Introduction to Deep Neural Network Verification

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Preface

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Neural Networks

1.1 Basics of Neural Networks

A *neural network* (**NN**) [23] consists of an input layer, multiple hidden layers, and an output layer. Each layer has a number of neurons, each connected to neurons in the next layer through a predefined set of weights (derived by training the network with data). A *Deep Neural Network* (**DNN**) is an NN with *two* or more hidden layers.

The output of an NN is obtained by iteratively computing the values of neurons in each layer. The value of a neuron in the input layer is the input data. The value of a neuron in the hidden layers is computed by applying an *affine transformation* (§1.2) to values of neurons in the previous layers, then followed by an *activation function* (§1.3) such as ReLU and Sigmoid. The value of a neuron in the output layer is computed similarly but may skip the activation function.

NN as a Function We can view an NN as a function that maps input vectors to output vectors:

$$f : \mathbb{R}^n \to \mathbb{R}^m \tag{1.1.1}$$

where n is the number of input neurons and m is the number of output neurons. The neurons in the input layer are the inputs to the function, and the neurons in the output layer are the outputs of the function. The neurons in the hidden layers are also functions that transform the inputs from the previous layer to produce outputs for the next layer.

Example 1.1.1. Fig. 1.1 shows an NN with two inputs $x_1, x_2 \in \mathbb{R}$, two hidden neurons x_3, x_4 in one hidden layer, and one output neuron x_5. The connections between the neurons are weighted edges, and the biases are shown below each neuron.

- The hidden neurons compute:

$$x_3 = \mathrm{ReLU}\left(-0.5x_1 + 0.5x_2 + 1.0\right), \quad x_4 = \mathrm{ReLU}\left(0.5x_1 + -0.5x_2 + -1.0\right),$$

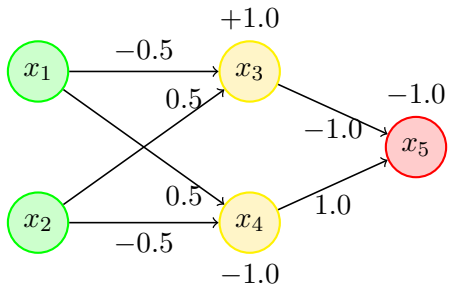


Figure 1.1: A simple DNN with two inputs x_1, x_2, two hidden neurons x_3, x_4, and one output neuron x_5.

where $\text{ReLU}(x) = \max(x, 0)$ is the ReLU activation function.

- The output neuron computes:

$$x_5 = -1.0 \cdot x_3 + 1.0 \cdot x_4 - 1.0.$$

Thus, this NN computes a function $f : \mathbb{R}^2 \to \mathbb{R}$ where:

$$f(x_1, x_2) = -\text{ReLU}(-0.5x_1 + 0.5x_2 + 1.0) + \text{ReLU}(0.5x_1 - 0.5x_2 - 1.0) - 1.0.$$

1.2 Affine Transformation

The affine transformation (AF) of a neuron consists of a *linear combination*—a weighted sum[1]—of its inputs, followed by the addition of a bias term. More specifically, for a neuron with weights $w_1, \ldots, w_n$, bias b, and inputs $v_1, \ldots, v_n$ from the previous layer, the AF computes:

$$f(v_1, v_2, \ldots, v_n) = \sum_{i=1}^{n} w_i v_i + b. \tag{1.2.1}$$

Example 1.2.1. In Fig. 1.1, neuron x_3 receives inputs x_1 and x_2 with weights -0.5, 0.5, and bias 1.0, so its AF is $x_3 = -0.5x_1 + 0.5x_2 + 1.0$.

1.3 Activation Functions

Popular activation functions used in NNs include ReLU, Sigmoid, Tanh, and Softmax. All of these are non-linear[2] functions that introduce non-linearity to the network, allowing it to learn complex patterns in the data.

[1] A weighted sum is a sum of the form $\sum_{i=1}^{n} w_i v_i$, where w_i are weights and v_i are variables or terms.

[2] Non-linear means that the output of the function is not a linear combination of its inputs.

Table 1.1: Summary of Common Neural Network Activation Functions

Name	Equation	Output Range	Key Use
ReLU	$\max(0, x)$	$[0, \infty)$	Hidden layers, fast train
Sigmoid	$\frac{1}{1+e^{-x}}$	$(0, 1)$	Binary classification
Tanh	$\tanh(x)$	$(-1, 1)$	Hidden layers, zero-centered
Softmax	$\frac{e^{x_i}}{\sum_j e^{x_j}}$	$(0, 1), \sum_i = 1$	Multi-class output

Tab. 1.1 summarizes the most common activation functions used in NNs, their equations, output ranges, and key uses.

1.3.1 ReLU (Rectified Linear Unit)

ReLU is a widely used activation function in NNs. It is defined as:

$$\text{ReLU}(x) = \max(0, x) = \begin{cases} 0 & \text{if } x \leq 0 \\ x & \text{if } x > 0 \end{cases}$$

ReLU is **piecewise linear** because it consists of two linear segments as shown as in Fig. 1.2: (i) a constant function (0) when $x \leq 0$, (ii) and (ii) a linear function (x) when $x > 0$. A ReLU activated neuron is said to be *active* if its input is greater than zero and *inactive* otherwise.

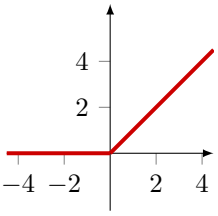


Figure 1.2: ReLU (Rectified Linear Unit) function.

Example 1.3.1. $\text{ReLU}(-1.2) = 0$ (inactive), $\text{ReLU}(0) = 0$ (inactive), and $\text{ReLU}(2.8) = 2.8$ (active).

Logical encoding ReLU can be encoded using the following logical formula:

$$y = \text{ReLU}(x) \iff (x \leq 0 \wedge y = 0) \vee (x > 0 \wedge y = x).$$

In other words, if $x \leq 0$, y must be zero; otherwise; otherwise, y must equal x.

Example 1.3.2. In Z3, we can declare ReLU using `If()`

```
import z3
def relu(x): return z3.If(x <= 0, 0, x)

relu(-1.2)  # returns 0
relu(0)     # returns 0
relu(2.8)   # returns 2.8
```

Nonlinear Property Despite being piecewise linear, ReLU is **nonlinear** because it does not satisfy the two core properties of a linear function

- *Additivity:* $\text{ReLU}(x+y) \neq \text{ReLU}(x) + \text{ReLU}(y)$ in general,
- *Homogeneity:* $\text{ReLU}(\alpha x) \neq \alpha \cdot \text{ReLU}(x)$ when $\alpha < 0$.

In simpler terms, ReLU is nonlinear because it does not form a straight line. It has a **kink** (a sharp bend) at $x = 0$, where the slope changes abruptly from 0 to 1. This discontinuity in the derivative prevents the function from being globally linear.

This non-linearity makes DNN verification difficult. In fact, verifying DNNs with ReLU has the NP-complete complexity as shown in §3.3. We will use ReLU throughout this book as the default activation function for hidden neurons in an NN.

1.3.2 Sigmoid

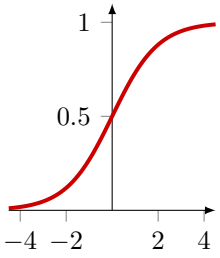


Figure 1.3: Sigmoid function.

Sigmoid, shown in Fig. 1.3, is a smooth—i.e., continuous and differentiable—non-linear activation function that maps any real value to the range (0,1). It is continuous, meaning that small changes in the input will result in small changes in the output, and differentiable, meaning that it has a well-defined derivative at every point. Sigmoid is often used in the output layer of a binary classification problem.

$$\text{sigmoid}\,(x) = \frac{1}{1+e^{-x}} \tag{1.3.1}$$

Example 1.3.3. $\text{sigmoid}\,(-1.2) \approx 0.23$, $\text{sigmoid}\,(0) = 0.5$, and $\text{sigmoid}\,(2.8) \approx 0.94$. This means that the sigmoid function maps -1.2 to a value close to 0, 0 to 0.5, and 2.8 to a value close to 1.

1.3.3 Hyperbolic Tangent (Tanh)

Tanh, shown in Fig. 1.4, is similar to sigmoid (§1.3.2) but maps any real value to the range (-1,1). It is often used in the output layer of a multi-class classification problem.

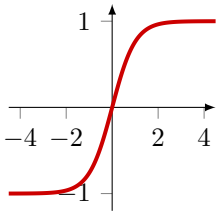


Figure 1.4: tanh (hyperbolic tangent) activation function.

$$\tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}} \tag{1.3.2}$$

Example 1.3.4. $\tanh(-1.2) \approx -0.83$, $\tanh(0) = 0$, and $\tanh(2.8) \approx 0.99$. This means that the tanh function maps -1.2 to a value close to -1, 0 to 0, and 2.8 to a value close to 1.

1.3.4 Softmax

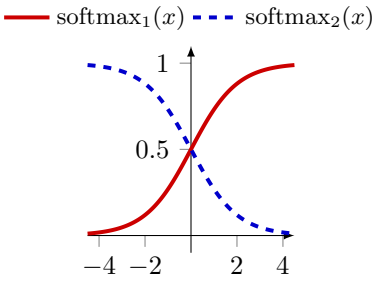


Figure 1.5: Softmax function for 2 classes.

Softmax, shown in Fig. 1.5, is a generalization of sigmoid (§1.3.2) that maps any real value to the range (0,1) and ensures that the sum of the output values is 1. It is often used in the output layer of a multi-class classification problem.

$$\text{softmax}\,(x)_i = \frac{e^{x_i}}{\sum_{j=1}^{n} e^{x_j}} \tag{1.3.3}$$

Example 1.3.5. For a vector $x = [2, 1, 0]$, softmax computes:

$$\begin{aligned}
\text{softmax}\,(x) &= \left[\frac{e^2}{e^2 + e^1 + e^0}, \frac{e^1}{e^2 + e^1 + e^0}, \frac{e^0}{e^2 + e^1 + e^0}\right] \\
&= \left[\frac{7.389}{7.389 + 2.718 + 1}, \frac{2.718}{7.389 + 2.718 + 1}, \frac{1}{7.389 + 2.718 + 1}\right] \\
&\approx [0.71, 0.24, 0.05]
\end{aligned}$$

This means that softmax maps the input vector x to a probability distribution over the three classes, where the first class has a probability of 0.71, the second class has a probability of 0.24, and the third class has a probability of 0.05.

Example 1.3.6. Use Z3 to encode the DNN in Fig. 1.1 and compute its output $x5$ for the input $(x_1, x_2) = (2.0, 0.5)$.

```
import z3

#setup the network
x1 = z3.Real('x1')
x2 = z3.Real('x2')
x3 = -0.5*x1 + 0.5*x2 + 1.0
x3_ = z3.If(x3 <= 0, 0, x3)  # ReLU
x4 = 0.5*x1 + -0.5*x2 + -1.0
x4_ = z3.If(x4 <= 0, 0, x4)  # ReLU
x5 = -1.0*x3_ + 1.0*x4_ - 1.0

#check output on given input
s = z3.Solver()
s.add(x1 == 2.0, x2 == 0.5)
if s.check() == z3.sat:
    m = s.model()
    print("Output x5 is ", m.evaluate(x5))
```

1.4 Neural Network Architectures and Layers

NNs vary in architecture depending on how information flows through them and how computations are structured. Most common models are variations of the *feed-forward network*, with additional structures or constraints layered on top. Tab. 1.2 summarizes several common NN architectures and their typical application domains.

Table 1.2: Popular NN Architectures and Applications

Name	Acronym	Typical Applications
Feedforward NN	FNN / MLP	General function approximation, tabular data
Convolutional NN	CNN	Image processing, video analysis
Residual NN	ResNet	Deep image recognition, medical imaging
Recurrent NN	RNN	Sequence modeling, NLP, time series
Transformer	–	NLP, summarization, code generation, vision
Graph NN	GNN	Graph-structured data, molecule modeling, recommendation

1.4.1 Feedforward Neural Networks (FNNs)

In an FNN, information flows in one direction: from the input layer, through one or more hidden layers, and finally to the output layer. There are no loops or cycles in the computation graph.

Widely used feedforward architectures include fully connected, convolutional, and residual networks. Each architecture has its own strengths and is suited for different types of tasks.

Fully Connected NNs (FCNs) In FCNs, each neuron in a layer is connected to every neuron in the next layer. Thus, every neuron in the input layer is connected to every neuron in the first hidden layer, every neuron in the first hidden layer is connected to every neuron in the second hidden layer, and so on, until the output layer. Fully connected NNs, sometimes called *dense networks*, are the most basic type of FNNs and are commonly used for tasks like classification.

Example 1.4.1. Fig. 1.1 earlier is an FCN with two inputs and one hidden layer with two neurons, and one output neuron. Fig. 1.6 below shows an FCN with four inputs, two hidden layers with five neurons each, and three output neurons (weights and biases not shown for simplicity).

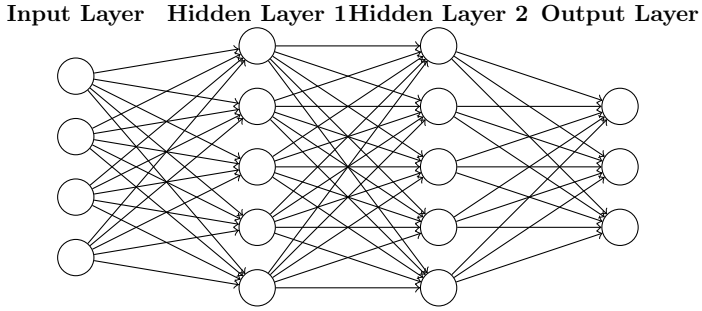


Figure 1.6: A fully connected NN with two hidden layers.

Example 1.4.2 (Classifier)**.** A common use case for FCNs is classification. They take an input, e.g., pixels of an image, and predict what the image is (e.g., cat, dog, car). The output layer represents the probabilities of each class (e.g., y_1 is the probability of cat, y_2 is the probability of dog). Moreover, the outputs are often passed through a softmax activation function (§1.3.4) to convert them into probabilities that sum to 1, and the class with the highest probability is chosen as the predicted label.

Convolutional NNs (CNNs) CNNs replace fully connected layers with *convolutional layers*, which apply local filters across the input space. In CNNs, each neuron receives several inputs, takes a weighted sum over them, passes it through an activation function, and responds with an output. CNNs are commonly used in computer vision and image processing. Despite their local structure, CNNs remain feedforward: data flows forward without cycles.

Example 1.4.3. Fig. 1.7 shows a simple CNN with four inputs, three hidden neurons, and three outputs. Given an input vector $\mathbf{x} = [x_1, x_2, x_3, x_4]$, the computation

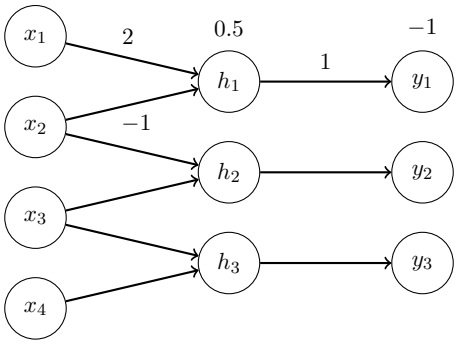


Figure 1.7: 1-dimensional CNN

of the first output proceeds as follows. The first hidden unit forms a linear combination of its inputs as $h_1 = 2x_1 - x_2 + 0.5$. This value is then passed through the ReLU activation function, resulting in $\hat{h}_1 = \text{ReLU}(h_1) = \max(0, 2x_1 - x_2 + 0.5)$. Finally, the first output is simply $y_1 = \hat{h}_1 - 1$.

Residual Networks (ResNets) Resnets extend FNNs by adding *skip connections*—direct links that bypass one or more layers. Resnets are often used in image recognition and classification.

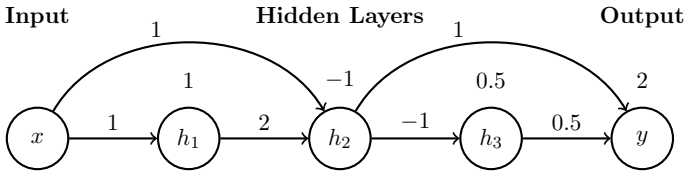


Figure 1.8: ResNet block with weights on all connections and biases above nodes. Each node is labeled and typical ReLU is applied after each hidden sum.

Example 1.4.4. Fig. 1.8 shows an example of a Resnet. Assume the input x and each node applies the ReLU activation. With the weights and biases shown in the diagram, the outputs are computed as follows:

$$h_1 = \text{ReLU}(x + 1) \quad h_2 = \text{ReLU}(2h_1 + x - 1)$$
$$h_3 = \text{ReLU}(-h_2 + 0.5) \quad y = 0.5h_3 + h_2 + 2$$

1.4.2 Other NN Architectures

Not all NNs are feedforward. Some architectures introduce cycles, dynamic connections, or non-Euclidean[3] data structures (e.g., graphs).

[3]Euclidean data refers to data that can be represented in a flat, two-dimensional space, such as images.

1.4.2.1 Recurrent Neural Networks (RNNs)

RNNs, often used in natural language processing (NLP) and speech recognition, are designed to recognize patterns in sequences of data. RNNs have *loops* in them, allowing information to be sent forward and backward.

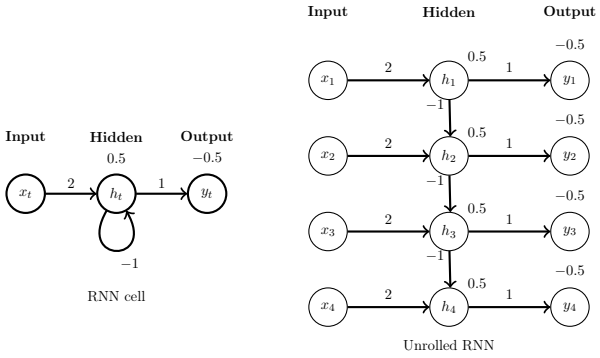


Figure 1.9: RNN cell (left) and unrolled RNN sequence structure (right). Weights on connections; biases above hidden and output nodes.

Example 1.4.5. Fig. 1.9 shows a simple RNN cell. Assume the input sequence is $\mathbf{x} = [x_1, x_2, x_3, x_4]$, and the initial hidden state is h_0. For the first time step, the hidden state is computed as $h_1 = \text{ReLU}\,(2x_1 - h_0 + 0.5)$, and the output is $y_1 = h_1 - 0.5$. For the second time step, the hidden state is $h_2 = \text{ReLU}\,(2x_2 - h_1 + 0.5)$, and the output is $y_2 = h_2 - 0.5$.

1.4.2.2 Transformers

Transformers are designed for long-range dependencies using *self-attention* rather than recurrence. They dominate applications in natural language processing and are increasingly used in vision and reinforcement learning.

1.4.2.3 Graph Neural Networks (GNNs)

operate on graphs, allowing each node to aggregate information from its neighbors. GNNs are used in applications involving structured data like molecules or social networks.

1.5 ONNX: Modelling Neural Networks

ONNX (Open Neural Network Exchange) [38] is an open source and widely adopted standard for representing neural networks. It provides a common format for representing the structure and parameters of neural networks, enabling interoperability between different ML frameworks and tools.

ONNX operators that cover most sequential feedforward networks include:

- `Add, Sub, Gemm, MatMul`: basic arithmetic and matrix operations.
- `ReLU, Sigmoid, SoftMax`: activation functions.
- `AveragePool, MaxPool, Flatten, Reshape`: tensor manipulation.
- `Conv, BatchNormalization, LRN`: CNN layers and normalizations.
- `Concat, Dropout, Unsqueeze`: tensor operations.

Example 1.5.1. For the network in Fig. 1.1, the ONNX representation would include:

- Input: x_1, x_2.
- Hidden layer: $x_3 = \text{ReLU}(-0.5x_1 + 0.5x_2 + 1.0)$, $x_4 = \text{ReLU}(0.5x_1 - 0.5x_2 + 1.0)$.
- Output: $x_5 = -x_3 + x_4 - 1$.

The ONNX representation would look like:

```
ir_version: 9
opset_import { version: 13 }
graph example_nn {
  input: "x"
  output: "x5"

  node { op_type: "Gemm" input: "x" input: "W1" input: "b1" output: "h1" }   # -0.5*x1+0.5*x2+1
  node { op_type: "Relu" input: "h1" output: "x3" }

  node { op_type: "Gemm" input: "x" input: "W2" input: "b2" output: "h2" }   # 0.5*x1-0.5*x2+1
  node { op_type: "Relu" input: "h2" output: "x4" }

  node { op_type: "Neg" input: "x3" output: "nx3" }
  node { op_type: "Add" input: "nx3" input: "x4" output: "s1" }
  node { op_type: "Add" input: "s1" input: "c_minus_1" output: "x5" }

  initializer { name: "W1" values: [-0.5, 0.5] }
  initializer { name: "b1" values: [1.0] }
  initializer { name: "W2" values: [0.5, -0.5] }
  initializer { name: "b2" values: [1.0] }
  initializer { name: "c_minus_1" values: [-1.0] }
}
```

Chapter 2

Properties

Similar to software programs, neural networks (NNs) have desirable properties to ensure the network behaves as expected. These could be specific to the applications modeled by the network, e.g., safety properties for a network modelling a collision avoidance system, or general properties that are desired by all networks, e.g., robustness to small perturbations in the input data.

Below we will discuss properties that are relevant to the verification of NNs. Specifically, these properties can be expressed in a formal language supported by a DNN verifier. Additional properties can be found in the literature [41].

2.1 Definition

As described in §1 NNs define functions of the form $f : \mathbb{R}^n \to \mathbb{R}^m$, where n is the dimension of the input and m is the dimension of the output. Thus, the properties or specifications of an NN—similarly to properties of software program—are defined in terms of its input and output:

> *For any input $x \in \mathbb{R}^n$ satisfying a precondition P, the neural network should produce an output $f(x) \in \mathbb{R}^m$ that satisfies a postcondition Q.*

This says that if the input x satisfies the precondition P, then the output $f(x)$ should satisfy the postcondition Q.

2.2 Common Properties in Neural Networks

We now define some commonly studied properties in NNs verification.

2.2.1 Robustness

Robustness ensures that small changes in the input do not drastically change the output. This is a desirable property for all neural networks, especially classifiers,

where we want to ensure that similar inputs yield similar outputs. For example, a slightly blurred image of a red light should still be classified as a red light.

There are two types of robustness properties: *local* (robustness around a chosen point) and *global* (robustness everywhere).

Local Robustness A neural network f is ϵ-locally-robust at point x with respect to norm $\|\cdot\|$ if

$$\forall x', \qquad \|x - x'\| \leq \epsilon \implies f(x) = f(x'). \tag{2.2.1}$$

where $\|x - x'\| \leq \epsilon$ indicates that the difference between the two points is within a certain (small) threshold ϵ.

Thus local robustness says that a network is robust if all nearby inputs x' (within radius ϵ) are classified the same as x. In other words, no small perturbation around this specific point x will fool the classifier."

Local robustness is what most adversarial robustness papers mean, e.g., checking whether an image of a cat is still classified as a cat under small pixel noise.

Example 2.2.1 (Local Robustness: Image Classification)**.** Consider a neural network f that classifies images into different categories (e.g., dog, cat, etc.). A robustness property requires that if an input image c is classified as a dog, then any perturbed image x that is visually similar to c should also be classified as a dog. This can be expressed as:

$$\forall x, \qquad \|c - x\| \leq \epsilon \implies f(x) = f(c)$$

Global Robustness A neural network f is ϵ-globally-robust with respect to norm $\|\cdot\|$ if

$$\forall x_1, x_2, \qquad \|x_1 - x_2\| \leq \epsilon \implies f(x_1) = f(x_2). \tag{2.2.2}$$

This says the property must hold for all pairs of inputs in the domain: whenever two points are within ϵ of each other, they must share the same label.

Global robustness is a very strong definition, and in practice, almost impossible unless the network is trivial (e.g., outputs the same label everywhere).

Problem 2.2.1. Suppose that an network classifies an input image x as digit 7. We want to ensure that if the image is slightly perturbed (e.g., brightness changed by a small amount ϵ), the network still outputs 7.

2.2.2 Safety

Safety properties ensure that the network conforms to certain safety constraints. This is particularly important in safety-critical applications, such as autonomous vehicles or medical diagnosis systems, where incorrect outputs can lead to catastrophic consequences.

Problem 2.2.2 (Collision Avoidance System)**.** A safety property in a collision avoidance system such as an autonomous vehicle might be that if the intruder is distant and significantly slower than us, then we stay below a certain velocity threshold. Formally, this can be expressed as:

$$d_{intruder} > d_{threshold} \land v_{intruder} < v_{threshold} \implies v_{us} < v_{threshold},$$

where $d_{intruder}$ is the distance to the intruder, $d_{threshold}$ is a predefined safe distance, $v_{intruder}$ is the speed of the intruder, and v_{us} is our speed.

Unlike robustness properties, which are often desirable in all networks, safety properties are often *specific* to the application domain. For example, a safety property for an autonomous vehicle may not be relevant for a surgical robot.

Problem 2.2.3 (Safety: Self-Driving Car)**.** A network controlling a self-driving car on a highway might require that: If the car in front is at least 160 meters away and moving slower than us, then we should not accelerate.

2.3 Other properties

2.3.1 Consistency

Consistency requires that a NN behaves consistently when given semantically equivalent or related inputs.

Example 2.3.1 (Logical Consistency in LLMs)**.** Consider queries q_1, q_2, and q_3 about a person's age:

$$q_1 : \text{``How old is person X?''}$$

$$q_2 : \text{``What year was X born if they are currently Y years old?''}$$

$$q_3 : \text{``Will X be Z years old in 2025?''}$$

Thus, if the LLM outputs age Y for q_1, then q_2 should output $\texttt{current\_year} - Y$, and the answer to q_3 should be logically consistent with the stated age. This prevents scenarios where an LLM claims someone is 30 years old but was born in 1985 when the current year is 2024.

2.3.2 Monotonicity

Monotonicity ensures that the NN maintains a consistent ordering relationship between inputs and outputs: an increase in certain input features always leads to a non-decreasing output value. This property is important in applications where domain knowledge dictates logical ordering constraints, such as fairness-aware systems, medical diagnosis, and scientific applications where physical laws impose natural ordering relationships.

Example 2.3.2 (Fairness)**.** A network modelling the probability of admission to a university should be monotonically non-decreasing with respect to GPA and test scores, regardless of gender. Formally, for applicants with profiles (p, s, g) and (p', s', g') where p, p' are GPAs, s, s' are test scores, and g, g' are gender indicators:

$$p \leq p' \land s = s' \land g \neq g' \implies f(p, s, g) \leq f(p', s', g'),$$

$$s \leq s' \land p = p' \land g \neq g' \implies f(p, s, g) \leq f(p, s', g'),$$

where f is the neural network computing admission probability. Additionally, for fairness:

$$f(p, s, \text{male}) = f(p, s, \text{female}) \text{ for all } p, s,$$

ensuring that applicants with identical academic qualifications receive the same treatment regardless of gender.

2.4 Counterexamples

A *counterexample* (**cex**) is a witness that falsifies the correctness property. Given the property defined in §2.1, a counterexample is an input x that satisfies the precondition P but produces an output $f(x)$ that violates the postcondition Q.

Example 2.4.1 (Counterexample to Robustness Property)**.** For local robustness property (§2.2.1):

$$f(x) \neq f(x') \land \|x - x'\| \leq \epsilon \implies x' \text{ is a counterexample.}$$

The goal of DNN verification (§3.1) is to either prove that a property holds—no cex exist—or find a cex that violates the property.

Example 2.4.2 (Counterexample: Monotonicity in Admission)**.** A network predicts admission probability to a university. Inputs: GPA p and test score s.

We want: a higher GPA with same score should not decrease admission probability.

But we observe a case violating this:

- A: GPA = 3.0, score = 1500, prediction = 0.8
- B: GPA = 3.5, score = 1500, prediction = 0.6

Using the numbers in this violating case, write the monotonicity requirement and show how this is a counterexample.

Monotonicity requirement:

$$p \leq p' \land s = s' \implies f(p, s) \leq f(p', s')$$

Counterexample:

$$3.0 \leq 3.5 \land 1500 = 1500 \quad \text{but} \quad f(3.0, 1500) = 0.8 > f(3.5, 1500) = 0.6$$

2.5 The VNN-LIB Specification Language

The VNN-LIB standard [16, 44] defines a format to describe neural networks and properties. Such a standard format enables the sharing of benchmarks across different tools and platforms, facilitating evaluations and comparisons of their performance. VNN-COMP [8] uses VNN-LIB to evaluate different neural network verification tools.

Specifically, VNN-LIB defines a common format for the following components:

- **Neural Network (or model) representation** in the ONNX format [38].
- **Property specification** in SMT-LIB format [4].

2.5.1 VNN-LIB: Property Specification Language

Verification tasks involve proving that the output of a network remains within some desired post-condition Σ, given inputs within a bounded set Π.

Formal Specification Let $\nu : D^{n_1 \times \cdots \times n_h} \to D^{m_1 \times \cdots \times m_k}$ be a neural network, and x and y its input and output tensors. A property is expressed as:

$$\forall x \in \Pi \to \nu(x) \in \Sigma$$

This includes:

- **Precondition** Π: constraints on inputs.
- **Postcondition** Σ: required properties of outputs.

Properties are encoded in **SMT-LIB2**, referencing input/output variable names consistent with ONNX.

Example 2.5.1. A typical ACAS XU network (§13.1.1) maps 5D input to 5D output via 6 layers of 50 ReLU neurons. A property is of the network is

$$-\varepsilon_i \leq x_i \leq \varepsilon_i \quad (0 \leq i < 5)$$

$$y_0 \leq y_1, \quad y_0 \leq y_2, \quad y_0 \leq y_3, \quad y_0 \leq y_4,$$

where x_i are the input variables, y_i are the output variables, and ε_i are small perturbation bounds for each input dimension. This property states that if the inputs are perturbed within the bounds ε_i, then the first output neuron y_0 is less than or equal to all other output neurons y_1, y_2, y_3, y_4.

The VNN-LIB code for this property is as follows:

```
; declaring the input variables
(declare-const X_0 Real)
(declare-const X_1 Real)
(declare-const X_2 Real)
(declare-const X_3 Real)
(declare-const X_4 Real)
(declare-const X_5 Real)
; declaring neuron outputs
(declare-const Y_0 Real)
(declare-const Y_1 Real)
(declare-const Y_2 Real)
(declare-const Y_3 Real)
(declare-const Y_4 Real)
; asserting the input relations
(assert (<= X_0 eps0))
(assert (>= X_0 -eps0))
(assert (<= X_1 eps1))
(assert (>= X_1 -eps1))
(assert (<= X_2 eps2))
(assert (>= X_2 -eps2))
(assert (<= X_3 eps3))
(assert (>= X_3 -eps3))
(assert (<= X_4 eps4))
(assert (>= X_4 -eps4))
; asserting the output relations
(assert (<= Y_0 Y_1))
(assert (<= Y_0 Y_2))
(assert (<= Y_0 Y_3))
(assert (<= Y_0 Y_4))
```

2.6 Problems

Problem 2.6.1 (Robustness + Safety: Drone Controller)**.** An autonomous drone computes its thrust level using a network controller $f(w, d)$, where w is winds speed and d the distance to nearest obstacle. We want two properties:

1. Robustness: If the wind speed reading changes by at most 1 unit ($|w - w'| \leq 1$) and distance remains the same, the thrust decision should remain the same.

2. Safety: If the obstacle distance is less than 5 meters, then thrust must not be greater than 2.

Problem 2.6.2 (Global Consistency: Celsius and Fahrenheit)**.** An NN answers two related questions: Q1: "What is the temperature in Celsius?" (input t_C) Q2: "What is the temperature in Fahrenheit?" (input t_F)

We want consistency: If Q1 outputs y, then Q2 must output $1.8y + 32$.

Problem 2.6.3 (Counterexample: Safety in Vehicles)**.** A NN computes car acceleration a. We want a safety property: if distance to obstacle $d < 10$, then $a \leq 0$. But we observe a scenario where $d = 5$ but $a = +2$.

Write the safety requirement and show how this is a counterexample.

Problem 2.6.4. Consider the NN in Fig. 2.1. Note that in this network the hidden neurons $(v_1 \dots v_4)$ use ReLU activation, but the output neurons (y_1, y_2) just use affine transformation.

- Encode this network using Z3.
  - Try to use Z3 to evaluate the network on various inputs.
- Come up with **three** properties that this network *does not* have. Recall that a property often has the form in §2.1.

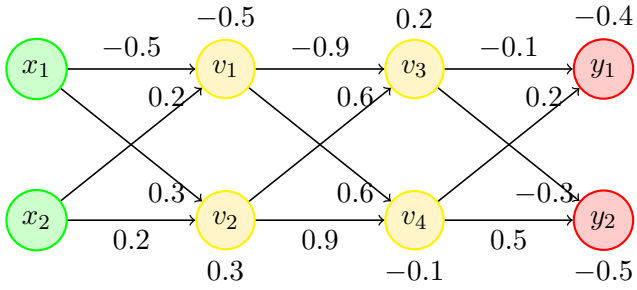


Figure 2.1: A simple NN with 2 inputs, 4 hidden ReLU neurons, and 2 outputs.

  - Argue why each property does not hold by providing a counterexample (§2.4).
  - (Optional, Easy) Try to use Z3 to show that the properties you came up with do not hold by asking Z3 to find counterexamples (one for each property).

- Come up with **three** properties that that this network has (i.e., as long as the precondition holds, the postcondition holds).
  - Argue why each property always holds (e.g., for any input satisfying the range X, the first layer outputs values in range Y, etc).
  - (Optional, A bit harder) Try to use Z3 to show that the properties you came up will always hold by asking Z3 to prove that no counterexample exists (i.e., `unsat`).

Chapter 3

Verification of Neural Networks

This chapter discusses the problem of verifying neural networks, i.e., checking if a given property holds for a neural network. We define the NN verification (NNV) problem in §3.1 and its satisfiability formulation, which is commonly used by DNN verifiers.

3.1 The Neural Network Verification (NNV) Problem

Definition 3.1.1 (NNV)**.** Given a DNN N and a property ϕ, the *NN verification* (NNV) problem asks if ϕ is a valid property[1] of N.

Typically, ϕ is a formula of the form

$$\phi_{in} \Rightarrow \phi_{out},$$

where ϕ_{in} is the *precondition*, i.e., a condition over the inputs of N, and ϕ_{out} is the *postcondition*, i.e., a condition over the outputs of N.

A DNN verifier attempts to find a *counterexample* input to N that satisfies ϕ_{in} but violates ϕ_{out}. If no such counterexample exists, ϕ is a valid property of N. Otherwise, ϕ is not valid and the counterexample can be used to retrain or debug the DNN [25].

Example 3.1.1 (Safety Property for Collision Avoidance System)**.** In Prob. 2.2.2, we defined a safety property (§2.2.2) for a collision avoidance system:

$$d_{intruder} > d_{threshold} \wedge v_{intruder} < v_{threshold} \implies v_{us} < v_{threshold},$$

where $d_{intruder}$ is the distance to the intruder, $d_{threshold}$ is a predefined safe distance, $v_{intruder}$ is the speed of the intruder, and v_{us} is our speed.

Here, the precondition is

$$\phi_{in} = d_{intruder} > d_{threshold} \wedge v_{intruder} < v_{threshold},$$

[1] §2 provides various examples of properties.

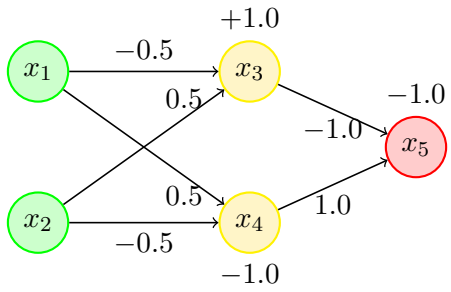


Figure 3.1: A simple DNN (similar to Fig. 1.1).

and the postcondition is

$$\phi_{out} = v_{us} < v_{threshold}.$$

Example 3.1.2. For the DNN in Fig. 3.1 a *valid* property is that the output is $x_5 \leq 0$ for any inputs $x_1 \in [-1, 1], x_2 \in [-2, 2]$.

An *invalid* property is that $x_5 > 0$ for those similar inputs. A counterexample showing this property violation is $\{x_1 = -1, x_2 = 2\}$, from which the network evaluates to $x_5 = -3.5$.

3.2 Satisfiability Formulation and Checking

As with traditional software verification, DNN verification is often represented as a satisfiability problem, which can be solved using an SMT solver (e.g., Z3 [14]) or a MILP solver (e.g., Gurobi [24]).

Formulation To formulate the problem, we first define a formula α to represent the network. Typically α is a conjunction ($\bigwedge$) of constraints representing the affine transformation (§1.2) and activation function (§1.3) of each neuron in the network. For example, for a fully-connected neural network (§1.4.1) with L layers, N ReLU neurons per layer, this formula is:

$$\alpha = \bigwedge_{\substack{i\in[1,L]\\ j\in[1,N]}} v_{i,j} \equiv \text{ReLU}\left(\sum_{k\in[1,N]} (w_{i-1,j,k} \cdot v_{i-1,j}) + b_{i,j}\right) \tag{3.2.1}$$

where $v_{i,j}$ is the output of the j-th neuron in layer i, $w_{i-1,j,k}$ is the weight connecting the k-th neuron in layer $i-1$ to the j-th neuron in layer i, and $b_{i,j}$ is the bias of the j-th neuron in layer i. The input layer is layer 0, i.e., $v_{0,j}$ are the input variables.

With this the NNV problem (Def. 3.1.1) can be formulated as checking the validity of the following formula:

$$\alpha \implies (\phi_{in} \implies \phi_{out}). \tag{3.2.2}$$

Formula Eq. 3.2.2 checks if network N satisfies (implies) the property $\phi_{in} \implies \phi_{out}$. This validity checking can be reduced to checking the satisfiability of the formula:

$$\alpha \wedge \phi_{in} \wedge \neg\phi_{out} \tag{3.2.3}$$

If Eq. 3.2.3 is unsatisfiable, then ϕ is a valid property of N. Otherwise, ϕ is not valid. Moreover, we can extract a counterexample for the original problem from the satisfying assignment of Eq. 3.2.3.

Problem 3.2.1. Let α represent our network and the robustness property $|x - x| \leq \epsilon \implies f(x) = f(y)$. Form the satisfiability formula (Eq. 3.2.3) that we need to check. Check them using Z3.

Problem 3.2.2. Let α represent our network and the property $y > 0$ for any input $x_1 \in [r_1, r_2], x_2 \in [r_3, r_4]$. Form the satisfiability formula (Eq. 3.2.3) that we need to check. Check them using Z3.

Problem 3.2.3 (Validity Formulation)**.** Show that $\alpha \implies (\phi_{in} \implies \phi_{out})$ (Eq. 3.2.2) is valid if and only if $\alpha \wedge \phi_{in} \wedge \neg\phi_{out}$ (Eq. 3.2.3) is unsatisfiable. First, do this by hand by explicitly writing out the logical equivalences step by step. Then, verify your result using Z3, i.e., show that the negation of the first formula is equivalent to the second formula.

Example 3.2.1. We represent the network in Fig. 3.1 as a formula α:

$$\begin{aligned} x_3 &= \text{ReLU}\left(-0.5x_1 + 0.5x_2 + 1.0\right) \ \wedge \\ x_4 &= \text{ReLU}\left(0.5x_1 - 0.5x_2 - 1.0\right) \ \wedge \\ x_5 &= -x_3 + x_4 - 1.0, \end{aligned}$$

and the property $x_5 > 0$ for any inputs $x_1 \in [-1, 1], x_2 \in [-2, 2]$ as:

$$\phi_{in} = (-1 \leq x_1 \leq 1) \wedge (-2 \leq x_2 \leq 2); \qquad \phi_{out} = (x_5 > 0)$$

Satisfiability Solving We can check the satisfiability of $\alpha \wedge \phi_{in} \wedge \neg\phi_{out}$ using constraint solving. §4.1 shows how to perform symbolic execution and an SMT solver (e.g., Z3) to automatically generate this formula from a given DNN and property, and check its satisfiability. §4.2 shows how to encode the problem as a MILP constraints, solvable using a MILP solver (e.g., Gurobi).

In this case, the formula is satisfiable, i.e., the property is invalid, and the solver returns `sat`. Any satisfying assignment, e.g., $x_1 = -1$ and $x_2 = 2$, is a counterexample (§2.4) to the property, as it satisfies the precondition ϕ_{in} but violates the postcondition ϕ_{out}, i.e., $x_5 = -3.5$, which is < 0.

Problem 3.2.4. Use Z3 to do Ex. 3.2.1. You might find Ex. 1.3.6 useful. Make sure that you also ask Z3 to find a counterexample violating the property (does not have to be the same as above).

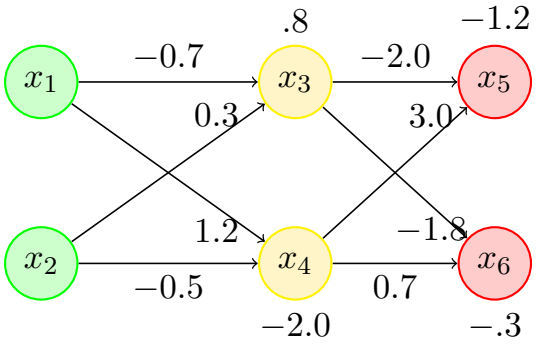


Figure 3.2: A simple DNN with 2 inputs, 2 hidden ReLU neurons, and 2 outputs.

Problem 3.2.5. Consider the DNN in Fig. 3.2. Do the following:

- Write the formula α representing the network.
- Create the property ϕ that the output $x_5 \geq x_6$ for any inputs $x_1 \in [-1, 1], x_2 \in [-1, 1]$.
- Generate the satisfiability formula (Eq. 3.2.3). DO NOT use Z3 to check it.

3.3 Complexity

ReLU-based NNV is NP-complete as shown in [26,40] by reducing the 3-SAT problem to it. This means that the problem of checking whether a given ReLu-based DNN satisfies a property is computationally hard, and no polynomial-time algorithm is known to solve it in the general case.

Part II

Constraint Solving and Abstraction

Chapter 4

Constraint Solving

4.1 Symbolic Execution and SMT Solving

As described in §3.2 the Neural Network Verification (NNV) problem can be represented as a satisfiability problem. Specifically, we encode the network as a logical formula, and use a constraint solver to check that formula satisfies the property of interest.

A straightforward and automated way to do this encoding is using *symbolic execution* (SE) [2, 29], a well-known software testing technique for finding bugs. SE executes a program on symbolic inputs, i.e., inputs represented as symbols rather than concrete values, and tracks the reachability of program state as symbolic expressions, i.e., logical formulae over symbolic inputs. The satisfiability of these formulae is then checked using an SMT solver, and satisfying assignments represent inputs leading to the undesirable (buggy) program state.

4.1.1 Symbolic Execution

We can adapt traditional SE to our problem by treating the DNN as a program and neurons as variables and executing the DNN on symbolic inputs. Affine transformations can easily be represented as logical formulae because they are linear functions. Activation functions such as ReLUs are translated to disjunctions of linear functions or if-then-else statements, i.e., $\text{ReLU}\,(x) \;=\; \max(x, 0) \;=\; x \geq 0 \wedge x \vee 0 \wedge \neg x$.

Example 4.1.1. To create a logical formula representing the DNN in Fig. 4.1, we can symbolically execute the DNN on symbolic inputs x_1, x_2 and track the values of the neurons x_3, x_4, x_5 as a set (conjunction) of logical formulae. SE starts with the inputs x_1 and x_2 and computes the values of the neurons in the hidden layer, x_3 and x_4, using the affine transformations, followed by ReLUs. Finally, SE computes the output neuron x_5 as a linear combination of the hidden layer neurons.

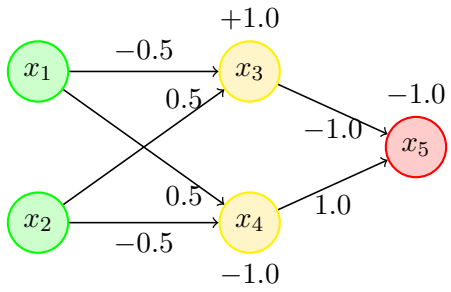


Figure 4.1: A simple DNN (similar to Fig. 1.1).

$$
\begin{aligned}
x_5 &= -x_3 + x_4 - 1.0 \wedge \\
x_3 &= \max(-0.5x_1 + 0.5x_2 + 1.0, 0) \wedge \\
x_4 &= \max(0.5x_1 - 0.5x_2 - 1.0, 0)
\end{aligned} \tag{4.1.1}
$$

4.1.2 SMT Solving

After obtaining the symbolic representation of the DNN, we can use an SMT solver [4] to check the satisfiability of the formula $\alpha \wedge \phi_{in} \wedge \neg\phi_{out}$, where α is the symbolic representation of the DNN, ϕ_{in} is the precondition on the inputs, and ϕ_{out} is the postcondition on the outputs. The solver checks if there exists an assignment to the symbolic inputs that satisfies the formula. If such an assignment exists, it means that the property is violated, and we can extract a counterexample from the satisfying assignment. Otherwise, if no such assignment exists, the property is valid

Example 4.1.2. To check that the DNN in Fig. 4.1 satisfies the property $x_5 > 0$ for any inputs $x_1 \in [-1, 1], x_2 \in [-2, 2]$ (Ex. 3.2.1), represented as:

$$\phi_{in} = (x_1 \geq -1) \wedge (x_1 \leq 1) \wedge (x_2 \geq -2) \wedge (x_2 \leq 2); \quad \phi_{out} = (x_5 > 0)$$

We check the satisfiability of $\alpha \wedge \phi_{in} \wedge \neg\phi_{out}$:

$$
\begin{aligned}
x_5 &= -x_3 + x_4 - 1.0 \wedge \\
x_3 &= \max(-0.5x_1 + 0.5x_2 + 1.0, 0) \wedge \\
x_4 &= \max(0.5x_1 - 0.5x_2 - 1.0, 0) \wedge \\
&\quad (x_1 \geq -1) \wedge (x_1 \leq 1) \wedge (x_2 \geq -2) \wedge (x_2 \leq 2) \quad \wedge (x_5 \leq 0)
\end{aligned}
$$

In this case, the SMT solver returns `sat` and a satisfying assignment, e.g., $x_1 = -1$ and $x_2 = 2$, which is a counterexample to the property. This means that for these inputs, the output $x_5 = -3.5$ violates the property $x_5 > 0$.

4.1.3 Limitations

While using symbolic execution and SMT solving is a straightforward way to verify DNNs, it has several practical limitations:

- **Path Explosion and Scalability**: the number of paths that the solver has to analyze can grow exponentially with the number of ReLU-based neurons and layers as each ReLU, represented as a disjunction of linear functions, has two possible outputs for any input (i.e., the input value itself or 0). This leads to the notorious *path explosion* problem and becoming intractable for large DNNs. Programming assignment 1 (§B.1) demonstrates this issue.
- **Non-linearity:** Other non-linear activation functions (§1.3), such as Sigmoid or Tanh, might not be easily representable as disjunctions of linear functions as ReLU. This can lead to complex formulae that are hard to reason about and/or result in a large search space for the SMT solver.
- **Precision Issues:** SMT solvers may struggle with precision issues when dealing with floating-point arithmetic, which is common in DNNs. This can lead to incorrect results or false positives/negatives in the verification process.

For these reasons, SMT solving is mostly used on toy examples, e.g., in a classroom setting. Modern-based DNN verification tools do not use SMT solving, and instead, rely on more efficient techniques such as abstraction (§5).

4.2 MILP

Instead of using SMT solving, we can encode the NNV problem as a Mixed Integer Linear Programming (MILP) constraints (§C.1), and then invoke an MILP solver such as Gurobi [24] to check their *feasibility* or satisfiability (§C.3.1).

4.2.1 ReLU Encoding

We first encode non-linear activation functions like ReLU using *binary indicator* variables and linear constraints. For each neuron, we introduce a binary variable (§C.2.1) that indicates whether the neuron is "active" (output equals input) or "inactive" (output is zero). This transforms the non-linear $\max(z, 0)$ operation into a set of linear inequalities controlled by the binary variable. We define

- z: the pre-activation value, i.e., the value that goes into ReLU
- $\hat{z}$: the post-activation value, i.e., the output of ReLU
- $a \in \{0, 1\}$: a binary indicator variable encoding whether the neuron is active ($z \geq 0$) or inactive ($z < 0$)

- l, u: lower and upper bounds on z ($l \leq z \leq u$) over the input region

The MILP encoding of $\hat{z} = \max(z, 0)$ is then (Ex. C.2.3 shows a simpler example that does not involve bounds):

$$\begin{aligned}
&\hat{z} \geq z \\
&\hat{z} \geq 0 \\
&\hat{z} \leq a \cdot u \\
&\hat{z} \leq z - l(1-a) \\
&a \in \{0, 1\}
\end{aligned}$$

These constraints enforce $\hat{z} = z$ when $a = 1$ (active) and $\hat{z} = 0$ when $a = 0$ (inactive), which captures the two possible ReLU outputs (0 or z). Note that constraints are linear and involve both continuous variable $\hat{z}$ and binary variable a.

Importance upper and lower bounds These bounds are critical not only for making the MILP encoding tight, but also for ensuring that the binary indicator a can only take on values that are valid given the possible range of z. For example, if $u < 0$, then z can never be non-negative, so the active phase ($a = 1$) is infeasible (the constraints are not satisfiable) and should be ruled out by the MILP encodin. Similarly, if $l \geq 0$, only the active phase is possible. Being able to eliminate infeasible cases is crucial for the efficiency of the MILP solver, as it significantly reduces the search space.

In general, the tightness of the bounds l and u is crucial for the efficiency of the MILP solver and a major focus of DNN reasoning is developing techniques to capture these bounds more precisely (§5).

Computing Bounds $l \leq e \leq u$ Given a linear expression e

$$e = a_1 x_1 + a_2 x_2 + \ldots + b,$$

where each variable x_i ranges over $[l_i, u_i]$, a simple way to compute the bounds $l \leq e \leq u$ is using *interval* arithmetic (§5.2.1):

- **For the lower bound** (l_3): For each x_i, use its upper bound u_i if $a_i < 0$, and use its lower bound l_i if $a_i \geq 0$.
- **For the upper bound** (u_3): For each x_i, use l_i if $a_i < 0$, and use u_i if $a_i \geq 0$.

This guarantees that the extreme values of e are achieved at some corner of the input box.

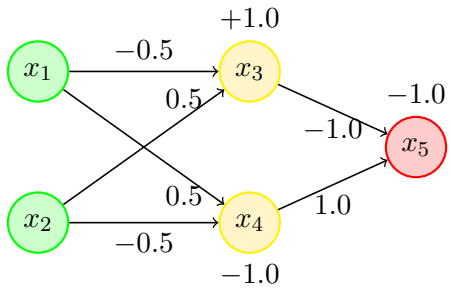


Figure 4.2: A simple DNN (similar to Fig. 1.1).

Example 4.2.1. Consider neuron x_3 in the DNN in Fig. 4.2. We have $x_3 = -0.5x_1 + 0.5x_2 + 1.0$ as the pre-activation value of x_3. The upper u_3 and lower l_3 bounds on x_3 over the input region $x_1 \in [-1, 1]$ and $x_2 \in [-2, 2]$ are:

$$\begin{aligned} z_3 &= -0.5x_1 + 0.5x_2 + 1.0 \\ l_3 &= -0.5(1) + 0.5(-2) + 1.0 = -0.5 \\ u_3 &= -0.5(-1) + 0.5(2) + 1.0 = 2.5 \end{aligned}$$

Notice that we use different pairs of values to compute the lower (1,-2) and upper (-1,2) bounds.

With the computed bounds, we encode the ReLU output of x_3:

$$\begin{aligned} &\hat{x}_3 \geq x_3 \\ &\hat{x}_3 \geq 0 \\ &\hat{x}_3 \leq a_3 \cdot u_3 \\ \implies &\hat{x}_3 \leq a_3 \cdot 2.5 \\ &\hat{x}_3 \leq x_3 - l_3(1 - a_3) \\ \implies &\hat{x}_3 \leq x_3 - (-0.5)(1 - a_3) \\ \implies &\hat{x}_3 \leq x_3 + 0.5(1 - a_3) \\ &a_3 \in \{0, 1\} \end{aligned}$$

Note that because $l_3 = -0.5$ and $u_3 = 2.5$, a_3 can be either 0 or 1, depending on the value of x_3. This is actually a worst-case scenario for the MILP solver, as it has to consider both cases. If we had different bounds, e.g., $l_3 = 0.1$, then a_3 would be forced to be 1, as x_3 can never be less than 0.1, and the MILP solver would only have to consider the active case.

4.2.2 DNN encoding

More generally, we can encode the DNN as a set of MILP linear constraints as follows:

$$
\begin{aligned}
&\text{(a)} \quad z^{(i)} = W^{(i)}\hat{z}^{(i-i)} + b^{(i)};\\
&\text{(b)} \quad y = z^{(L)}; x = \hat{z}^{(0)};\\
&\text{(c)} \quad \hat{z}_j^{(i)} \geq z_j^{(i)}; \hat{z}_j^{(i)} \geq 0;\\
&\text{(d)} \quad a_j^{(i)} \in \{0,1\};\\
&\text{(e)} \quad \hat{z}_j^{(i)} \leq a_j^{(i)} u_j^{(i)}; \hat{z}_j^{(i)} \leq z_j^{(i)} - l_j^{(i)}(1 - a_j^{(i)});
\end{aligned}
\tag{4.2.1}
$$

where x is input, y is output, and $z^{(i)}$, $\hat{z}^{(i)}$, $W^{(i)}$, and $b^{(i)}$ are the pre-activation, post-activation, weight, and bias vectors for layer i.

(a) defines the affine transformation computing the pre-activation value for a neuron in terms of outputs in the preceding layer;

(b) defines the inputs and outputs in terms of the adjacent hidden layers;

(c) asserts that post-activation values are non-negative and no less than pre-activation values;

(d) defines that the neuron activation status indicator variables that are either 0 or 1; and

(e) defines constraints on the upper, $u_j^{(i)}$, and lower, $l_j^{(i)}$, bounds of the pre-activation value of the jth neuron in the ith layer.

Deactivating a neuron, $a_j^{(i)} = 0$, simplifies the first of the (e) constraints to $\hat{z}_j^{(i)} \leq 0$, and activating a neuron simplifies the second to $\hat{z}_j^{(i)} \leq z_j^{(i)}$, which is consistent with the semantics of $\hat{z}_j^{(i)} = max(z_j^{(i)}, 0)$.

Example 4.2.2 (Full example)**.** We use MILP to formulate and check if the DNN in Fig. 4.2 satisfies the property $x_5 > 0$ for any inputs $x_1 \in [-1, 1], x_2 \in [-2, 2]$. We do this by checking the feasibility of the MILP constraints encoding $\alpha \wedge \phi_{in} \wedge \neg\phi_{out}$, where α is the MILP encoding of the DNN, ϕ_{in} is the precondition on the inputs, and ϕ_{out} is the postcondition on the outputs. We do this in several steps:

1. Encoding precondition ϕ_{in} representing input bounds and the postcondition $\neg\phi_{out}$ representing the negation of the postcondition:

$$
\begin{aligned}
\phi_{in} &: -1 \leq x_1 \leq 1; \quad -2 \leq x_2 \leq 2\\
\neg\phi_{out} &: x_5 \leq 0
\end{aligned}
$$

2. Encoding the DNN Hidden layer (pre- and post-activation):

$$
\begin{aligned}
z_3 &= -0.5x_1 + 0.5x_2 + 1.0 \\
z_4 &= 0.5x_1 - 0.5x_2 - 1.0 \\
\hat{z}_3 &\geq z_3, \quad \hat{z}_3 \geq 0 \\
\hat{z}_4 &\geq z_4, \quad \hat{z}_4 \geq 0 \\
a_3, a_4 &\in \{0, 1\} \\
\hat{z}_3 &\leq a_3 \cdot u_3, \quad \hat{z}_3 \leq z_3 - l_3(1 - a_3) \\
\hat{z}_4 &\leq a_4 \cdot u_4, \quad \hat{z}_4 \leq z_4 - l_4(1 - a_4)
\end{aligned}
$$

Output layer:

$$x_5 = -\hat{z}_3 + \hat{z}_4 - 1.0$$

3. Computing upper and lower bounds over given input ranges. Here, with $x_1 \in [-1, 1]$ and $x_2 \in [-2, 2]$, we have:

$$
\begin{aligned}
z_3 &\in [-0.5 \cdot 1 + 0.5 \cdot (-2) + 1, -0.5 \cdot (-1) + 0.5 \cdot 2 + 1] = [-0.5, 2.5] \\
z_4 &\in [0.5 \cdot (-1) - 0.5 \cdot 2 - 1, 0.5 \cdot 1 - 0.5 \cdot (-2) - 1] = [-2.5, 0.5]
\end{aligned}
$$

So we set $l_3 = -0.5, u_3 = 2.5$, and $l_4 = -2.5, u_4 = 0.5$.

4. **Substituting bounds into the constraints:**

$$
\begin{aligned}
\hat{z}_3 &\leq a_3 \cdot 2.5, \quad \hat{z}_3 \leq z_3 - (-0.5)(1 - a_3) = z_3 + 0.5(1 - a_3) \\
\hat{z}_4 &\leq a_4 \cdot 0.5, \quad \hat{z}_4 \leq z_4 - (-2.5)(1 - a_4) = z_4 + 2.5(1 - a_4)
\end{aligned}
$$

5. **The final MILP encoding:**

$$
\begin{aligned}
& -1 \leq x_1 \leq 1; \quad -2 \leq x_2 \leq 2; \\
& z_3 = -0.5x_1 + 0.5x_2 + 1.0; \\
& z_4 = 0.5x_1 - 0.5x_2 - 1.0; \\
& \hat{z}_3 \geq z_3, \quad \hat{z}_3 \geq 0; \\
& \hat{z}_4 \geq z_4, \quad \hat{z}_4 \geq 0; \\
& a_3, a_4 \in \{0, 1\}; \\
& \hat{z}_3 \leq a_3 \cdot 2.5, \quad \hat{z}_3 \leq z_3 + 0.5(1 - a_3); \\
& \hat{z}_4 \leq a_4 \cdot 0.5, \quad \hat{z}_4 \leq z_4 + 2.5(1 - a_4); \\
& x_5 = -\hat{z}_3 + \hat{z}_4 - 1.0; \\
& x_5 \leq 0; \\
& \text{where } z_3 \in [-0.5, 2.5], z_4 \in [-2.5, 0.5], \hat{z}_3 \in [0, 2.5], \hat{z}_4 \in [0, 0.5].
\end{aligned}
$$

6. **Solving** From the MILP formulation, the MILP solver attempts to find a feasible (§C.3.1) or satisfying assignment representing a counterexample violating the property. In this example, it might find $x_1 = -1, x_2 = 2$, which leads to:

$$
\begin{aligned}
z_3 &= -0.5(-1) + 0.5(2) + 1.0 = 2.5 \\
z_4 &= 0.5(-1) - 0.5(2) - 1.0 = -2.5 \\
a_3 &= 1, \hat{z}_3 = 2.5 \quad \text{(neuron active)} \\
a_4 &= 0, \hat{z}_4 = 0 \quad \text{(neuron inactive)} \\
x_5 &= -2.5 + 0 - 1.0 = -3.5
\end{aligned}
$$

Since $x_5 = -3.5 \leq 0$, this assignment satisfies our search for $x_5 \leq 0$ and thus is a counterexample.

4.2.3 Limitations

- **Scalability:** While MILP is more efficient than SMT solving[TVN]: is it? due to what?, it still cannot be applied directly to real-world DNNs due to the exponential growth of the search space. Each ReLU introduces a binary variable, leading to 2^n possible branches, and realistic DNNs can have millions of ReLUs, making the search space intractable.

- **Limited exploitation of network structure and modern hardware** General MILP solvers are designed for arbitrary MILP problems and do not exploit DNN-specific structures such as[TVN]: Hai, like what? mention those that DNN verification tools exploit.

  Moreover, MILP solvers, even industrial-strength ones such as Gurobi [24], are primarily CPU-based and does not leverage the massive parallelism provided by modern GPUs.

- **Advanced Abstraction and Heuristics** Interval analysis is efficient and commonly used for computing neuron bounds, but cannot capture dependencies between neurons, leading to precision loss in deeper networks. SOTA DNN verification tools (and in general program analyses) employ more advanced abstract domains such as zonotopes (which capture linear relationships) and polytopes (which represent arbitrary linear constraints) to improve precision.

  Modern DNN verification tools also employ heuristics to decide which neurons to branch on and to determine stable neurons to avoid unnecessary branching. These heuristics are not available in general MILP solvers.

[TVN]: Hai, above you mention MILP also employs BaB algorithm, could you write a paragraph or so about how MILP solvers use BaB and briefly show how that would apply to example 4.2.2 (just briefly, no need a full step by step demonstration). Is this BaB algorithm used by MILP very similar to the one used by DNN verification

tools (minus the DNN specific optimizations and heuristics)? like the BaB algorithm described in Alg. 1

Chapter 5

Abstractions

As mentioned in §4.2, and DNN verification in general, we need to compute the bounds of the neurons. However, computing these bounds precisely is often infeasible due to the complexity of the DNN structure and non-linear activation functions such as ReLU. To address this, modern DNN verifiers use *abstraction* techniques to approximate the set of possible values that a post-ReLU neuron can have.

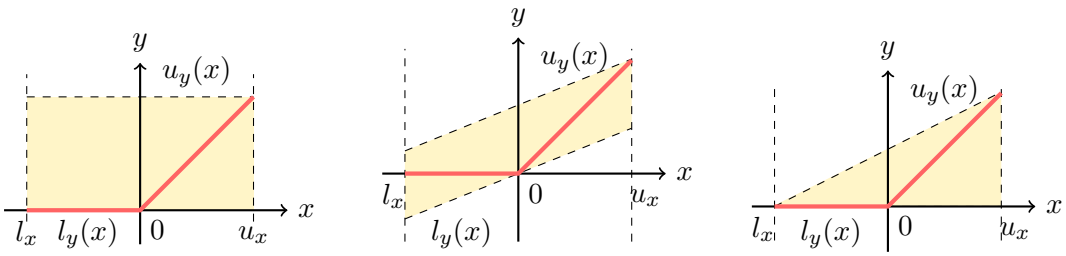
5.1 Overview of Abstractions for ReLU

We will focus on ReLU (§1.3.1) activation functions, which are the most common in DNNs. The goal is to compute the bounds of a post-ReLU neuron $\hat{z}$ given the bounds of its pre-ReLU value z over the input region. For example, for a ReLU neuron $y = \max(0, x)$, we want to compute the bounds $[l_y(x), u_y(x)]$ of y given the bounds $[l_x, u_x]$ on x.

We want to compute the bounds to be as tight as possible, i.e., they should be the largest lower and lowest upper values that $\hat{z}$ can take given the bounds on z. This computation is called *abstraction* and is crucial for DNN verification, as it allows us to reason about the behavior of the network without having to enumerate all possible values of the neurons. There are several abstraction techniques that can be used to compute these bounds, each with its own trade-offs in terms of precision and computational complexity.

5.1.1 Common Abstractions for ReLU

Fig. 5.1 illustrates common abstractions (or *over-approximations*) for the ReLU function $y = \max(0, x)$, where $x \in [l_x, u_x]$ and $y \in [l_y(x), u_y(x)]$. The values of ReLU are shown as points on the red line, which is non-convex and consists of two linear segments: one for $x < 0$ (where $y = 0$) and another for $x \geq 0$ (where $y = x$). To compute the bounds $l_y(x)$ and $u_y(x)$, we can use different abstractions:



(a) Interval (b) Zonotope (c) Polytope (lower flat)

Figure 5.1: Abstractions of $\text{ReLU}(x) = \max(0, x)$ over $x \in [l_x, u_x]$: (a) interval, (b) zonotope, (c–d) polytope abstractions with different lower bounds.

- **Interval Abstraction:** Interval represents the output of the post-ReLU neuron as intervals $[l_y(x), u_y(x)]$ where $l_y(x) = 0$ and $u_y(x) = u_x$. It does not capture the relationship between the input and output of ReLU, and simply assumes that the output can take any value between 0 and the upper bound of the input. Interval is a simple and efficient abstraction, but it can be *too imprecise* for many cases.

  In Fig. 5.1a, the yellow rectangle represents the interval $[0, u_x]$. As can be seen, this interval region is too large of an over-approximation (too coarse or loose), as it includes many points that are not achievable by ReLU, e.g., the point $(0.5, 0.0)$ is not on the red line.

- **Zonotope Abstraction:** Zonotopes can capture linear relationships between variables more effectively. We can represent ReLU as a zonotope that includes the linear segments. The lower bound $l_y(x)$ is $y = \lambda x$ and the upper bound $u_y(x)$ is $y = \lambda x + u_x(1 - \lambda)$ for some slope $\lambda \in [0, \frac{u_x}{u_x - l_x}]$. If we set $\lambda = 0$, the zonotope is a rectangle, which is the same as the interval abstraction. If we set $\lambda = \frac{u_x}{u_x - l_x}$, the zonotope's is upper bound is the same as polytope's upper bound in Fig. 5.1c.

  In Fig. 5.1b, the zonotope, depicted as a a parallelogram, is arguably tighter than the interval in Fig. 5.1a. It captures the linear relationship between x and y and excludes points that are not achievable by ReLU, e.g., the point $(0.5, 0.0)$ that was included in the interval abstraction is not included in the zonotope. However, it still includes non-ReLU points and is also not strictly better than interval, e.g., the point $(0.5, -0.5)$ is included in the zonotope but not in the interval abstraction (or ReLU).

- **Polytope Abstraction:** Polytopes can represent arbitrary linear constraints and provide very precise bounds. We can construct a polytope that tightly encloses the non-convex shape of the ReLU function.

In Fig. 5.1c, the polytope is shown as a trapezoid that captures the linear segments of ReLU. The lower bound is $l_y(x) = 0$ and the upper bound is $u_y(x) = u_x$.

5.1.2 Transformer Functions

The concept of computing abstractions is central to program analysis, e.g., through *abstract interpretation* techniques. It allows us reason about the behavior of a program without evaluating it on all concrete inputs—which may be infinite. Instead, we use an *abstract domain*, such as interval, to summarize sets of concrete values, enabling sound and scalable approximation.

5.1.2.1 Abstraction Functions

In abstraction interpretation, we have the *abstraction function*

$$\alpha : D \to D^a,$$

which maps a concrete value from the domain D to an element in a finite or simpler abstract domain D^a.

Example 5.1.1 (Odd/Even)**.** The `odd/even` or parity abstraction is defined as:

$$\alpha_{\texttt{parity}}(x \in \mathbb{Z}) = \begin{cases} \texttt{even} & \text{if } x \bmod 2 = 0 \\ \texttt{odd} & \text{if } x \bmod 2 = 1 \end{cases}$$

Even though $\mathbb{Z}$ is infinite, this abstraction maps all integers to a finite set $\{\texttt{odd}, \texttt{even}\}$.

5.1.2.2 Transformer Functions

Once we have values in the abstract domains, we often define an *abstract transformer function*

$$f^a : D^a \to D^a,$$

for each operation f to reason about its behavior on abstract values.

Example 5.1.2. Consider the function $f(x) = x + 1$. We define the abstract transformers f^a for different abstract domains D^a:

- **Odd/Even abstraction**: $D^a = \{\texttt{odd}, \texttt{even}\}$. Then:

$$f^a(\texttt{odd}) = \texttt{even}, \quad f^a(\texttt{even}) = \texttt{odd}$$

- **Sign abstraction**: $D^a = \{\texttt{neg}, \texttt{zero}, \texttt{pos}\}$. Then:

$$f^a(\texttt{neg}) = \{\texttt{neg}, \texttt{zero}\}, \quad f^a(\texttt{zero}) = \texttt{pos}, \quad f^a(\texttt{pos}) = \texttt{pos}$$

- **Interval abstraction**: $D^a = \{[a, b] \mid a \leq b \in \mathbb{Z} \cup \{-\infty, +\infty\}\}$. Then:

$$f^a([a, b]) = [a + 1, b + 1]$$

5.2 Abstract Domains

We now introduce several abstract domains that are commonly used in DNN verification. Each domain has its own abstract transformer functions to compute the bounds of neurons.

5.2.1 Interval

Interval is a very simple abstraction for DNN verification. Instead of keeping a single value for each variable, it maintains a lower and upper bound for it. Thus, we can use it to estimate the range of values that a neuron can take using a lower and upper bound $[l, u]$, e.g., an interval over the set of values $\{-2.5, -8.2, -10.7, 2, 4.7, 5.1\}$ can be represented as $[-10.7, 5.1]$.

Interval is very efficient, but treats each variable independently, so it cannot capture correlations between variables such as $x_2 = -x_1$.

Definition The interval for one variable v is defined as:

$$v \in [l, u] = \{v \in \mathbb{R} \mid l \leq v \leq u\}$$

For n variables, the interval becomes a box (like a rectangle in 2D, a cuboid in 3D, or a hyperrectangle in nD):

$$[v_1, v_2, \ldots, v_n] \in [l_1, u_1] \times [l_2, u_2] \times \cdots \times [l_n, u_n]$$

5.2.1.1 Affine Transformer

For the linear or affine function f in §1.2

$$f(v_1, v_2, ..., v_n) = \sum_{i=1}^{n} w_i v_i + b$$

where w_i is the weight for the input v_i, n is the number of output nodes from the previous layer and b is the bias term, the abstract transformer f^a is:

$$f^a([l_1, u_1], ..., [l_n, u_n]) = [f_L^a, f_U^a] = \left[b + \sum_{i=1}^{n} \big(\min(w_i l_i, w_i u_i), \; b + \sum_{i=1}^{n} \big(\max(w_i l_i + w_i u_i) \right].$$

Example 5.2.1. Consider the DNN in Fig. 5.2 with inputs $x_1 \in [1, 2]$ and $x_2 \in [-1, 3]$. The affine function for the neuron x_3 is given by:

$$f(x_1, x_2) = -0.5\, x_1 + 0.5\, x_2 + 1.0$$

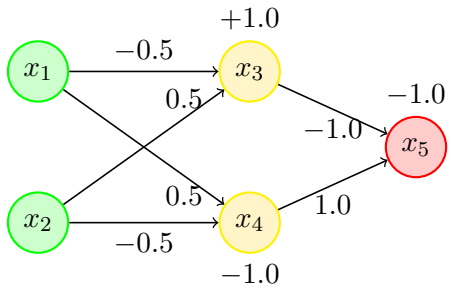


Figure 5.2: A simple DNN (similar to Fig. 1.1).

Then

$$f^a([1,2],[-1,3]) = \Big[1 + \min(-0.5 \cdot 1, 0.5 \cdot 2) + \min(-0.5 \cdot -1, 0.5 \cdot 3)$$
$$1 + \max(-0.5 \cdot 1, 0.5 \cdot 2) + \max(-0.5 \cdot -1, 0.5 \cdot 3)\Big]$$
$$= [-0.5, 2.0]$$

5.2.1.2 ReLu Transformer

For $\text{ReLU}(x) = \max(0, x)$, the abstract transformer is defined as:

$$\text{ReLU}^a([l,u]) = [\text{ReLU}(l), \text{ReLU}(u)] = [\max(0,l), \max(0,u)]$$

This is equivalent to three cases:

1. If $u < 0$, then $\text{ReLU}^a([l,u]) = [0,0]$. If inputs are negative, the output is also negative.
2. If $l \geq 0$, then $\text{ReLU}^a([l,u]) = [l,u]$. If inputs are positive, the output is exactly the same.
3. If $l < 0 < u$, then $\text{ReLU}^a([l,u]) = [0,u]$. If inputs are mixed, the output is approximated to $[0,u]$

Example 5.2.2. For the example in Ex. 5.2.1, applying ReLU to the output bounds of neuron x^3 gives:

$$\text{ReLU}^a([-0.5, 2.0]) = [\text{ReLU}(-0.5), \text{ReLU}(2.0)] = [0, 2.0].$$

5.2.1.3 Efficiency and Precision

Intervals is very *efficient* and scales very well to large networks. The affine transformer only requires a linear number of multiplications and min/max operations, and ReLU reduces to only three matching cases. However, the cost of efficiency is precision. Intervals approximate each variable independently, which can lead to over-approximation errors when variables are correlated.

Example 5.2.3. Suppose we have $v_1 \in [0, 1]$, $v_2 = -v_1$, and $z = v_1 + v_2$[TVN: Hai, do we have these kinds of correlation in DNN verification?. The concrete value of z is always 0, but the interval abstraction gives $z \in [-1, 1]$, which is a very loose over-approximation.

Moreover, if we apply ReLU, then the true output is $\text{ReLU}(z) = \text{ReLU}(0) = 0$, but the interval abstraction gives $\text{ReLU}^a([-1, 1]) = [0, 1]$, which is again a loose over-approximation.

This overapproximation error grows quickly as we propagate through many layers of a large network, i.e., it keeps "inflating" the bounds, leading to a very loose approximation of the output and becomes useless for verification tasks. For example, if we want to verify that $z \leq 0$, the interval, which gives $z \in [0, 1]$, cannot provide a tight enough bound to prove this property.

Nonetheless, interval-based methods remain popular due to their simplicity and efficiency. In some cases, despite being too coarse, they can still successfully verify properties of neural networks, e.g., if we want to verify that $z \leq 2$, then the interval result $[-1, 1]$ would suffice.

5.2.2 Zonotope

Zonotopes extend intervals (§5.2.1) by introducing *generators* that represent linear dependencies between variables. This allows zonotopes to capture correlations between variables, leading to more precise approximations compared to intervals.

A **zonotope** $\mathcal{Z}$ in $\mathbb{R}^n$ is formally defined as:

$$\mathcal{Z} = \left\{ c + \sum_{i=1}^{m} \epsilon_i g_i \mid \epsilon_i \in [-1, 1] \right\}$$

where :

- $c \in \mathbb{R}^n$ is the *center* (like the midpoint of intervals),
- $g_i \in \mathbb{R}^n$ are *generator vectors* (directions of variability), and
- ϵ_i are independent coefficients in $[-1, 1]$.

5.2.2.1 Affine Transformer

For the affine function f in §1.2

$$f(x) = Wx + b$$

where W is a weight matrix and b is a bias vector. Given an input zonotope $\mathcal{Z} = (c, G)$ where $G = [g_1, g_2, \ldots, g_m]$ is the generator matrix, the abstract transformer f^a for zonotope is:

$$f^a(\mathcal{Z}) = (Wc + b, WG)$$

The new center becomes $Wc + b$ and the new generator matrix becomes WG. Since affine transformations preserve zonotope structure, this transformation is exact with no over-approximation.

Example 5.2.4. Consider the DNN in Fig. 5.2 with inputs $x_1 \in [1, 2]$ and $x_2 \in [-1, 3]$. The affine function for neuron x_3 is given by:

$$f(x_1, x_2) = -0.5\, x_1 + 0.5\, x_2 + 1.0$$

The center c represents the midpoint of each input interval:

$$c_1 = \frac{1+2}{2} = 1.5, \quad c_2 = \frac{(-1)+3}{2} = 1.0$$

The generator matrix G captures the half-widths of each interval as diagonal entries:

$$G_{11} = \frac{2-1}{2} = 0.5, \quad G_{22} = \frac{3-(-1)}{2} = 2.0$$

This construction ensures the zonotope exactly represents the input box: $x_1 \in [1.5 - 0.5, 1.5 + 0.5] = [1, 2]$ and $x_2 \in [1.0 - 2.0, 1.0 + 2.0] = [-1, 3]$. Thus, the input box can be encoded as a zonotope with center and generator matrix:

$$c = \begin{bmatrix} 1.5 \\ 1.0 \end{bmatrix}, \quad G = \begin{bmatrix} 0.5 & 0 \\ 0 & 2.0 \end{bmatrix}$$

For the weight $w = [-0.5, 0.5]^\top$ and bias $b = 1.0$, applying the zonotope transformer:

$$\begin{aligned} c' &= w^\top c + b = [-0.5, 0.5] \begin{bmatrix} 1.5 \\ 1.0 \end{bmatrix} + 1.0 = -0.75 + 0.5 + 1.0 = 0.75 \\ g_1' &= w^\top g_1 = [-0.5, 0.5] \begin{bmatrix} 0.5 \\ 0 \end{bmatrix} = -0.25 \\ g_2' &= w^\top g_2 = [-0.5, 0.5] \begin{bmatrix} 0 \\ 2.0 \end{bmatrix} = 1.0 \end{aligned} \tag{5.2.1}$$

The output zonotope for x_3 is $(0.75, [-0.25, 1.0])$, thus the concrete bounds are:

$$\begin{aligned} f_L^a &= c' - |g_1'| - |g_2'| = 0.75 - 0.25 - 1.0 = -0.5 \\ f_U^a &= c' + |g_1'| + |g_2'| = 0.75 + 0.25 + 1.0 = 2.0 \end{aligned} \tag{5.2.2}$$

Note that, for this single affine operation over a box input, both interval and zonotope abstractions yield identical bounds $[-0.5, 2.0]$. The advantage of zonotopes becomes apparent when propagating through multiple layers, where zonotopes preserve linear correlations that intervals lose.

5.2.2.2 ReLU Transformer

Activation functions like ReLU are non-affine and do not preserve zonotope structure. For the ReLU function $\text{ReLU}(x) = \max(0, x)$, we must use conservative approximations. Given an input zonotope, we first compute its interval bounds $[l, u]$, then consider three cases:

- **Active case** ($l \geq 0$): All values are non-negative, so $\text{ReLU}^a(\mathcal{Z}) = \mathcal{Z}$ (identity).
- **Inactive case** ($u \leq 0$): All values are negative, so $\text{ReLU}^a(\mathcal{Z}) = \{0\}$ (zero zonotope).
- **Unstable case** ($l < 0 < u$): The range crosses zero, requiring over-approximation using a parallelogram that bounds the ReLU function over $[l, u]$.

For the unstable case, the zonotope approximation introduces a new generator to capture the ReLU's piecewise-linear behavior, typically using the slope $\lambda = \frac{u}{u-l}$ for the lower bound and maintaining the upper bound $y = u$.

Example 5.2.5 (ReLU on zonotope)**.** Continuing from the previous example, applying ReLU to the zonotope output $(0.75, [-0.25, 1.0])$ with bounds $[-0.5, 2.0]$:

Since $l = -0.5 < 0 < 2.0 = u$, this is an unstable neuron. The ReLU approximation introduces over-approximation, typically resulting in bounds $[0, 2.0]$ with additional generators to model the ReLU constraint.

5.3 Polytope

In the previous section, we have seen the abstract domain of zonotopes, which is more expressive than the interval domain. Specifically, instead of approximating functions using a hyper-rectangle, the zonotope domain allows us to approximate functions using a zonotope, e.g., a parallelogram, capturing relations between different dimensions. In this section, we look at an even more expressive abstract domain, the polyhedron (or polytope) domain.

Unlike the zonotope domain, the polyhedron domain allows us to approximate functions using arbitrary convex polyhedra. A polyhedron in $\mathbb{R}^n$ is a region made of

straight (as opposed to curved) faces; a convex shape is one where the line between any two points in the shape is completely contained in the shape. Convex polyhedra can be specified as a set of linear inequalities of the form:

$$Ax \leq b$$

where $A \in \mathbb{R}^{m \times n}$ and $b \in \mathbb{R}^m$ for some m, specifying m half-spaces whose intersection forms the polyhedron.

Using a set of convex polyhedra, we can more precisely approximate activation functions like ReLU. For instance, to approximate ReLU, we can describe the tightest convex over-approximation by the following constraints:

$$x \leq y, \quad 0 \leq y, \quad y \leq \lambda x + \mu$$

where λ and μ are parameters chosen based on the bounds of x.

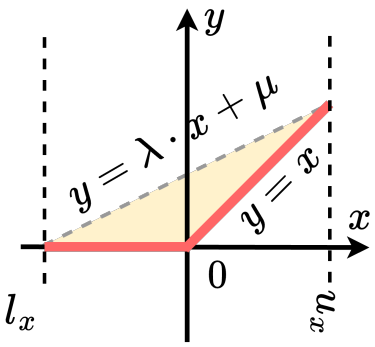


Figure 5.3: The tightest Convex Polyhedral Approximation of ReLU.

This is the smallest convex polyhedron that soundly approximates ReLU, and is strictly more precise than the interval and zonotope abstractions, as can be seen visually.

5.3.1 Affine Functions

Affine transformations map convex polyhedra to convex polyhedra. Given an affine transformation $f(x) = Wx + b$, where W is a matrix and b is a bias vector, we can transform a polyhedron $\{x \mid Ax \leq b\}$ through f by substitution:

$$\{x \mid A(W^{-1}(x - b)) \leq b\}$$

if W is invertible. More commonly in practice, when applying affine transformations in neural networks (layer-wise), we modify the constraints accordingly by propagating through the weights and biases.

Thus, affine layers can be handled exactly under polyhedral abstraction without any need for relaxation or over-approximation.

5.3.2 Activation Functions

Handling non-linear activation functions, such as ReLU, with polyhedral abstraction is challenging because non-linearities generally map polytopes to non-convex shapes. Therefore, over-approximations are required.

The key idea is to approximate the graph of the non-linear function by a convex polyhedron that covers all possible cases. For ReLU, the previously mentioned three constraints:

$$x \leq y, \quad 0 \leq y, \quad y \leq \lambda x + \mu \tag{5.3.1}$$

construct a tight convex relaxation.

For other activations like sigmoid or tanh, the approximation involves linearizing the curve between the lower and upper bounds of the input variable, but the number of constraints can quickly grow, increasing computational complexity.

DeepPoly. By containing two lower polyhedra constraints for y, the approximation in 5.3.1 inherently suffers from a potential blow-up in number of constraints as the analysis proceeds. Due to scalability issues associated with general polyhedral representations, DeepPoly [43] was proposed as a precise and scalable abstract domain. DeepPoly introduces a specialized form of polyhedral abstraction combined with interval bounds.

More specifically, DeepPoly only allows for one lower bound in 5.3.1, the selection of which lower constraint depends on which constraint provides the tighter approximation.

Returning to our example, the area of the approximation in Fig. 4(b) is given by $0.5 \cdot u \cdot (u - l)$, while the area in Fig. 4(c) is given by $0.5 \cdot (-l_i) \cdot (u_i - l_i)$. To achieve a tighter relaxation, we select the approximation with the smaller area. Specifically, when $u \leq -l$, we apply the constraints and bounds derived from $x \leq y$. In addition, each neuron x_j is bounded above and below by affine expressions of the input neurons:

$$l_j(x) \leq x_j \leq u_j(x)$$

where l_j and u_j are affine functions.

5.3.3 DeepPoly Transformers

The DeepPoly abstract domain defines a scalable and precise framework for verifying deep neural networks by combining interval and polyhedral abstractions. Each neuron is bounded from above and below using affine expressions of the input neurons:

$$l_j(x) \leq x_j \leq u_j(x)$$

where $l_j(x)$ and $u_j(x)$ are affine functions representing lower and upper bounds respectively. DeepPoly then defines **abstract transformers** to propagate these bounds through different types of neural network layers.

5.3.3.1 Affine Layer Transformer

Given an affine transformation:

$$x^{(l+1)} = Wx^{(l)} + b$$

we define the transformation of the bounds by propagating the affine expressions directly:

$$l_j^{(l+1)}(x) = \sum_i w_{ji}^+ \cdot l_i^{(l)}(x) + w_{ji}^- \cdot u_i^{(l)}(x) + b_j$$
$$u_j^{(l+1)}(x) = \sum_i w_{ji}^+ \cdot u_i^{(l)}(x) + w_{ji}^- \cdot l_i^{(l)}(x) + b_j$$

Here, $w_{ji}^+ = \max(w_{ji}, 0)$, and $w_{ji}^- = \min(w_{ji}, 0)$, ensuring correct handling of sign-dependent propagation.

5.3.3.2 ReLU Transformer

The ReLU transformer in DeepPoly uses a convex relaxation that is tighter than previous abstractions by selecting only one lower bound constraint depending on the sign and tightness. Suppose $x_j = \text{ReLU}(x_i)$. Let $[l_i, u_i]$ be the lower and upper bounds for x_i.

- If $l_i \geq 0$: ReLU is linear, so

$$l_j(x) = l_i(x), \quad u_j(x) = u_i(x)$$

- If $u_i \leq 0$: ReLU is constant 0, so

$$l_j(x) = u_j(x) = 0$$

- If $l_i < 0 < u_i$: ReLU is approximated with:

$$u_j(x) = \frac{u_i}{u_i - l_i} \cdot (x_i - l_i)$$

and only one lower bound is selected:

$$l_j(x) = \begin{cases} 0, & \text{if area under lower 0 line is smaller} \\ x_i, & \text{if area under identity line is smaller} \end{cases}$$

The decision is made based on which convex region has smaller area to achieve a tighter abstraction, following the principle:

$$\text{Choose constraint with smaller area:} \quad 0.5 \cdot u_i \cdot (u_i - l_i) \quad \text{vs} \quad 0.5 \cdot (-l_i) \cdot (u_i - l_i)$$

By maintaining only upper and lower affine bounds, DeepPoly avoids the full complexity of manipulating arbitrary polytopes while retaining significantly more precision than intervals or zonotopes.

...

Thus, DeepPoly achieves a practical balance between precision and scalability for verifying deep neural networks.

5.3.4 Example

Consider again the DNN in Fig. 1.1. Suppose the input set is defined by box constraints $x_1 \in [-1, 1]$ and $x_2 \in [-2, 2]$. These can be represented initially by 4 inequalities.

Applying the affine transformation for the hidden layer, we obtain a new set of inequalities describing the hidden layer nodes. Upon applying ReLU, we would use the convex polyhedral relaxation as depicted in **??**. The output layer similarly results from affine operations on the polyhedra describing the hidden layer.

In a DeepPoly setting, instead of carrying full inequalities, we track only the lower and upper affine bounds per neuron, leading to an efficient verification process.

5.3.5 Comparison to Zonotope Abstraction

While zonotope abstraction captures dependencies between variables better than intervals, it still assumes symmetrical dependencies around a center point and cannot easily model arbitrary convex shapes.

Polyhedral abstraction, on the other hand, allows representing arbitrary convex shapes precisely, enabling much tighter approximations, especially after ReLU activations.

However, traditional polyhedral methods suffer from:

- High computational complexity,
- Rapid growth in the number of constraints,
- Difficulty scaling to large networks.

DeepPoly addresses these challenges by:

- Restricting to simple upper and lower affine bounds,
- Maintaining polynomial scalability,

- Achieving higher precision than zonotopes or intervals,
- Providing efficient transformers for common layers in DNNs.

Therefore, DeepPoly achieves a balance, combining the expressiveness of polyhedral domains with the efficiency required for deep network verification.

5.4 Abstractions for Other Activation Functions

5.5 problems

5.5.1 Interval Abstraction

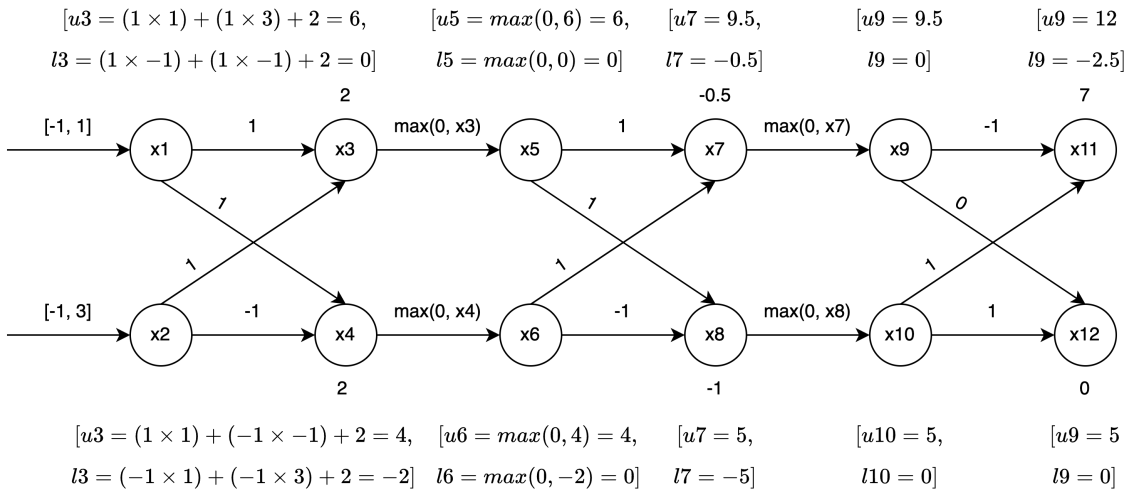


Figure 5.4: Feed-forward neural network with 6 layers and 2 neurons per layer.

Example 5.5.1 (Full Example of Interval Abstraction)**.** In Fig. 5.4, we aim to verify whether $x_{11} \geq x_{12}$ given a bounded input range on x_1 and x_2. To do this using interval abstraction, we propagate intervals layer by layer.

Suppose the inputs x_1 and x_2 satisfy:

$$x_1 \in [-1, 1], \quad x_2 \in [-1, 2]$$

Let an affine neuron (e.g., x_3) compute:

$$x_3 = 1x_1 + 1x_2 + 2$$

Then we apply the affine abstract transformer:

$$\begin{aligned} x_3 \in [&\min(1 \times -1, 1 \times 1) + \min(1 \times -1, 1 \times 3) + 2, \\ &\max(1 \times -1, 1 \times -1) + \max(-1 \times -1, -1 \times 3) + 2] = \\ &[0, 6] \end{aligned} \tag{5.5.1}$$

So we over-approximate x_3 as:

$$x_3 \in [0, 6]$$

This process is repeated for each layer until we reach the output layer. Here we can see that by using Interval abstraction, the property $x_{11} \geq x_{12}$ or $x_{11} - x_{12} \geq 0$ is $UNSAT$[HD]: seems incorrect due to

$$-2.5 - 0 \leq x_{11} - x_{12} \leq 12 - 5$$

Part III

DNN Verification Algorithms

Chapter 6

The Branch and Bound Search Algorithm

As we have seen in **??**, the NNV verification problem can be formulated as a satisfiability problem, solvable using constraint solving. However, constraint solvers, e.g., SMT and MILP solvers, often struggle to scale to large DNNs due to the complexity of the underlying problem. Thus, modern DNN verification techniques reframe the problem to search for *activation patterns* that satisfy the constraints, and use the Branch-and-Bound (BaB) algorithm to explore the space of possible activation patterns.

6.1 Activation Pattern Search

DNNs with piecewise linear activation functions have a special structure that can be exploited for verification. For example, each ReLU (§1.3.1) function partitions the input space into two regions—active and inactive. Within each region, the DNN behavior can be encoded as *a linear constraint*, which can be efficiently analyzed.

Thus, verifying a DNN reduces to checking that none of these linear regions contains a counterexample. More specifically, we can rewrite Eq. 3.2.3 as:

$$\bigvee_{p \in P} (\alpha_p \wedge \phi_{in} \wedge \neg \phi_{out}) \tag{6.1.1}$$

where P is the set of all possible activation patterns—boolean assignments of activation statuses of all neurons– of the DNN, and α_p is the formula α restricted to the linear region defined by the activation pattern p. This means that α_p includes additional constraints that fix the activation status of each neuron according to p. For example, if p specifies that neuron n_i is active, then α_p includes the constraint $z_i \geq 0$, indicating that the pre-activation value z_i of neuron n_i is non-negative. Similarly, if n_i is inactive, then α_p includes $z_i < 0$.

As long as one of the disjuncts in Eq. 6.1.1 is satisfiable, i.e., we could find a counterexample in one of the linear regions, the entire formula is satisfiable, indicating that the property is invalid. Conversely, if all disjuncts are unsatisfiable, the property is valid.

This allows us to break down the verification problem into smaller subproblems, each searches for *activation pattern*, or boolean assignment of activation statuses of all neurons, that satisfies the formula in Eq. 3.2.3. Modern DNN verification techniques [1, 10, 17, 19, 21, 28, 39, 47] all adopt this idea and search for a satisfying activation pattern to find a counterexample.

6.1.1 Activation Patterns

Definition 6.1.1 (Activation Pattern)**.** Let N be a DNN with ReLU neurons $n_1, \ldots, n_m$. An *activation pattern* is a Boolean assignment of the activation status of a subset (or all) of the neurons. If a neuron n_i is active, we set $b_i = \texttt{true}$ (meaning $z_i \geq 0$); if it is inactive, $b_i = \texttt{false}$ (meaning $z_i < 0$).

Definition 6.1.2 (Complete Activation Pattern)**.** A *complete activation pattern* assigns an activation status to *every* neuron in the DNN:

$$p = \langle b_1, b_2, \ldots, b_m \rangle \in \{\texttt{true}, \texttt{false}\}^m.$$

Definition 6.1.3 (Partial Activation Pattern)**.** A *partial activation pattern* assigns activation statuses to only a *subset* of the neurons.

$$q = \langle b_1, b_2, *, b_4, *, \ldots, b_m \rangle \in \{\texttt{true}, \texttt{false}, *\}^m,$$

where $*$ means "undetermined" or "don't care". Each partial activation pattern represents multiple complete activation patterns.

Example 6.1.1. Consider a DNN with three ReLU neurons n_1, n_2, n_3. A complete activation pattern might be

$$p = \langle \texttt{true}, \texttt{false}, \texttt{true} \rangle,$$

which means n_1 and n_3 are active while n_2 is inactive.

In contrast, a partial activation pattern such as

$$q = \langle \texttt{true}, \texttt{false}, * \rangle$$

represents *both* complete patterns $\langle \texttt{true}, \texttt{false}, \texttt{true} \rangle$ and $\langle \texttt{true}, \texttt{false}, \texttt{false} \rangle$.

Problem 6.1.1 (Pattern Enumeration)**.** Consider an NN with 3 ReLU neurons:

1. How many complete activation patterns are there?

2. How many partial patterns of size 2 (i.e., fixing 2 neurons but leaving 1 unspecified) are there?

3. Give an explicit example of one partial pattern and list all the complete patterns it represents.

Problem 6.1.2 (Counting Complete Patterns Compatible with a Partial Pattern)**.** Suppose we have a DNN with $m = 10$ ReLU neurons. Consider a partial pattern p' that fixes 4 neurons.

1. How many complete patterns extend p'?

2. Suppose we restrict p' further by adding 2 more neuron assignments. How many extensions now?

3. Generalize: If p' fixes k neurons out of m, how many complete patterns extend it?

6.1.1.1 Activation Patterns and LP Constraints

Once having an activation pattern p, we can simplify the formula α representing the DNN by replacing each ReLU function with a linear constraint according to the activation status specified in p. For example, if p specifies that neuron n_i is active, we replace $\text{ReLU}(z_i)$ with z_i and add the constraint $z_i \geq 0$; if n_i is inactive, we replace $\text{ReLU}(z_i)$ with 0 and add the constraint $z_i < 0$. This gives us the formula α_p corresponding to the linear region defined by p.

A complete activation pattern p defines a unique linear region of the DNN. This is because with a complete pattern p, α_p becomes a purely linear formula. In contrast, a partial activation pattern q defines multiple linear regions, one for each complete pattern it represents. With q, α_q may still contain some ReLU functions that are not fixed by q. However, since q fixes the status of some neurons, we can simplify α by replacing the ReLU functions of those neurons with linear constraints.

In any case, given an activation pattern, we can reduce the complexity of the satisfiability check by fixing the activation status of some neurons. Thus, checking the satisfiability of $\alpha_p \wedge \phi_{in} \wedge \neg\phi_{out}$ is easier than checking that of $\alpha \wedge \phi_{in} \wedge \neg\phi_{out}$.

Example 6.1.2. Recall the DNN from Fig. 3.1 can be represented as the formula α

$$
\begin{aligned}
&\hat{x}_3 = -0.5x_1 + 0.5x_2 + 1.0 \wedge \\
&\hat{x}_4 = 0.5x_1 - 0.5x_2 + 1.0 \wedge \\
&x_3 = \text{ReLU}(\hat{x}_3) \wedge \\
&x_4 = \text{ReLU}(\hat{x}_4) \wedge \\
&x_5 = -x_3 + x_4 - 1.0,
\end{aligned}
$$

Here $\hat{x}_3$ and $\hat{x}_4$ are the pre-activation values of the ReLU neurons x_3 and x_4, respectively. Thus, if we fix the activation status of x_3 and x_4, we can simplify α by replacing the ReLUs with linear constraints.

- **Complete activation pattern.** A complete activation pattern specifies the status of both ReLU neurons. For instance,

  $$p = \langle \texttt{true}, \texttt{false} \rangle$$

  means that $\hat{x}_3 \geq 0$ (so $x_3 = \hat{x}_3$) while $\hat{x}_4 < 0$ (so $x_4 = 0$). In this case, the network reduces to a single linear constraint (region):

  $$x_5 = -(-0.5x_1 + 0.5x_2 + 1.0) + 0 - 1.0 = 0.5x_1 - 0.5x_2 - 2.0.$$

- **Partial activation pattern.** A partial pattern specifies only some activation statuses. For example,

  $$q = \langle \texttt{true}, * \rangle$$

  means $\hat{x}_3 \geq 0$ but places no restriction on $\hat{x}_4$. Here, the network reduces to

  $$\begin{aligned} \hat{x}_4 &= 0.5x_1 - 0.5x_2 + 1.0 \ \wedge \\ x_4 &= \text{ReLU}\,(\hat{x}_4) \ \wedge \\ x_5 &= -(-0.5x_1 + 0.5x_2 + 1.0) + x_4 - 1.0, \end{aligned}$$

  Because q does not fix the status of x_4, we cannot simplify the ReLU for x_4. Thus, the formula still contains a ReLU function which splits the input space into two linear regions corresponding to the two possible activation statuses of x_4.

Problem 6.1.3. Consider the DNN in Fig. 3.1. Suppose we fix the activation pattern

$$p = \{\mathsf{true}, \mathsf{true}\}.$$

1. Provide the constraints represented by the network induced by p.
2. Consider an invalid property $x_5 > 0$ for inputs $x_1 \in [-1, 1], x_2 \in [-2, 2]$. Find an activation pattern that satisfies the formula $\alpha_p \wedge \phi_{in} \wedge \neg\phi_{out}$. In other words, find a pattern that contains a counterexample to the property.

6.2 Branch and Bound

Modern DNN verifiers typically adopt the Branch-and-Bound (BaB) approach to explore the space of possible neuron activation patterns. The BaB algorithm systematically splits (*branch*) the verification problem into smaller subproblems by deciding

Algorithm 1. The $\texttt{BaB}_{\texttt{NV}}$ algorithm.

input : DNN $\mathcal{N}$, property $\phi_{in} \Rightarrow \phi_{out}$
output : unsat if property is valid, otherwise (sat, cex)

```
1 ActPatterns ← {∅} // initialize verification problems
2 while ActPatterns do // main loop
3     σ_i ← Select(ActPatterns) // process problem i-th
4     if Deduce(N, φ_in, φ_out, σ_i) then
5         (cex, v_i) ← Decide(N, φ_in, φ_out, σ_i)
6         if cex then // found a valid counter-example
7             return (sat, cex)
          // create new activation patterns
8         ActPatterns ← ActPatterns ∪ {σ_i ∧ v_i ; σ_i ∧ ¬v_i}
9 return unsat
```

the activation status (active/inactive) of neurons, and uses abstraction (bound) techniques to compute upper and lower bounds on the output values for these subproblems. If a subproblem's bounds indicate that it cannot contain a counterexample, it is pruned from the search space. This process continues until either a counterexample is found or all subproblems are exhausted, proving the property holds.

Alg. 1 shows $\texttt{BaB}_{\texttt{NV}}$, a reference BaB architecture [35] for modern DNN verifiers. $\texttt{BaB}_{\texttt{NV}}$ takes as input a ReLU-based DNN $\mathcal{N}$ and a formulae $\phi_{in} \Rightarrow \phi_{out}$ representing the property of interest. $\texttt{BaB}_{\texttt{NV}}$ maintains a set of activation patterns (`ActPatterns`) that represent the current activation pattern of the DNN. Initially, `ActPatterns` is initialized with an empty activation pattern (line 1). In each iteration, $\texttt{BaB}_{\texttt{NV}}$ selects and removes an activation pattern σ_i from `ActPatterns`. It then calls `Deduce` to check the feasibility of the problem based on the current activation pattern. (Note that we do this even on the empty activation pattern, which is the initial state of the search, because the problem might be trivially infeasible.)

If `Deduce` determines that the problem is feasible (using the current activation pattern σ_i), it calls `Decide` to select a neuron v_i to split, which essentially means the problem is split into two independent subproblems: one with v_i (active) and the other with $\overline{v_i}$ (inactive). $\texttt{BaB}_{\texttt{NV}}$ then adds the two new activation patterns $\sigma_i \wedge v_i$ and $\sigma_i \wedge \overline{v_i}$ to `ActPatterns`. $\texttt{BaB}_{\texttt{NV}}$ then loops back to line 6 to process the next activation pattern. [TVN]: briefly describe what Decide do? in particular what does it do to determine/create an cex when the activation pattern is partially assigned?

If `Deduce` determines that the problem is infeasible, it loops back to line 6 to process the next activation pattern. $\texttt{BaB}_{\texttt{NV}}$ terminates when there are no more activation patterns to process, at which point it returns `unsat`, indicating that the property is valid.

[TVN]: shows that $\texttt{BaB}_{\texttt{NV}}$ often does not exhaust all activation patterns, but rather prunes the search space by deducing infeasibility of some activation patterns. May be use a tree example to illustrate this?

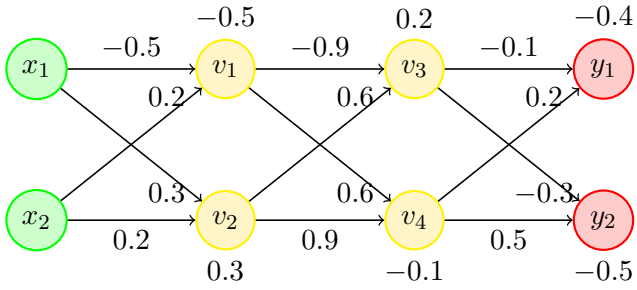


Figure 6.1: A simple DNN (similar to Fig. 2.1)

Example 6.2.1. [TVN]: We should change this example to the 5-neuron DNN we have always been using.Fig. 6.1a illustrates a DNN and how $\texttt{BaB}_{\texttt{NV}}$ verifies that this DNN has the property

$$(x_1, x_2) \in [-2.0, 2.0] \times [-1.0, 1, 0] \Rightarrow (y_1 > y_2).$$

First, $\texttt{BaB}_{\texttt{NV}}$ initializes the activation pattern set `ActPatterns` with an empty activation pattern $\emptyset$ (line 1). Then $\texttt{BaB}_{\texttt{NV}}$ enters a loop (line 6–line 20) to search for a satisfying assignment. In the first iteration, $\texttt{BaB}_{\texttt{NV}}$ selects the only available activation pattern $\emptyset \in$ `ActPatterns`. It calls `Deduce` to check the feasibility of the problem based on the current activation pattern. `Deduce` uses abstraction to approximate that from the input constraints the output values are feasible for the given network. Since `Deduce` cannot decide infeasibility, $\texttt{BaB}_{\texttt{NV}}$ randomly selects a neuron to split (`Decide`). Let us assume that it chooses v_4 to split, which essentially means the problem is split into two independent subproblems: one with v_4 active and the other with v_4 inactive. $\texttt{BaB}_{\texttt{NV}}$ then adds $\{v_4\}$ and $\{\overline{v_4}\}$ to `ActPatterns`.

In the second iteration, $\texttt{BaB}_{\texttt{NV}}$ has two subproblems (that can be processed in parallel). For the first subproblem with v_4, `Deduce` cannot decide infeasibility, so it selects v_2 to split. It then conjoins v_4 with v_2 and then with $\overline{v_2}$ and adds both conjuncts to `ActPatterns`. For the second subproblem with $\overline{v_4}$ inactive, `Deduce` determines that the problem is unsatisfiable.

In the third iteration, $\texttt{BaB}_{\texttt{NV}}$ has two subproblems for $v_4 \wedge v_2$ and $v_4 \wedge \overline{v_2}$. For the first subproblem, `Deduce` cannot decide infeasibility, so it selects v_1 to split. It then conjoins v_1 and then $\overline{v_1}$ to the current activation pattern and adds them to `ActPatterns`. For the second subproblem, `Deduce` determines that the problem is unsatisfiable.

In the fourth iteration, $\texttt{BaB}_{\texttt{NV}}$ has two subproblems for $v_4 \wedge v_2 \wedge v_1$ and $v_4 \wedge v_2 \wedge \overline{v_1}$. Both subproblems are determined to be unsatisfiable.

Finally, $\texttt{BaB}_{\texttt{NV}}$ has an empty `ActPatterns`, stops the search, and returns `unsat`—the property is valid.

6.2.1 Beyond the Basic

What described above is the basic and minimal BaB algorithm. However, modern DNN verifiers implement many optimizations and strategies to improve the performance of the search. For example, they apply various engineering tricks to eliminate easy cases or find easy counterexamples (§7) before running the full BaB search.

Even the BaB search itself is optimized to avoid exploring the entire search space. For example, if `Deduce` step determines infeasibility, a smarter $\texttt{BaB}_{\texttt{NV}}$ variant (e.g., the `NeuralSAT` tool described in §8) can analyze the conflict and add a new clause to the set of clauses (`clauses`) to prevent the same activation pattern from being selected again. This is similar to conflict-driven clause learning (CDCL) in modern SAT solvers and is implemented in the `NeuralSAT` DNN verification tool [18]. In addition, heuristics are also used to select, e.g., which neuron to split next (`Decide`). We explore these optimizations and strategies in Part VI.

Chapter 7

Common Engineerings and Optimizations

A full branch and bound (BaB search (§6) is typically expensive and slow. Thus, DNN verifiers often begin by applying a range of optimizations and engineering techniques that aim to quickly eliminate easy cases, such as when the network has a small number of inputs.

7.1 Input Splitting

Modern DNN verifiers [1, 18, 27, 28] often use a technique called *input splitting* to quickly deal with networks with verification problems involving low-dimensional networks, such as those in the ACAS Xu benchmark §13.1.1 where the networks have a small number of inputs. Currently many work set the threshold to 50 inputs, i.e., if the network has more than 50 inputs, it is considered large and input splitting is not applied.

The idea is to split the original verification problem into subproblems, each checking whether the DNN produces the desired output from a smaller input region and returns `unsat` if all subproblems are verified and `sat` if a counterexample is found in any subproblem. Input splitting avoids BaB search—also called *neuron splitting* and focuses on individual neurons—and is often used as a fast-path optimization to quickly eliminate easy cases.

Example 7.1.1. Given k available threads, `NeuralSAT` splits the original input region to obtain subproblems as described and and runs DPLL(T) on k subproblems in parallel. `NeuralSAT` returns `unsat` if it verifies all subproblems and `sat` if it found a counterexample in any subproblem. For example, we split the input region $\{x_1 \in [-1, 1], x_2 \in [-2, 2]\}$ into four subregions $\{x_1 \in [-1, 0], x_2 \in [-2, 0]\}$, $\{x_1 \in [-1, 0], x_2 \in [0, 2]\}$, $\{x_1 \in [0, 1], x_2 \in [-2, 0]\}$, and $\{x_1 \in [0, 1], x_2 \in [0, 2]\}$. Note that the formula $-1 \leq x_1 \leq 1 \wedge -2 \leq x_2 \leq 2$ representing the original input region

is equivalent to the formula $(-1 \leq x_1 \leq 0 \vee 0 \leq x \leq 1) \wedge (-2 \leq x_2 \leq 0 \vee 0 \leq x_2 \leq 2)$ representing the combination of the created subregions.

7.2 Input Bounds Tightening

For networks with small inputs, DNN verification tools use a more aggressive abstraction process to achieve more precise computation. Specifically, they use LP solving to compute the tightest bounds for all input variables from the generated linear constraints. This computation is efficient when the number of inputs is small.

After tightening input bounds DNN verification tools apply abstraction to approximate the output bounds, which can be more precise with better input bounds. For networks with large number of inputs, we obtain input bounds from the input property ϕ_{in}.[TVN]: Vu: to rewrite

7.3 Adversarial Attacks (§B)

Like other DNN verifiers [21, 51], `NeuralSAT` tool implements a fast-path optimization that attempts to disprove or falsify the property before running DPLL(T). `NeuralSAT` uses two *adversarial attack* algorithms to find counterexamples to falsify properties. First, we try a randomized attack approach [12], which is a derivative-free sampling-based optimization [50], to generate a potential counterexample. If this approach fails, we then use a gradient-based approach [32] to create another potential counterexample.

If either attack algorithm gives a valid counterexample, `NeuralSAT` returns `sat`, indicating that property is invalid. If both algorithms cannot find a counterexample or they exceed a predefined timeout, `NeuralSAT` continues with its DPLL(T) search.

7.4 Multiprocessing

[TVN]: Do we still use this? or we use the Parallel DPLL(T) in §8.3.1.1 instead? For networks with small inputs, `NeuralSAT` uses a simple approach to create and solve subproblems in parallel. Given a verification problem $N_{orig} = (\alpha, \phi_{in}, \phi_{out})$, where α is the DNN and $\phi_{in} \Rightarrow \phi_{out}$ is the desired property, `NeuralSAT` creates subproblems $N_i = (\alpha, \phi_{in_i}, \phi_{out})$, where ϕ_{in_i} is the i-th subregion of the input region specified by ϕ_{in}. Intuitively, each subproblem checks if the DNN produces the output ϕ_{out} from a smaller input region ϕ_{in_i}. The combination of these subproperties $\bigwedge \phi_{in_i} \Rightarrow \phi_{out}$ is logically equivalent to the original property $\phi_{in} \Rightarrow \phi_{out}$.

Given k available threads, `NeuralSAT` splits the original input region to obtain subproblems as described and and runs DPLL(T) on k subproblems in parallel. `NeuralSAT` returns `unsat` if it verifies all subproblems and `sat` if it found a counterexample in any subproblem. For example, we split the input region $\{x_1 \in [-1, 1], x_2 \in$

$[-2, 2]\}$ into four subregions $\{x_1 \in [-1, 0], x_2 \in [-2, 0]\}$, $\{x_1 \in [-1, 0], x_2 \in [0, 2]\}$, $\{x_1 \in [0, 1], x_2 \in [-2, 0]\}$, and $\{x_1 \in [0, 1], x_2 \in [0, 2]\}$. Note that the formula $-1 \leq x_1 \leq 1 \wedge -2 \leq x_2 \leq 2$ representing the original input region is equivalent to the formula $(-1 \leq x_1 \leq 0 \vee 0 \leq x \leq 1) \wedge (-2 \leq x_2 \leq 0 \vee 0 \leq x_2 \leq 2)$ representing the combination of the created subregions.

7.5 GPU Processing

[TVN]: Hai, talk about how modern tools like crown and neuralsat leverage GPU. Give details. Provide small CUDO code and examples as needed.

Chapter 8

The NeuralSAT Algorithm

NeuralSAT [18, 19] is a relatively late competitor in the DNN verification space, but it has quickly become a strong contender, consistently placed among the top tools at DNN verification competitions §14.

At its core, NeuralSAT is BaB, but follows a DPLL(T) framework [13] and includes unique optimizations and heuristics to improve the search performance. Thus, NeuralSAT is essentially an SMT solver with respect to a theory, in this case, the theory of DNNs.

8.1 Overview

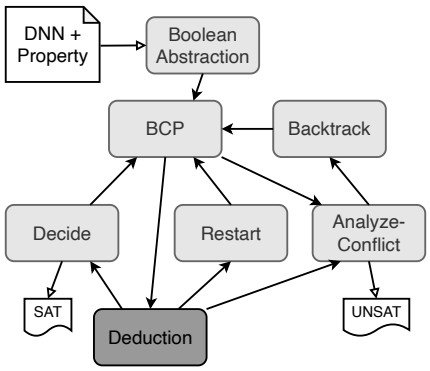


Figure 8.1: The NeuralSAT DPLL(T) Algorithm.

Fig. 8.1 gives an overview of NeuralSAT, which consists of standard DPLL components (light shades) and the theory solver (dark shade). NeuralSAT first constructs a propositional formula over Boolean variables that represent the activation status of neurons (*Boolean Abstraction*). Clauses in the formula assert that each neuron, e.g., neuron i, is active or inactive, e.g., $v_i \vee \overline{v_i}$. This representation enables using standard DPLL to search for truth values satisfying these clauses and a DNN-specific theory solver to check the feasibility of truth assignments with respect to the constraints

encoding the DNN and the property of interest.

`NeuralSAT` now enters an iterative process to find a truth assignment—*activation pattern* (§6.1)—satisfying the activation clauses. First, `NeuralSAT` assigns a truth value to an unassigned variable (*Decide*), detects unit clauses caused by this assignment, and infers additional assignments (*Boolean Constraint Propagation*). Next, `NeuralSAT` invokes the theory solver or T-solver (*Deduction*), which uses LP solving and abstraction to check the satisfiability of the constraints of the current assignment with the property of interest.

If the T-solver confirms satisfiability, `NeuralSAT` continues with new assignments (*Decide*). Otherwise, `NeuralSAT` detects a conflict (*Analyze Conflict*) and learns clauses to remember it and backtrack to a previous decision (*Backtrack*). If `NeuralSAT` detects local optima, it would restart (*Restart*) the search by clearing all decisions that have been made, but save the conflict clauses learned so far to avoid reaching the same state in the next runs. Restarting especially benefits challenging DNN problems by enabling better clause learning and exploring different decision orderings.

This iterative process repeats until `NeuralSAT` can no longer backtrack, and returns `unsat`, indicating the DNN has the property, or it finds a total assignment for all boolean variables, and returns `sat`.

§A provides more details on the `NeuralSAT` algorithm, describing the main components of `NeuralSAT` and how they work together to verify DNNs.

8.2 Illustration

Example 8.2.1. We use `NeuralSAT` to prove that for inputs $x_1 \in [-1, 1], x_2 \in [-2, 2]$ the DNN in Fig. 1.1 produces the output $x_5 \leq 0$. `NeuralSAT` takes as input the formula α representing the DNN:

$$\begin{aligned} x_3 &= \text{ReLU}\left(-0.5x_1 + 0.5x_2 + 1\right) \ \wedge \\ x_4 &= \text{ReLU}\left(x_1 + x_2 - 1\right) \ \wedge \\ x_5 &= -x_3 + x_4 - 1.0 \end{aligned}$$

and the formula ϕ representing the property:

$$\phi : -1 \leq x_1 \leq 1 \wedge -2 \leq x_2 \leq 2 \quad \Rightarrow \quad x_5 \leq 0.$$

To prove $\alpha \Rightarrow \phi$, `NeuralSAT` needs to show that *no* values of x_1, x_2 satisfying the input properties would result in $x_5 > 0$. In other words, `NeuralSAT` needs to return `unsat` for:

$$\alpha \ \wedge \ -1 \leq x_1 \leq 1 \ \wedge \ -2 \leq x_2 \leq 2 \ \wedge \ x_5 > 0. \tag{8.2.1}$$

Notation: In the following, we write $x \mapsto v$ to denote that the variable x is assigned with a truth value $v \in \{T, F\}$. This assignment can be either decided by

Table 8.1: `NeuralSAT`'s run producing `unsat`.

Iter	**BCP**	**DEDUCTION**		**DECIDE**	**ANALYZE-CONFLICT**	
		Constraints	Bounds		Bt	Learned Clauses
Init	-	$I = -1 \leq x_1 \leq 1;$ $-2 \leq x_2 \leq 2$	$-1 \leq x_1 \leq 1;$ $-2 \leq x_2 \leq 2$	-	-	$C = \{v_3 \vee \overline{v_3};\ v_4 \vee \overline{v_4}\}$
1	-	I	$x_5 \leq 1$	$\overline{v_4}$@1	-	-
2	-	$I; x_4 =$ `off`	$x_5 \leq -1$	-	0	$C = C \cup \{v_4\}$
3	v_4@0	$I; x_4 =$ `on`	$x_3 \geq 0.5; x_5 \leq 0.5$	v_3@0	-	-
4	-	$I; x_3 =$ `on`$; x_4 =$ `on`	-	-	**-1**	$C = C \cup \{\overline{v_4}\}$

`Decide` or inferred by `BCP`. We also write $x@dl$ and $\overline{x}@dl$ to indicate the respective assignments $x \mapsto T$ and $x \mapsto F$ at decision level dl.

Boolean Abstraction First, `NeuralSAT` creates two Boolean variables v_3 and v_4 to represent the activation status of the hidden neurons x_3 and x_4, respectively. For example, $v_3 = T$ means x_3 is `active` and thus gives the constraint $-0.5x_1 + 0.5x_2 + 1 > 0$. Similarly, $v_3 = F$ means x_3 is `inactive` and therefore gives $-0.5x_1 + 0.5x_2 + 1 \leq 0$. Next, `NeuralSAT` forms two clauses $\{v_3 \vee \overline{v_3}\ ;\ v_4 \vee \overline{v_4}\}$ ensuring that these variables are either `active` or `inactive`.

DPLL(T) Iterations `NeuralSAT` searches for a satisfying *activation pattern*—truth assignment for the Boolean variables to satisfy the clauses and the constraints they represent with respect to the formula in Eq. 8.2.1. For this example, `NeuralSAT` uses four iterations, summarized in Tab. 8.1, to determine that no such assignment exists and the problem is thus `unsat`.

In *iteration 1*, as shown in Fig. 8.1, `NeuralSAT` starts with `BCP`, which has no effects because the current clauses and (empty) assignment produce no unit clauses. In `Deduction`, `NeuralSAT` uses an LP solver to determine that the current set of constraints, which contains just the initial input bounds, is feasible[1]. `NeuralSAT` then uses abstraction to approximate an output upper bound $x_5 \leq 1$ and thus deduces that satisfying the output $x_5 > 0$ might be feasible. `NeuralSAT` continues with `Decide`, which uses a heuristic to select the unassigned variable v_4 and sets $v_4 = F$—essentially a *guess* that neuron x_4 is inactive. `NeuralSAT` increments the decision level (dl) to 1 and associates $dl = 1$ to the assignment, i.e., $\overline{v_4}$@1.

In *iteration 2*, `BCP` again has no effect because it does not detect any unit clauses. In `Deduction`, `NeuralSAT` determines that current set of constraints, which contains $x_1 + x_2 - 1 \leq 0$ due to the assignment $v_4 \mapsto F$ (i.e., $x_4 =$ `off`), is feasible. `NeuralSAT` then approximates a new output upper bound $x_5 \leq -1$, which means satisfying the output $x_5 > 0$ constraint is *infeasible*.

[1]We use the terms feasible, from the LP community, and satisfiable, from the SAT community, interchangeably.

`NeuralSAT` now enters `AnalyzeConflict` and determines that v_4 causes the conflict (v_4 is the only variable assigned so far). From the assignment $\overline{v_4}$@1, `NeuralSAT` learns a "backjumping" clause v_4, i.e., v_4 must be T. `NeuralSAT` now backtracks to dl 0 and erases all assignments decided *after* this level. Thus, v_4 is now unassigned and the constraint $x_1 + x_2 - 1 \leq 0$ is also removed.

In *iteration 3*, `BCP` determines that the learned clause is also a unit clause v_4 and infers v_4@0. In `Deduction`, we now have the new constraint $x_1 + x_2 - 1 > 0$ due to $v_4 \mapsto T$ (i.e., $x_4 =$ `on`). With the new constraint, `NeuralSAT` approximates the output upper bound $x_5 \leq 0.5$, which means $x_5 > 0$ might be satisfiable. Also, `NeuralSAT` computes new bounds $0.5 \leq x_3 \leq 2.5$ and $0 < x_4 \leq 2.0$, and deduces that x_3 must be positive because its lower bound is 0.5. Thus, `NeuralSAT` has a new assignment v_3@0 (dl stays unchanged due to the implication). This new assignment inference from the T-solver is known as *theory propagation* in DPLL(T).

In *iteration 4*, `BCP` has no effects because we have no new unit clauses. In `Deduction`, `NeuralSAT` determines that the current set of constraints, which contains the new constraint $-0.5x_1 + 0.5x_2 + 1 > 0$ (due to $v_3 \mapsto T$), is *infeasible*. Thus, `NeuralSAT` enters `AnalyzeConflict` and determines that v_4, which was set at $dl = 0$ (by `BCP` in iteration 3), causes the conflict. `NeuralSAT` then learns a clause $\overline{v_4}$ (the conflict occurs due to the assignment $\{v_3 \mapsto T; v_4 \mapsto T\}$, but v_3 was implied and thus making v_4 the conflict). However, because v_4 was assigned at decision level 0, `NeuralSAT` can no longer backtrack and thus sets $dl = -1$ and returns `unsat`, i.e , the property is valid.

8.3 `NeuralSAT`'s Optimizations

`NeuralSAT`implements several optimizations to improve the performance of the search. First are the common optimizations used by other DNN verifiers, such as input splittings (§7) and adversarial attacks (§B). In addition, `NeuralSAT` implements several unique optimizations [19] to improve the performance of the search. These are neuron stability, restart tree, and restart.

8.3.1 Neuron Stability

A neuron is *stable* if its activation status does not change regardless of the input values. In contrast, a neuron is *unstable* if its activation status can change depending on the input values. For example, in the DNN in Fig. 1.1, [TVN]: any neuron stable? or they are all unstable?

The key idea in using neuron stability is that if we can determine that a neuron is stable, we can assign the exact truth value for the corresponding Boolean variable instead of having to guess. This has a similar effect as `BCP`—reducing mistaken assignments by `Decide`—but it operates at the theory level instead of the propositional Boolean level.

Algorithm 2. `Stabilize`

input : DNN α, property $\phi_{in} \Rightarrow \phi_{out}$, current assignment σ, number of neurons for stabilization k

output : Tighten bounds for variables **not** in σ (unassigned variables)

```
model ← MIP(α, φ_in, φ_out, σ) // create model ( Eq. 12.3.1) with current assignment
[v_1, ..., v_m] ← GetUnassignedVariable(σ) // get all m current unassigned variables
[v'_1, ..., v'_m] ← Sort([v_1, ..., v_m]) // prioritize tightening order
[v'_1, ..., v'_k] ← Select([v'_1, ..., v'_m], k) // select top-k unassigned variables, k ≤ m
// stabilize k neurons in parallel
parfor v_i in [v'_1, ..., v'_k] do
    if (v_i.lower + v_i.upper) ≥ 0 then // lower is closer to 0 than upper, optimize lower first
        Maximize(model, v_i.lower) // tighten lower bound of v_i
        if v_i.lower < 0 then // still unstable
            Minimize(model, v_i.upper) // tighten upper bound of v_i
    else // upper is closer to 0 than lower, optimize upper first
        Minimize(model, v_i.upper) // tighten upper bound of v_i
        if v_i.upper > 0 then // still unstable
            Maximize(model, v_i.lower) // tighten lower bound of v_i
```

Stabilization involves the solution of a mixed integer linear program (MILP) system [45]:

$$
\begin{aligned}
&\text{(a)} \quad z^{(i)} = W^{(i)}\hat{z}^{(i-i)} + b^{(i)};\\
&\text{(b)} \quad y = z^{(L)}; x = \hat{z}^{(0)};\\
&\text{(c)} \quad \hat{z}_j^{(i)} \geq z_j^{(i)}; \hat{z}_j^{(i)} \geq 0;\\
&\text{(d)} \quad a_j^{(i)} \in \{0, 1\};\\
&\text{(e)} \quad \hat{z}_j^{(i)} \leq a_j^{(i)} u_j^{(i)}; \hat{z}_j^{(i)} \leq z_j^{(i)} - l_j^{(i)}(1 - a_j^{(i)});
\end{aligned}
\tag{8.3.1}
$$

where x is input, y is output, and $z^{(i)}$, $\hat{z}^{(i)}$, $W^{(i)}$, and $b^{(i)}$ are the pre-activation, post-activation, weight, and bias vectors for layer i. The equations encode the semantics of a DNN as follows: (a) defines the affine transformation computing the pre-activation value for a neuron in terms of outputs in the preceding layer; (b) defines the inputs and outputs in terms of the adjacent hidden layers; (c) asserts that post-activation values are non-negative and no less than pre-activation values; (d) defines that the neuron activation status indicator variables that are either 0 or 1; and (e) defines constraints on the upper, $u_j^{(i)}$, and lower, $l_j^{(i)}$, bounds of the pre-activation value of the jth neuron in the ith layer. Deactivating a neuron, $a_j^{(i)} = 0$, simplifies the first of the (e) constraints to $\hat{z}_j^{(i)} \leq 0$, and activating a neuron simplifies the second to $\hat{z}_j^{(i)} \leq z_j^{(i)}$, which is consistent with the semantics of $\hat{z}_j^{(i)} = max(z_j^{(i)}, 0)$.

Alg. 5 describes Stabilize solves this equation system. First, a MILP problem is

created from the current assignment, the DNN, and the property of interest using formulation in Eq. 12.3.1. Note that the neuron lower ($l_j^{(i)}$) and upper bounds ($u_j^{(i)}$) can be quickly computed by polytope abstraction.

Next, it collects a list of all unassigned variables which are candidates being stabilized (line 2). In general, there are too many unassigned neurons, so `Stabilize` restricts consideration to k candidates. Because each neuron has a different impact on abstraction precision we prioritize the candidates. In `Stabilize`, neurons are prioritized based on their interval boundaries (line 3) with a preference for neurons with either lower or upper bounds that are closer to zero. The intuition is that neurons with bounds close to zero are more likely to become stable after tightening.

We then select the top-k (line 4) candidates and seek to further tighten their interval bounds. The order of optimizing bounds of select neurons is decided by its boundaries, e.g., if the lower bound is closer to zero than the upper bound then the lower bound would be optimized first. These optimization processes, i.e., `Maximize` (line 11 or line 17) and `Minimize` (line 13 or line 15), are performed by an external LP solver (e.g., Gurobi [24]).

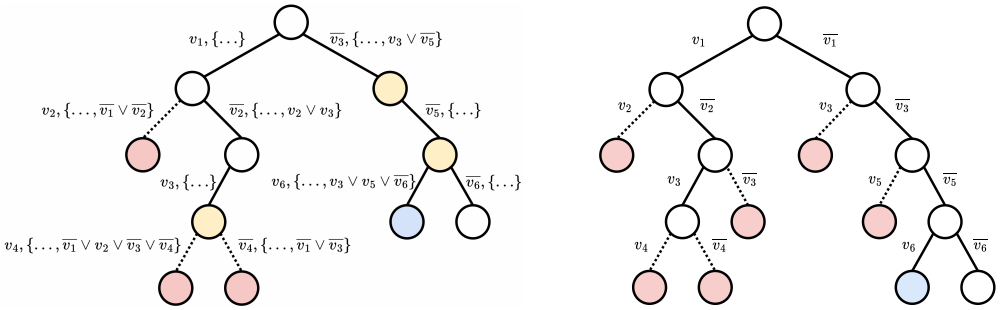
Example 8.3.1. [TVN]: Need a concrete example here. Use the DNN in Fig. 1.1 and create the MILP system in Eq. 12.3.1.

8.3.1.1 Parallel Search

The DPLL(T) process in `NeuralSAT` is designed as a tree-search problem where each internal node encodes an *activation pattern* defined by the variable assignments from the root. To parallelize DPLL(T), we adopt a beam search-like strategy which combines distributed search from Distributed Tree Search (DTS) algorithm [20] and Divide and Conquer (DNC) [**?**] paradigms for splitting the search space into disjoint subspaces that can be solved independently. At every step of the search algorithm, we select up to n nodes of the DPLL(T) search tree to create a beam of width n. This splits (like DNC) the search into n subproblems that are independently processed. Each subproblem extends the tree by a depth of 1.

Our approach simplifies the more general DNC scheme since the n bodies of the **parfor** on line **??** of Alg. 6 are roughly load balanced. While this is a limited form of parallelism, it sidesteps one of the major roadblocks to DPLL parallelism – the need to efficiently synchronize across load-imbalanced subproblems [**?**, 31].

In addition to raw speedup due to multiprocessing, parallelism accelerates the sharing of information across search subspaces, in particular learned clause information for DPLL. In `NeuralSAT`, we only generate independent subproblems which eliminates the need to coordinate their solution. When all subproblems are complete, their conflicts are accumulated, Alg. 6 line **??**, to inform the next round of search. As we show in S**??**, the engineering of this form of parallelism in DPLL(T) leads to substantial performance improvement.



(a) `NeuralSAT` (b) Others

Figure 8.2: Search tree explored by `NeuralSAT` (a) and other verifiers (b) during a verification run. [TVN]: Hai, instead of other verifiers can we say this search tree is for a native/general BaB approach? The notation {...} indicates learned clauses; red is infeasibility; white is feasibility; yellow is BCP application; and blue is current consideration. The search tree of `NeuralSAT` is smaller than the tree of the other techniques because `NeuralSAT` was able to prune various branches, e.g., through BCPs (e.g., v_3 and $\overline{v_5}$) and non-chronological backtracks (e.g., $\overline{v_3}$).

8.3.2 Restart

As with any stochastic algorithm, `NeuralSAT` would perform poorly if it gets into a subspace of the search that does not quickly lead to a solution, e.g., due to choosing a bad sequence of neurons to split [15,21,47]. This problem, which has been recognized in early SAT solving, motivates the introduction of restarting the search [22] to avoid being stuck in such a *local optima*.

`NeuralSAT` uses a simple restart heuristic that triggers a restart when either the number of processed assignments (nodes) exceeds a pre-defined number or the number of remaining assignments that need be checked exceeds a pre-defined threshold. After a restart, `NeuralSAT` avoids using the same decision order of previous runs (i.e., it would use a different sequence of neuron splittings). It also resets all internal information except the learned conflict clauses, which are kept and reused as these are *facts* about the given constraint system. This allows a restarted search to quickly prune parts of the space of assignments. Although restarting may seem like an engineering aspect, it plays a crucial role in stochastic algorithms, and helps `NeuralSAT` reduce verification time for challenging problemsk.

8.4 `NeuralSAT` vs. BaB

[TVN]: TODO: talk about how `NeuralSAT` is BaB but has things such as CDCL to help prune the search space.

[TVN]: rewrite: technically we don't split if the guess was right Note that this process of selecting and assigning (guessing) values to variables representing neurons is the *branching* phase in BaB. It is also commonly called *neuron splitting* because

it splits the search tree into subtrees corresponding into the assigned values (e.g., see §8.4).

As mentioned in §3.3, ReLU-based DNN verification is NP-complete, and for difficult problem instances DNN verification tools often have to exhaustively search a very large space, making scalability a main concern for modern DNN verification.

Fig. 8.2 shows the difference between `NeuralSAT` and another DNN verification tool (e.g., using the popular Branch-and-Bound (BaB) approach) in how they navigate the search space. We assume both tools employ similar abstraction and neuron splitting. Fig. 8.2b shows that the other tool performs splitting to explore different parts of the tree (e.g., splitting v_1 and explore the branches with $v_1 = T$ and $v_1 = F$ and so on). Note that the other tool needs to consider the tree shown regardless if it runs sequentially or in parallel.

In contrast, `NeuralSAT` has a smaller search space shown in Fig. 8.2a. `NeuralSAT` follows the path v_1, v_2 and then $\overline{v_2}$ (just like the tool on the right). However, because of the learned clause $v_2 \vee v_3$, `NeuralSAT` performs a BCP step that sets v_3 (and therefore prunes the branch with $\overline{v_3}$ that needs to be considered in the other tree). Then `NeuralSAT` splits v_4, and like the other tool, determines infeasibility for both branches. Now `NeuralSAT`'s conflict analysis determines from learned clauses that it needs to backtrack to v_3 (yellow node) instead of v_1. Without learned clauses and non-chronological backtracking, `NeuralSAT` would backtrack to decision v_1 and continues with the $\overline{v_1}$ branch, just like the other tool in Fig. 8.2b.

Thus, `NeuralSAT` was able to generate non-chronological backtracks and use BCP to prune various parts of the search tree. In contrast, the other tool would have to move through the exponential search space to eventually reach the same result as `NeuralSAT`.

Chapter 9

The Reluplex Algorithm

Reluplex [26] is a classical BaB (§6) approach for verifying neural networks. The technique extends the simplex method [36] to support the ReLU activation function (**Reluplex** = **Relu** + Sim**plex**). Reluplex has been succeeded by the Marabou [28] tool, which are more efficient and scalable. However, the core ideas of Reluplex are still relevant and therefore we present it here.

9.1 Illustration

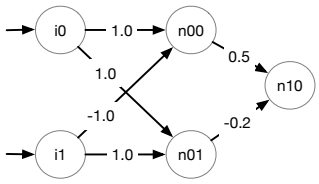


Figure 9.1: A DNN example

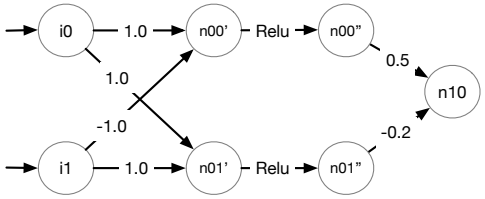


Figure 9.2: Separating nodes to represent RELU

Example 9.1.1. We use the DNN in Fig. 9.1 to demonstrate Reluplex. Assume we want to check that the DNN has the property

$$(0 \leq i_0 \leq 0.5 \wedge -2 \leq i_1 \leq -1) \implies (n_{10} < 0 \vee n_{10} > 0.5). \tag{9.1.1}$$

That is, when the inputs i_0, i_1 fall within certain ranges, then the result n_{10} has certain values. As mentioned in 3.2, we turn this into a satisfiability problem by negating the property and checking if the negation is unsatisfiable. In this case, we want to check if the negation of Eq. 9.1.1 is unsat:

$$(0 \leq i_0 \leq 0.5 \wedge -2 \leq i_1 \leq -1) \wedge 0 \leq n_{10} \leq 0.5. \tag{9.1.2}$$

If Eq. 9.1.2 is unsat, then the DNN satisfies the property in Eq. 9.1.1—there exists no assignment of the inputs i_0, i_1 such that the output n_{10} is within the

range $[0, 0.5]$. Otherwise, the DNN does not have the property and we can return a counterexample.

Problem Encoding A DNN can be encoded as a conjunctions of constraints. The ReLU node v can be encoded as a pair of variables v' and v'', where v' is used to connect the nodes of previous layers to v, and v'' is used to connect v to the next layer.

For example, in Fig. 9.1, the ReLU node $n00 = \max(i0 - 1i1, 0)$ is encoded using two variables $n00' = i0 - 1i1$ and $n00'' = \max(n00', 0)$. The DNN inFig. 9.2 shows the network in Fig. 9.1 with additional nodes representing ReLU encoding.

The first step to use Repluplex is to encode the constraints representing the DNN and the problem into a format that Reluplex accepts. The DNN in Fig. 9.1 can be encoded as a conjunction of equalities:

$$\begin{aligned} n00' &= i_0 - i_1, \quad n00'' = \max(n00', 0), \\ n01' &= i_0 + i_1, \quad n01'' = \max(n01', 0), \\ n_{10} &= 0.5n00'' - 0.2n01'' \end{aligned}$$

Basic Variables We also introduce three new *basic* (auxilliary or slack) variables to store the relationships of the DNN's constraints:

$$a_1 = i_0 - v_{12}^b - n00', \tag{9.1.3}$$

$$a_2 = i_0 + v_{12}^b - n01', \tag{9.1.4}$$

$$a_3 = 0.5n00'' - 0.2n01'' - n_{10} \tag{9.1.5}$$

In simplex terminology, a basic variable is a variable that is used to represent the relationship between other variables in the constraints. For example, a_1 represents the difference between i_0, v_{12}^b, and $n00'$. The basic variables are used to maintain the relationships between the variables in the constraints and are updated during the search process.

In contrast, a *non-basic* variable is a variable that is not used to represent the relationship between other variables in the constraints. For example, i_0 and i_1 are non-basic because they are not used to represent the relationship between other variables in the constraints. Non-basic variables are typically the input variables of the DNN.

Iteration `Reluplex` first assigns 0 to all [TVN]: basic? variables in the constraints in Eq. 9.1.3– Eq. 9.1.5. This assignment—essentially an initial guess—would likely cause issues such as variables violating their bounds. `Reluplex` works by iteratively fixing these invalid values until it finds a feasible assignment (and returns `sat`) or cannot do so (and returns `unsat`).

This iterative updating process can be demonstrated through a sequence of configuration updates over the variables. Tab. 9.1 shows the initial configuration with all values assigned to 0. Observe that the lower and upper bounds of the inputs i_0, i_1 and output n_{10} are specified in the property in Eq. 9.1.2, the lower bounds of v_f's representing ReLU are 0, and the other hidden variables are unbounded.

	i_0	i_1	$n00'$	$n00''$	$n01'$	$n01''$	n_{10}	a_1	a_2	a_3
LB	0	-2	$-\infty$	0	$-\infty$	0	0	0	0	0
Val	0	0	0	0	0	0	0	0	0	0
UP	0.5	-1	∞	∞	∞	∞	0.5	0	0	0

Table 9.1: Configuration #1

Tab. 9.1 shows that i_1 is out-of-bounds because $0 \notin [-2, -1]$. To fix i_1, which is non-basic, Reluplex simply updates it to a valid value, e.g., i_1`+=` $-1.0 = -1.0$, which means adding -1.0 to the current value of i_1 and thus having $i_1 = -1.0$. Now, because a_1, a_2 depend on i_1 as shown in Eq. 9.1.3 and Eq. 9.1.4, respectively, this update to i_1 also changes a_1, a_2:

$$a_1 \mathrel{+}= 1.0 = 1.0 \text{ because } a_1 = i_0 - i_1 - n00',$$
$$a_2 \mathrel{+}= -1.0 = -1.0 \text{ because } a_2 = i_0 + i_1 - n01'.$$

Tab. 9.2 shows the new configuration. Tab. 9.2 also shows a_1, a_2 violate their bounds and need to be fixed. Assume Reluplex picks a_1. To fix a_1, which is a basic variable, Reluplex pivots (swaps) it with one of the variables it depends on as shown in the constraint $a_1 = i_0 - v_{12}^b - n00'$ in Eq. 9.1.3. Assume Reluplex pivots a_1 with $n00'$, we get

$$n00' = i_0 - v_{12}^b - a_1. \tag{9.1.6}$$

	i_0	i_1	$n00'$	$n00''$	$n01'$	$n01''$	n_{10}	a_1	a_2	a_3
LB	0	-2	$-\infty$	0	$-\infty$	0	0	0	0	0
Val	0	**-1**	0	0	0	0	0	**1**	**-1**	0
UP	0.5	-1	∞	∞	∞	∞	0.5	0	0	0

Table 9.2: Configuration #2

Reluplex now updates the non-basic a_1 to 0 ($a_1 \mathrel{+}= -1.0 = 0$). This also changes $n00'$ to 1.0 ($n00' \mathrel{+}= 1.0 = 1.0$) because $n00'$ depends on a_1 as shown in Eq. 9.1.6.

Tab. 9.3 shows the new configuration. Tab. 9.3 also shows the basic variable a_2 is out-of-bound. To fix it, Reluplex pivots a_2 with a variable it depends on as shown in the constraint $a_2 = i_0 + v_{12}^b - n01'$ in Eq 9.1.4. Assume Reluplex pivots a_2 with $n01'$, we get

$$n01' = i_0 + v_{12}^b - a_2 \tag{9.1.7}$$

	i_0	i_1	$n00'$	$n00''$	$n01'$	$n01''$	n_{10}	a_1	a_2	a_3
LB	0	-2	$-\infty$	0	$-\infty$	0	0	0	0	0
Val	0	-1	**1**	0	0	0	0	**0**	-1	0
UP	0.5	-1	∞	∞	∞	∞	0.5	0	0	0

Table 9.3: Configuration #3

Now a_2 becomes non-basic and is updated to 0 through $a_2 += 1.0 = 0$. As $n01'$ depends on a_1 as shown in Eq. 9.1.7, we make the change $n01'$ `-=` $1.0 = -1.0$.

	i_0	i_1	$n00'$	$n00''$	$n01'$	$n01''$	n_{10}	a_1	a_2	a_3
LB	0	-2	$-\infty$	0	$-\infty$	0	0	0	0	0
Val	0	-1	1	0	**-1**	0	0	0	**0**	0
UP	0.5	-1	∞	∞	∞	∞	0.5	0	0	0

Table 9.4: Configuration #4

Tab. 9.4 shows the new configuration. At this point, we no longer have out-of-bound variables, but have inconsistent values for the pair of RELU variables $n00', n00''$. This is because $n00'' = \max(n00', 0)$ but we have $n00' = 1$ thus $\max(1, 0) = 1$, which is not $n00'' = 0$. Thus, Reluplex needs to fix either $n00''$ or $n00'$.

Assume Reluplex picks $n00''$. Because $n00''$ is non-basic, we simply update it, i.e., $n00'' = +1 = 1$. As a_3 depends on $n01''$, i.e., $a_3 = 0.5n00'' - 0.2n01'' - n_{10}$, Reluplex also makes the change $a_3 += 0.5 \times 1.0 = 0.5$.

	i_0	i_1	$n00'$	$n00''$	$n01'$	$n01''$	n_{10}	a_1	a_2	a_3
LB	0	-2	$-\infty$	0	$-\infty$	0	0	0	0	0
Val	0	-1	1	**1**	-1	0	0	0	0	**0.5**
UP	0.5	-1	∞	∞	∞	∞	0.5	0	0	0

Table 9.5: Configuration #5

Tab. 9.5 shows the new configuration. In the new configuration, a_3 is out-of-bound. To fix this basic variable, we pivot a_3 with one of the variables $n00'', n01'', n_{10}$ because of the constraint $a_3 = 0.5n00'' - 0.2n01'' - n_{10}$ in Eq. 9.1.5. Assume we pivot a_3 with n_{10}, we get

$$n_{10} = 0.5n00'' - 0.2n01'' - a_3 \tag{9.1.8}$$

Now, a_3 becomes non-basic and we update it to 0 through $a_3 += -0.5 = 0$. As n_{10} depends on a_3 as shown in Eq 9.1.8, we make the change $n_{10} += 0.5 = 0.5$.

Tab. 9.6 shows the new configuration. At this point, Reluplex no longer has any out-of-bound or inconsinstent values, and thus stops and returns `sat` with the values

	i_0	i_1	$n00'$	$n00''$	$n01'$	$n01''$	n_{10}	a_1	a_2	a_3
LB	0	-2	$-\infty$	0	$-\infty$	0	0	0	0	0
Val	0	-1	1	**1**	-1	0	**0.5**	0	0	**0**
UP	0.5	-1	∞	∞	∞	∞	0.5	0	0	0

Table 9.6: Configuration #6

in the **Val** row in Tab. 9.6 as the satisfying assignment for the formula in Eq 9.1.2.

Thus, in this example, we conclude that property in Eq. 9.1.1 is *not valid* for the DNN in Fig. 9.1 because for the inputs $i_0 = 0, v_{-12} = -1$, the DNN gives the output $n_{10} = 0.5$, which violates the property in Eq. 9.1.1.

9.2 Excercises

Problem 9.2.1. Consider the DNN in Fig. 9.1 and the property in Eq. 9.1.1. Use `Reluplex` to verify the property. If you find a counterexample, provide it. You will need to provide all the steps in the `Reluplex` algorithm, e.g., DNN encoding, basic variable encoding, and the `Reluplex` search through a series of configurations as shown in Ex. 9.1.1.

Chapter 10

GPU and Multicore Parallelism

Part IV

Survey of DNN Verification Tools

Chapter 11

Popular Techniques and Tools

Part V

Advanced Topics

Chapter 12

Proof Generation and Checking

As DNN tools become more complex (e.g., SOTA tools have 20K LoCs), they are more prone to bugs. VNN-COMP'23 [9] showed that 3 of the top 7 participants produced unsound results by claiming unsafe DNNs are safe, i.e., they produce `unsat` on problems that are actually `sat`. This is a serious issue, as it can lead to unsafe DNNs being deployed in safety-critical applications, such as autonomous driving and medical diagnosis.

While checking counterexamples is relatively straightforward (we can just evaluate the DNN on the input), checking `unsat` results—proving no counterexample exists—is far more challenging. This would require verifiers to track their decision steps, which are often complex and large.

12.1 Proof Generation

A proof of satisfiability (sat) is an input that violates the property, i.e., a counterexample. We can easily check such a counterexample c by evaluating $\phi(c, N(c))$ (i.e., running the DNN on the counterexample). In fact, VNN-COMPs already requires competing DNN verification tools to return counterexamples demonstrating satisfiability.

In contrast, the proof of an unsatisfiability result (which explains why *no possible inputs* can violate the property) is inherently more complex to generate (§12.1), requires a more sophisticated encoding (§12.2), and an efficient checking algorithm (§12.3). We are mainly interested in `unsat` proofs.

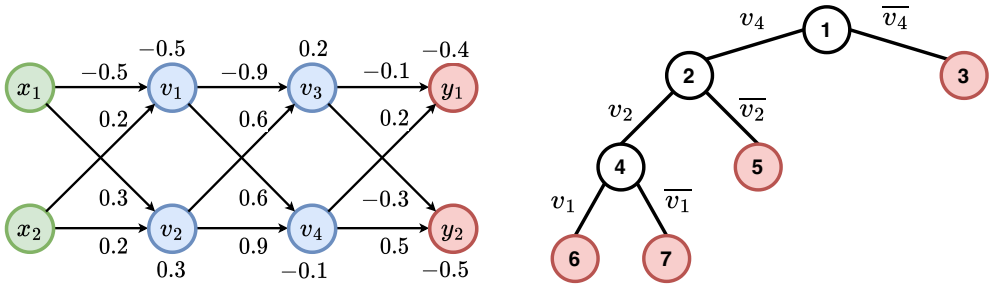
12.1.1 Proof Generation for Branch and Bound (BaB) Algorithms

As mentioned in §6, major DNN verification techniques share the common "branch and bound" (BaB) search algorithm. The BaB structure, shown in Alg. 1, splits the problem into smaller subproblems and use abstraction to compute bounds to prune

Algorithm 3. The $\texttt{BaB}_{\texttt{ProofGen}}$ DNN verification with proof generation.

input : DNN $\mathcal{N}$, property $\phi_{in} \Rightarrow \phi_{out}$
output : (unsat, proof) if property is valid, otherwise (sat, cex)

```
1  ActPatterns ← {∅} // initialize verification problems
2  proof ← { } // initialize proof tree
3  while ActPatterns do // main loop
4      σ_i ← Select(ActPatterns) // process problem i-th
5      if Deduce(N, φ_in, φ_out, σ_i) then
6          (cex, v_i) ← Decide(N, φ_in, φ_out, σ_i)
7          if cex then // found a valid counter-example
8              return (sat, cex)
           // create new activation patterns
9          ActPatterns ← ActPatterns ∪ {σ_i ∧ v_i ; σ_i ∧ ¬v_i}
10     else // detect a conflict
11         proof ← proof ∪ {σ_i} // build proof tree
12 return (unsat, proof)
```



(a) (b)

Figure 12.1: (a) A simple DNN (a redrawn of Fig. 6.1), and (b) A proof tree produced verifying the property $(x_1, x_2) \in [-2.0, 2.0] \times [-1.0, 1, 0] \Rightarrow (y_1 > y_2)$.

the search space. This commonality allows us to bring proof generation capabilities with minimal overhead to existing DNN verification tools.

Alg. 3 extends Alg. 1 to show $\texttt{BaB}_{\texttt{ProofGen}}$, a BaB-based DNN verification algorithm with proof generation capability. The key idea is to introduce a proof tree (line 2) and recording the branching decisions to the proof tree (line 11). The proof tree is a binary tree structure, where each node represents a neuron and its left and right edges represent its activation decision (active or inactive). At the end of the verification process, the proof tree is returned as the proof of `unsat` result.

Example We reuse the example in §6 to illustrate $\texttt{BaB}_{\texttt{ProofGen}}$. Recall the goal is to verify that the DNN in Fig. 12.1(a) (a redraw of Fig. 6.1) has the property $(x_1, x_2) \in [-2.0, 2.0] \times [-1.0, 1, 0] \Rightarrow (y_1 > y_2)$. $\texttt{BaB}_{\texttt{ProofGen}}$ generates the proof tree

in Fig. 12.1(b) to show unsatisfiability, i.e., the property is valid.

First, $\texttt{BaB}_{\texttt{ProofGen}}$ initializes the activation pattern set `ActPatterns` with an empty activation pattern $\emptyset$. Then $\texttt{BaB}_{\texttt{ProofGen}}$ enters a loop (line 6-line 20) to search for a satisfying assignment or a proof of unsatisfiability. In the first iteration, $\texttt{BaB}_{\texttt{ProofGen}}$ selects the only available activation pattern $\emptyset \in$ `ActPatterns`. It calls `Deduce` to check the feasibility of the problem based on the current activation pattern. `Deduce` uses abstraction to approximate that from the input constraints the output values are feasible for the given network. Since `Deduce` cannot decide infeasibility, $\texttt{BaB}_{\texttt{ProofGen}}$ randomly selects a neuron to split (`Decide`). Let us assume that it chooses v_4 to split, which essentially means the problem is split into two independent subproblems: one with v_4 active and the other with v_4 inactive. $\texttt{BaB}_{\texttt{ProofGen}}$ then adds v_4 and $\overline{v_4}$ to `ActPatterns`.

In the second iteration, $\texttt{BaB}_{\texttt{ProofGen}}$ has two subproblems (that can be processed in parallel). For the first subproblem with v_4, `Deduce` cannot decide infeasibility, so it selects v_2 to split. It then conjoins v_4 with v_2 and then with $\overline{v_2}$ and adds both conjuncts to `ActPatterns`. For the second subproblem with $\overline{v_4}$ inactive, `Deduce` determines that the problem is unsatisfiable and $\texttt{BaB}_{\texttt{ProofGen}}$ saves the node v_4 to the proof tree, as node 3, to indicate one unsatisfiable pattern, i.e., whenever the network has v_4 being inactive, the problem is unsatisfiable.

In the third iteration, $\texttt{BaB}_{\texttt{ProofGen}}$ has two subproblems for $v_4 \wedge v_2$ and $v_4 \wedge \overline{v_2}$. For the first subproblem, `Deduce` cannot decide infeasibility, so it selects v_1 to split. It then conjoins v_1 and then $\overline{v_1}$ to the current activation pattern and adds them to `ActPatterns`. For the second subproblem, `Deduce` determines that the problem is unsatisfiable and $\texttt{BaB}_{\texttt{ProofGen}}$ saves the node $v_4 \wedge \overline{v_2}$ to the proof tree, as node 5.

In the fourth iteration, $\texttt{BaB}_{\texttt{ProofGen}}$ has two subproblems for $v_4 \wedge v_2 \wedge v_1$ and $v_4 \wedge v_2 \wedge \overline{v_1}$. Both subproblems are determined to be unsatisfiable, and $\texttt{BaB}_{\texttt{ProofGen}}$ saves them to the proof tree as nodes 6 and 7, respectively.

Finally, $\texttt{BaB}_{\texttt{ProofGen}}$ has an empty `ActPatterns`, stops the search, and returns `unsat` and the proof tree.

12.2 Proof Language

In §12.1 we have shown that the BaB class of DNN verification techniques can generate a binary tree that represents a proof of unsatisfiability. Rather than record such proofs in an verifier-specific format, it is more desirable to have a standard format that is human-readable, is compact, can be efficiently generated by verification tools, and can be efficiently and independently processed by proof checkers.

To meet this goal, we introduce $\texttt{BaB}_{\texttt{ProofLang}}$, a proof language to specify DNN proofs. This language is inspired by the SMTLIB format [4] used for SMT solving, which has also been adopted by the VNNLIB language [44] to specify DNNs and their properties for verification.

$$
\begin{aligned}
\langle \textit{proof} \rangle &::= \langle \textit{declarations} \rangle\ \langle \textit{assertions} \rangle \\
\langle \textit{declarations} \rangle &::= \langle \textit{declaration} \rangle \mid \langle \textit{declaration} \rangle\ \langle \textit{declarations} \rangle \\
\langle \textit{declaration} \rangle &::= (\textbf{declare-const}\ \langle \textit{input-vars} \rangle\ \textbf{Real}) \\
&\quad \mid (\textbf{declare-const}\ \langle \textit{output-vars} \rangle\ \textbf{Real}) \\
&\quad \mid (\textbf{declare-pwl}\ \langle \textit{hidden-vars} \rangle\ \langle \textit{activation} \rangle) \\
\langle \textit{input-vars} \rangle &::= \langle \textit{input-var} \rangle \mid \langle \textit{input-var} \rangle\ \langle \textit{input-vars} \rangle \\
\langle \textit{output-vars} \rangle &::= \langle \textit{output-var} \rangle \mid \langle \textit{output-var} \rangle\ \langle \textit{output-vars} \rangle \\
\langle \textit{hidden-vars} \rangle &::= \langle \textit{hidden-var} \rangle \mid \langle \textit{hidden-var} \rangle\ \langle \textit{hidden-vars} \rangle \\
\langle \textit{activation} \rangle &::= \text{ ReLU} \mid \text{Leaky ReLU} \mid \ldots \\
\langle \textit{assertions} \rangle &::= \langle \textit{assertion} \rangle \mid \langle \textit{assertion} \rangle\ \langle \textit{assertions} \rangle \\
\langle \textit{assertion} \rangle &::= (\textbf{assert}\ \langle \textit{formula} \rangle) \\
\langle \textit{formula} \rangle &::= (\langle \textit{operator} \rangle\ \langle \textit{term} \rangle\ \langle \textit{term} \rangle) \\
&\quad \mid (\textbf{and}\ \langle \textit{formula} \rangle +) \mid (\textbf{or}\ \langle \textit{formula} \rangle +) \\
\langle \textit{term} \rangle &::= \langle \textit{input-var} \rangle \mid \langle \textit{output-var} \rangle \\
&\quad \mid \langle \textit{hidden-var} \rangle \mid \langle \textit{constant} \rangle \\
\langle \textit{operator} \rangle &::= < \mid \leq \mid > \mid \geq \\
\langle \textit{input-var} \rangle &::= \text{X\_}\langle \textit{constant} \rangle \\
\langle \textit{output-var} \rangle &::= \text{Y\_}\langle \textit{constant} \rangle \\
\langle \textit{hidden-var} \rangle &::= \text{N\_}\langle \textit{constant} \rangle \\
\langle \textit{constant} \rangle &::= \textbf{Int} \mid \textbf{Real}
\end{aligned}
$$

Figure 12.2: The $\texttt{BaB}_{\texttt{ProofLang}}$ proof language.

```
; Declare variables
(declare-const X_0 X_1 Real)
(declare-const Y_0 Y_1 Real)
(declare-pwl N_1 N_2 N_3 N_4 ReLU)

; Input constraints
(assert (>= X_0 -2.0))
(assert (<= X_0  2.0))
(assert (>= X_1 -1.0))
(assert (<= X_1  1.0))

; Output constraints
(assert (<= Y_0 Y_1))

; Hidden constraints
(assert (or
    (and (<  N_4 0))
    (and (<  N_2 0) (>= N_4 0))
    (and (>= N_2 0) (>= N_1 0) (>= N_4 0))
    (and (>= N_2 0) (<  N_1 0) (>= N_4 0))))
```

Figure 12.3: $\texttt{BaB}_{\texttt{ProofLang}}$ example format of the proof tree in Fig. 12.1b.

Fig. 12.2 outlines the $\texttt{BaB}_{\texttt{ProofLang}}$ syntax and grammar, represented as production rules. A proof is composed of *declarations* and *assertions*. Declarations define the variables and their types within the proof. Specifically, *input variables* (prefixed with `X`) and *output variables* (prefixed with `Y`) are declared as real numbers, representing the inputs and outputs of the neural network, respectively. Additionally, *hidden variables* are declared with specific piece-wise linear (PWL) activation functions, such as ReLU or Leaky ReLU. These hidden variables correspond to the internal nodes of the neural network that process the input data through various activation functions.

Assertions are logical statements that specify the conditions or properties that must hold within the proof. Assertions over input variables are *preconditions* and those over output variables are *post-conditions*. Each assertion is composed of a *formula*, which can involve terms and logical operators. Formulas include simple comparisons between terms (e.g., less than, greater than) or more complex logical combinations using `and` and `or` operators. The terms used in these formulas can be input variables, output variables, hidden variables, or constants.

The `declare-*` statements declare input, output, and hidden variables, while the `assert` statements specify the constraints on these variables (i.e., the pre and postcondition of the desired property). The hidden constraints represent the activation patterns of the hidden neurons in the network (i.e., the proof tree). Each `and` statement represents a tree path that represents an activation pattern.

Example 12.2.1. The proof in Fig. 12.3 corresponds to the proof tree in Fig. 12.1b. The statement `(and (< N_4 0))` corresponds to the rightmost path of the tree with $\overline{v_4}$ decision (leaf 3). The statement `(and (< N_2 0) (>= N_4 0))` corresponds to

the path with $v_4 \wedge \overline{v_2}$ (leaf 5).

The $\texttt{BaB}_{\texttt{ProofLang}}$ language is intentionally designed to (a) not explicitly include weights/bias terms to minimize size of the proof structure, and (b) explicitly reflect a DNF structure to enable easy parallelization. The DNN weight and bias terms are readily available in the standard ONNX [38] format, which is typically used to represent the DNN input to a $\texttt{BaB}_{\texttt{ProofGen}}$-based DNN verification tool and can be accessed by any $\texttt{BaB}_{\texttt{ProofLang}}$ checker like the one described next in §12.3.

12.3 Proof Checker

Finally, we need to check that the generated proof is correct and that the original NN verification problem is indeed unsatisfiable. The checker must be efficient to handle large proofs and trusted of its results (if it verifies the proof, then the original NNV problem is proved).

To achieve this, we present $\texttt{BaB}_{\texttt{ProofCheck}}$, a proof checker for $\texttt{BaB}_{\texttt{ProofLang}}$ proofs. $\texttt{BaB}_{\texttt{ProofCheck}}$ is verifier-independent and support $\texttt{BaB}_{\texttt{ProofLang}}$ proofs generated by different verification tools. $\texttt{BaB}_{\texttt{ProofCheck}}$ also has several optimizations to handle large proofs efficiently.

12.3.1 The Core $\texttt{BaB}_{\texttt{ProofCheck}}$ Algorithm

The goal of $\texttt{BaB}_{\texttt{ProofCheck}}$ is to verify that the $\texttt{BaB}_{\texttt{ProofLang}}$ tree generated by a DNN verification tool is correct (i.e., the proof tree is a proof of unsatisfiability of the DNN verification problem). $\texttt{BaB}_{\texttt{ProofCheck}}$ thus must verify that the constraint represented by each *leaf* node in the proof tree is unsatisfiable. To check each node, $\texttt{BaB}_{\texttt{ProofCheck}}$ forms an MILP problem (§4.2) consisting of the constraint in Eq. 3.2.3 (the DNN, the input condition, and the negation of the output) with the constraints representing the activation pattern encoded by the tree path to the leaf node. $\texttt{BaB}_{\texttt{ProofCheck}}$ then invokes an LP solver to check that the MILP problem is infeasible, which indicates unsatisfiability of the leaf node.

Alg. 4 shows a minimal (core) $\texttt{BaB}_{\texttt{ProofCheck}}$ algorithm, which takes as input a DNN $\mathcal{N}$, a property $\phi_{in} \Rightarrow \phi_{out}$, a proof tree proof, and returns certified if the proof tree is valid and uncertified otherwise. $\texttt{BaB}_{\texttt{ProofCheck}}$ first checks the validity of the proof tree (line 3), i.e., the input must represent a proper $\texttt{BaB}_{\texttt{ProofLang}}$ proof tree (§12.2). If the proof tree is invalid, $\texttt{BaB}_{\texttt{ProofCheck}}$ raises an error. $\texttt{BaB}_{\texttt{ProofCheck}}$ next creates a MILP model (line 3) representing the input. $\texttt{BaB}_{\texttt{ProofCheck}}$ then enters a loop (line 5) that selects a (random) leaf node from the proof tree (line 6) and adds its MILP constraint to the model (line 7). It then checks the model using an LP solver to determine whether the leaf node is unsatisfiable. If the LP solver returns feasibility, $\texttt{BaB}_{\texttt{ProofCheck}}$ returns uncertified, i.e., it cannot verify the input proof tree. $\texttt{BaB}_{\texttt{ProofCheck}}$ continues until all leaf nodes are checked and returns certified, indicating the proof tree is valid.

Algorithm 4. $\texttt{BaB}_{\texttt{ProofCheck}}$ algorithm.

```
input  : DNN 𝒩, property ϕ_in ⇒ ϕ_out, proof
output : certified if proof is valid, otherwise uncertified
if ¬ RepOK (proof) then
    RaiseError(Invalid proof tree)
// initialize MILP model with inputs
model ← CreateStabilizedMILP(𝒩, ϕ_in, ϕ_out)
node ← null // initialize current processing node
while proof do
    node ← Select(proof, node) // get next node to check
    model ← AddConstrs(model, node) // add constraints
    if CheckFeasibility(model) then
        return uncertified // cannot certify
return certified
```

Example 12.3.1. For the $\texttt{BaB}_{\texttt{ProofLang}}$ proof in Fig. 12.3, we need to check that the four leaf nodes 3, 5, 6, and 7 of the proof tree in Fig. 12.1b are unsatisfiability. Assume $\texttt{BaB}_{\texttt{ProofCheck}}$ first selects node 3, it forms the MILP problem for leaf node 3 by conjoining the constraint representing $0.6v_1 + 0.9v_2 - 0.1 \leq 0$ (i.e., $\overline{v_4}$) with the constraints in Eq. 3.2.3 representing the input ranges and the DNN with the objective of optimizing the output. $\texttt{BaB}_{\texttt{ProofCheck}}$ then invokes an LP solver, which determines that this MILP is infeasible, i.e., leaf node 3 indeed leads to unsatisfiability. $\texttt{BaB}_{\texttt{ProofCheck}}$ continues this process for the other three leaf nodes and returns certified as all leaf nodes are unsatisfiable.

12.3.1.1 MILP Formulation

$\texttt{BaB}_{\texttt{ProofCheck}}$ formulates MILP problems [45] and check for feasible solutions using off-the-shelf LP solving. Formally, the MILP problem is defined as:

$$\begin{aligned}
&\text{(a)} \quad z^{(i)} = W^{(i)}\hat{z}^{(i-i)} + b^{(i)};\\
&\text{(b)} \quad y = z^{(L)}; x = \hat{z}^{(0)};\\
&\text{(c)} \quad \hat{z}_j^{(i)} \geq z_j^{(i)}; \hat{z}_j^{(i)} \geq 0;\\
&\text{(d)} \quad a_j^{(i)} \in \{0,1\};\\
&\text{(e)} \quad \hat{z}_j^{(i)} \leq a_j^{(i)} u_j^{(i)}; \hat{z}_j^{(i)} \leq z_j^{(i)} - l_j^{(i)}(1 - a_j^{(i)});
\end{aligned} \tag{12.3.1}$$

where x is input, y is output, and $z^{(i)}$, $\hat{z}^{(i)}$, $W^{(i)}$, and $b^{(i)}$ are the pre-activation, post-activation, weight, and bias vectors for layer i, respectively. This encodes the semantics of a ReLU-based DNN: (a) the affine transformation computing the pre-activation value for a neuron in terms of outputs in the preceding layer; (b) the inputs and outputs in terms of the adjacent hidden layers; (c) assertion that post-activation values are non-negative and no less than pre-activation values; (d) neuron

activation status indicator variables that are either 0 or 1; and (e) constraints on the upper, $u_j^{(i)}$, and lower, $l_j^{(i)}$, bounds of the pre-activation value of the jth neuron in the ith layer. Deactivating a neuron, $a_j^{(i)} = 0$, simplifies the first of the (e) constraints to $\hat{z}_j^{(i)} \leq 0$, and activating a neuron simplifies the second to $\hat{z}_j^{(i)} \leq z_j^{(i)}$, which is consistent with the semantics of $\hat{z}_j^{(i)} = max(z_j^{(i)}, 0)$.

12.3.1.2 Correctness

Alg. 4 returns certified iff the input $\texttt{BaB}_{\texttt{ProofLang}}$ proof tree is unsatisfiable. This proof tree encodes a disjunction of constraints, one per tree path, where each constraint represents an activation pattern of the network (the leaf node). The algorithm checks each constraint using LP solving and only returns certified iff every one of them is unsatisfiable. We note that this correctness argument assumes that the LP solver is correct – in practice multiple solvers could be used to guard against errors in that component. We note that it is standard for proof checkers to assume the correctness of a small set of external tools, e.g., checkers that use theorem provers assume the correctness of the underlying prover [**?**].

12.3.2 Optimizations

While the core $\texttt{BaB}_{\texttt{ProofCheck}}$ algorithm in Alg. 4 is minimal, it can be inefficicient for large proofs. $\texttt{BaB}_{\texttt{ProofCheck}}$ employs several optimizations to improve its efficiency. These are crucial for checking large proof trees generated by DNN verification tools for challenging problems.

12.3.2.1 Neuron Stabilization

A primary challenge in DNN analysis is the presence of large numbers of piecewise-linear constraints (e.g., ReLU) which generate a large number of branches and yield large proof trees. In the MILP formulation, this creates many disjunctions which are hard to solve. To reduce the number of disjunctions, $\texttt{BaB}_{\texttt{ProofCheck}}$ uses *neuron stabilization* [19] to determine neurons that are *stable*, either active or inactive, for all inputs defined by the property pre-condition. For all stable neurons, the disjunctive ReLU constraint is replaced with a linear constraint that represents the neuron's value. This simplifies the MILP problem.

$\texttt{BaB}_{\texttt{ProofCheck}}$ uses the algorithm in Alg. 5 to traverse the DNN and compute stable neurons. The algorithm initializes the MILP model with input constraints (line 1) and then iterates over each layer of the network. Next, for each layer, it creates constraints (line 4 or line 6) depending on the layer type. Moreover, it uses approximation to estimate bounds of neuron values to determine neuron stability (line 7). Next, it filters unstable neurons (line 8) and attempt to make them stable by optimizing either their lower (`Maximize`) or upper (`Minimize`) bounds.

Algorithm 5. `CreateStabilizedMILP` procedure.

input : DNN $\mathcal{N}$, property $\phi_{in} \Rightarrow \phi_{out}$, parallel factor k
output : MILP model

```
model ← AddInputConstrs(φ_in) // input property
// Add MILP constraints for each layer of network
for layer in 𝒩 do
    if isPiecewiseLinear(layer) then
        // add constraints Eq. 12.3.1 (c), (d), (e)
        model ← AddConstrsPWL(layer, φ_in, φ_out)
    else // this layer is linear
        // add constraints Eq. 12.3.1 (a), (b)
        model ← AddConstrsLinear(layer, φ_in, φ_out)
        // estimate upper and lower bounds
        layer_bounds ← EstimateBounds(layer)
        // select unstable neurons to be stabilized
        [v_1, ..., v_k] ← GetUnstableNeurons(layer_bounds)
        // stabilize selected neurons in parallel
        parfor v_i in [v_1, ..., v_k] do
            // optimize lower first
            if (v_i.lower + v_i.upper) ≥ 0 then
                Maximize(model, v_i.lower)
                if v_i.lower < 0 then // still unstable
                    Minimize(model, v_i.upper)
            else // optimize upper first
                Minimize(model, v_i.upper)
                if v_i.upper > 0 then // still unstable
                    Maximize(model, v_i.lower)
model ← AddObjectives(model, φ_out) // output property
return model
```

12.3.2.2 Pruning Leaf Nodes

Another optimization $\texttt{BaB}_{\texttt{ProofCheck}}$ employs is that it does not check child nodes if the parent node is unsatisfiable. In an $\texttt{BaB}_{\texttt{ProofLang}}$ proof tree, a child node adds constraints to the parent (e.g., node 6 adds the constraint of v_1 to node 4, which adds the constraint of v_2 to node 2 in Fig. 12.1b). Thus, if we determine that the constraint of the parent is unsatisfiable, we can skip the child nodes, which must also be unsatisfiable.

$\texttt{BaB}_{\texttt{ProofCheck}}$ uses a backtracking mechanism to check the parent node only when the child nodes are infeasible. Specifically, it starts checking a leaf node l. If it determines unsatisfiability it will check the parent p of l. If p is unsatisfiable it immediately removes the children of p (more specifically the sibling of l). Next it backtracks to the parent of p and repeats until meeting a stopping criteria. This optimization reduces the number of LP problems that need to be solved, making the

proof checking process more efficient.

We implement a backjumping strategy that allows for backtracking multiple levels, N, rather than a single level at a time. A large value of N offers the chance for greater pruning if an unsatisfiable node is found by backjumping, but such nodes also represent less constrained, and therefore, more complex MILP problems and are less likely to be unsatisfiable. The default value in $\texttt{BaB}_{\texttt{ProofCheck}}$ is $N = 2$ is selected to enable a modest degree of pruning, while being close enough to a proven unsatisfiable node that it has a reasonable chance of itself being unsatisfiable. Future work will explore tuning N to a given verification problem.

12.3.2.3 Parallelization

Finally, the structure of $\texttt{BaB}_{\texttt{ProofLang}}$ proof tree is designed to be easily parallelized. Each tree path is an independent sub-proof and partitions of the tree allow checker to leverage multiprocessing to check large proof trees efficiently. $\texttt{BaB}_{\texttt{ProofCheck}}$ uses a parameter k to control the number of leaf nodes to be checked in parallel.

12.4 Rounding Errors

[TVN]: Give concrete examples of rounding errors in VNN-COMP

Chapter 13

DNN Verification Benchmarks

Here we survey the latest benchmarks in DNN verification and how SOTA tools perform on them. These results are taken from the Verification Neural Network Competitions (VNN-COMP) [8] and the recent work by Duong et al. [19].

13.1 VNN-COMP Benchmarks

[TVN]: check this table with VNN-COMP'24 reports. The Report seems to have a lot more benchmarks for regular tracks. Also many numbers don't quite match. We should probably use the benchmarks from VNN-COMP'24 report. I also ? on place for you to fill in

13.1.1 ACAS Xu

Networks The ACASXu benchmark consists of 10 properties defined over 45 neural networks used to issue turn advisories to aircraft to avoid collisions. The neural

Table 13.1: Benchmark instances. U: `unsat`, S: `sat`, ?: `unknown`.

Benchmarks	**Networks**			**Per Network**		**Tasks**	
	Type	Networks	Neurons	Parameters	Input Dim	Properties	Instances (U/S/?)
cGan	Conv. + Vision Trans.			500K–68M	5		
NN4Sys	ReLU + Sigmoid			33k–37M	1–308		
LinearizeNN	FC. + Conv. + Vision Trans. + Res. + ReLU			203k	4		
Collins RUL CNN	Conv. + ReLU, Dropout			60k–262k	400–800		
cifar100	FC + Conv. + Res., ReLU + BatchNorm			2.5M–3.8M	3072		
tinyimagenet	FC + Conv. + Res., ReLU + BatchNorm			3.6M	9408		
Metaroom	Conv. + FC, ReLU			466k–7.4M	5376		
TLL Verify Bench	Two-Level Lattice NN (FC. + ReLU)			17k–67M	2		
Acas XU	FC. + ReLU	45	300	13k	5	10	139/47/0
Dist Shift	FC. + ReLU + Sigmoid			342k – 855k	792		
safeNLP	FC. + ReLU			4k	30		
CORA	FC. + ReLU			575k, 1.1M	784, 3072		

networks have 300 neurons arranged in 6 layers, with ReLU activation functions. There are 5 inputs corresponding to the aircraft states, and 5 network outputs, where the minimum output is used as the turn advisory the system ultimately produces.

Specifications VNN-COMP uses the original 10 properties [26], where properties 1–4 are checked on all 45 networks as was done in later work by the original authors [28]. Properties 5–10 are checked on a single network. The total number of benchmarks is therefore 186.[TVN]: does not match table

13.1.2 Cifar2020

Motivation This benchmark combines two convolutional CIFAR10 networks from last year's VNN-COMP 2020 with a new, larger network with the goal to evaluate the progress made by the whole field of Neural Network verification.

Networks The two ReLU networks `cifar_10_2_255` and `cifar_10_8_255` with two convolutional and two fully-connected layers were trained for ℓ_∞ perturbations of $\epsilon = \frac{2}{255}$ and $\frac{8}{255}$, respectively, using COLT [**?**] and the larger `ConvBig` with four convolutional and three fully-connected networks, was trained using adversarial training [**?**] and $\epsilon = \frac{2}{255}$.

Specifications We draw the first 100 images from the CIFAR10 test set and for every network reject incorrectly classified ones. For the remaining images, the specifications describe a correct classification under an ℓ_∞-norm perturbation of at most $\frac{2}{255}$ and $\frac{8}{255}$ for `cifar_10_2_255` and `ConvBig` and `cifar_10_8_255`, respectively and allow a per sample timeout of 5 minutes.

13.1.3 VGGNET16

Proposed by Stanley Bak, Stony Brook University

Motivation This benchmark tries to scale up the size of networks being analyzed by using the well-studied VGGNET-16 architecture [**?**] that runs on ImageNet. Input-output properties are proposed on pixel-level perturbations that can lead to image misclassification.

Networks All properties are run on the same network, which includes 138 million parameters. The network features convolution layers, ReLU activation functions, as well as max pooling layers.

Specifications Properties analyzed ranged from single-pixel perturbations to perturbations on all 150528 pixles (L-infinity perturbations). A subset of the images was used to create the specifications, one from each category, which was randomly chosen to attack. Pixels to perturb were also randomly selected according to a random seed.

Link https://github.com/stanleybak/vggnet16_benchmark2022/

13.1.4 cGAN

Proposed by Feiyang Cai, Ali Arjomandbigdeli, Stanley Bak (Stony Brook Univ.). Link: https://github.com/feiyang-cai/cgan_benchmark2023

This benchmark targets robustness verification for generative models—an area often overlooked compared to discriminative networks. It uses conditional GANs trained to generate images of vehicles at specific distances. The generator takes a 1D distance input and a 4D noise vector; the discriminator outputs a real/fake score and a predicted distance. Models vary in architecture (CNNs, vision transformers) and image size (32×32, 64×64). The verification task checks whether the predicted distance from the generated image matches the input condition, under small input perturbations.

Motivation While existing neural network verification benchmarks focus on discriminative models, the exploration of practical and widely used generative networks remains neglected in terms of robustness assessment. This benchmark introduces a set of image generation networks specifically designed for verifying the robustness of the generative networks.

Networks The generative networks are trained using conditional generative adversarial networks (cGAN), whose objective is to generate camera images that contain a vehicle obstacle located at a specific distance in front of the ego vehicle, where the distance is controlled by the input distance condition. The network to be verified is the concatenation of a generator and a discriminator. The generator takes two inputs: 1) a distance condition (1D scalar) and 2) a noise vector controlling the environment (4D vector). The output of the generator is the generated image. The discriminator takes the generated image as input and outputs two values: 1) a real/fake score (1D scalar) and 2) a predicted distance (1D scalar). Several different models with varying architectures (CNN and vision transformer) and image sizes (32x32, 64x64) are provided for different difficulty levels.

Specifications The verification task is to check whether the generated image aligns with the input distance condition, or in other words, verify whether the input distance condition matches the predicted distance of the generated image. In each specification, the inputs (condition distance and latent variables) are constrained in

small ranges, and the output is the predicted distance with the same center as the condition distance but with slightly larger range.

Chapter 14

VNN-COMPs

Chapter 15

Benchmarks Generation

Chapter 16

Conclusion

Appendix A

Schedule and Assignments

1. Week 1 (Aug 27): Introduction (videos of neural networks, basic terminologies and concepts).
2. Week 2 (Sept 3):
   - HW due: Post a short introduction about yourself on Canvas
   - Topics: Background on Logic §B and Linear Programming §C
   - Quiz: no quiz this week
3. Week 3 (Sept 10):
   - HW due: MILP problem Prob. C.3.3
   - Topics: DNN and Properties and their formal representation (§1 and §2)
   - Quiz: Prob. C.3.4
4. Week 4 (Sept 17):
   - HW due: Neural Networks and Properties Prob. 2.6.4
   - Topics: DNN Verification (§3)
   - Quiz: Prob. 2.6.1
5. Week 5 (Sept 24): No class this week (prof not available). No quiz or HW due.
   - Programming Assignment 1 (PA1): Symbolic Execution of Neural Networks §B.1. Due date Monday October 6, 2024 11:59pm.
6. Week 6 (Oct 1):
   - HW due: Prob. 3.2.3, Prob. 3.2.4, and Prob. 6.1.1.
   - Topics: Activation Pattern Search (§6.1) and Symbolic Execution (§4.1)
   - Quiz: Prob. 3.2.5

7. Week 7 (Oct 8):
    - No HW due because of PA1.
8. Week 8 (Oct 15):
9. Week 9 (Oct 22):
10. Week 10 (Oct 29):

Appendix B

Programming Assignments

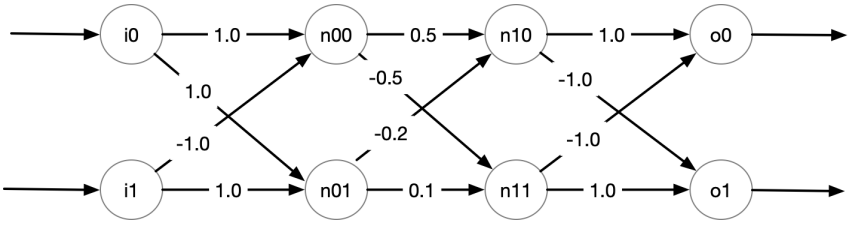
B.1 PA1: Symbolic Execution of Neural Networks

In this PA you will implement an neural network (NN) verifier using symbolic execution (SE) as described in §4.1. You can consider NNs as a specific type of programs and thus can "execute" it. SE runs the NN on symbolic inputs and returns symbolic outputs, i.e., a constraint representation. You will represent the symbolic outputs as a logical formula and use a constraint solver to check *assertions*, i.e., properties about the DNN. This PA has two parts: (1) implement SE on a given DNN, and (2) evaluate the scalability of your SE on various DNNs.

You will use Python and the Z3 SMT solver (§B.2.2) for this assignment. **Do not** use external libraries or any extra tools (other than `z3-solver`).

B.1.1 Part1: Symbolic Execution

Consider the following fully-connected DNN with 2 inputs, 2 hidden layers, and 2 outputs.



1. **DNN Encoding**: We can encode this DNN using Python:

```
# (weights, bias, use activation function relu or not)
n00 = ([1.0, -1.0], 0.0, True)
n01 = ([1.0, 1.0], 0.0, True)
hidden_layer0 = [n00,n01]

n10 = ([0.5, -0.2], 0.0, True)
```

```
n11 = ([-0.5, 0.1], 0.0, True)
hidden_layer1 = [n10, n11]

# don't use relu for outputs
o0 = ([1.0, -1.0], 0.0, False)
o1 = ([-1.0, 1.0], 0.0, False)
output_layer = [o0, o1]

dnn = [hidden_layer0, hidden_layer1, output_layer]
```

In this DNN, the outputs of the neurons in the hidden layers (prefixed with `n`) are applied with the `relu` activation function, but the outputs of the DNN (prefixed with `o`) are not. These settings are controlled by the `True`, `False` parameters as shown above. Also, this example does not use `bias`, i.e., bias values are all 0.0's as shown.

Note that all of these settings are parameterized and I deliberately use this example to show these how these parameters are used (e.g., `relu` only applies to hidden neurons, but not outputs).

2. **Symbolic States**: After performing symbolic execution on `dnn`, we obtain symbolic states, represented by a logical formula relating input and output variables.

```
# my_symbolic_execution is something you implement,
# it returns a single (but large) formula representing the symbolic states.
symbolic_states = my_symbolic_execution(dnn)
...
``done, obtained symbolic states for DNN in 0.1s''
assert z3.is_expr(symbolic_states)  #symbolic_states is a Z3 expression

# your symbolic states should look something like this
print(symbolic_states)
# And(n0_0 == If(i0 + -1*i1 <= 0, 0, i0 + -1*i1),
#     n0_1 == If(i0 + i1 <= 0, 0, i0 + i1),
#     n1_0 ==
#     If(1/2*n0_0 + -1/5*n0_1 <= 0, 0, 1/2*n0_0 + -1/5*n0_1),
#     n1_1 ==
#     If(-1/2*n0_0 + 1/10*n0_1 <= 0, 0, -1/2*n0_0 + 1/10*n0_1),
#     o0 == n1_0 + -1*n1_1,
#     o1 == -1*n1_0 + n1_1)
```

3. **Constraint Solving**: We will use `Z3` to query various things about this DNN from the obtained symbolic states. Examples include:

   (a) Generating random inputs and obtain outputs. Note that these are random values (that satisfy the symbolic states), so your results might look different.

```
z3.solve(symbolic_states)
[n0_1 = 15/2,
    o1 = 1/2,
    o0 = -1/2,
    i1 = 7/2,
```

```
n1_1 = 1/2,
n1_0 = 0,
i0 = 4,
n0_0 = 1/2]
```

(b) Simulating a concrete execution.

```
i0, i1, n0_0, n0_1, o0, o1 = z3.Reals("i0 i1 n0_0 n0_1 o0 o1")

# finding outputs when inputs are fixed [i0 == 1, i1 == -1]
g = z3.And([i0 == 1.0, i1 == -1.0])
z3.solve(z3.And(symbolic_states, g))  # you should get o0, o1 = 1, -1
[n0_1 = 0,
o1 = -1,
o0 = 1,
i1 = -1,
n1_1 = 0,
n1_0 = 1,
i0 = 1,
n0_0 = 2]
```

(c) Checking assertions, i.e., verifying/proving properties about the DNN or disproving/finding counterexamples

```
print("Prove that if (n0_0 > 0.0 and n0_1 <= 0.0) then o0 > o1")
g = z3.Implies(z3.And([n0_0 > 0.0, n0_1 <= 0.0]), o0 > o1)
print(g)  #  Implies (And(n0_0 > 0, n0_1 <= 0), o0 > o1)
z3.prove(z3.Implies(symbolic_states, g))  # proved

print("Prove that when (i0 - i1 > 0 and i0 + i1 <= 0), then o0 > o1")
g = z3.Implies(z3.And([i0 - i1 > 0.0, i0 + i1 <= 0.0]), o0 > o1)
print(g)  # Implies(And(i0 - i1 > 0, i0 + i1 <= 0), o0 > o1)
z3.prove(z3.Implies(symbolic_states, g))
# proved

print("Disprove that when i0 - i1 >0, then o0 > o1")
g = z3.Implies(i0 - i1 > 0.0, o0 > o1)
print(g)  # Implies(And(i0 - i1 > 0, i0 + i1 <= 0), o0 > o1)
z3.prove(z3.Implies(symbolic_states, g))
# counterexample  (you might get different counterexamples)
# [n0_1 = 15/2,
# i1 = 7/2,
# o0 = -1/2,
# o1 = 1/2,
# n1_0 = 0,
# i0 = 4,
# n1_1 = 1/2,
# n0_0 = 1/2]
```

B.1.2 TIPS

1. It is strongly recommend that you do symbolic execution on this DNN example **by hand** first before attempt any coding. This example is small enough that you can work out step by step. For example, you can do these two steps

   (a) First, obtain the symbolic states by hand (e.g., on a paper) for the given DNN

(b) Then, put what you have in code but also for the given DNN. Use Z3 format (e.g., you would declare the inputs as symbolic values `i0 = z3.Real("i0")`, then compute the neurons and outputs, etc)

(c) Finally, convert what you have into a general program that would work for any DNN inputs.

2. You can use the below method to construct Z3 formula for ReLU

```
@classmethod
def relu(cls, v):
   return z3.If(0.0 >= v, 0.0, v)
```

3. Two ways of doing symbolic execution to obtain symbolic states

   (a) You can follow the traditional SE method which produces the symbolic execution trees in which each condition representing ReLU forks into two paths. You can decide whether to do a depth-first search or breadth-first search here (they will have the same results). At the end, the symbolic states are a disjunction of the path conditions (i.e., `z3.And[path_conds]`).

   (b) But since we are using Z3, a much much simpler way, is to encode all those forked paths directly as a formula. For example

```
if (x + y > 0):
   r = 3
else:
   r = 4
```

   Using traditional SE, you would have 2 paths, e.g., path 1: `x+y > 0 && r = 3` and path 2 : `x+y <= 0 && r ==4`, from which you take the disjunction and get `(x+y > 0 && r == 3) || (x+y <= 0 && r ==4)`. But for this assignment, instead of having to fork into two paths, you can use Z3 to encode both branches using the `If` function, e.g., `If(x+y>0, r==3, r==4)` or `r==If(x+y>0,3,4)`. The results of these two methods are exactly the same at the end, just that the prior, traditional one you do more work while the later you do less. It is up to you.

4. When `bias` is none-zero, then it will simply be added to the neuron computation, i.e., `neuron = relu(sum(value_i * weight_i) + bias)`. For example, if `bias` is `0.123` then for neuron `n0_0` we would obtain `n0_0 == If(i0 + -1*i1 + 0.123 <= 0, 0, i0 + -1*i1 + 0.123)`.

5. Using `Tensorflow Keras` (or `Pytorch`)

   In my example above, I create a DNN using simple Python lists. But you can also use `Tensorflow Keras` (or `Pytorch`) to create a DNN. It might be simpler that way as then you can reuse existing methods from these Python packages. You will still need to implement symbolic execution, just that instead the input DNN being Python lists, they are now Tensorflow or Pytorch. Also note that

if you use `tensorflow` or `pytorch`, then be sure to indicate what packages are needed to run your program in the **README** file, i.e., `pip install ...`.

Below is the tensorflow representation of the DNN example above.

```
import tensorflow as tf
from tensorflow import keras
from tensorflow.keras.models import Sequential
from tensorflow.keras.layers import Dense
from tensorflow.keras import activations

model = Sequential()

# layer 0: nodes n00, n01
model.add(Dense(units=2,
                input_shape=(2, ),    # 2 inputs (i.e., i0, i1 in the Figure)
                activation=activations.relu,  # relu activation
                kernel_initializer=tf.constant_initializer(
                    [[1.0, 1.0],  # weights of n00
                    [-1.0, 1.0]  # weights of n01
                    ]),
                bias_initializer=tf.constant_initializer(
                    [[0.0],  # bias of n00
                    [0.0]]  # bias of n01
                ),
                dtype='float64'
                ))

# layer 1: nodes n10, n11
model.add(Dense(units=2,
                activation=activations.relu,
                kernel_initializer=tf.constant_initializer(
                    [[0.5, -0.5], [-0.2, 0.1]]),
                bias_initializer=tf.constant_initializer([[0.0], [0.0]]),
                dtype='float64'
                ))

# last layer: nodes represent outputs o0, o1
model.add(Dense(units=2,
                activation=None,  # no activation function for output nodes
                kernel_initializer=tf.constant_initializer(
                    [[1.0, -1.0], [-1.0, 1.0]]), # weights of o0, o1
                bias_initializer=tf.constant_initializer([[0.0], [0.0]]),
# bias of o0, o1
                dtype='float64'
                ))
```

B.1.3 Part:2: Evaluation

In this part you will show that symbolic execution *does not* scale on large DNNs.

1. You will create a function `create_random` that takes as input a list of positive integers representing the sizes of the neurons `[#inputs, #ofnumbers, #ofneurons, ..., #outputs]`, and create a neural network of that size with *random* weights and bias (e.g., between say -5 and 5).

2. You will run symbolic execution on this network as you did in PA1, get its results, and time the solving process.

3. You will do this for various sizes of neurons until you feel that your computer cannot handle it anymore (e.g., until it takes more than a minute or two).

4. You will **save these networks** because you will reuse them to measure and compare execution time using abstraction in Part 2.

5. Finally, you will plot the results: the x-axis will show the size of the neurons (for simplicity, the product of all numbers in the input list) and the y-axis shows the time.

Feel free to be creative in this process (e.g., play around with different sizes/layers), and discuss your findings in the `README` file. Below gives some code example:

```
# Create a random network from a given
# number of inputs, hidden neurons, and outputs
l = [2,3,4,3,3]   # 2 inputs, 3 hidden layers (with 3,4,3 hidden neurons for
                  # respective hidden layer 1, 2, 3), and 3 outputs.
dnn = create_random_nn(l)

symbolic_state = my_symbolic_execution(dnn)

# time the execution
import time
st = time.time()
_ = z3.solve(symbolic_state)
print('time to solve: ', time.time() - st)
```

B.1.4 Conventions and Requirements

Your program must have the following:

Part 1

1. a function `my_symbolic_execution(dnn)` that

   - takes as input the DNN, whose specifications are given as example above (or using `tensorflow` or `pytorch`)
     - This goes without saying: do not hard-code the DNN in your program (e.g., do not hardcode the example given above in your code). Your program should work with any DNN input.
   - returns *symbolic states* of the DNN represented as a Z3 expression (a formula) as shown above
   - this goes without saying but do NOT write this function only to work with the given example, i.e., do not hard-code the weight values etc in your program. This function should work with any DNN input (though it could be slow for big DNN's).

2. in your resulting formula, you must name
    - the nth input as i_n (e.g., the first input is i_0)
    - the nth output as o_n (e.g., the second output is o_1)
    - the jth neuron at the ith layer as n_{i_j}. Note that the first layer is the 0th layer
3. a testing function `test()` where you copy and paste pretty much the complete examples given above to demonstrate that your SE works for the given example. In summary, your `test` will include
    - the specification of the 2x2x2x2 DNN in the Figure
    - run the symbolic execution on the dnn (as shown above, it should output the dimension of the dnn and runtime)
    - output the symbolic states results
    - apply Z3 to the symbolic states to obtain
        - random inputs and associated outputs
        - simulate concrete execution
        - checking the 3 assertions as shown
4. another testing function `test2()` where you create another DNN:
    - The DNN will have
        - the same number of 2 inputs and 2 outputs, but 3 hidden layers where each layer has 4 neurons, i.e., a 2x4x4x4x2 DNN.
        - non-0.0 bias values.
    - then on this DNN, do every single tasks you did in `test()` (run SE on it, output results, apply Z3 etc). You will need to have 2 assertions that are true and 1 assertion that is false (just like above).
        - Initially you might randomly generate weights and bias values, but it is likley that you will need to manually adjust them so that you can prove some correct assertions (randomly generated values probably will not give you a meaningful DNN with any asserted properties).

You can be as creative as you want, but your SE must not run for too long and must not take up too much space (e.g., do not generate over 50MB of files). Use the `README` to tell me exactly how to compile/run your program, e.g., `python3 se.py`.

Part 2

1. a function `create_random(sizes:int)` that

- takes as input the list `sizes` and returns a DNN of that size as descibed above.

2. a testing function `test3()` that runs `create_random` on various sizes of DNNs, runs `my_symbolic_execution` on them as you did with `test()` and `test2()` above, and time the execution.

3. a plot (in pdf, png, or jpeg) showing the scalability of `my_symbolic_execution` on various DNNs

4. in the `README`, write your observation and conclusion about the scalability of symbolic execution. You must refer to the plot and describe it to support your conclusion.

5. **BONUS**: as you will see, SE does not scale. Come up with ways to improve it and implement it in a new function `my_symbolic_execution_optimize(dnn)`. Then compare its scalability with `my_symbolic_execution(dnn)` using the same DNNs created in `test3()`. Discuss your new SE and result findings in the `README` file (see below for details).

B.1.5 What to Turn In

You must submit a **zip file** containing the following files. Use the following names:

1. the zip file must be named `pa1-yourname.zip` (1 submission per group)

2. One single main source file `se.py`. Indicate in the `README` file on how I can run it.

   - your file should include at least a `my_symbolic_execution` function and the test functions `test`, `test2()`, and `test3()` as indicated above

3. a `README.txt` or `README.md` file

4. 2 screen shots showing how (1) you start your program (e.g., the commands used to run your program) and (2) the end of the run (e.g., of your program on the terminal screen)

5. Nothing else, do not include any binary files or anything else.

The `README` file should be a *plain ASCII text file* or *Markdown file*. DO NOT submit a Word, RTF, HTML, etc. The `README` should include the following:

1. **Complete run** show how you run your program **AND** its complete outputs, e.g.,

```
python3 se.py    # this should execute both test() and test2 and show all outputs
....             # (something similar to the outputs for the complete example above)
```

2. **Answer the following questions about your SE** in your `README` file

   (a) Briefly describe your SE algorithm

   (b) What do you think the most difficult part of this assignment? (e.g., programming symbolic execution, using Z3, dealing with scalability,etc)

   (c) What advice do you give other students (e.g., students in this class next year) about this PA?

3. **BONUS**: if you implement the bonus part, then include `my_symbolic_execution_optimize(dnn)` in `se.py`, and include in your `README` file:

   (a) Briefly describe your new SE algorithm

   (b) Discuss your findings and results (e.g., plots, runtime differences, etc)

B.2 PA2: Abstract Domain Analysis of Neural Networks

In this PA you will implement neural network (NN) verification using *zonotope abstraction* as described in §5.2.2. While symbolic execution (PA1, §B.2) computes exact symbolic representations, abstract interpretation uses over-approximations to make verification more scalable at the cost of some precision. You will implement zonotope abstract transformers and compare their precision-scalability trade-offs with symbolic execution.

You will use Python and PyTorch for this assignment. **Do not** use external verification libraries (other than standard numerical libraries like `torch`, `numpy`).

This PA has two main parts: (1) implement zonotope abstract transformers for linear layers and ReLU activations, and (2) evaluate the precision and scalability compared to symbolic execution from PA1.

B.2.1 Part 1: Zonotope Representation

B.2.1.1 From Bounds to Zonotope

A zonotope is represented by a tuple of a center vector and a generator matrix. Given the bounds of a zonotope, we can convert it to a zonotope.

```
def zonotope(lb, ub):
    """
    Computes zonotope from interval bounds [l, u].
    """
    center = (lb + ub) / 2
    generator = (ub - lb) / 2
    return center, generator
```

B.2.1.2 From Zonotope to Bounds

Given the center and generators of a zonotope, we can concretize the bounds of the zonotope.

```
def concrete(center, generator):
    """
    Computes interval bounds [l, u] from zonotope (center, generator).

    A zonotope Z = {c + sum_{i=1}^{m} ε_i g_i | ε_i ∈ [-1, 1]} can be converted to interval bounds:
    Lower bound: l = c - sum_{i=1}^{m} |g_i| (when all ε_i = -sign(g_i))
    Upper bound: u = c + sum_{i=1}^{m} |g_i| (when all ε_i = +sign(g_i))

    Args:
        center: Center vector c of the zonotope
        generator: Generator matrix G

    Returns:
        (lb, ub): Interval bounds for each dimension

    # TODO: compute interval bounds from zonotope
    # 1. compute lower bound
    # 2. compute upper bound
    """
    return lb, ub
```

B.2.2 Part 2: Zonotope for Linear Layers

Linear (affine) transformations can be handled exactly in zonotope abstraction. You will implement the missing components in the provided zonotope framework.

```
class LinearTransformer(nn.Module):
    def __init__(self, W, b):
        # TODO: store weights and bias

    def forward(self, center, generator):
        """
        Apply affine transformation f(x) = Wx + b to zonotope Z = (c, G)
        Result: f^a(Z) = (Wc + b, WG)

        Args:
            center: center vector c of input zonotope
            generator: generator matrix G of input zonotope

        Returns:
            (new_center, new_generator): transformed zonotope
        """
        # TODO:
        # 1. Transform center using weight matrix and bias
        # 2. Transform generator matrix using weight matrix
        # 3. Return transformed (center, generator)

        return new_center, new_generator
```

B.2.3 Part 3: Zonotope for ReLU Activations

ReLU activations are non-linear and require over-approximation in zonotope abstraction. For each neuron with bounds $[l, u]$, there are three cases to handle.

```
class ReluTransformer(nn.Module):

    def forward(self, center, generator):
        """
        Apply ReLU abstraction to zonotope representation: ReLU(x) = max(0, x)

        Three cases for each neuron i with bounds [l_i, u_i]:
        1. Active case (l_i >= 0): ReLU is identity, Z' = Z
        2. Inactive case (u_i <= 0): ReLU outputs 0, Z' = {0}
        3. Unstable case (l_i < 0 < u_i): requires over-approximation

        Args:
            center: center vector of input zonotope
            generator: generator matrix of input zonotope

        Returns:
            (new_center, new_generator): over-approximated zonotope after ReLU
        """
        # TODO:
        # 1. Compute current bounds using concrete(center, generator)
        # 2. Create new generator matrix with extra row for ReLU error
        # 3. For each neuron, handle based on bounds [l, u]:
        #    - Active (l >= 0): keep unchanged
        #    - Inactive (u <= 0): set to zero
        #    - Unstable (l < 0 < u): apply slope approximation
        # 4. Return transformed (center, generator)

        return new_center, new_generator
```

B.2.4 Part 4: Putting It All Together

```
    class ZonotopeAbstraction(nn.Module):

        def __init__(self, DNN):
            # TODO: convert DNN to corresponding zonotope abstraction transformers
            self.transformers = ...

        def forward(self, lb, ub):
            # 1. convert bounds to zonotope
            center, generator = ...
            # 2. propagate zonotope through layers
            for transformer in self.transformers:
                center, generator = ...

            # 3. convert zonotope to bounds
            lb, ub = ...
            return (lb, ub)
```

B.2.5 Part 5: Evaluation

```
# (weights, bias, use activation function relu or not)
n00 = ([1.0, 1.0], 2.0, True)
n01 = ([1.0, -1.0], 2.0, True)
hidden_layer0 = [n00, n01]

n10 = ([1.0, 1.0], -0.5, True)
n11 = ([1.0, -1.0], -1.0, True)
hidden_layer1 = [n10, n11]

n20 = ([-1.0, 1.0], 7.0, False)
n21 = ([0.0, 1.0], 0.0, False)
hidden_layer2 = [n20, n21]

o0 = ([1.0, -1.0], 0.0, False)
output_layer = [o0]

dnn = [hidden_layer0, hidden_layer1, hidden_layer2, output_layer]
```

In this DNN, the outputs of the neurons in the hidden layers (prefixed with `n`) are applied with the `relu` activation function, but the outputs of the DNN (prefixed with `o`) are not. These settings are controlled by the `True`, `False` parameters as shown above. Also, this example does not use `bias`, i.e., bias values are all 0.0's as shown.

Note that all of these settings are parameterized and I deliberately use this example to show these how these parameters are used (e.g., `relu` only applies to hidden neurons, but not outputs).

```
net = ZonotopeAbstraction(dnn)
input_lower = torch.tensor([-1, -1], dtype=torch.float)
input_upper = torch.tensor([1, 3], dtype=torch.float)
output_lower, output_upper = net(input_lower, input_upper)
print(f'{output_lower=}')
print(f'{output_upper=}')
# output_lower=tensor([1.5000])
# output_upper=tensor([5.5000])
```

Grading Rubric

Grading (out of 30 points):

- 15 points — for a complete SE as described
  - 10 points if your SE works for the given example (e.g., `test()` produces expected results)
  - 3 points if your SE works for the addition example you created
  - 2 points if your SE works on my own example (not provided). This means you should try to generalize your work and test it on various scenarios.
- 10 points - for complete scalability analysis and plots (part 1 and part 2) as described

  - 5 points for `create_random` code and testing function `test3()`
  - 5 points for scalability plots and explanations

- 5 points — for the answers in the README
  - 5 — clear explanations on running the program and thorough answers for the given questions
  - 2 — vague or hard to understand; omits important details
  - 0 — little to no effort, or submitted an RTF/DOC/PDF file instead of plain TXT

- **BONUS** (up to 5 extra points) — for the new SE algorithm and its analysis as described
  - 3 points for the new SE algorithm
  - 2 points for the analysis and results

Background A

Comparing neural networks with software

Table A.1: Similarities

Aspect	Description
Representation	Represented using if-then-else statements
Input-Output Mapping	Take Inputs and produce outputs
Determinism	Can produce deterministic outputs
Execution Path	Paths from input to output
Specifications	Can have specifications involving preconditions over inputs and postconditions over outputs
Logical Constraints	Can be represented as logical constraints
Bugs and Errors	Can have bugs that violate specifications

Table A.2: Differences

Aspect	Traditional Software	Neural Networks
Explainability	Can be explained through code inspection	Lacks explicit explainability mechanisms
Designing	Written by human	Created by machine through learning from training
Size	Small to medium-sized codebases	Large number of neurons and layers
Error Causing	arise from bugs in logic or implementation	arise from insufficient training data, overfitting, etc
Error Incurring	Can cause crashes, incorrect outputs, or unexpected behavior	Can cause incorrect predictions or unexpected beha
Error Handling	try-catch blocks for exception handling	Lacks explicit error-handling mechanisms

Background B

Logics

The field of neural network verification (NNV) relies heavily on two fundamental areas: *logic* (to formalize and reason about properties as logical formulae) and *optimization* (to formulate and reason about numerical constraints). This chapter and the next (§C) provides the necessary background on both topics in detail, starting with propositional logic and satisfiability, and then moving to linear and mixed-integer programming.

B.1 Propositional Logic and Satisfiability

Propositional, or Boolean, logic is the branch of logic that studies formulae built from Boolean variables, where each variable can take only the values `True` or `False`. These formulae are combined using logical connectives such as `and`, `or`, and `not`, and their evaluation always reduces to a single truth value.

B.1.1 Syntax

A *propositional variable* is a symbol (e.g., x, y, z). Logical formulae are built *inductively* from these variables using logical connectives as follows:

- Variables: Any propositional variable p is a formula.
- Constants: $\top$ and $\bot$ are formulae.
- Negation: If ϕ is a formula, then so is $\neg\phi$.
- Binary connectives: If ϕ, ψ are formulae, then so are $(\phi \wedge \psi)$, $(\phi \vee \psi)$, and $(\phi \to \psi)$.

Example B.1.1.

$$(x \vee y) \wedge (\neg x \vee z)$$

is a formula involving three variables x, y, z.

Special connectives In addition to the standard connectives, we define some special connectives that are often useful:

- *Implication*: $\phi \to \psi \equiv \neg\phi \vee \psi$
- *Biconditional* (or *equivalence*): $\phi \leftrightarrow \psi \equiv (\phi \to \psi) \wedge (\psi \to \phi)$

Convert to Conjunctive Normal Form (CNF) A formula is in CNF if it is a conjunction of disjunctions of literals, where a literal is either a variable p or its negation $\neg p$.

Any formula can be transformed into CNF. The process generally involves the following steps:

1. Eliminate biconditionals and implications.
2. Move negations inward using De Morgan's laws.
3. Distribute disjunctions over conjunctions.

Problem B.1.1. Transform the formula

$$(x \to y) \wedge (y \to z)$$

into CNF.

> Notice here that we purely define the syntax of propositional logic, which allows us to construct valid formulae. We will discuss the semantics or meanings of formulae next (§B.1.2).

B.1.2 Semantics

A logical formula in propositional logic has a truth value, which can be either `True` or `False`. For example, the formula $x \vee \neg x$ is always `True`, while the formula $x \wedge y$ is `True` if both x and y are `True`, and `False` otherwise. This is the *semantics* of the formula.

An *assignment* α maps each formula to `True` or `False`. The truth value of a formula is defined recursively

$$\begin{aligned}
\alpha(\top) &= \texttt{True}, \\
\alpha(\bot) &= \texttt{False}, \\
\alpha(p) &\text{ iff } \alpha(p) = \texttt{True}, \\
\alpha(\neg\phi) = \texttt{True} &\text{ iff } \alpha(\neg\phi) = \texttt{True}, \\
\alpha(\phi \wedge \psi) = \texttt{True} &\text{ iff } \alpha(\phi) = \texttt{True} \text{ and } \alpha(\psi) = \texttt{True}, \\
\alpha(\phi \vee \psi) = \texttt{True} &\text{ iff } \alpha(\phi) = \texttt{True} \text{ or } \alpha(\psi) = \texttt{True}, \\
\alpha(\phi \to \psi) = \texttt{True} &\text{ iff } \alpha(\phi) = \texttt{False} \text{ or } \alpha(\psi) = \texttt{True}.
\end{aligned}$$

Problem B.1.2. For the formula

$$(x \vee y) \wedge (\neg x \vee z),$$

evaluate its truth value under all $2^3 = 8$ possible assignments of x, y, z.

B.1.3 Satisfiability and Validity

Definition B.1.1 (Satisfiability)**.** A formula ϕ

- is *satisfiable* if there exists **some** α such that $\alpha(\phi) = \texttt{True}$.
- is *unsatisfiable* if **no** assignment satisfies it.
- is *valid* if **all** assignments satisfy it.

Example B.1.2. The formula

$$x$$

is satisfiable (e.g., $\alpha(x) = \texttt{True}$).

$$(x) \wedge (\neg x)$$

is unsatisfiable (no assignment works). In contrast,

$$(x \vee \neg x)$$

is valid.

Problem B.1.3. Show that $(\phi \to \psi)$ is equivalent to $(\neg\phi \vee \psi)$. (Hint: construct a truth table.)

B.1.4 SAT Solving

A SAT solver takes a propositional formula as input and determines its satisfiability by searching for a satisfying assignment. If one exists, it returns the assignment; otherwise, it reports `unsat`.

Example B.1.3.

$$\phi_1 = (x \vee y) \wedge (\neg x \vee z) \quad \Rightarrow \texttt{sat}$$
$$\phi_2 = (x) \wedge (\neg x) \quad \Rightarrow \texttt{unsat}$$

Problem B.1.4. Use the Z3 solver to check whether

$$(x \vee y) \wedge (\neg x \vee y) \wedge (x \vee \neg y)$$

is satisfiable. Provide a satisfying assignment if it exists.

Conjunctive Normal Form (CNF) In practice, SAT solvers do not take arbitrary formulae as input. Instead, they require the formula to be in *Conjunctive Normal Form (CNF)*.

Example B.1.4.

$$(x \vee y) \wedge (\neg x \vee z)$$

is in CNF. Each clause $(x \vee y)$, $(\neg x \vee z)$ is a disjunction of literals.

B.1.5 Validity Checking

By Def. B.1.1, a formula α is valid if all assignments satisfy it. This is equivalent to saying that its negation $\overline{\alpha}$ is unsatisfiable (no assignment satisfies it), i.e.,

$$\text{valid}(\alpha) \iff \text{unsat}(\overline{\alpha})$$

Thus, to check the validity of α, we can use a SAT solver to check that $\overline{\alpha}$ is `unsat`.

B.2 Satisfiability Modulo Theories (SMT)

SAT solvers only reason about propositional formulae, which only contain Boolean variables and logical operators such as $\wedge, \vee$. However, in verification problems, we often need to reason about arithmetic constraints $2x + 3y \leq 7; x \geq 0; x, y \in \mathbb{Z}$.

This leads to *Satisfiability Modulo Theories (SMT)*:

- SMT generalizes SAT by adding background theories (e.g., linear arithmetic, bit-vectors, arrays).
- An SMT formula mixes Boolean structure with constraints from these theories.

Example B.2.1. Is the formula $2x = 1$ satisfiable?

The answer depends on the chosen theory. Here, over real numbers ($\mathbb{R}$), it is SAT (e.g., $x = 0.5$), but over integers ($\mathbb{Z}$) it is UNSAT.

B.2.1 SMT Solvers

Popular SMT solvers include Z3 (Microsoft Research), CVC5, and dReal. They combine:

- A SAT solver for the Boolean skeleton.
- A *theory solver* or T-solver (e.g., linear arithmetic) for the numeric parts.

The SAT solver guesses a truth assignment for the Boolean structure. The T-solver checks whether the corresponding arithmetic constraints are feasible. This loop continues until either a satisfying assignment is found or `unsat` is proven.

Problem B.2.1. Decide the satisfiability of:

$$(x > 3) \wedge (y < 2) \wedge (x + y < 1).$$

First, do the reasoning informally by hand, and then confirm with an SMT solver such as Z3.

B.2.2 Z3 SMT Solver

Z3 [14] is a well-known SMT solver developed by Microsoft Research. Here we'll show how to use it for various logical and arithmetic problems.

Installing You can install Z3 using your package manager, for example

```
brew install z3        # using homebrew
pip install z3-solver   # using pip
apt install z3 python3-z3 # using apt (on Debian-based Linux systems)
conda install z3solver # using conda
```

Then try its Python interface:

```
from z3 import *
x = Int('x')
y = Int('y')
solve(x > 2, y < 10, x + 2*y == 7)
```

Example B.2.2 (Propositional Logic)**.** We use Z3 to check satisfiability of propositional formulae and generate counterexamples.

```
from z3 import *

x, y = Bools('x y')
formula = And(Or(x, y), Or(Not(x), y))
s = Solver()
s.add(formula)
print(s.check())   #output: sat
print(s.model())   #a possible model is {x=True, y=True}
```

Problem B.2.2. Modify the code in Ex. B.2.2 to check

$$(x \wedge \neg x).$$

Confirm that the result is `unsat`.

Example B.2.3 (Linear Constraints.)**.** We now use Z3 as an SMT solver to check linear constraints.

```
from z3 import *
x, y = Reals('x y')

# example 1
s = Solver()
s.add(x > 0, y > 0, 2*x + y <= 1)
print(s.check())  # Output: unsat
```

```
# example 2
s = Solver()
s.add(x + y <= 4, x >= 0, y >= 0)
print(s.check()) # Output: sat
print(s.model())  # Output: {x=0, y=0}


# example 3
x, y = Ints('x y')
s = Solver()
s.add(Implies(x > 3, y > 2))
print(s.check()) # Output: sat
print(s.model()) # Output: {x=0, y=0}
```

Problem B.2.3. Use Z3 to check whether the constraints

$$x + y = 5, \quad x \geq 0, \quad y \geq 0$$

are satisfiable, and if so, ask Z3 for a model.

Problem B.2.4. Use Z3 to check the formula given in Ex. B.2.1. Do it for both the reals and integers.

Problem B.2.5. Use Z3 to formulate and check the statement "`If` $x > 3$ `then` $y > 2$ `AND` $x \leq 1$". Is it satisfiable? What model does Z3 return?

Example B.2.4 (DNN-style checking)**.** Consider a one-neuron ReLU: $y = \max(0, x-1)$. We want to check if the property "`For all` $x \leq 0$`, we have` $y = 0$" holds.

```
x, y = Reals('x y')
s = Solver()

# y = max(0, x-1)
s.add(y >= x-1, y >= 0)
s.add(Or(y == x-1, y == 0)) # ReLU
s.add(x <= 0, y != 0) # Negation of property

print(s.check()) # Output: unsat, property holds
```

Problem B.2.6. Modify the above to check property: "`For all` $x \geq 2$`, we have` $y \geq 1$." What does Z3 return?

B.3 SAT and SMT Solving Algorithms

Here we briefly discuss SAT and SMT solving algorithms, which are used to determine the satisfiability (and therefore validity) of SAT and SMT formulae.

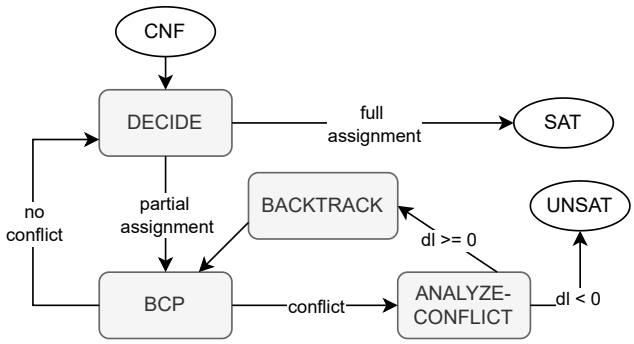


Figure B.1: The classicial DPLL Algorithm.

B.3.1 Satisfiability (SAT) Problem

The classical satisfiability (SAT) problem asks if a given propositional formulae (§B.1) can be satisfied [7]. Given a formula CNF f, an SAT solver returns `sat` if it can find a satisfying assignment that maps truth values to variables of f that makes f evaluate to true, and `unsat` if it cannot find any satisfying assignments.

The SAT problem is NP-Complete and research into methods for efficiently solving problem instances has been ongoing for multiple decades.

B.3.2 DPLL

Fig. B.1 gives an overview of **DPLL**, a SAT solving technique introduced in 1961 by Davis, Putnam, Logemann, and Loveland [13]. DPLL is an iterative algorithm that takes as input a propositional formula and (i) decides an unassigned variable and assigns it a truth value, (ii) performs Boolean constraint propagation (BCP or also called Unit Propagation), which detects single literal clauses that either force a literal to be true in a satisfying assignment or give rise to a conflict; (iii) analyzes the conflict to backtrack to a previous decision level `dl`; and (iv) erases assignments at levels greater than `dl` to try new assignments.

These steps repeat until DPLL finds a satisfying assignment and returns `sat`, or decides that it cannot backtrack (`dl`=-1) and returns `unsat`.

B.3.3 CDCL

Modern DPLL solving improves the original version with Conflict-Driven Clause Learning (*CDCL* [6, 33, 34]). DPLL with CDCL can *learn new clauses* to avoid past conflicts and backtrack more intelligently (e.g., using non-chronologically backjumping). Due to its ability to learn new clauses, CDCL can significantly reduce the search space and allow SAT solvers to scale to large problems. In the following, whenever we refer to DPLL, we mean DPLL with CDCL.

B.3.4 DPLL(T)

DPLL(T) [37] extends DPLL for propositional formulae to check SMT formulae involving non-Boolean variables, e.g., real numbers and data structures such as strings, arrays, lists. DPLL(T) combines DPLL with dedicated *theory solvers* to analyze formulae in those theories[1]. For example, to check a formula involving linear arithmetic over the reals (LRA), DPLL(T) may use a theory solver that uses linear programming to check the constraints in the formula.

Modern DPLL(T)-based SMT solvers such as Z3 [14] and CVC4 [3] include solvers supporting a wide range of theories including linear arithmetic, nonlinear arithmetic, string, and arrays [30].

[1] SMT is Satisfiability Modulo Theories and the T in DPLL(T) stands for Theories.

Background C

Linear Programming (LP)

Linear Programming (LP) and its generalization Mixed-Integer Linear Programming (MILP) form the optimization backbone of many neural network verification techniques. This chapter provides an overview of LP and MILP that are related to DNN verification.

C.1 Linear Constraints and Objectives

At a high level, LP is a method for optimizing an objective with respect to certain constraints. For example, we want to maximize profit while keeping production costs within budget. In LP, both the objective and constraints are *linear*.

Linear Constraints Linear constraints are inequalities that involve linear combinations of variables. A linear inequality has the general form

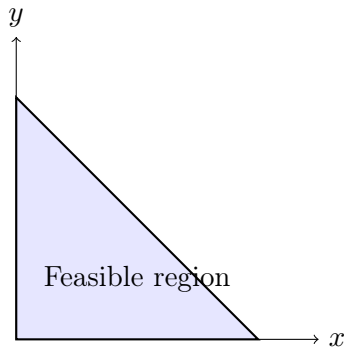
$$c_1x_1 + c_2x_2 + \cdots + c_nx_n \leq b,$$

where $c_i, b \in \mathbb{R}$. These constraints limit the feasible values that the variables x_i can take. The set of points satisfying all constraints is called the *feasible region*.

Example C.1.1. Consider the following linear constraints:

$$x + y \leq 4, \qquad x \geq 0, \qquad y \geq 0.$$

The feasible region is a triangle with vertices at $(0, 0), (4, 0), (0, 4)$.



Linear Objective Functions A linear objective function z has the general form

$$z(x_1, x_2, \ldots, x_n) = c_1x_1 + c_2x_2 + \cdots + c_nx_n,$$

where $c_i \in \mathbb{R}$ are coefficients, and $x_i \in \mathbb{R}$ are decision variables.

Optimizing Goals Our goal is to optimize (maximize or minimize) z with respect to a set of linear constraints over the decision variables.

$$\begin{aligned}&\text{maximize } z\\&\text{subject to}\\&\{c_1x_1 + c_2x_2 + \cdots + c_nx_n \leq b, \ldots\}\end{aligned}$$

Example C.1.2. Maximize

$$1.5x + 2y$$

subject to:

$$\{x + y \leq 4, x \geq 0, y \geq 0\}.$$

First, we can solve for the intersection points of the constraints:

$$\begin{aligned}x + y &= 4\\x &= 0\\y &= 0\end{aligned}$$

Solving these equations gives us the corner points or vertices of the feasible region:

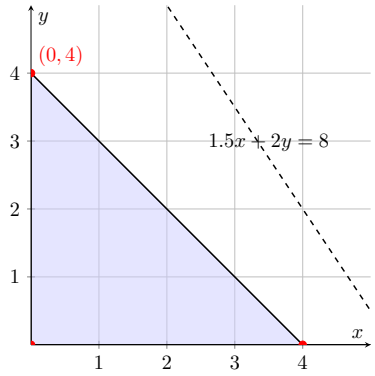
$$\begin{aligned}&(0, 0)\\&(4, 0)\\&(0, 4)\end{aligned}$$

Now, we can evaluate the objective function $z = 1.5x + 2y$ at each vertex:

x	y	z
0	0	0
4	0	6
0	4	8

Thus, the maximum value of z is 8, achieved at the vertex $(0, 4)$.

Geometric interpretation The constraints represent the feasible region as a triangle with vertices at $(0, 0)$, $(4, 0)$, and $(0, 4)$:



The objective function $z = 1.5x + 2y$ is maximized at vertex $(0, 4)$.

Problem C.1.1. Maximize $z = 4x + 5y$ subject to $\{x + y \leq 20,\ 2x + 4y \leq 72\}$.

1. Identify the corner points.
2. Evaluate the objective function at each corner point.

C.2 Mixed-Integer Linear Programming (MILP)

LP (§C.1) assumes continuous variables over real numbers. A mixed-integer linear program (MILP) extends LP by requiring some variables to be integers (often binary 0 or 1). This is useful because it allows for modeling discrete decisions and logical constraints, e.g., on/off decisions, yes/no choices, and active/inactive ReLU.

Linear Constraints In MILP, a linear constraint can involve both integer and continuous decision variables, and have the general form

$$c_1x_1 + c_2x_2 + \cdots + c_nx_n + d_1y_1 + d_2y_2 + \cdots + d_my_m \leq b,$$

where $x_i \in \mathbb{R}$ are continuous variables, $y_j \in \mathbb{Z}$ are integer variables, and $c_i, d_j, b \in \mathbb{R}$.

Objective Function A linear objective function z in MILP can be expressed as:

$$z(x_1, \ldots, x_n, y_1, \ldots, y_m) = c_1x_1 + c_2x_2 + \cdots + c_nx_n + d_1y_1 + d_2y_2 + \cdots + d_my_m,$$

where $x_i \in \mathbb{R}$ are continuous variables, $y_j \in \mathbb{Z}$ are integer variables, and $c_i, d_j \in \mathbb{R}$.

Optimizing Goals In MILP, the goal is to find the optimal values of the decision variables x and y that maximize or minimize the objective function z, while satisfying all linear constraints.

$$\begin{aligned}
&\text{maximize } z(x_1, \ldots, x_n, y_1, \ldots, y_m) \\
&\text{subject to} \\
&\{c_1x_1 + c_2x_2 + \cdots + c_nx_n + d_1y_1 + d_2y_2 + \cdots + d_my_m \leq b\}
\end{aligned}$$

Example C.2.1. A company sells a chair for \$50 and a table for \$120. The production costs of the chair and the table are \$20 and \$70, respectively. It also takes 3 hours to produce a chair and 1 hour to produce a table. Moreover, it takes 5 units of wood to produce a chair and 20 units of wood to produce a table.

How many chairs and tables should the company produce to *maximize* profit within a week without exceeding its monthly budget of 200 units of woods, 80 hours of labor, and \$800 in production costs?

First, the decision variables are defined as follows:

- x: the number of chairs produced.
- y: the number of tables produced.

The objective function to maximize profit P is given by:

$$P = 50x + 120y - 20x - 70y = 30x + 50y$$

with subject to the constraints:

$$\begin{aligned}
&5x + 20y \leq 200 \implies x + 4y \leq 40 \\
&3x + y \leq 80 \\
&20x + 70y \leq 800 \implies 2x + 7y \leq 80 \\
&x \geq 0 \\
&y \geq 0.
\end{aligned}$$

Solving First, we can find the corner points from the constraints

$$\begin{aligned}
&x + 4y = 40 \\
&3x + y = 80 \\
&2x + 7y = 80 \\
&x = 0 \\
&y = 0
\end{aligned}$$

Solving these equations gives us the corner points or vertices of the feasible region: (0,0); (0, 10); $(\frac{80}{3}, 0)$; and $(\frac{280}{11}, \frac{40}{11})$ (from x + 4 y = 40 & 3x + y = 80). Note that all of these are feasible with $2x + 7y \leq 800$.

Now, we can evaluate the objective function P at each vertex:

x	y	P = 30x + 50y
0	0	0
0	10	500
$\frac{80}{3}$	0	800
$\frac{280}{11}$	$\frac{40}{11}$	945.45

Thus, the maximum value of P is 945.45, achieved at the vertex $(\frac{280}{11}, \frac{40}{11})$.

Of course, since we cannot produce fractional chairs or tables, we need to round these numbers to the nearest integers. This means the company should produce 24 chairs and 4 tables per week, and get a profit of $920.00

C.2.1 Encoding Binary Variables

MILP problems often involve disjunction or condition where the answer depends on some condition. We can encode such condition using binary variables (0-1 integers), e.g., using $z \in \{0, 1\}$ to indicate whether a certain condition is met. Moreover, we also use a "trick" with a large constant M, e.g., ∞, to encode logical implications.

Example C.2.2. To encode "if $z =$ `True` then $x \geq 5$", use:

$$x \geq 5 - M(1 - z), \quad z \in \{0, 1\}$$

This works because

- $z = 1 \implies x \geq 5 - M(0) \implies x \geq 5$.
- $z = 0 \implies x \geq 5 - M \implies x \geq -\infty$ (because M is large this is vacuously true and can be discarded).

Problem C.2.1. Encode the disjunction $x \geq 5 \vee x \leq 3$ in MILP.

Example C.2.3 (Encoding ReLU in MILP)**.** To encode the ReLU (§1.3.1) activation function $y = \max(0, x)$, use

$$\begin{aligned} &y \geq x, \\ &y \geq 0, \\ &y \leq x + M(1 - z), \\ &y \leq Mz, \quad z \in \{0, 1\}. \end{aligned}$$

This works because

- $z = 1 \implies y = x$.
- $z = 0 \implies y = 0$.

Problem C.2.2. Consider again the ReLU example in Ex. C.2.3 but now x has the bounds $L \leq x \leq U$. Modify the MILP encoding so that L and U are used *directly* instead of a large constant M.

C.3 Using Z3 to Solve LP and MILP

We can use Z3's optimization capabilities to solve both LP and MILP problems. Note that in practice, we often use dedicated solvers such as Gurobi or CPLEX for large problems, but Z3 is effective for demonstration purposes.

Example C.3.1. We can model and solve Ex. C.1.2 using Z3 as follows:

```
from z3 import *

x, y = Reals("x y")
opt = Optimize() # setup the optimization problem
opt.add(x + y <= 4, x >= 0, y >= 0)

# Objective
z = 1.5*x + 2*y
h = opt.maximize(z)

# Solve
if (opt.check() == sat):
    print("Optimal sol:", opt.model())  # output [x = 0, y = 4]
    print("Max value:", opt.upper(h))   # output 8
```

Problem C.3.1. Do Prob. C.1.1 using Z3.

Problem C.3.2. Do Ex. C.2.1 using Z3.

Problem C.3.3. For this problem, you will find some interesting MILP problem online, formulate it, and solve it using Z3. Specifically, do the following:

- Find *two* interesting MILP problems online. These can be from textbooks, research papers, or online resources (Youtube, Google, online tutorials).

  Note: Interesting here means the problem has a non-trivial structure, resembles real-world applications (like the table and chair example in Ex. C.2.1), or involves complex constraints.

- For each problem:
  - Write down the problem and *cite* the sources (e.g., exact URL or Author(s)/Title/Year if from a paper).

- Formulate the problem as a MILP (clearly indicate the objective and constraints).
- Solve them by hand (you can type this out, but show all the steps, if possible, draw the graph showing the feasible region).
- Implement the formulation in Z3 and solve it.

Problem C.3.4. Minimize $z = x + y$ subject to:

$$\begin{aligned} x + 2y &\geq 3, \\ 3x + y &\geq 3, \\ x, y &\geq 0, \\ x, y &\in \mathbb{R}. \end{aligned}$$

You can either do this by hand on paper (and take picture) or write Python code with Z3. Either way, show all the steps (e.g., as comments in the Z3 code):

1. The constraints and objective function.
2. The corner or candidate points (this problem is very simple that you do need an algorithm like Simplex to solve. You can simply "guess" these points, e.g., the intersection of the given constraints)
3. The objective value at each corner point.
4. The optimal solution.

—

C.3.1 Using LP as Feasibility Checking

In addition to optimization, LP can be used for *feasibility* (or satisfiability) checking of linear constraints, i.e., are there any values for the variables that satisfy all the constraints? This is achieved by running an LP solver with a constant objective (e.g., "minimize 0"), in which case it simply tries to find *any* point in the feasible region or shows that none exists (infeasible). This thus makes it usefful for property checking and verification (e.g., showing that no counterexample exists).

The main difference between LP feasibility and SMT satisfiability is the type of constraints they can handle. SMT satisfiability can handle richer logics involving booleans, integers, nonlinear arithmetic, and other theories while LP feasibility is limited to linear equalities/inequalities over real numbers. But for problems that involve only linear real arithmetic, LP feasibility is sufficient and often more efficient. For problems involving more complex logic or theories, SMT solvers are necessary.

Example C.3.2. For the constraints in Ex. C.1.1:

$$x + y \leq 4, \quad x \geq 0, \quad y \geq 0 \tag{C.3.1}$$

Running an LP solver with objective $\min 0$ will return a point, e.g., (x=0,y=0), within the feasible region.

Background D

Software vs DNN Verification

General Software verification and DNN verification share the common goal of ensuring the correctness and reliability of their respective systems. Both fields aim to identify and eliminate potential errors or vulnerabilities before deployment, ultimately enhancing user trust and system robustness.

Similarities

Differences Software verification typically deals with discrete systems and logical properties, while DNN verification focuses on continuous input spaces and the behavior of neural networks under various conditions. Additionally, the techniques used in each field differ significantly, with software verification relying on formal methods and testing, whereas DNN verification often employs specialized techniques such as adversarial training and robustness analysis.

Table D.1: Comparison of Software Verification and DNN Verification

Aspect	Software Verification	DNN Verification
Input	Source code, specifications	DNN model, input space
Output	Verification results, counterexamples	Verification results, adversarial examples
Techniques	Model checking, theorem proving	Formal methods, testing
Challenges	State explosion, incomplete specifications	High dimensionality, non-convexity

Table D.2: Similarities of Software Verification and DNN Verification

Aspect	**Software Verification**	**DNN Verification**
Input	Source code, specifications	DNN model, input space
Output	Verification results, counterexamples	Verification results, adversarial examples
Techniques	Model checking, theorem proving	Formal methods, testing
Challenges	State explosion, incomplete specifications	High dimensionality, non-convexity

Table D.3: Differences of Software Verification and DNN Verification

Aspect	**Software Verification**	**DNN Verification**
Input	Source code, specifications	DNN model, input space
Output	Verification results, counterexamples	Verification results, adversarial examples
Techniques	Model checking, theorem proving	Formal methods, testing
Challenges	State explosion, incomplete specifications	High dimensionality, non-convexity

Advanced Topics A

NeuralSAT Algorithm

Alg. 6 shows the NeuralSAT algorithm, which takes as input the formula α representing the ReLU-based DNN N and the formulae $\phi_{in} \Rightarrow \phi_{out}$ representing the property ϕ to be proved. Internally, NeuralSAT checks the satisfiability of the formula given in Eq. 3.2.3

$$\alpha \wedge \phi_{in} \wedge \overline{\phi_{out}}.$$

NeuralSAT returns unsat if the formula unsatisfiable, indicating that ϕ is a valid property of N, and sat if it is satisfiable, indicating the N is not a valid property.

NeuralSAT uses a DPLL(T)-based algorithm to check unsatisfiability. First, the input formula in Eq. 3.2.3 is abstracted to a propositional formula with variables encoding neuron activation status (BooleanAbstraction). Next, NeuralSAT assign values to Boolean variables (Decide) and checks for conflicts the assignment has with the real-valued constraints of the DNN and the property of interest (BCP and Deduction). If conflicts arise, NeuralSAT determines the assignment decisions causing the conflicts (AnalyzeConflict), backtracks to erase such decisions (Backtrack), and learns clauses to avoid those decisions in the future. NeuralSAT repeats these decisions and checking steps until it finds a total or full assignment for all Boolean variables, in which it returns sat, or until it no longer can backtrack and returns unsat.

A.1 Boolean Abstraction

BooleanAbstraction (Alg. 6 line 1) encodes the DNN verification problem into a Boolean constraint to be solved by DPLL. This step creates Boolean variables to represent the *activation status* of hidden neurons in the DNN. Observe that when evaluating the DNN on any concrete input, the value of each hidden neuron *before* applying ReLU is either > 0 (the neuron is *active* and the input is passed through to the output) or ≤ 0 (the neuron is *inactive* because the output is 0). This allows partial assignments to these variables to represent neuron activation patterns within the DNN.

Algorithm 6. The `NeuralSAT` DPLL(T) algorithm.

input : DNN α, property $\phi_{in} \Rightarrow \phi_{out}$
output : `unsat` if the property is valid and `sat` otherwise

```
1  clauses ← BooleanAbstraction(α)
2  while true do
3      σ ← ∅ // initial assignment
4      dl ← 0 // initial decision level
5      igraph ← ∅ // initial implication graph
6      while true do
7          is_conflict ← true
8          if BCP(clauses, σ, dl, igraph) then
9              if Deduction(σ, dl, α, φ_in, φ_out) then
10                 is_sat, v_i ← Decide(α, φ_in, φ_out, dl, σ) // decision heuristic
11                 if is_sat then return sat // total assignment
12                 σ ← σ ∧ v_i
13                 dl ← dl + 1
14                 is_conflict ← false // mark as no conflict
15         if is_conflict then
16             if dl ≡ 0 then return unsat // conflict at decision level 0
17             clause ← AnalyzeConflict(igraph)
18             dl ← Backtrack(σ, clause)
19             clauses ← clauses ∪ {clause} // learn conflict clauses
20         if Restart() then break // restart heuristic
```

From the given network, `NeuralSAT` first creates Boolean variables representing the activation status of neurons. Next, `NeuralSAT` forms a set of initial clauses ensuring that each status variable is either `T` or `F`, indicating that each neuron is either active or inactive, respectively. A truth assignment over the variable v_i creates a constraint on the pre-ReLU neuron x_i.

Example A.1.1. For the DNN in Fig. 1.1, `NeuralSAT` creates two status variables v_3, v_4 for neurons x_3, x_4, respectively, and two initial clauses $v_3 \vee \overline{v_3}$ and $v_4 \vee \overline{v_4}$. The assignment $\{x_3 = T, x_4 = F\}$ creates the constraint $0.5x_1 - 0.5x_2 - 1 > 0 \wedge x_1 + x_2 - 2 \leq 0$.

A.2 DPLL

After `BooleanAbstraction`, `NeuralSAT` iteratively searches for an assignment satisfying the status clauses (Alg. 6, lines 6– 20). `NeuralSAT` combines DPLL components (e.g., `Decide`, `BCP`, `AnalyzeConflict`, `Backtrack` and `Restart`) to assign truth values with a theory solver (SA.3), consisting of abstraction and linear programming solving, to check the feasibility of the constraints implied by the assignment with

respect to the network and property of interest.

`NeuralSAT` maintains several variables (Alg. 6, lines 1– 5). These include clauses, a set of *clauses* consisting of the initial activation clauses and learned clauses; σ, a *truth assignment* mapping status variables to truth values; *igraph*, an *implication graph* used for analyzing conflicts; and *dl*, a non-zero *decision level* used for assignment and backtracking.

A.2.1 Decide

From the current assignment, `Decide` (Alg. 6, line 10) uses a heuristic to choose an unassigned variable and assigns it a random truth value at the current decision level. `NeuralSAT` applies the Filtered Smart Branching (FSB) heuristic [11, 15]. For each unassigned variable, FSB assumes that it has been decided (i.e., the corresponding neuron has been split) and computes a fast approximation of the lower and upper-bounds of the network output variables. FSB then prioritizes unassigned variables with the best differences among the bounds that would help make the input formula unsatisfiable (which helps prove the property of interest). Note that if the current assignment is full, i.e., all variables have assigned values, `Decide` returns `False` (from which `NeuralSAT` returns `sat`).

A.2.2 Boolean Constraint Propagation (BCP)

From the current assignment and clauses, `BCP` (Alg. 6, line 8) detects *unit clauses*[1] and infers values for variables in these clauses. For example, after the decision $a \mapsto F$, `BCP` determines that the clause $a \vee b$ becomes unit, and infers that $b \mapsto T$. Moreover, each assignment due to `BCP` is associated with the current decision level because instead of being "guessed" by `Decide` the chosen value is logically implied by other assignments. Moreover, because each BCP implication might cause other clauses to become unit, `BCP` is applied repeatedly until it can no longer find unit clauses. BCP returns `False` if it obtains contradictory implications (e.g., one BCP application infers $a \mapsto F$ while another infers $a \mapsto T$), and returns `True` otherwise.

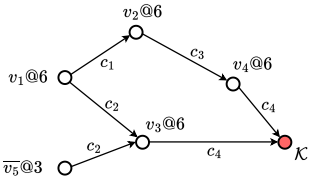
Implication Graph `BCP` uses an *implication graph* [5] to represent the current assignment and the reason for each BCP implication. In this graph, a node represents the assignment and an edge $i \xrightarrow{c} j$ means that `BCP` infers the assignment represented in node j due to the unit clause c caused by the assignment represented by node i. The implication graph is used by both BCP, which iteratively constructs the graph on each BCP application and uses it to determine conflict, and `AnalyzeConflict` (§A.2.3), which analyzes the conflict in the graph to learn clauses.

Example A.2.1. Assume we have the clauses in Fig. A.1(a), the assignments $\overline{v_5}@3$ and $v_1@6$ (represented in the graph in Fig. A.1(b) by nodes $\overline{v_5}@3$ and $v_1@6$, re-

[1] A unit clause is a clause that has a single unassigned literal.

$c_1 = (\overline{v_1} \vee v_2)$
$c_2 = (\overline{v_1} \vee v_3 \vee$
$c_3 = (\overline{v_2} \vee v_4)$
$c_4 = (\overline{v_3} \vee \overline{v_4})$

(a)



(b)

name	cl	lit	var	ante
c_4	$\overline{v_3} \vee \overline{v_4}$	$\overline{v_3}$	v_3	c_2
	$\overline{v_4} \vee \overline{v_1} \vee v_5$	$\overline{v_4}$	v_4	c_3
	$\overline{v_1} \vee v_5 \vee \overline{v_2}$	$\overline{v_2}$	v_2	c_1
c_5	$\overline{v_1} \vee v_5$			

(c)

Figure A.1: (a) A set of clauses, (b) an implication graph, and (c) learning a new clause.

spectively), and are currently at decision level *dl* 6. Because of assignment v_1@6, `BCP` infers v_2@6 from the unit clause c_1 and captures that implication with edge v_1@6 $\xrightarrow{c_1}$ v_2@6. Next, because of assignment v_2@6, `BCP` infers v_4@6 from the unit clause c_3 as shown by edge v_2@6 $\xrightarrow{c_3}$ v_4@6.

Similarly, `BCP` creates edges v_1@6 $\xrightarrow{c_2}$ v_3@6 and $\overline{v_5}$@ $\xrightarrow{c_2}$ v_3@6 to capture the inference v_3@6 from the unit clause c_2 due to assignments $\overline{v_5}$@3 and v_1@6. Now, `BCP` detects a conflict because clause $c_4 = \overline{v_3} \vee \overline{v_4}$ cannot be satisfied with the assignments v_4@6 and v_3@6 (i.e., both v_3 and v_4 are T) and creates two edges to the (red) node κ: v_4@6 $\xrightarrow{c_4}$ κ and v_3@6 $\xrightarrow{c_4}$ κ to capture this conflict.

Note that in this example `BCP` has the implication order v_2, v_4, v_3 (and then reaches a conflict). In the current implementation, `NeuralSAT` makes an arbitrary decision and thus could have a different order, e.g., v_3, v_4, v_2.

A.2.3 Conflict Analysis

Given an implication graph with a conflict (e.g., Fig. A.1b), `AnalyzeConflict` learns a new *clause* to avoid past decisions causing the conflict. The algorithm traverses the implication graph backward, starting from the conflicting node κ, while constructing a new clause through a series of resolution steps. `AnalyzeConflict` aims to obtain an *asserting* clause, which is a clause that will force an immediate BCP implication after backtracking.

`AnalyzeConflict`, shown in Alg. 7, first extracts the conflicting clause *cl* (line 1), represented by the edges connecting to the conflicting node κ in the implication graph. Next, the algorithm refines this clause to achieve an asserting clause (lines 2– 6). It obtains the literal *lit* that was assigned last in *cl* (line 3), the variable *var* associated with *lit* (line 4), and the antecedent clause *ante* of that *var* (line 5), which contains

Algorithm 7. AnalyzeConflict

input : implication graph igraph
output : clause

```
1 clause ← CurrentConflictClause(igraph)
2 while ¬StopCriterion(clause) do
3     lit ← LastLiteral(igraph, clause)
4     var ← LiteralToVariable(lit)
5     ante ← Antecedent(igraph, lit)
6     clause ← BinRes(clause, ante, var)
7 return clause
```

$\overline{lit}$ as the only satisfied literal in the clause. Now, `AnalyzeConflict` resolves cl and $ante$ to eliminate literals involving var (line 6). The result of the resolution is a clause, which is then refined in the next iteration.

Resolution. We use the standard *binary resolution rule* to learn a new clause implied by two (*resolving*) clauses $a_1 \vee ... \vee a_n \vee \beta$ and $b_1 \vee ... \vee b_m \vee \overline{\beta}$ containing complementary literals involving the (*resolution*) variable β:

$$\frac{(a_1 \vee ... \vee a_n \vee \beta) \qquad (b_1 \vee ... \vee b_m \vee \overline{\beta})}{(a_1 \vee ... \vee a_n \vee b_1 \vee ... \vee b_m)} \quad \text{(Binary-Resolution)} \qquad \text{(A.2.1)}$$

The resulting (*resolvant*) clause $a_1 \vee ... \vee a_n \vee b_1 \vee ... \vee b_m$ contains all the literals that do not have complements β and $\neg\beta$.

Example A.2.2. Fig. A.1(c) demonstrates `AnalyzeConflict` using the example in §A.2.2 with the BCP implication order v_2, v_4, v_3 and the conflicting clause cl (connecting to node κ in the graph in Fig. A.1(b)) $c_4 = \overline{v_3} \vee \overline{v_4}$. From c_4, we determine the last assigned literal is $lit = \overline{v_3}$, which contains the variable $var = v_3$, and the antecedent clause containing v_3 is $c_2 = \overline{v_1} \vee v_3 \vee v_5$ (from the implication graph in Fig. A.1(b), we determine that assignments $v_1@6$ and $\overline{v_5}@3$ cause the BCP implication $v_3@6$ due to clause c_2). Now we resolve the two clauses cl and c_2 using the resolution variable v_3 to obtain the clause $\overline{v_4} \vee \overline{v_1} \vee v_5$. Next, from the new clause, we obtain $lit = \overline{v_4}, var = v_4, ante = c_3$ and apply resolution to get the clause $\overline{v_1} \vee v_5 \vee \overline{v_2}$. Similarly, from this clause, we obtain $lit = \overline{v_2}, var = v_2, ante = c_1$ and apply resolution to obtain the clause $v_1 \vee v_5$.

At this point, `AnalyzeConflict` determines that this is an asserting clause, which would force an immediate BCP implication after backtracking. As will be shown in §A.2.4, `NeuralSAT` will backtrack to level 3 and erases all assignments after this level (so the assignment $\overline{v_5}@3$ is not erased, but assignments after level 3 are erased). Then, `BCP` will find that c_5 is a unit clause because $\overline{v_5}@3$ and infers $\overline{v_1}$. Once obtaining the asserting clause, `AnalyzeConflict` stops the search, and `NeuralSAT` adds $v_1 \vee v_5$ as the new clause c_5 to the set of existing four clauses.

The process of learning clauses allows `NeuralSAT` to learn from its past mistakes. While such clauses are logically implied by the formula in Eq. 3.2.3 and therefore do not change the result, they help prune the search space and allow DPLL and therefore `NeuralSAT` to scale. For example, after learning the clause c_5, together with assignment $v_5@3$, we immediately infer $v_1 \mapsto F$ through BCP instead of having to guess through `Decide`.

A.2.4 Backtrack

From the clause returned by `AnalyzeConflict`, `Backtrack` (Alg. 6, line 18) computes a backtracking level and erases all decisions and implications made after that level. If the clause is *unary* (containing just a single literal), then we backtrack to level 0.

Currently, NeuralSAT uses the standard *conflict-drive backtracking* strategy [5], which sets the backtracking level to the *second most recent* decision level in the clause. Intuitively, by backtracking to the second most recent level, which means erasing assignments made *after* that level, this strategy encourages trying new assignments for more recently decided variables.

Example A.2.3. From the clause $c_5 = \overline{v_1} \vee v_5$ learned in AnalyzeConflict, we backtrack to decision level 3, the second most recent decision level in the clause (because assignments v_1@6 and $\overline{v_5}$@3 were decided at levels 6 and 3, respectively). Next, we erase all assignments from decision level 4 onward (i.e., the assignments to v_1, v_2, v_3, v_4 as shown in the implication graph in Fig. A.1). This thus makes these more recently assigned variables (after decision level 3) available for new assignments (in fact, as shown by the example in §A.2.2, BCP will immediately infer $v_1 = T$ by noticing that c_5 is now a unit clause).

A.2.5 Restart

As with any stochastic algorithm, NeuralSAT can perform poorly if it gets into a subspace of the search that does not quickly lead to a solution, e.g., due to choosing a bad sequence of neurons to split [11, 15]. This problem, which has been recognized in early SAT solving, motivates the introduction of restarting the search [22] to avoid being stuck in such a *local optima*.

NeuralSAT uses a simple restart heuristic (Alg. 6, line 20) that triggers a restart when either the number of processed assignments (nodes) exceeds a pre-defined number (e.g., 300 nodes) or the current runtime exceeds a pre-defined threshold (e.g., 50 seconds). After a restart, NeuralSAT avoids using the same decision order of previous runs (i.e., it would use a different sequence of neuron splittings). It also resets all internal information (e.g., decisions and implication graph) except the learned conflict clauses, which are kept and reused as these are *facts* about the given constraint system. This allows a restarted search to quickly prune parts of the space of assignments.

We found the combination of clause learning and restarts effective for DNN verification. In particular, while restart resets information it keeps learned clauses, which are *facts* implied by the problem, and therefore enables quicker BCP applications and non-chronological backtracking (e.g., as illustrated in Fig. 8.2).

A.3 Deduction (Theory Solving)

Deduction (Alg. 6, line 9) is the theory or T-solver, i.e., the T in DPLL(T). The main purpose of the T-solver is to check the feasibility of the constraints represented by the current propositional variable assignment; as shown in the formalization in S?? this amounts to just *linear equation* solving for verifying piecewise linear DNNs. However, NeuralSAT is able to leverage specific information from the DNN problem, including

Algorithm 8. DEDUCTION

input : DNN α, input property ϕ_{in}, output property ϕ_{out}, decision level dl and current assignment σ

output : false if infeasibility occurs, true otherwise

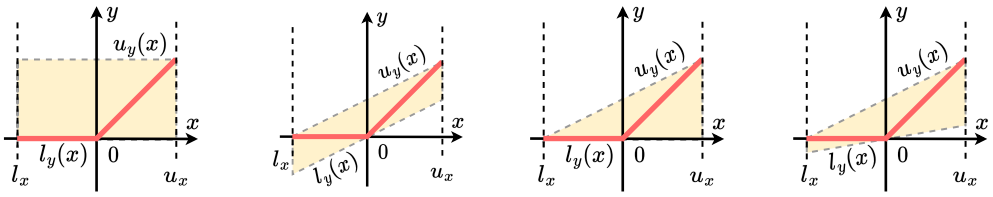
```
1  solver ← LPSolver(σ, α ∧ φ_in ∧ ¬φ_out)
2  if Solve(solver) ≡ INFEASIBLE then return false
3  if isTotal(σ) then return true // orig prob ( Eq. 3.2.3) is satisfiable
4  input_bounds ← TightenInputBounds(solver, φ_in)
5  output_bounds, hidden_bounds ← Abstract(α, σ, input_bounds)
6  if Check(output_bounds, ¬φ_out) ≡ INFEASIBLE then return false
7  for v ∈ hidden_bounds do
8      x ← ActivationStatus(v)
9      if x ∈ σ ∨ ¬x ∈ σ then continue
10     if LowerBound(v) > 0 then σ ← σ ∪ x@dl
11     else if UpperBound(v) ≤ 0 then σ ← σ ∪ x̄@dl
12 return true
```

input and output properties, for more aggressive feasibility checking. Specifically, `Deduction` has three tasks: (i) checking feasibility using linear programming (LP) solving, (i) further checking feasibility with input tightening and abstraction, and (iii) inferring literals that are unassigned and are implied by the abstracted constraint.

Alg. 8 describes `Deduction`, which returns `False` if infeasibility occurs and `True` otherwise. First, it creates a linear constraint system from the input assignment σ and $\alpha \wedge \phi_{in} \wedge \overline{\phi_{out}}$, i.e., the formula in Eq. 3.2.3 representing the original problem (line 1). The key idea is that we can remove ReLU activation for hidden neurons whose activation status have been decided. For constraints in α associated with variables that are not in the σ, we ignore them and just consider the cutting planes introduced by the partial assignment. For example, for the assignment $v_3 \mapsto T, v_4 \mapsto F$, the non-linear ReLU constraints $x_3 = ReLU(-0.5x_1 + 0.5x_2 + 1)$ and $x_4 = ReLU(x_1 + x_2 - 1)$ for the DNN in Fig. 1.1 become linear constraints $x_3 = -0.5x_1 + 0.5x_2$ and $x_4 = 0$, respectively.

Next, an LP solver checks the feasibility of the linear constraints (line 2). If the solver returns infeasible, `Deduction` returns `False` so that `NeuralSAT` can analyze the assignment and backtrack. If the constraints are feasible, then there are two cases to handle. First, if the assignment is total (i.e., all variables are assigned), then that means that the original problem is satisfiable (line 3) and `NeuralSAT` returns `sat`.

ReLU Abstraction. Second, if the assignment is not total then `Deduction` applies abstraction to check satisfiability (lines 4–6). Specifically, we over-approximate ReLU computations to obtain the upper and lower bounds of the output values and check if the output properties are feasible with respect to these bounds. For example, the output $x_5 > 0$ is *not* feasible if the upperbound is $x_5 \leq 0$ and *might be*



(a) interval (b) zonotope (c) DeepPoly (d) LiRPA

Figure A.2: Abstractions for ReLU: (a) interval, (b) zonotope, and (c-d) polytopes. Notice that ReLU is a non-convex region (red line) while all abstractions are convex regions. Note that (c) and (d) are both polytopes.

feasible if the upperbound is $x_5 \leq 0.5$ ("might be" because this is an upper-bound). If abstraction results in infeasibility, then `Deduction` returns `False` for `NeuralSAT` to analyze the current assignment (line 6).

`NeuralSAT` uses abstraction to approximate the lower and upper bounds of hidden and output neurons. Fig. A.2 compares the (a) interval [46], (b) zonotope [42], and (c, d) polytope [43,47,49] abstraction domains to compute the lower $l_y(x)$ and upper $u_y(x)$ bounds of a ReLU computation $y =$ `ReLU(x)` (non-convex red line). `NeuralSAT` can employ any existing abstract domains, though currently it adopts the *LiRPA* polytope (Fig. A.2d) [47–49] because it has a good trade-off between precision and efficiency.

Inference If abstraction results in feasible constraints, `Deduction` next attempts to infer implied literals (lines 7– 11). To obtain the bounds of the output neurons, abstraction also needs to compute the bounds of hidden neurons, including those with undecided activation status (i.e., not yet in σ). This allows us to assign the activation variable of a hidden neuron the value `True` if the lowerbound of that neuron is greater than 0 (the neuron is active) and `False` otherwise. Since each literal is considered, this would be considered exhaustive theory propagation. Whereas the literature [30,37] suggests that this is an inefficient strategy, we find that it does not incur significant overhead (average overhead is about 4% and median is 2%).

Example A.3.1. For the illustrative example in Ex. 8.2.1, in iteration 3, the current assignment σ is $\{v_4 = 1\}$, corresponding to a constraint $x_1 + x_2 - 1 > 0$. With the new constraint, we optimize the input bounds and compute the new bounds for hidden neurons $0.5 \leq x_3 \leq 2.5$, $0 < x_4 \leq 2.0$ and output neuron $x_5 \leq 0.5$ (and use this to determine that the postcondition $x_5 > 0$ might be feasible). We also infer $v_3 = 1$ because of the positive lower bound $0.5 \leq x_3$.

Part VI

Optimizations and Strategies

Advanced Topics B

Adversarial Attacks

Modern DNN verifiers such as $\alpha\beta$-`CROWN` and `NeuralSAT` often first run an adversarial attack technique to check for obvious counterexamples. If one is found, the property is violated (and the verifier returns `sat`). If no counterexample is found, the verifier proceeds to the more expensive search-based verification algorithm (e.g., $\texttt{BaB}_{\texttt{NV}}$ as shown in §6).

Thus, in the first phase of running adversarial attacks, the goal to *falsify* the property, i.e., find a counterexample that violates the property. If this fails, then the goal is to *verify* the property, i.e., prove that no counterexample exists. Of course, during the verification phase, the verifier may also discover counterexamples that the falsify phase misses.

B.1 Random Search Attack

Random search (RS) is a simple method for adversarial attack. It randomly samples points in the allowed input ranges and checks if any samples violate the property; if so, a counterexample is found.

Example B.1.1. Suppose the DNN input ranges are:

$$-1 \leq x_1 \leq 1, \quad -2 \leq x_2 \leq 2$$

and the output is:

$$y = 2x_1 - 1.5x_2 + 1.$$

We wish to use RS to find a counterexample to the property $y > 0$; i.e., trying random inputs (x_1, x_2) satisfying the given ranges and producing $y \leq 0$.

- Try 1: $x_1 = 0.2,\ x_2 = -0.5$

  $$y = 2 \times 0.2 - 1.5 \times (-0.5) + 1 = 0.4 + 0.75 + 1 = 2.15 > 0$$

  Not a violation.

- Try 2: $x_1 = -1,\ x_2 = 2$

$$y = 2 \times (-1) - 1.5 \times 2 + 1 = -2 - 3 + 1 = -4 < 0$$

Counterexample found: $(x_1 = -1,\ x_2 = 2)$.

2. Projected Gradient Descent (PGD)

Projected Gradient Descent (PGD) is a strong first-order adversarial attack that iteratively moves the input in the direction that maximizes property violation, while projecting (clipping) the input back into the allowed domain after every step.

1. **Initialize** at a valid input, e.g., $(x_1^{(0)}, x_2^{(0)}) = (0, 0)$.
2. **For each step t:**
   (a) Compute the gradient:

$$\nabla_x x_5 = \left(\frac{\partial x_5}{\partial x_1}, \frac{\partial x_5}{\partial x_2} \right)$$

   For our example,

$$\nabla_x x_5 = (2, -1.5)$$

   (b) Update:

$$x_1^{(t+1)} = x_1^{(t)} - \eta \cdot 2$$
$$x_2^{(t+1)} = x_2^{(t)} - \eta \cdot (-1.5)$$

   (c) **Project (Clip)**:

$$x_1^{(t+1)} = \max(-1, \min(x_1^{(t+1)}, 1))$$
$$x_2^{(t+1)} = \max(-2, \min(x_2^{(t+1)}, 2))$$

   (d) If $x_5 \leq 0$, **return** $(x_1^{(t+1)}, x_2^{(t+1)})$ as a counterexample.

Example:
Let $\eta = 0.5$, initial point $(x_1, x_2) = (0, 0)$.

$$x_1^{(1)} = 0 - 0.5 \times 2 = -1$$
$$x_2^{(1)} = 0 - 0.5 \times (-1.5) = 0.75$$

Clip to the ranges: $x_1^{(1)} = -1$, $x_2^{(1)} = 0.75$.
Compute:

$$x_5 = 2 \times (-1) - 1.5 \times 0.75 + 1 = -2 - 1.125 + 1 = -2.125 < 0$$

So, the PGD attack finds a counterexample at $(x_1 = -1,\ x_2 = 0.75)$.

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