation³⁴ uses SMT solvers to construct a reachable set in step 1 and build a search tree in step 2. For simplicity, our implementation in algorithm 8.7 does not involve SMT solvers. For step 1, we may compute the reachable set using any reachability method discussed in section 5. In algorithm 8.7, we use interval arithmetic by directly calling MaxSens using the function `get_bounds` in algorithm 5.5. The considerations in building the search tree in step 2 and the satisfiability check in step 3 are discussed below.

Search tree To build a search tree, we may explore all possible directions as shown in figure 19a. However, the complexity grows exponentially with k_i , the number of nodes in layer i . The authors of DLV suggest that we decompose the high-dimensional search space into several perpendicular low-dimensional search spaces, and only build search trees in those low-dimensional search spaces. Here, we simplify the search to element-wise exploration, *i.e.*, we sample every hidden node separately as shown in figure 19b. The construction of the search tree for a new layer needs to ensure that the tree is finer in the new layer. A set of conditions that precisely define “finer” are discussed in the DLV paper [18]. The problem of finding a search tree is then solved by calling an SMT solver.

For simplicity, our implementation takes equidistant samples for every hidden node. The sampling interval for node $z_{i,j}$ is denoted $\epsilon_{i,j}$. The sample intervals are refined layer by layer. For the input node, the sampling intervals $\epsilon_{0,j}$ for all $j \in \{1, \dots, k_0\}$ are set to a solver-specified value. The sample interval at layer $i-1$ indeed defines a hyperrectangle spanned by the following vectors

$$\mathbf{v}_{i-1,1} := [\epsilon_{i-1,1}, 0, \dots, 0], \mathbf{v}_{i-1,2} := [0, \epsilon_{i-1,2}, 0, \dots, 0], \dots, \mathbf{v}_{i-1,k_{i-1}} := [0, \dots, 0, \epsilon_{i-1,k_{i-1}}]. \quad (119)$$

No point, with the exception of the vertices of the hyperrectangle, are evaluated at layer $i-1$. In layer i , we need to ensure that we evaluate points inside the hyperrectangle, as shown in figure 18. The vertices of the hyperrectangle are mapped to $\mathbf{W}_i \mathbf{v}_{i-1,j'}$ at layer i for all $j' \in \{1, \dots, k_{i-1}\}$. For the j th node in layer i , the projected sampling interval given the hyperrectangle at layer $i-1$ is $\max_{j'} \sigma_{i,j}(|\mathbf{w}_{i,j} \mathbf{v}_{i-1,j'}|) = \max_{j'} \sigma_{i,j}(|w_{i,j,j'}| \epsilon_{i-1,j'})$.³⁵ We then set the sample interval to

Figure 18. Illustration of the DLV approach. DLV uses layer-by-layer analysis. At layer i , it computes an over-approximated reachable set and a finer search tree based on the reachable set and the search tree in layer $i-1$. For each point on the search tree, DLV first checks whether it violates the output constraint \mathcal{Y} using the forward map. For a point that violates the output constraint, DLV then checks whether it is reachable given the input constraint \mathcal{X} using the backward map. If such a point is reachable, then the corresponding input value is taken as a counter example.

³⁴ <https://github.com/VeriDeep/DLV>

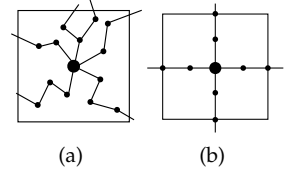


Figure 19. Illustration of a search tree in a 2D hidden space. (a) Complex search tree that explores all directions. (b) Simplified search tree for element-wise exploration.

³⁵ $\sigma_{i,j}$ is the activation function for node j at layer i . $\mathbf{w}_{i,j}$ is the j th row in the weight matrix \mathbf{W}_i . $w_{i,j,k}$ is the k th entry in $\mathbf{w}_{i,j}$.

```

struct DLV
  optimizer
   $\epsilon$ ::Float64
end

function solve(solver::DLV, problem::Problem)
   $\eta$  = get_bounds(problem)
   $\delta$  = Vector{Vector{Float64}}(undef, length( $\eta$ ))
   $\delta[1]$  = fill(solver. $\epsilon$ , dim( $\eta[1]$ ))
  if issubset(last( $\eta$ ), problem.output)
    return CounterExampleResult(:holds)
  end
  output = compute_output(problem.network, problem.input.center)
  for (i, layer) in enumerate(problem.network.layers)
     $\delta[i+1]$  = get_manipulation(layer,  $\delta[i]$ ,  $\eta[i+1]$ )
    if i == length(problem.network.layers)
      mapping = x -> (x  $\in$  problem.output)
    else
      forward_nnet = Network(problem.network.layers[i+1:end])
      mapping = x -> (compute_output(forward_nnet, x)  $\in$  problem.output)
    end
    var, y = bounded_variation( $\eta[i+1]$ , mapping,  $\delta[i+1]$ )
    if var
      backward_nnet = Network(problem.network.layers[1:i])
      status, x = backward_map(y, backward_nnet,  $\eta[1:i+1]$ )
      if status
        return CounterExampleResult(:violated, x)
      end
    end
  end
  return ReachabilityResult(:violated, [last( $\eta$ )])
end

```

Algorithm 8.7. Main code for DLV. First, the reachable set η for each layer is computed by calling `get_bounds`. Then the sampling intervals for the input layer are initialized. The solver first checks for counter examples in the input layer by calling `bounded_variation`. If no counter example is found, the solver then proceeds to the hidden layers. For every hidden layer, the desired sampling intervals are computed by calling `get_manipulation`. Then the solver checks for hidden values that do not map to \mathcal{Y} by calling `bounded_variation`. For those hidden values, the solver then maps back to the input layer by calling `backward_map`. If a corresponding input is found, it returns the input as a counter example for the problem. Otherwise, it goes to the next layer. The details of the functions `get_manipulation` and `bounded_variation` are not included.

be a value smaller than the projected sampling interval:

$$\epsilon_{i,j} := \gamma \max_{j'} \sigma_{i,j}(|w_{i,j,j'}| \epsilon_{i-1,j'}), \quad (120)$$

where $\gamma \in (0, 1)$ is set by the solver. This function is implemented in `get_manipulation`.

Given the sampling interval ϵ_i , the search tree \mathcal{T}_i consists of $2k_i$ chain branches. All branches are centered at $\mathbf{f}_{1 \rightarrow i}(\mathbf{x}_0)$. Then chains move along $\mathbf{v}_{i,j}$ in either the positive direction or the negative direction,

$$\mathbf{f}_{1 \rightarrow i}(\mathbf{x}_0) \rightarrow \mathbf{f}_{1 \rightarrow i}(\mathbf{x}_0) + 1 \cdot \mathbf{v}_{i,j} \rightarrow \mathbf{f}_{1 \rightarrow i}(\mathbf{x}_0) + 2 \cdot \mathbf{v}_{i,j} \rightarrow \dots \quad (121a)$$

$$\mathbf{f}_{1 \rightarrow i}(\mathbf{x}_0) \rightarrow \mathbf{f}_{1 \rightarrow i}(\mathbf{x}_0) - 1 \cdot \mathbf{v}_{i,j} \rightarrow \mathbf{f}_{1 \rightarrow i}(\mathbf{x}_0) - 2 \cdot \mathbf{v}_{i,j} \rightarrow \dots \quad (121b)$$

Since $j \in \{1, \dots, k_i\}$, we then have $2k_i$ chain branches. For example, in figure 19b, the search tree in two-dimensional space contains four branches. We don't need to explicitly construct the search tree. The search tree will be implicitly traversed when we check for satisfiability in step 3.

The original implementation of DLV is always complete and is sound when the search tree obtained by SMT solvers is minimal [18]. The tree nodes on a minimal search tree effectively cover all branches of a network. However, the search tree in our implementation is built heuristically and may not be minimal. To still make it sound, we only return holds when the output reachable set belongs to the output constraint. Otherwise, even if a counter example is not found, we return a violated reachability result. Hence, our implementation is sound but not complete.

Satisfiability check For every sampled value \mathbf{z}_i in the search tree, we first check if the corresponding output belongs to \mathcal{Y} . The function is implemented in `bounded_variation`, which outputs the points on the search tree that violate the output constraint. The original paper [18] indeed computes the maximum bounded variation of the search tree, *i.e.*, the maximum number of links that connect one satisfying node and one unsatisfying node along any tree path. As only one counter example is needed to falsify our problem, our implementation only checks for the existence of such a link.

If such a \mathbf{z}_i is found, we solve the following optimization problem to see if \mathbf{z}_i is reachable from \mathcal{X} :³⁶

$$\min_{\mathbf{x}} \|\mathbf{x} - \mathbf{x}_0\|_{\infty}, \quad (122a)$$

$$\text{s.t. } \mathbf{x} \in \mathcal{X}, \mathbf{f}_{1 \rightarrow i}(\mathbf{x}) = \mathbf{z}_i. \quad (122b)$$

³⁶ The point \mathbf{z}_i may lie in the over-approximated area that is not reachable from the input set \mathcal{X} .

The optimization problem is solved using a MILP encoding in `backward_map`. The method is similar to NSVerify. If we find such an \mathbf{x} , then it is a counter example.

9 Search and Optimization

This section discusses methods that combine search with optimization approaches. These methods leverage the piecewise linearity in the activation functions to develop efficient algorithms. Sherlock [10] uses local and global search to compute bounds on the output, solving different optimization problems during the local search and the global search. BaB [7] uses branch and bound to compute bounds on the output, where the branch step corresponds to search and the bound step corresponds to optimization. Planet [13] formulates the verification problem as a

satisfiability problem, searching for an activation pattern such that a feasible input is mapped to an infeasible output. Reluplex [20] uses a simplex algorithm that searches for a feasible activation pattern that leads to an infeasible output.

9.1 Sherlock

Sherlock [10] estimates the output range for a network with a single output, *i.e.*, $k_n = 1$. If $k_n > 1$, the method works for each individual variable. Given the input domain \mathcal{X} , we compute the tightest output bounds

$$\ell_n = \min_{\mathbf{x} \in \mathcal{X}} f(\mathbf{x}), \quad u_n = \max_{\mathbf{x} \in \mathcal{X}} f(\mathbf{x}). \quad (123)$$

Sherlock solves (123) by combining local search and global search. In local search, it solves a linear program to find the optimal value in a given line segment of the function f . In global search, it solves a feasibility program to check whether the current local optimal bound can be improved. To find the global optimal bound, the solver iteratively does local search and global search. This approach is illustrated in figure 20. The main process is implemented in algorithm 9.1.

```

struct Sherlock
    optimizer
     $\epsilon :: \text{Float64}$ 
end

function solve(solver::Sherlock, problem::Problem)
    ( $x_u$ ,  $u$ ) = output_bound(solver, problem, :max)
    ( $x_l$ ,  $l$ ) = output_bound(solver, problem, :min)
    bound = Hyperrectangle(low = [ $l$ ], high = [ $u$ ])
    reach = Hyperrectangle(low = [ $l$  - solver. $\epsilon$ ], high = [ $u$  + solver. $\epsilon$ ])
    return interpret_result(reach, bound, problem.output,  $x_l$ ,  $x_u$ )
end

function output_bound(solver::Sherlock, problem::Problem, type::Symbol)
    opt = solver.optimizer
     $x$  = sample(problem.input)
    while true
        ( $x$ , bound) = local_search(problem,  $x$ , opt, type)
        bound_ $\epsilon$  = bound + ifelse(type == :max, solver. $\epsilon$ , -solver. $\epsilon$ )
        ( $x_{\text{new}}$ , bound_new, feasible) = global_search(problem, bound_ $\epsilon$ ,
                                                    opt, type)

        feasible || return ( $x$ , bound)
        ( $x$ , bound) = ( $x_{\text{new}}$ , bound_new)
    end
end

```

Algorithm 9.1. The main function in Sherlock. Sherlock computes both the upper and the lower bound of the output node through the function `output_bound` and then interprets the result with respect to the given output constraint. The function `output_bound` performs iterative local and global search in the while loop. The global search step needs to improve the bound by at least ϵ . The while loop is broken if the global search fails. The value ϵ is specified by the solver, which affects the tightness of the bound.

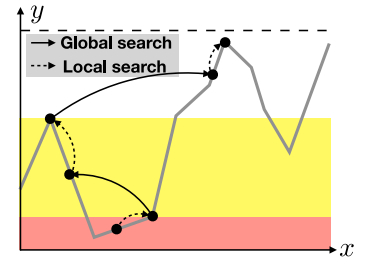


Figure 20. Illustration of the Sherlock approach. Sherlock combines local and global search. For a network with ReLU activations, the function represented by the network is piecewise linear. Local search improves the bound in a linear segment. Global search finds a point that improves the local bound by ϵ , which lies in another linear segment.

Local search Starting from a sampled point \mathbf{x}^* in the input domain. Local search tries to find a better solution that has the same activation pattern as \mathbf{x}^* , *i.e.*, in the same line segment of f . Denote the activation pattern with respect to \mathbf{x}^* as $\delta_{i,j}^*$ for all layers i and nodes j . The network

is encoded using (43). The local optimization problem for the upper bound is formulated as

$$\max_{\mathbf{z}_0, \dots, \mathbf{z}_n, \hat{\mathbf{z}}_1, \dots, \hat{\mathbf{z}}_n} \nabla f(\mathbf{x}^*)^\top \mathbf{z}_0, \quad (124a)$$

$$\text{s.t. } \mathbf{z}_0 \in \mathcal{X}, \quad (124b)$$

$$z_{i,j} = \hat{z}_{i,j} \geq 0, \text{ if } \delta_{i,j}^* = 1, \forall i \in \{1, \dots, n\}, j \in \{1, \dots, k_i\}, \quad (124c)$$

$$z_{i,j} = 0, \hat{z}_{i,j} \leq 0, \text{ if } \delta_{i,j}^* = 0, \forall i \in \{1, \dots, n\}, j \in \{1, \dots, k_i\}, \quad (124d)$$

$$\hat{\mathbf{z}}_i = \mathbf{W}_i \mathbf{z}_{i-1} + \mathbf{b}_i, \forall i \in \{1, \dots, n\}, \quad (124e)$$

where $\nabla f(\mathbf{x}^*)$ is the gradient at \mathbf{x}^* computed by (18). The optimal solution is denoted as \mathbf{x}^l . The corresponding bound is $u_n^l := f(\mathbf{x}^l)$. Similarly we can compute the lower bound by changing the max to min. The local search is implemented in algorithm 9.2.

```
function local_search(problem::Problem, x, optimizer, type::Symbol)
    nnet = problem.network
    act_pattern = get_activation(nnet, x)
    gradient = get_gradient(nnet, x)
    model = Model(with_optimizer(optimizer))
    neurons = init_neurons(model, nnet)
    add_set_constraint!(model, problem.input, first(neurons))
    encode_network!(model, nnet, neurons, act_pattern, StandardLP())
    o = gradient * neurons[1]
    index = ifelse(type == :max, 1, -1)
    @objective(model, Max, index * o[1])
    optimize!(model)
    x_new = value(neurons[1])
    bound_new = compute_output(nnet, x_new)
    return (x_new, bound_new[1])
end
```

Algorithm 9.2. Local search in Sherlock, which solves equation (124). The network is encoded as a set of linear constraints according to the given activation pattern. Those constraints confine the function f to the line segment that \mathbf{x}^* lies on. The slope of the line segment equals the gradient of f at \mathbf{x}^* . Hence, the solution of the local search is a local optimum of the function f .

Global search Given the bound from local search, a global search aims to improve the bound by ϵ , a solver-specified value. The global search problem is a feasibility problem. For example, for the upper bound, it tries to find a solution that satisfies

$$\mathbf{x} \in \mathcal{X}, f(\mathbf{x}) \geq u_n^l + \epsilon. \quad (125)$$

This problem is solved by calling NSVerify. If a solution \mathbf{x}^g is found, then the upper bound is updated to $u_n^g = f(\mathbf{x}^g)$. The global search is implemented in algorithm 9.3.

Since global search only solves a feasibility problem, the solution is not guaranteed to be a local optimum. Once a new global bound is found, local search will be called again to obtain the local optimum with respect to the new result. The reference point in the local search is set to $\mathbf{x}^* := \mathbf{x}^g$. After the local search, the global search will be called again. If there is no solution for the global search, we conclude that the upper bound is the bound obtained by the last local search, i.e., $u_n := u_n^l$. Similarly, we can compute the global lower bound.

```

function global_search(problem::Problem, bound, optimizer, type::Symbol)
    index = ifelse(type == :max, 1.0, -1.0)
    h = HalfSpace([index], index * bound)
    output_set = HPolytope([h])
    problem_new = Problem(problem.network, problem.input, output_set)
    solver = NSVerify(optimizer)
    result = solve(solver, problem_new)
    if result.status == :violated
        x = result.counter_example
        bound = compute_output(problem.network, x)
        return (x, bound[1], true)
    else
        return ([], 0.0, false)
    end
end

```

Algorithm 9.3. Global search in Sherlock. It calls NSVerify to solve equation (125) to determine if the bound can be improved by ϵ or not. If there is such a point that improves the bound by at least ϵ , the point and the new bound are returned. If there does not exist such a point, the problem is determined infeasible by returning a false flag.

Result interpretation The original purpose of Sherlock is only to obtain tight bounds. To fit into our problem formulation (4), the obtained bounds are compared against the output constraint \mathcal{Y} . The bounding set $\mathcal{B} := [\ell_n, u_n]$ is tight with at most ϵ uncertainty. The reachable set is defined as $\tilde{\mathcal{R}} := [\ell_n - \epsilon, u_n + \epsilon]$. The solution of the problem can be determined by

$$\tilde{\mathcal{R}} \in \mathcal{Y} \Rightarrow \text{holds}, \quad (126a)$$

$$\mathcal{B} \notin \mathcal{Y} \Rightarrow \text{violated}, \quad (126b)$$

$$\text{otherwise} \Rightarrow \text{Undetermined}. \quad (126c)$$

The three conditions are illustrated in figure 21 and implemented in algorithm 9.4. When the reachable set belongs to the output constraint, the property holds. When either bound u_n or ℓ_n exceeds the output constraint, the property is violated. In this case, we can output the counter example, which is the point that achieves either u_n or ℓ_n that violates the constraint. Otherwise, the problem is undetermined. The smaller the ϵ , the more accurate the result, as the problem is less likely to be undetermined. It is worth noting that the key advantage of Sherlock is to output tight bounds. It calls optimization solvers multiple times during the search for bounds. If the purpose is only to verify a given output constraint, it would be more computationally efficient to solve a feasibility problem using NSVerify, which corresponds to one global search step in Sherlock.

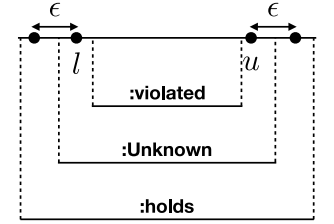


Figure 21. Interpreting results. The upper line illustrates the computed bound $[l, u]$ and the potential reachable set $[l - \epsilon, u + \epsilon]$. The bottom three lines illustrate three different output constraints \mathcal{Y} . If \mathcal{Y} does not cover either ℓ or u , the solver returns violated. If \mathcal{Y} covers the reachable set, the solver returns holds. Otherwise, the solver returns unknown.

```

function interpret_result(reach, bound, output, x_l, x_u)
    if high(reach) > high(output) && low(reach) < low(output)
        return ReachabilityResult(:holds, reach)
    end
    high(bound) > high(output) && return CounterExampleResult(:violated, x_u)
    low(bound) < low(output) && return CounterExampleResult(:violated, x_l)
    return ReachabilityResult(:Unknown, reach)
end

```

Algorithm 9.4. Interpretation of results. The code implements equation (126) and outputs corresponding counter examples when there is a violation. The input `reach` corresponds to $[\ell_n - \epsilon, u_n + \epsilon]$. The input `bound` corresponds to $[\ell_n, u_n]$. The input `output` is the output constraint \mathcal{Y} . The last two inputs are the points that achieve ℓ_n and u_n respectively.

9.2 BaB

BaB [7] uses branch and bound to estimate the output bounds of a network.³⁷ The main loop is shown in algorithm 9.5. For simplicity, we assume that the network only has one output node. Similar to Sherlock, the solver tries to compute the lower and upper bounds of the output in (123). The bounds are computed using the function `output_bound`. The results are interpreted by `interpret_result` in algorithm 9.4. BaB is different from Sherlock mainly in the method to estimate bounds. In the following discussion, we discuss the approach to estimate the upper bound u_n . Estimation of ℓ_n follows easily.

We maintain a global upper bound \bar{u}_n of u_n , and a global lower bound \underline{u}_n of u_n . The lower bound \underline{u}_n is computed by sampling for a concrete input, hence it is also called the concrete bound. The upper bound \bar{u}_n is computed with respect to a relaxation of the problem, hence it is called the approximated bound. The concrete bound always provides an under-estimation, while the upper bound always provides an over-estimation. For the lower bound ℓ_n , its lower bound $\underline{\ell}_n$ is the approximated bound, while its upper bound $\bar{\ell}_n$ is the concrete bound. These two possibilities are encoded by the `:max` and `:min` symbols in algorithm 9.5.

If $\bar{u}_n - \underline{u}_n < \epsilon$ for some small ϵ specified by the solver, the over-estimation is small. Then we conclude u_n is found. To minimize the over-approximation, the bounds \bar{u}_n and \underline{u}_n are improved by iterative interval refinement (a search process) similar to the procedure discussed in ReluVal in section 8.1.

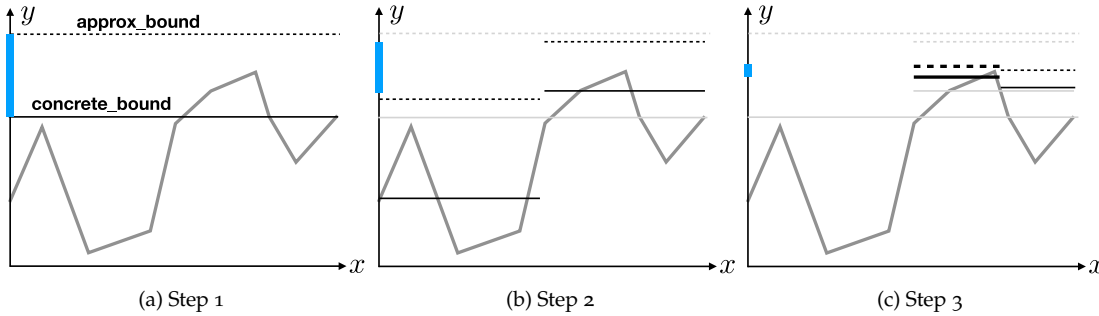


Figure 22. Illustration of branch and bound to estimate the upper bound of y . In step 1, an approximated upper bound (dashed line) and a concrete lower bound (solid line) are computed for the whole input interval. As there is a large gap between the two bounds (blue range), the input interval is split in two. In step 2, approximated upper bounds and concrete lower bounds are computed for the two intervals respectively. As the upper bound of the left interval is smaller than the lower bound of the right interval, the left interval is pruned out. The new global bounds are updated to be the bounds of the right interval. In step 3, the right interval is further split into two intervals. The previous process is repeated. The new bounds are close to each other. Hence, the global upper bound of y is found.

Search strategy During the search process, a list of input subsets $\{\mathcal{X}_i\}_i$ are recorded. In addition, the approximated bound of that subset \mathcal{X}_i is recorded, which is used to prioritize the list. For the estimation of u_n , we record $\bar{u}_n(\mathcal{X}_i)$. The list satisfies that $\bar{u}_n(\mathcal{X}_1) \geq \bar{u}_n(\mathcal{X}_2) \geq \dots$. For the estimation of ℓ_n , we record $\underline{\ell}_n(\mathcal{X}_i)$. The list satisfies that $\underline{\ell}_n(\mathcal{X}_1) \leq \underline{\ell}_n(\mathcal{X}_2) \leq \dots$.

At each iteration, the first domain in the priority queue, *i.e.*, the domain with the largest upper bound $\bar{u}_n(\mathcal{X}_1)$ or the domain with the smallest lower bound $\underline{\ell}_n(\mathcal{X}_1)$, is picked out and split into two domains. In ReluVal, we split the index that corresponds to the greatest smear value. In BaB, we split the index that has the longest interval. The resulting two domains are denoted \mathcal{X}_1^j for $j \in \{1, 2\}$.

For the two domains, we compute their approximated and concrete bounds $\bar{u}_n(\mathcal{X}_1^j)$ and $\underline{u}_n(\mathcal{X}_1^j)$ for $j \in \{1, 2\}$. The global lower bound $\underline{u}_n(\mathcal{X})$ is updated to $\max_j \underline{u}_n(\mathcal{X}_1^j)$ if it is greater than the previous global lower bound. If the upper bound $\bar{u}_n(\mathcal{X}_1^j)$ is greater than the global

lower bound, the corresponding sub domain \mathcal{X}_1^j needs further splits. Then \mathcal{X}_1^j is pushed back to the priority list. The current global upper bound $\bar{u}_n(\mathcal{X})$ is $\bar{u}_n(\mathcal{X}_1)$ in the new list.

The search terminates if the global concrete and approximated bounds are close to each other, i.e., $\bar{u}_n(\mathcal{X}) - \underline{u}_n(\mathcal{X}) < \epsilon$. The search process is illustrated in figure 22.

```

struct BaB
    optimizer
     $\epsilon::\text{Float64}$ 
end

function solve(solver::BaB, problem::Problem)
    (u_approx, u, x_u) = output_bound(solver, problem, :max)
    (l_approx, l, x_l) = output_bound(solver, problem, :min)
    bound = Hyperrectangle(low = [l], high = [u])
    reach = Hyperrectangle(low = [l_approx], high = [u_approx])
    return interpret_result(reach, bound, problem.output, x_l, x_u)
end

function output_bound(solver::BaB, problem::Problem, type::Symbol)
    nnet = problem.network
    global_concrete, x_star = concrete_bound(nnet, problem.input, type)
    global_approx = approx_bound(nnet, problem.input, solver.optimizer, type)
    doms = [(global_approx, problem.input)]
    index = ifelse(type == :max, 1, -1)
    while index * (global_approx - global_concrete) > solver. $\epsilon$ 
        dom = pick_out(doms)
        subdoms = split_dom(dom[2])
        for i in 1:length(subdoms)
            dom_concrete, x = concrete_bound(nnet, subdoms[i], type)
            dom_approx = approx_bound(nnet, subdoms[i], solver.optimizer, type)
            if index * (dom_concrete - global_concrete) > 0
                (global_concrete, x_star) = (dom_concrete, x)
            end
            if index * (dom_approx - global_concrete) > 0
                add_domain!(doms, (dom_approx, subdoms[i]), type)
            end
        end
        global_approx = doms[1][1]
    end
    return (global_approx, global_concrete, x_star)
end

```

Algorithm 9.5. The main function in BaB. BaB computes both the upper and the lower bound of the output node through the function `output_bound` and then interprets the result with respect to the given output constraint. The function `output_bound` performs branch and bound in the while loop. The solver keeps track of a concrete under-estimation and an approximated over-estimation in the search process. The search terminates once the two bounds are close to each other. The value ϵ is specified by the solver, which affects the tightness of the bound.

Concrete bounds The concrete bounds $\underline{u}_n(\mathcal{X}_i)$ and $\bar{\ell}_n(\mathcal{X}_i)$ are computed by sampling in the domain \mathcal{X}_i .³⁸ Heuristically, we only check three points in a domain, the upper and lower bounds of the domain, and the center point. Hence, an upper bound is always accompanied with a concrete sample input that achieves that bound. Computation of concrete bounds is implemented in the function `concrete_bound` in algorithm 9.6.

Approximated bounds The approximated bounds $\bar{u}_n(\mathcal{X}_i)$ and $\bar{\ell}_n(\mathcal{X}_i)$ are computed by minimizing the output given the Δ -relaxation of the network. For example, $\bar{u}_n(\mathcal{X}_i)$ is computed by

³⁸ ReluVal uses a similar approach to search for violations in `check_inclusion`.

$$\max_{z_0, \dots, z_n, \hat{z}_1, \dots, \hat{z}_n} z_n, \quad (127a)$$

$$\text{s.t. } z_{i,j} = \hat{z}_{i,j}, \forall i \in \{1, \dots, n-1\}, j \in \Gamma_i^+, \quad (127b)$$

$$z_{i,j} = 0, \forall i \in \{1, \dots, n-1\}, j \in \Gamma_i^-, \quad (127c)$$

$$z_{i,j} \geq \hat{z}_{i,j}, z_{i,j} \geq 0, z_{i,j} \leq \frac{\hat{u}_{i,j}(\hat{z}_{i,j} - \hat{\ell}_{i,j})}{\hat{u}_{i,j} - \hat{\ell}_{i,j}}, \forall i \in \{1, \dots, n-1\}, j \in \Gamma_i, \quad (127d)$$

$$\hat{z}_i = \mathbf{W}_i \mathbf{z}_{i-1} + \mathbf{b}_i, \forall i \in \{1, \dots, n-1\}, \quad (127e)$$

$$\mathbf{z}_0 \in \mathcal{X}_i. \quad (127f)$$

The approximated bound $\ell_n(\mathcal{X}_i)$ can be computed by changing the maximization to minimization in (127). ConvDual solves a similar optimization problem in (73), though it transforms it to the dual problem and then obtains a heuristic solution. Due to relaxation, the above optimization overestimates the true bounds, *i.e.*, $\bar{u}_n(\mathcal{X}_i) \geq u_n(\mathcal{X}_i)$ and $\ell_n(\mathcal{X}_i) \leq \ell_n(\mathcal{X}_i)$. The finer \mathcal{X}_i , the closer the approximated bound is to the true value. Hence, the approximated bound is improved during iterative refinement. Computation of the approximated bounds is implemented in the function `approx_bound` in algorithm 9.6.

```
function concrete_bound(nnet::Network, subdom::Hyperrectangle, type::Symbol)
    points = [subdom.center, low(subdom), high(subdom)]
    values = Vector{Float64}(undef, 0)
    for p in points
        push!(values, sum(compute_output(nnet, p)))
    end
    value, index = ifelse(type == :min, findmin(values), findmax(values))
    return (value, points[index])
end

function approx_bound(nnet::Network, dom::Hyperrectangle, optimizer, type)
    bounds = get_bounds(nnet, dom)
    model = Model(with_optimizer(optimizer))
    neurons = init_neurons(model, nnet)
    add_set_constraint!(model, dom, first(neurons))
    encode_network!(model, nnet, neurons, bounds, TriangularRelaxedLP())
    index = ifelse(type == :max, 1, -1)
    o = sum(last(neurons))
    @objective(model, Max, index * o)
    optimize!(model)
    termination_status(model) == OPTIMAL && return value(o)
end
```

Algorithm 9.6. Compute bounds in BaB. The concrete bound is computed by sampling in the domain. Heuristically, we sample three points: lower bound of domain, upper bound of domain, and center of domain. The approximated bound is computed by minimizing the output constrained on Δ -relaxation of the network.

Result interpretation Similar to Sherlock, the original purpose of BaB is only to obtain tight bounds. To fit into our problem formulation (4), the obtained bounds are compared against the output constraint \mathcal{Y} . Define the bounding set $\mathcal{B} := [\bar{\ell}_n, \bar{u}_n]$, which considers only the concrete bounds, and are tight with at most ϵ uncertainty. The reachable set is defined as $\tilde{\mathcal{R}} := [\ell_n, \bar{u}_n]$, which considers only the approximated bounds. Then the solution to the problem can be determined following the conditions in (126).

9.3 Planet

Planet [13] formulates the problem (4) as a satisfiability problem, which consists of trying to find an assignment for δ_i for all i such that a point in the input set can be mapped to the complement of the output set. The search in Planet can be understood as a binary tree search as the assignment is either 0 or 1 as illustrated in figure 23. The novelty of Planet is that it uses linear programming to 1) infer tighter bounds on the nodes, 2) filter out conflicting assignments, and 3) infer more assignments given a partial assignment of δ_i . In this way, the search can be more efficient.

The original implementation³⁹ is eager, which modifies the main loop in a state-of-the-art SAT solver (*i.e.*, MiniSAT) to impose network constraints during the search phase with partial assignments for δ_i . If conflicts are detected in the partial assignments, the solver performs back-tracking.

For simplicity, we didn't follow the original eager implementation. Instead, we only check for conflicts when all δ have been assigned. We call PicoSAT.jl⁴⁰ to solve the SAT problem for assignment. In this way, we can leave the SAT solver untouched. The main loop in algorithm 9.7 is different from the Planet paper. In the non-eager implementation, the node-wise bounds are computed first. Planet introduces an optimization approach to compute tighter bounds, which will be discussed below. Then a clause Ψ is initialized with respect to the bounds. The clause can be understood as a pruned search tree. A full assignment of all δ 's according to the clause is computed by calling PicoSAT. The feasibility of this assignment is checked by elastic filtering, which returns conflicts in the assignment if the assignment is not feasible. Then the conflicts are added to the clause, which helps further pruning the search tree. If the assignment is feasible, that means there is an activation pattern that maps a desired input to an undesired output. Then the property is violated. If no such assignment exists, the property holds.

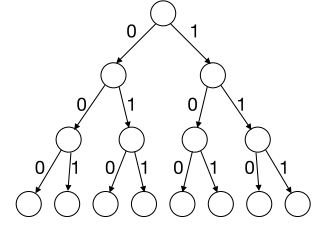


Figure 23. Illustration of binary tree search to assign values to $\delta_{i,j}$ for all nodes j in layer i .

³⁹ <https://github.com/progirep/planet>

⁴⁰ <https://github.com/jakebolewski/PicoSAT.jl>

```

struct Planet
    optimizer
    eager::Bool
end

function solve(solver::Planet, problem::Problem)
    status, bounds = tighten_bounds(problem, solver.optimizer)
    status == OPTIMAL || return CounterExampleResult(:holds)
     $\Psi$  = init_ $\Psi$ (problem.network, bounds)
     $\delta$  = PicoSAT.solve( $\Psi$ )
    opt = solver.optimizer
    while  $\delta$  != :unsatisfiable
        status, conflict = elastic_filtering(problem,  $\delta$ , bounds, opt)
        status == INFEASIBLE || return CounterExampleResult(:violated, conflict)
        push!( $\Psi$ , conflict)
         $\delta$  = PicoSAT.solve( $\Psi$ )
    end
    return CounterExampleResult(:holds)
end

```

Algorithm 9.7. Main loop in Planet. This is a non-eager implementation. First, tight bounds of node values are computed through `tighten_bounds`. Then the clause Ψ is initialized with respect to the bounds. A full assignment according to the clause is computed by calling `PicoSAT`. The feasibility of this assignment is checked by `elastic_filtering`, which returns conflicts in the assignment if the assignment is not feasible. Then the conflicts are added to the clause. The while loop repeats previous steps. If the assignment is feasible, that means there is an activation pattern that maps a desired input to an undesired output. Then the property is violated. If no such assignment exists, the property is violated.

Computing tight bounds We first compute the bounds through `tighten_bounds` in algorithm 9.8. This function first gets relatively loose bounds ℓ_i and \mathbf{u}_i from `get_bounds` in algorithm 5.5. Then

the following optimization problem is solved

$$\min_{\mathbf{z}_0, \dots, \mathbf{z}_n, \hat{\mathbf{z}}_1, \dots, \hat{\mathbf{z}}_n} q \sum_{i=1}^n \sum_{j=1}^{k_i} z_{i,j}, \quad (128a)$$

$$\text{s.t. } \mathbf{z}_0 \in \mathcal{X}, \mathbf{z}_n \notin \mathcal{Y}, \quad (128b)$$

$$z_{i,j} = \hat{z}_{i,j}, \forall i \in \{1, \dots, n-1\}, j \in \Gamma_i^+, \quad (128c)$$

$$z_{i,j} = 0, \forall i \in \{1, \dots, n-1\}, j \in \Gamma_i^-, \quad (128d)$$

$$z_{i,j} \geq \hat{z}_{i,j}, z_{i,j} \geq 0, z_{i,j} \leq \frac{\hat{u}_{i,j}(\hat{z}_{i,j} - \hat{\ell}_{i,j})}{\hat{u}_{i,j} - \hat{\ell}_{i,j}}, \forall i \in \{1, \dots, n-1\}, j \in \Gamma_i, \quad (128e)$$

$$\hat{\mathbf{z}}_i = \mathbf{W}_i \mathbf{z}_{i-1} + \mathbf{b}_i, \forall i \in \{1, \dots, n\}, \quad (128f)$$

where $q \in \{-1, 1\}$. When $q = -1$, we compute the tighter upper bounds. When $q = 1$, we get the lower bounds. Here we use Δ -relaxation in (46). If there is no solution in (128), that means the constraints are infeasible. Hence, for all $\mathbf{x} \in \mathcal{X}$, $\mathbf{y} = \mathbf{f}(\mathbf{x}) \in \mathcal{Y}$. Then the property is satisfied.

```

function tighten_bounds(problem::Problem, optimizer)
    bounds = get_bounds(problem)
    network = problem.network
    model = Model(with_optimizer(optimizer))
    neurons = init_neurons(model, network)
    add_set_constraint!(model, problem.input, first(neurons))
    add_complementary_set_constraint!(model, problem.output, last(neurons))
    encode_network!(model, network, neurons, bounds, TriangularRelaxedLP())

    min_sum!(model, neurons)
    optimize!(model)
    termination_status(model) == OPTIMAL || return (INFEASIBLE, bounds)
    lower = value.(neurons)

    max_sum!(model, neurons)
    optimize!(model)
    termination_status(model) == OPTIMAL || return (INFEASIBLE, bounds)
    upper = value.(neurons)

    new_bounds = Vector{Hyperrectangle}(undef, length(neurons))
    for i in 1:length(neurons)
        new_bounds[i] = Hyperrectangle(low = lower[i], high = upper[i])
    end
    return (OPTIMAL, new_bounds)
end

```

Algorithm 9.8. Obtaining tighter bounds using optimization. The solution is tighter than `get_bounds` in algorithm 5.5. The implementation encodes equation (128) and solves the optimization problem by calling the JuMP solver.

Solving the SAT problem A clause Ψ corresponds to a search tree, which encodes a set of binary conditions. According to the bounds computed earlier, the clause can be initialized as

$$\Psi = \bigwedge_{\hat{\ell}_{i,j} \leq 0 \leq \hat{u}_{i,j}} [\{\delta_{i,j} = 1\} \vee \{\delta_{i,j} = 0\}] \bigwedge_{0 < \hat{\ell}_{i,j}} [\delta_{i,j} = 1] \bigwedge_{\hat{u}_{i,j} < 0} [\delta_{i,j} = 0]. \quad (129)$$

Solving the SAT problem means finding an assignment of δ 's such that the clause Ψ is true. The case that $\Psi = \bigwedge_{i,j} [\{\delta_{i,j} = 1\} \vee \{\delta_{i,j} = 0\}]$ corresponds to a full search tree shown in figure 23. As more conditions are added to the clause, we are essentially pruning the search tree. Elastic filtering, to be discussed below is used to help the pruning. There may be more than one solution that satisfies the clause Ψ . We only consider one solution at a time. PicoSAT is called to find a feasible assignment for δ 's.

Elastic filtering Given an assignment of $\delta_{i,j}$'s, we check for conflicts using `elastic_filtering` in algorithm 9.9. The problem is defined as

$$\min_{\mathbf{z}_0, \dots, \mathbf{z}_n, \hat{\mathbf{z}}_1, \dots, \hat{\mathbf{z}}_n, \mathbf{s}_1, \dots, \mathbf{s}_n} q \sum_{i=1}^n \sum_{j=1}^{k_i} s_{i,j}, \quad (130a)$$

$$\text{s.t. } \mathbf{z}_0 \in \mathcal{X}, \mathbf{z}_n \notin \mathcal{Y}, \quad (130b)$$

$$z_{i,j} = \hat{z}_{i,j}, \forall i \in \{1, \dots, n-1\}, j \in \Gamma_i^+, \quad (130c)$$

$$z_{i,j} = 0, \forall i \in \{1, \dots, n-1\}, j \in \Gamma_i^-, \quad (130d)$$

$$z_{i,j} \geq \hat{z}_{i,j}, z_{i,j} \geq 0, z_{i,j} \leq \frac{\hat{u}_{i,j}(\hat{z}_{i,j} - \hat{\ell}_{i,j})}{\hat{u}_{i,j} - \hat{\ell}_{i,j}}, \forall i \in \{1, \dots, n-1\}, j \in \Gamma_i, \quad (130e)$$

$$\hat{\mathbf{z}}_i = \mathbf{W}_i \mathbf{z}_{i-1} + \mathbf{b}_i, \forall i \in \{1, \dots, n\}, \quad (130f)$$

$$z_{i,j} = \hat{z}_{i,j} + s_{i,j} \geq 0, \text{ for } \delta_{i,j} = 1, \forall i \in \{1, \dots, n\}, j \in \{1, \dots, k_i\}, \quad (130g)$$

$$z_{i,j} = 0, \hat{z}_{i,j} - s_{i,j} \leq 0, \text{ for } \delta_{i,j} = 0, \forall i \in \{1, \dots, n\}, j \in \{1, \dots, k_i\}, \quad (130h)$$

which uses both Δ -relaxation (given bounds) and slack relaxation (given activation). If the assignment of $\delta_{i,j}$'s are feasible, then all the slack variables should be non-positive. If some slack variables are positive, we fix the node with the largest slack value by adding a condition $s_{i,j} = 0$. Then the optimization problem is solved again and again until there is no feasible solution. The list of node $\{(i^{(1)}, j^{(1)}), (i^{(2)}, j^{(2)}), \dots, (i^{(k)}, j^{(k)})\}$ and their δ assignments that we fixed during the process is a conflict. A conflict means that the δ assignments of those nodes cannot be satisfied simultaneously. The intuition behind elastic filtering is that we can find conflicts faster by fixing the most violated constraints.

Once a conflict is determined with respect to an assignment, we can add the conflict back to the clauses and solve the SAT problem again. If there is no feasible solution of Ψ , the property holds. If no conflict is found for a specific assignment, the property is violated. Our implementation is still sound and complete, though it is less efficient than the original eager implementation. Our implementation requires that input set \mathcal{X} be a `Hyperrectangle` and the output set \mathcal{Y} be a `PolytopeComplement`.

9.4 Reluplex

Reluplex [20] applies a simplex algorithm to ReLU networks. It searches for a counter example (10).

For each node (i, j) , Reluplex optimizes over two variables $z_{i,j}$ and $\hat{z}_{i,j}$. There are three possible statuses for each node (i, j) , active (denoted $(i, j) \in \mathcal{A}$), inactive (denoted $(i, j) \in \mathcal{N}$), and undetermined (denoted $(i, j) \in \mathcal{U}$). Reluplex tries to find a feasible assignment for undetermined nodes through depth-first search. The basic constraints in Reluplex without considering the

```

function elastic_filtering(problem::Problem,  $\delta$ , bounds, optimizer)
    network = problem.network
    model = Model(with_optimizer(optimizer))
    neurons = init_neurons(model, network)
    add_set_constraint!(model, problem.input, first(neurons))
    add_complementary_set_constraint!(model, problem.output, last(neurons))
    encode_network!(model, network, neurons, bounds, TriangularRelaxedLP())
    SLP = encode_network!(model, network, neurons,  $\delta$ , SlackLP())
    min_sum!(model, SLP.slack)
    conflict = Vector{Int64}()
    act = get_activation(network, bounds)
    while true
        optimize!(model)
        termination_status(model) == OPTIMAL || return (INFEASIBLE, conflict)
        (m, index) = max_slack(value.(SLP.slack), act)
        m > 0.0 || return (:Feasible, value.(neurons[1]))
        coeff =  $\delta$ [index[1]][index[2]] ? -1 : 1
        node = coeff * get_node_id(network, index)
        push!(conflict, node)
        @constraint(model, SLP.slack[index[1]][index[2]] == 0.0)
    end
end

```

Algorithm 9.9. Elastic filtering is used to determine conflicts in an assignment of all δ 's. It iteratively solves equation (130). At each iteration, it fixes the largest slack variable to zero. The conflicting sequence is found once the optimization becomes infeasible.

undetermined nodes are

$$\mathcal{B} = \{\mathbf{z}_i, \hat{\mathbf{z}}_i : \mathbf{z}_0 \in \mathcal{X}, \mathbf{z}_n \notin \mathcal{Y}, \quad (131a)$$

$$z_{i,j} \geq 0, z_{i,j} \geq \hat{z}_{i,j}, \hat{\ell}_{i,j} \leq \hat{z}_{i,j} \leq \hat{u}_{i,j}, \quad (131b)$$

$$z_{i,j} = \hat{z}_{i,j}, \hat{z}_{i,j} \geq 0, \forall (i, j) \in \mathcal{A}, \quad (131c)$$

$$z_{i,j} = 0, \hat{z}_{i,j} < 0, \forall (i, j) \in \mathcal{N}, \quad (131d)$$

$$\hat{\mathbf{z}}_i = \mathbf{W}_i \mathbf{z}_{i-1} + \mathbf{b}_i, \forall i \in \{1, \dots, n\}, \quad (131e)$$

At each search step, Reluplex either finds a counter example, or determines that there is no such counter example (then does backtracking), or assigns one node $(i^*, j^*) \in \mathcal{U}$ to be active or inactive. The set $\mathcal{B}^0 := \mathcal{B}$, $\mathcal{A}^0 := \mathcal{A}$, $\mathcal{N}^0 := \mathcal{N}$, and $\mathcal{U}^0 := \mathcal{U}$ are initialized at the beginning of the search. At search depth k , we have a set of constraints \mathcal{B}^k , which is an intersection of the basic constraint \mathcal{B} and the constraint induced by the assignments of nodes in \mathcal{U}^0 during the search. \mathcal{B}^k can be represented in the form of (131) by adding superscript k to \mathcal{B} , \mathcal{A} , and \mathcal{N} . The relationships among the sets at different depths are

$$\mathcal{A}^0 \subseteq \mathcal{A}^1 \subseteq \dots \subseteq \mathcal{A}^k, \quad (132a)$$

$$\mathcal{N}^0 \subseteq \mathcal{N}^1 \subseteq \dots \subseteq \mathcal{N}^k, \quad (132b)$$

$$\mathcal{U}^0 \supset \mathcal{U}^1 \supset \dots \supset \mathcal{U}^k. \quad (132c)$$

At each search step k , we first solve a feasibility problem to check if there is a solution of \mathcal{B}^{k-1} . If there is no feasible solution that satisfies \mathcal{B}^{k-1} , we do back tracking. If there exists a solution that satisfies \mathcal{B}^{k-1} , we consider the following two possibilities.

- If all ReLU constraints are satisfied, *i.e.*, $z_{i,j} = \max\{\hat{z}_{i,j}, 0\}$, then we indeed find a counter example for the problem (4).

- If some ReLU constraints are not satisfied, *i.e.*, $z_{i,j} \neq \max\{\hat{z}_{i,j}, 0\}$, then we need to fix those broken nodes during the search. We pick such a broken node (i^k, j^k) from \mathcal{U}^{k-1} . Then $\mathcal{U}^k = \mathcal{U}^{k-1} \setminus \{(i^k, j^k)\}$. We may assign the node to be either active or inactive. In the active case, $\mathcal{A}^k = \mathcal{A}^{k-1} \cup \{(i^k, j^k)\}$, $\mathcal{N}^k = \mathcal{N}^{k-1}$, and

$$\mathcal{B}^k := \mathcal{B}^{k-1} \cap \{\mathbf{z}_i, \hat{\mathbf{z}}_i : z_{i^k, j^k} = \hat{z}_{i^k, j^k} \geq 0\}. \quad (133)$$

In the inactive case, $\mathcal{A}^k = \mathcal{A}^{k-1}$, $\mathcal{N}^k = \mathcal{N}^{k-1} \cup \{(i^k, j^k)\}$, and

$$\mathcal{B}^k := \mathcal{B}^{k-1} \cap \{\mathbf{z}_i, \hat{\mathbf{z}}_i : z_{i^k, j^k} = 0, \hat{z}_{i^k, j^k} \leq 0\}. \quad (134)$$

During the search, we either end up finding a counter example or concluding that there is no such counter example. The worst case scenario complexity is $2^{|\mathcal{U}|}$, *i.e.*, we traverse a depth $|\mathcal{U}|$ binary tree, where $|\mathcal{U}|$ computes the cardinality of the set \mathcal{U} . It is possible to use elastic filtering introduced in Planet to help detect conflicts faster.

Our implementation supports input sets \mathcal{X} of type `Hyperrectangle` and output sets \mathcal{Y} of type `PolytopeComplement` and is shown in algorithm 9.10.⁴¹ The depth-first search is performed in the function `reluplexStep`. The construction of \mathcal{B}^k at each search step is done by `encode` in algorithm 9.11. The inputs to `reluplexStep` include,

- `model`, which encodes the constraint \mathcal{B}^k similar to (131).
- `b_vars` and `f_vars`, which are $\hat{\mathbf{z}}$'s and \mathbf{z} 's.
- `relu_status`, which can be either 0, 1 or 2. If it is 0, the corresponding node belongs \mathcal{U}^k . If it is 1, the corresponding node belongs \mathcal{A}^k . If it is 2, the corresponding node belongs \mathcal{N}^k .

⁴¹ The original Reluplex uses a data structure called Tableau to encode new LP constraints. Conceptually, our Julia implementation is the same as the original implementation, but in a less efficient way.

10 Comparison and Results

This section presents experimental results for our implementation of the algorithms.⁴² Different algorithms handle problems with different specifications as shown in table 1. As described previously, the objects used to represent the input set \mathcal{X} and the output set \mathcal{Y} vary along with the characteristics of the sets that each of the algorithms support. Additionally, different algorithms output different types of results. We have, consequently, split the algorithms in six groups such that the same verification problem can be solved by all the algorithms within a group, facilitating a comparison of the implementations provided with this work. The groups are as follows:

1. Ai2, ExactReach, and maxSens - Input: `HPolytope`, Output: `HPolytope` (bounded).
2. ILP, MIPVerify, and NSVerify - Input: `Hyperrectangle`, Output: `PolytopeComplement`.
3. Duality and convDual - Input: `Hyperrectangle` (uniform radius), Output: `Halfspace`.
4. FastLin, FastLip, ILP, and MIPVerify - Input: `Hyperrectangle`, Output: `Halfspace`.
5. BaB, DLV, ReluVal, and Sherlock - Input: `Hyperrectangle`, Output: `Hyperrectangle` (1-D).
6. Planet, Reluplex, and ReluVal - Input: `Hyperrectangle`, Output: `PolytopeComplement` and `Hyperrectangle`.

Despite having different problem specifications, the exact same property can be encoded across Groups 2, 3, 4, and 6 by using their corresponding input and output sets to represent the same constraints.

⁴² In our implementations, readability was favored over speed. Some of our implementations are simplified versions of the original ones that still output the same results but can be slower.

```

struct Reluplex
  optimizer
end

function solve(solver::Reluplex, problem::Problem)
  initial_model = Model(solver)
  bs, fs = encode(solver, initial_model, problem)
  layers = problem.network.layers
  initial_status = [zeros(Int, n) for n in n_nodes.(layers)]
  insert!(initial_status, 1, zeros(Int, dim(problem.input)))

  return reluplex_step(solver, problem, initial_model, bs, fs, initial_status)
end

function reluplex_step(solver::Reluplex,
  problem::Problem,
  model::Model,
   $\hat{z}$ ::Vector{Vector{VariableRef}},
  z::Vector{Vector{VariableRef}},
  relu_status::Vector{Vector{Int}})
  optimize!(model)
  if termination_status(model) == OPTIMAL
    i, j = find_relu_to_fix( $\hat{z}$ , z)
    i == 0 && return CounterExampleResult(:violated, value.(first( $\hat{z}$ )))
    for repair_type in 1:2
      relu_status[i][j] = repair_type
      new_m = Model(solver)
      bs, fs = encode(solver, new_m, problem)
      enforce_repairs!(new_m, bs, fs, relu_status)
      result = reluplex_step(solver, problem, new_m, bs, fs, relu_status)
      relu_status[i][j] = 0
      result.status == :violated && return result
    end
  end
  return CounterExampleResult(:holds)
end

function enforce_repairs!(model::Model,  $\hat{z}$ , z, relu_status)
  for i in 1:length(relu_status), j in 1:length(relu_status[i])
     $\hat{z}_{ij}$  =  $\hat{z}$ [i][j]
     $z_{ij}$  = z[i][j]
    if relu_status[i][j] == 1
      type_one_repair!(model,  $\hat{z}_{ij}$ ,  $z_{ij}$ )
    elseif relu_status[i][j] == 2
      type_two_repair!(model,  $\hat{z}_{ij}$ ,  $z_{ij}$ )
    end
  end
end

function type_one_repair!(model,  $\hat{z}_{ij}$ ,  $z_{ij}$ )
  @constraint(model,  $\hat{z}_{ij}$  ==  $z_{ij}$ )
  @constraint(model,  $\hat{z}_{ij}$  >= 0.0)
end

function type_two_repair!(model,  $\hat{z}_{ij}$ ,  $z_{ij}$ )
  @constraint(model,  $\hat{z}_{ij}$  <= 0.0)
  @constraint(model,  $z_{ij}$  == 0.0)
end

```

Algorithm 9.10. Main loop in Reluplex. The function `reluplexStep` performs depth-first search. At every search step, it first solves a feasibility problem encoded in `model`. If the problem is infeasible, meaning that no counter example can be found, we output `:holds`. If there is a solution of the problem, we find the first node such that the ReLU activation is broken, *i.e.*, $z_{i,j} \neq [\hat{z}_{i,j}]_+$. If no such broken node is found, meaning that we have found a counter example, we output `:violated` with the counter example. For the broken node, we can either change its status to 1 or 2, which corresponds to the two branches in the search. For each branch, a new constrained problem is formulated. New constraints are added through `enforce_repairs!`, which encode constraints according to `relu_status`. With the new model, the search continues into the next depth.

```

function encode(solver::Reluplex, model::Model, problem::Problem)
    layers = problem.network.layers
     $\hat{z}$  = init_neurons(model, layers)
    z = init_neurons(model, layers)
    activation_constraint!(model,  $\hat{z}$ [1], z[1], Id())
    bounds = get_bounds(problem)
    for (i, L) in enumerate(layers)
        @constraint(model, affine_map(L, z[i]) .==  $\hat{z}$ [i+1])
        add_set_constraint!(model, bounds[i],  $\hat{z}$ [i])
        activation_constraint!(model,  $\hat{z}$ [i+1], z[i+1], L.activation)
    end
    add_complementary_set_constraint!(model, problem.output, last(z))
    feasibility_problem!(model)
    return  $\hat{z}$ , z
end

```

Algorithm 9.11. Encoding the optimization problem in Reluplex. The optimization problem has zero objective and is constrained on \mathcal{B} in equation (131). In the search process, more constraints are to be added by `enforce_repairs!`, which encode constraints according to `relu_status`.

10.1 Experiments

We used different neural networks to benchmark the performance of the algorithms in different scenarios. We focused on three contexts: networks of varying sizes trained to classify hand-written digits from the MNIST dataset [21], the Aircraft Collision Avoidance System (ACAS) network [20].⁴³ and we created a tiny toy network (small nnet) for which we analytically derived its transfer function.

Small nnet We manually specified a toy network and analytically derived the one dimensional function that it represents. We evaluated simple properties corresponding to upper and lower bounds of the image of this function for a small interval in the input set. The network has two hidden layers of two units each.

MNIST For the MNIST networks, we constructed properties that encode regions centered around a point corresponding to a hand-written digit in the original dataset. We verified a property associated to the correct classification of the image. The property requires that the logits (outputs of the final layer) do not vary significantly from those of the original image when the image is perturbed within a region in the input space. This corresponds to an ℓ_1 ball centered around the point that corresponds to a sample hand-written image of the number 1 digit. The output set \mathcal{V} is an ℓ_1 ball built around the original output of the network corresponding to that input. For algorithms that only support halfspace or polytopeComplement output sets, we encoded the region where the logit of the digit 0 is less than the logit of the digit 1. The networks have the following characteristics:

- mnist1. Input size: 748, 1 hidden layer of size: 25, output size: 10 (0.9009 test accuracy).
- mnist2. Input size: 748, 1 hidden layer of size: 100, output size: 10 (0.9463 test accuracy).
- mnist3. Input size: 748, 4 hidden layers of size: 25, output size: 10 (0.9555 test accuracy).
- mnist4. Input size: 748, 6 hidden layers of size: 50, output size: 10 (0.9664 test accuracy).

⁴³ This network is based on a neural network trained on a very early prototype of ACAS Xu, targeted for unmanned aircraft. Details can be found in the article by Julian, Kochenderfer, and Owen [19].

ACAS For the ACAS network, we verified property 10 introduced by Katz et al. [20]. Property 10 corresponds to the situation where the intruder aircraft is far away from the ownship and the desired output is that the advisory is clear-of-conflict. To make the property faster to verify, we reduced the volume of the input region by fixing the last three inputs of the network to specific values instead of the ranges originally defined for the property. This property has been verified in prior work [20], [40]. For the algorithms that can only support halfspace or PolytopeComplement output sets, we encoded the region where the first output is less than the last output. The network has five input units, six hidden layers of 50 units each, and five output units.

The experiments in Group 5 required networks with a single output node. We used pruned versions of the exact same networks. We encoded the corresponding properties in the dimension of the preserved output node. For the MNIST networks this is the output corresponding to digit 1 and for the ACAS network this is the output corresponding to the cost of advising clear-of-conflict.

10.2 Results

In the following table, we summarize the results of evaluating the aforementioned properties with the different algorithms. For each experiment, we recorded the time that it took for each algorithm to terminate. Timed-out threshold is set to be 24 hours. We also recorded the result of each algorithm to identify cases in which incomplete algorithms failed to correctly identify properties that hold.

Group 1 supports hyperrectangle input sets. Groups 2, 3, 4, and 6 support H-polytope input sets. Group 5 supports hyperrectangle input sets and networks with only one output node.

| Algorithm | small_nnet | mnist1 | mnist2 | mnist3 | mnist4 | acas |
|------------|-------------|-------------|-------------|------------|-------------|-------------|
| ExactReach | 0.004070968 | - | - | - | - | - |
| Ai2 | 0.005170172 | - | - | - | - | - |
| maxSens | 0.000201878 | 16.06772067 | 16.20866383 | 16.1892307 | 15.93491465 | 0.006839497 |

| Algorithm | small_nnet | mnist1 | mnist2 | mnist3 | mnist4 | acas |
|-----------|--------------|--------------|--------------|---------------|---------------|---------------|
| NSVerify | 0.000437805 | 0.561558217 | 1.23185184 | 0.234906589 | - | - |
| MIPVerify | 0.422803839 | 0.236930468 | 1.055669556 | 46.36556919 | - | - |
| ILP | 0.423599637 | 0.374052375 | 0.65545287 | 0.951015935* | 4.866014534* | 0.108586473* |
| convDual | 0.001725546 | 0.374052375 | 0.02184014 | 0.001638679 | 0.005836024 | 0.002674586 |
| Duality | 0.001336414* | 21.60260384* | 130.7149674* | 37.3058392* | 52.87126159* | 0.020148564* |
| FastLin | 2.088460281 | 0.477470278 | 0.002369427 | 0.007551539 | 0.01564011 | 0.166508046** |
| FastLip | 9.179938173 | 0.130989072 | 0.059900531 | 0.051348471** | 0.091895366** | 0.001703324** |
| MIPVerify | 9.940695891 | 0.256747563 | 1.23054911 | 46.77128226 | - | - |
| ILP | 0.347950783 | 0.367925285 | 0.665364297 | 0.890090777* | 4.664959506* | 0.00834114* |
| Planet | 0.000247003 | 0.211006714 | 0.301637916 | 0.186482861 | - | - |
| Reluplex | 0.012245108 | 125.0347088 | 62582.48883 | - | - | 2952.784643 |
| Reluval | 0.000031296 | 0.646829741 | 0.008979679 | 0.008030365 | 0.824760803* | 0.196084517* |

Table 2. Experimental results for group 1. All results are in seconds, missing entries correspond to experiments that timed-out. An asterisk indicates the result was :unknown and two asterisks indicate that the algorithm incorrectly returned :violated.

Table 3. Experimental results for groups 2, 3, 4 and 6. All results are in seconds, missing entries correspond to experiments that timed-out. An asterisk indicates the result was :unknown and two asterisks indicate that the algorithm incorrectly returned :violated.

| Algorithm | small_nnet | mnist1 | mnist2 | mnist3 | mnist4 | acas |
|-----------|-------------|-------------|-------------|---------------|---------------|---------------|
| Reluval | 0.096123516 | 0.104757137 | 0.082225486 | 0.019977288 | 0.021589774* | 0.000375971* |
| DLV | 0.145483368 | 0.055010885 | 0.7606918** | 0.203945542** | 3.426374089** | 0.450508522** |
| Sherlock | 0.150546186 | - | - | - | - | - |
| BaB | 0.160190662 | - | - | - | - | - |

Table 4. Experimental results for group 5. All results are in seconds, missing entries correspond to experiments that timed-out. An asterisk indicates the result was :unknown and two asterisks indicate that the algorithm incorrectly returned :violated.

10.3 Analysis

The experimental results shown in the previous section demonstrate the capability of the pedagogical implementation to verify realistic networks. Many of the algorithms are able to verify properties for networks as large as the ACAS Xu networks, which has been used for prior benchmarks [20], [40]. Overall we observed that algorithms that are complete take a longer time to run. Consequently, complete algorithms are more amenable, at least at this point and this implementation, to verifying properties of smaller networks. Algorithms that are not complete usually rely on over-approximations or other schemes that significantly reduce their computational cost. Incomplete algorithms are faster and can more easily be used to verify properties on larger networks.

In particular, for Group 1, we can observe in table 2 that ExactReach and Ai2 timed out for most of the properties. Currently, our implementations of this algorithms require the conversion of sets from H-representation to V-representation which is computationally expensive in general. For example, converting a 700-dimensional polytope is an unreasonable task to perform. The original implementations of these algorithms are better equipped to handle larger networks. In particular, Ai2 was specifically designed to avoid this task by using zonotopes, in the near future we will update our implementation to incorporate this better approach.

For Groups 2, 3, 4 and 6, we can observe in table 3 that NSVerify, MIPVerify, Planet and Reluplex timed out for some of the properties associated to larger networks, this result is not surprising as completeness comes at a high computational cost. It is worth noting that 1) many of the algorithms that are not complete were able to terminate in significantly shorter amounts of time compared to their complete counterparts, but 2) many of them (the ones marked with two asterisks) exhibited their in-completeness by returning :violated for properties that, in fact, hold. Other algorithms, particularly in Group 3, were unable to reach a conclusion and returned :unknown as a result.

Algorithms in Group 5, as shown in table 4, either terminated very quickly but produced either incorrect or inconclusive results (Reluval and DLV respectively) or timed out for most networks such as Sherlock and BaB. Sherlock and BaB try to compute the exact bounds on the output even if the bounds already lie outside of the output constraint, which can explain why they timed-out for most networks as other approaches only check if a counter example can be found, hence should stop much earlier than Sherlock and BaB converge to precise-enough bounds.

Finally, algorithms that rely on optimization are susceptible to numerical stability issues and we observed this in the case of MIPVerify and Planet.

11 Conclusion

This article surveyed algorithms for verification of deep neural networks. A unified mathematical framework was introduced to verify satisfiability of a neural network given certain

input and output constraints. Three basic verification methods were identified: reachability, optimization, and search. We classified existing methods into five induced categories according to their core methodologies, and pointed out the connections among them. In particular, we reviewed the following methods: 1) reachability methods: ExactReach, Ai2, and MaxSens; 2) primal optimization methods: NSVerify, MIPVerify, and ILP; 3) dual optimization methods: Duality, ConvDual, and Certify; 4) search and reachability methods: ReluVal, FastLin, FastLip, and DLV; and 5) search and optimization methods: Sherlock, BaB, Planet, and Reluplex. In the numerical experiments, we compare methods that either use similar methodologies or can solve the same problems. In general, there is a trade-off between completeness of a verification algorithm and its scalability. Complete algorithms run slower on larger networks, while incomplete algorithms are more conservative. Pedagogical implementations of all these methods were provided in Julia. The connections and differences among different methods were pointed out. This article can serve as a tutorial for students and professionals interested in this emerging field as well as a benchmark to facilitate the design of new verification algorithms.

Acknowledgments

This work is partially supported by the Center for Automotive Research at Stanford (CARS). The authors would like to thank many of the authors of the referenced papers for their help in clarifying their algorithms and reviewing early drafts of this survey: Weiming Xiang, Taylor Johnson, Hoang-Dung Tran, Martin Vechev, Gagandeep Singh, Alessio Lomuscio, Michael Akintunde, Osbert Bastani, Zico Kolter, Shiqi Wang, Huan Zhang, Xiaowei Huang, Rudy Bunel, Reudiger Ehlers, and Guy Katz. The authors would also like to thank Christian Schilling and Marcelo Forets, the authors of LazySets.jl, for their implementation support, as well as Amelia Hardy and Zongzhang Zhang for their comments.

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