# VERIFIED DEEP LEARNING

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IN PROGRESS; DO NOT CIRCULATE

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# About This Book

## Why This Book

I believe that deep learning is here to stay and that we have only scratched the surface of what neural networks can actually do. The line between software 1.0 (that is, manually written code) and software 2.0 (learned neural networks) is getting fuzzier and fuzzier, and neural networks are participating in safety-critical, security-critical, and socially-critical tasks. Think, for example, healthcare, self-driving cars, malware detection, etc. But neural networks are fragile and so we need to prove that they are well-behaved when applied in critical settings.

Over the past few decades, the formal methods community has developed a plethora of techniques for automatically proving properties of programs, and, well, neural networks are programs. So there is a great opportunity to port verification ideas to the software 2.0 setting. This book offers the first introduction of foundational ideas from automated verification as applied to deep neural networks and deep learning. I hope that it will inspire verification researchers to explore correctness in deep learning and deep learning researchers to adopt verification technologies.

## Who Is This Book For

Given that the book's subject matter sits at the intersection of two pretty much disparate areas of computer science, one of my main design goals is to make it as self-contained as possible. This way the book can serve as an introduction to the field for first-year graduate students even if they have not been exposed to deep learning or verification.

## What Does This Book Cover

The book is divided into four parts:

**Part 1** defines neural networks as data-flow graphs of operators over real-valued inputs. This formulation will serve as our basis for the rest of the book. Additionally, we will survey a number of correctness properties that are desirable of neural networks and place them in a formal framework.

**Part 2** discusses *constraint-based* techniques for verification. As the name suggests, we construct a system of constraints and solve it to prove (or disprove) that a neural network satisfies some properties.

**Part 3** discusses *abstraction-based* techniques for verification. Instead of executing a neural network on a single input, we can actually execute it on an *infinite* set and show that all of those inputs satisfy desirable correctness properties.

**Part 4** Finally, we will discuss verification technology as applied to deep reinforcement learning tasks, where neural networks are used as controllers in a dynamical system.

Parts 2 and 3 are disjoint; the reader can go directly from Part 1 to Part 3.

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Part I

# Neural Networks & Correctness

Chapter 1

# A New Beginning

> He had become so caught up in building sentences that he had almost forgotten the barbaric days when thinking was like a splash of color landing on a page.
>
> —Edward St. Aubyn, *Mother's Milk*

## 1.1 It Starts With Turing

This book is about *verifying* that a *neural network* behaves according to some set of desirable properties. These fields of study, verification and neural networks, have been two distinct areas of computing research with no bridges between them, until very recently. Interestingly, however, both fields trace their genesis to a two-year period of Alan Turing's tragically short life.

In 1949, Turing wrote a little-known paper titled *Checking a Large Routine*. It was a truly forward-looking piece of work. In it, Turing asks how can we prove that the programs we write do what they are supposed to do? Then, he proceeds to provide a proof of correctness of a program implementing the factorial function. Specifically, Turing proved that his little piece of code always terminates and always produces the factorial of its input. The proof is elegant; it breaks down the program into single instructions, proves a lemma for every instruction, and finally stitches the lemmas together to prove correctness of the full program. Until this day, proofs of programs very much

Quote found in William Finnegan's *Barbarian Days*.

follow Turing's proof style from 1949. And, as we shall see in this book, proofs of neural networks will, too.

Just a year before Turing's proof of correctness of factorial, in 1948, Turing wrote a perhaps even more farsighted paper, *Intelligent Machinery*, in which he proposed *unorganized machines*. These machines, Turing argued, mimic the infant human cortex, and he showed how they can *learn* using what we now call a genetic algorithm. Unorganized machines are a very simple form of what we now know as neural networks.

## 1.2 **The Rise of Deep Learning**

The topic of training neural networks continued to be studied since Turing's 1948 paper. But it only recently exploded in popularity, thanks to a combination algorithmic developments, hardware developments, and a flood of data for training.

Modern neural networks are called *deep* neural networks, and the approach to training these neural networks is *deep learning*. Deep learning has enabled incredible improvements in complex computing tasks, most notably in computer vision and natural language processing, for example, in recognizing objects and people in an image and translating between languages. And, everyday, a growing research community is exploring ways to extend and apply deep learning to more challenging problems, from music generation to proving mathematical theorems.

The advances in deep learning have changed the way we think of what software is, what it can do, and how we build it. Modern software is increasingly becoming a menagerie of traditional, manually written code and automatically trained—sometimes constantly learning—neural networks. But deep neural networks can be fragile and produce unexpected results. As deep learning becomes used more and more in sensitive settings, like autonomous cars, it is imperative that we verify these systems and provide formal guarantees on their behavior. Luckily, we have decades of research on program verification that we can build upon, but what exactly do we verify?

## 1.3 What do We Expect of Neural Networks?

Remember Turing's proof of correctness of factorial? Turing was concerned that we will be programming computers to perform mathematical operations, but we could be getting them wrong. So in his proof he showed that his implementation of factorial is indeed equivalent to the mathematical definition. This notion of program correctness is known as *functional correctness*, meaning that a program is a faithful implementation of some mathematical function. Functional correctness is incredibly important in many settings—think of the disastrous effects of a buggy implementation of a cryptographic primitive.

In the land of deep learning, proving functional correctness is an unrealistic task. What does it mean to correctly recognize cats in an image or correctly translate English to Hindi? We cannot mathematically define these tasks. The whole point of using deep learning to do these tasks is because we cannot mathematically capture what exactly they entail.

So what now? Is verification out of the question for deep neural networks? No! While we cannot precisely capture what a deep neural network should do, we can often characterize some of its desirable or undesirable properties. Let us look at some examples of such properties.

### Robustness

The most-studied correctness property of neural networks is *robustness*, because it is generic in nature and deep learning models are infamous for their fragility. Robustness means that small perturbations to inputs should not result in changes to the output of the neural network. For example, changing a small number of pixels in my photo should not make the network think that I am a cupboard instead of a person, or adding inaudible noise to a recording of my lecture should not make the network think it is a lecture about the Ming dynasty in the 15th century. Funny examples aside, lack of robustness can be a safety and security risk. Take, for instance, an autonomous vehicle following traffic signs using cameras. It has been shown that a light touch of vandalism to the stop sign can cause the vehicle to miss it, potentially causing an accident. Or consider the case of a neural network for detecting malware.

We do not want a minor tweak to the malware's binary to cause the detector to suddenly deem it safe to install.

### Safety

Safety is a broad class of correctness properties stipulating that a program should not get to a *bad state*. The definition of *bad* depends on the task at hand. Consider a neural-network-operated robot working in a some kind of plant; we might be interested in ensuring that the robot does not exceed certain speed limits, to avoid endangering human workers, or that it does not go to a dangerous part of the plant. Another well-studied example is a neural network implementing a collision avoidance system for aircrafts. One property of interest is that if an intruding aircraft is approaching from the left, the neural network should decide to turn the aircraft right.

### Consistency

Neural networks learn about our world via examples, like images. As such, they may sometimes miss basic axioms, like physical laws, and assumptions about realistic scenarios. For instance, a neural network recognizing objects in an image and their relationships might say that object A is to the on top of object B, B is on top of C, and C is on top of A. But this cannot be!

For another example, consider a neural network tracking players on the soccer field using a camera. It should not in one frame of video say that Ronaldo is on the right side of the pitch and then in the next frame say that Ronaldo is on the left side of the pitch—Ronaldo is fast, yes, but he has slowed down in the last couple of seasons.

## Looking Ahead

I hope that I have convinced you of the importance of verifying properties of neural networks. In the next two chapters, we will formally define what neural networks look like (hint: they are ugly programs) and then build a language for formally specifying correctness properties of neural networks, paving the way for verification algorithms to prove these properties.

Chapter 2

# Neural Networks as Graphs

There is no rigorous definition of what deep learning is and what it is not. In fact, at the time of writing this, there is a raging debate in the artificial intelligence community about a clear definition. In this chapter, we will define neural networks generically as graphs of operations over real numbers. In practice, the shape of those graphs, called the *architecture*, is not arbitrary: Researchers and practitioners carefully construct new architectures to suit various tasks. For example, neural networks for image recognition typically look different from those for natural language tasks.

First, we will informally introduce graphs and look at some popular architectures. Then, we will formally define graphs and their semantics.

## 2.1 The Neural Building Blocks

A neural network is a graph where each node performs an operation. Overall, the graph represents a function from real numbers to real numbers, that is, $\mathbb{R}^n \to \mathbb{R}^m$. Consider the following very simple graph. The red node is an

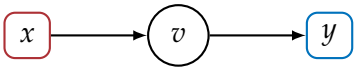



**Figure 2.1** A very simple network

*input* node; it just passes input $x$, a real number, to node $v$. Node $v$ performs some operation on $x$ and spits out a value that goes to the *output* node $y$. For example, $v$ might simply return $2x + 1$, which we will denote as the function

$f_v : \mathbb{R} \to \mathbb{R}$:

$$f_v(x) = 2x + 1$$

In our model, the output node may also perform some operation, for example,

$$f_y(x) = \max(0, x)$$

Taken together, this simple graph encodes the following function $f : \mathbb{R} \to \mathbb{R}$:

$$f(x) = f_y(f_v(x)) = \max(0, 2x + 1)$$

## Transformations and Activations

The function $f_v$ is an *affine transformation*. Simply, it multiplies inputs by constant values (in this case, $2x$) and adds constant values (1). The function $f_y$ is an *activation* function, because it turns on or off. When its input is negative, $f_y$ outputs 0, otherwise it outputs its input. Specifically, $f_y$ is called a *rectified linear unit* (ReLU), and it is a very popular activation function in modern deep neural networks.

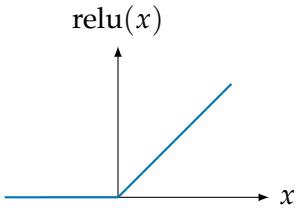



**Figure 2.2** Rectified linear unit

There are other popular activation functions, for example, sigmoid,

$$\sigma(x) = \frac{1}{1 + \exp(-x)}$$

whose output is bounded between 0 and 1, as shown in **??**.

Often, in the literature and practice, the affine transformation and the activation function are combined into a single operation. Our graph model of neural networks can capture that, but we usually prefer to distribute the two operations on two different nodes of the graph as it will simplify our life in later chapters when we start analyzing those graphs.

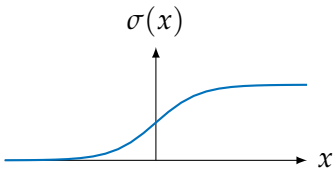



**Figure 2.3** Sigmoid activation function

### Universal approximation

What is so special about these activation functions? The short answer is they work in practice, in that they result in neural networks that are able to learn complex tasks. It is also very interesting to point out that you can construct a neural network comprised of ReLUs or sigmoids and affine transformations to approximate any function. This is known as the *universal approximation theorem*, and in fact the result is way more general than ReLUs and sigmoids—nearly any activation function you can think of works, as long as it is not polynomial!

## 2.2 Layers and Layers and Layers

In general, a neural network can be a crazy graph, with nodes and arrows pointing all over the place. In practice, networks are usually *layered*. Take the graph in **??**. Here we have 3 inputs and 3 outputs, $\mathbb{R}^3 \to \mathbb{R}^3$. Notice that

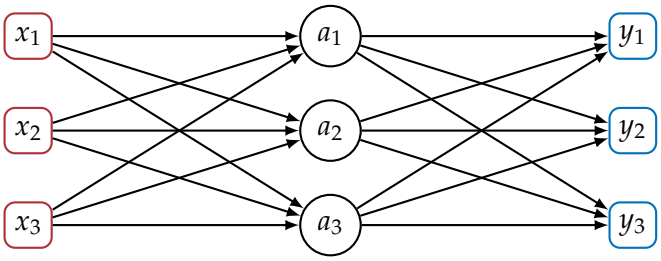



**Figure 2.4** A multilayer perceptron

the nodes of the graph form layers, the input layer, the output layer, and the

layer in the middle which is called the *hidden* layer. This form of graph—or architecture—has the grandiose name of *multilayer perceptron* (MLP). Usually, we have a bunch of hidden layers in an MLP, like in **??**. Layers in an MLP

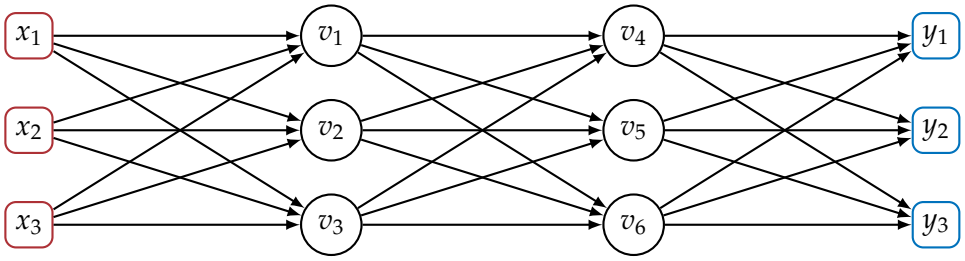



**Figure 2.5** A multilayer perceptron with two hidden layers

are called *fully connected* layers, since each node receives all outputs from the preceding layer.

When we are doing classification, the output layer of the MLP represents the probability of each class, for example, $y_1$ is the probability of the input being a chair, $y_2$ is the probability of a TV, and $y_3$ of a couch. To ensure that the probabilities are normalized, that is, between 0 and 1 and sum up to 1, the final layer employs a *softmax* function. Softmax, generically, looks like this for an output node $y_i$, where $n$ is the number of classes:

$$f_{y_i}(x_1, \ldots, x_n) = \frac{\exp(x_i)}{\sum_{k=1}^{n} \exp(x_k)}$$

To visualize why this actually works, please see Nielsen (2018, Chapter 3).

## 2.3 Convolutional Layers

Another kind of layer that you will find in a neural network is a *convolutional* layer. This kind of layer is widely used in computer vision tasks, but also has uses in natural language processing. The rough intuition is that if you are looking at an image, you want to scan it looking for patterns—the same thing is true of sentences in natural language. The convolutional layer gives you that: it defines an operation, a *kernel*, that is applied to every region of pixels in an image or every sequence of words in a sentence. For illustration,

let us consider an input layer of size 4, perhaps each input defines a word in a 4-word sentence, as shown in **??**. Here we have a kernel, nodes $v_i$, that is applied to every pair of consecutive words, $(x_1, x_2)$, $(x_2, x_3)$, and $(x_3, x_4)$. We say that this kernel has size 2, since it takes an input in $\mathbb{R}^2$. This kernel is 1-dimensional, since its input is a vector of real numbers. In practice, we work with 2-dimensional kernels or more; for instance, to scan blocks of pixels of a gray scale image where every pixel is a real number, we can use kernels that are functions in $\mathbb{R}^{10\times 10} \to \mathbb{R}$, meaning that the kernel is applied to every $10 \times 10$ sub-image in the input.

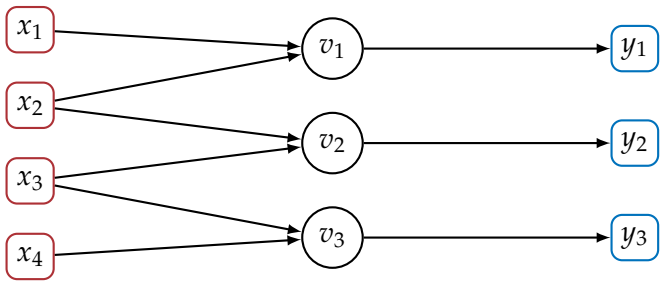



**Figure 2.6** 1-dimensional convolution

Typically, a *convolutional neural network* will apply a bunch of kernels to an input—and many layers of them—and aggregate (*pool*) the information from each kernel. We will formally define these operations in later chapters when we verify properties of such networks.

## 2.4 Where are the Loops?

All the neural networks we have seen so far seem to be a composition of a number mathematical functions, one after the other. So what about loops? Can we have loops in neural networks? In practice, neural network graphs are really just directed acyclic graphs (DAGs). This makes training the neural network possible using the *backpropagation* algorithm.

That said, there are popular classes of neural networks that appear to have loops, but they are very simple, in the sense that the number of iterations of the loop is just the size of the input. *Recurrent neural networks* (RNNs)

is the canonical class of such networks, which are usually used for sequence data, like text. You will often see the graph of an RNN rendered as follows, with the self loop on node $v$.

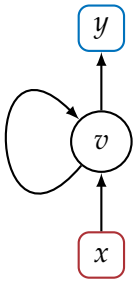



**Figure 2.7** Recurrent neural network

Effectively, this graph represents an infinite family of acyclic graphs that unroll this loop a finite number of times. For example, the following is an unrolling of length 3. Notice that this is an acyclic graph that takes 3 inputs. The idea is that if you receive a sentence, say, with $n$ words, you unroll the RNN to length $n$ and apply it to the sentence.

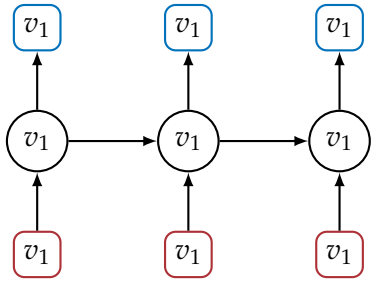



**Figure 2.8** Unrolled recurrent neural network

Thinking of it through a programming lens, given an input, we can easily statically determine—i.e., without executing the network—how many loop iterations it will require. This is in contrast to, say, a program where the number of loop iterations is a complex function of its input, and therefore we do not know how many loop iterations it will take until we actually run

it. With this in mind, in what follows, we will formalize neural networks as acyclic graphs.

## 2.5 Structure and Semantics of Networks

We are done with looking at pretty graphs. Let us now look at pretty symbols. We will now formally define graphs and discuss some of their properties.

### Networks as DAGs

A neural network is a directed acyclic graph $G = (V, E)$, where

- $V$ is a finite set of nodes.
- $E \subseteq V \times V$ is a set of edges.
- $V^{\text{in}} \subseteq V$ is a non-empty set of input nodes.
- $V^{\text{o}} \subset V$ is a non-empty set of output nodes.
- Each non-input node $v$ is associated with a function $f_v : \mathbb{R}^n \to \mathbb{R}$, where $n$ is the number of edges whose target is $v$. Notice that we assume, for simplicity but without loss of generality, that a node $v$ only outputs a single real value. The vector of real values $\mathbb{R}^n$ that $v$ takes as input is all the outputs of nodes $v'$ such that $(v', v) \in E$.

To make sure that a graph $G$ does not have any dangling nodes and that semantics are clearly defined, we will assume the following structural properties:

- All nodes are reachable, via directed edges, from some input node.
- Every node can reach an output node.
- There is fixed total ordering on edges $E$ and another one on nodes $V$.

### Semantics of DAGs

A network $G = (V, E)$ defines a function in $\mathbb{R}^n \to \mathbb{R}^m$ where

$$n = |V^{\mathsf{in}}| \qquad m = |V^{\mathsf{o}}|$$

That is, $G$ maps the values of the input nodes to those of the output nodes.

Specifically, for every non-input node $v \in V$, we recursively define the value in $\mathbb{R}$ that it produces as follows. Let $(v_1, v), \ldots, (v_n, v)$ be an ordered sequence of all edges whose target is $v$. Then,

$$\mathsf{out}(v) = f_v(x_1, \ldots, x_n)$$

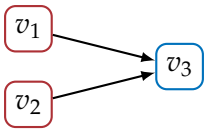
where $x_i = \mathsf{out}(v_i)$, for $i \in [1, n]$.

The base case of this definition is input nodes, since they have no edges incident on them. Suppose we are given an input $\boldsymbol{x} \in \mathbb{R}^n$, where we will use $\boldsymbol{x}$ to denote a vector and $x_i$ to denote its $i$th element. Let $v_1, \ldots, v_n$ be an ordered sequence of all input nodes. Then,

$$\mathsf{out}(v_i) = x_i$$

### A simple example

Let us look at an example graph $G$




We have $V^{\mathsf{in}} = \{v_1, v_2\}$ and $V^{\mathsf{o}} = \{v_3\}$. Now assume that

$$f_{v_3}(x_1, x_2) = x_1 + x_2$$

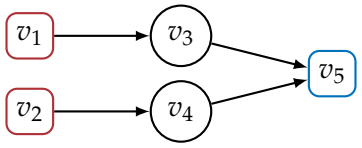
and that we are given the input vector $(11, 79)$ to the network, where node $v_1$ gets the value 11 and $v_2$ the value 79. Then, we have

$$\begin{aligned}
&\mathsf{out}(v_1) = 11 \\
&\mathsf{out}(v_2) = 79 \\
&\mathsf{out}(v_3) = \mathsf{out}(v_1) + \mathsf{out}(v_2) = 11 + 79 = 90
\end{aligned}$$

### Data flow and control flow

The graphs we have defined are known in the field of program analysis as *data-flow* graphs; this is in contrast to *control-flow* graphs.[1] Control-flow graphs dictate the *order* in which operations need be performed—the flow of who has *control* of the CPU. Data-flow graphs, on the other hand, only tell us what node needs what data to perform its computation, but not how to order the computation. This is best seen through a small example.

Consider the following graph




Viewing this graph as an imperative program, one way to represent it is as follows, where $\leftarrow$ is the assignment symbol.

$$\begin{aligned}
\mathsf{out}(v_3) &\leftarrow f_{v_3}(\mathsf{out}(v_1)) \\
\mathsf{out}(v_4) &\leftarrow f_{v_4}(\mathsf{out}(v_2)) \\
\mathsf{out}(v_5) &\leftarrow f_{v_5}(\mathsf{out}(v_3), \mathsf{out}(v_4))
\end{aligned}$$

This program dictates that the value of $v_3$ is computed before $v_4$. But this need not be, as the output of one does not depend on the the other. Therefore, an equivalent implementation of the same graph can swap the first two operations:

$$\begin{aligned}
\mathsf{out}(v_4) &\leftarrow f_{v_4}(\mathsf{out}(v_2)) \\
\mathsf{out}(v_3) &\leftarrow f_{v_3}(\mathsf{out}(v_1)) \\
\mathsf{out}(v_5) &\leftarrow f_{v_5}(\mathsf{out}(v_3), \mathsf{out}(v_4))
\end{aligned}$$

Formally, we can compute the values $\mathsf{out}(\cdot)$ in any *topological* ordering of graph nodes. This ensures that all inputs of a node are computed before its own operation is performed.

[1] In deep learning frameworks like TensorFlow, they call graphs *computation graphs*.

### Properties of operations

So far, we have assumed that a node $v$ can implement any operation $f_v$ it wants over real numbers. In practice, to enable efficient training of neural networks, these operations need be *differentiable* or differentiable *almost everywhere*. The ReLU activation function, **??**, that we have seen earlier is differentiable almost everywhere, since at $x = 0$, there is a sharp turn in the function and the gradient is undefined.

Many of the operations we will be concerned with are *linear* or *piecewise linear*. Formally, a function $f : \mathbb{R}^n \to \mathbb{R}$ is linear if it can be defined as follows:

$$f(\boldsymbol{x}) = \sum_i c_i x_i + b$$

where $c_i, b \in \mathbb{R}$. A function is piecewise linear if it can be written in the form

$$f(\boldsymbol{x}) = \begin{cases} \sum_i c_i^1 x_i + b^1, & \boldsymbol{x} \in S_1 \\ \vdots & \\ \sum_i c_i^m x_i + b^m, & \boldsymbol{x} \in S_m \end{cases}$$

where $S_i$ are mutually disjoint subsets of $\mathbb{R}^n$ and $\cup_i S_i = \mathbb{R}^n$. ReLU, for instance, is a piecewise linear function, as it is of the form:

$$\text{relu}(x) = \begin{cases} 0, & x < 0 \\ x, & x \geqslant 0 \end{cases}$$

Another important property that we will later exploit is *monotonicity*. A function $f : \mathbb{R} \to \mathbb{R}$ is monotone if for any $x \geqslant y$, we have $f(x) \geqslant f(y)$. Both activation functions we saw earlier in the chapter, ReLUs and sigmoids, are monotone. You can verify this in **????**: the functions never decrease with increasing values of $x$.

## Looking Ahead

Now that we have formally defined neural networks, we are ready to pose questions about their behavior. In the next chapter, we will formally define a language for posing those questions. Then, in the chapters that follow, we will look at algorithms for answering those questions.

Chapter 3

# Correctness Properties

In this chapter, we will come up with a *language* for specifying properties of neural networks. The specification language is a formulaic way of making statements about the behavior of a neural network (or sometimes multiple neural networks). Our concerns in this chapter are solely about specifying properties, not about automatically verifying them. So we will take liberty in specifying complex properties, ridiculous ones, and useless ones. In later parts of the book, we will constrain the properties of interest to fit certain verification algorithms—for now, we have fun.

## 3.1 Properties, Informally

Remember that a neural network defines a function $f : \mathbb{R}^n \to \mathbb{R}^m$. The properties we will consider here are of the form:

> **for any input** $x$, the neural network **produces an output** that ...

In other words, properties dictate the input–output behavior of the networ, but not the internals of the network—how it comes up with the answer.

Sometimes, our properties will be more involved, talking about multiple inputs, and perhaps multiple networks:

> **for any inputs** $x, y$, ... **that** ... the neural networks **produce outputs** that ...

The first part of these properties, the one talking about inputs, is called the *precondition*; the second part, talking about outputs, is called the *postcondition*.

In what follows, we will continue our informal discussion of properties using examples.

### Images

Let's say we have a neural network $f$ that takes in an image and predicts a label from *dog*, *zebra*, etc. An important property that we may be interested in checking is *robustness* of such classifier. A classifier is robust if its prediction does not change with small variations in input. For example, changing the brightness slightly or damaging a few pixels should not change classification.

Let us fix some image $\boldsymbol{c}$ that is classified as *dog* by $f$. To make sure that $\boldsymbol{c}$ is not an *adversarial image* of a dog that is designed to fool the neural network, we will check the following property:

> for any image $\boldsymbol{x}$ that is slightly brighter or darker than $\boldsymbol{c}$, $f(\boldsymbol{x})$ predicts *dog*

Notice here that the precondition specified a set of images $\boldsymbol{x}$ that are brighter or darker than $\boldsymbol{c}$, and the postcondition specified that the classification of $f$ remain unchanged.

That's a desirable property: you don't want classification to change with a small movement in the brightness slider. But there are many other other things you desire—robustness to changes in contrast, rotations, instagram filters, white balance, and the list goes on. This hits at the crux of the specification problem: we often cannot specify every possible thing that we desire, so we have to choose some. (More on this later.)

### Natural language

Suppose now that $f$ takes an English sentence and decides whether it represents a a positive or negative sentiment. This problem arises, for example, in automatically analyzing online reviews. We are also interested in robustness in this setting. For example, say we have fixed a sentence $\boldsymbol{c}$ with positive sentiment, then we might specify the following property:

> for any sentence $\boldsymbol{x}$ that is $\boldsymbol{c}$ with a few spelling mistakes added, $f(\boldsymbol{x})$ should predict positive sentiment

For another example, instead of spelling mistakes, imagine replacing words with synonyms:

> for any sentence $\boldsymbol{x}$ that is $\boldsymbol{c}$ with some words replaced by synonyms, then $f(\boldsymbol{x})$ should predict positive sentiment

We could also combine the two properties above to get a stronger property specifying that prediction should not change in the presence of synonyms or spelling mistakes.

### Source code

Say that our neural network $f$ is a malware classifier, taking a piece of code and deciding whether it is malware or not. A malicious entity may try to modify a malware $\boldsymbol{x}$ to sneak it past the neural network by fooling it to think that it's a good program. One trick the attacker may use is adding a piece of code to $\boldsymbol{x}$ that does not change its operation but that fools the neural network. We can state this property as follows: Say we have piece of malware $\boldsymbol{c}$, then we can state the following property:

> for any program $\boldsymbol{x}$ that is equivalent to $\boldsymbol{c}$ and syntactically similar, then $f(\boldsymbol{x})$ predicts malware

### Controllers

All of our examples so far have been robustness problems. Let us now look at a slightly different property. Say you have a controller deciding on the actions of a robot. The controller looks at the state of the world and decides whether to move left, right, forward, or backward. We, of course, do not want the robot to move into an obstacle, whether it is a wall, a human, or another robot. As such, we might specify the following property:

> for any state $\boldsymbol{x}$, if there is an obstacle to the right of the robot, then $f(x)$ should *not* predict right

We can state one such property per direction.

## 3.2 A Specification Language

We are now ready to fully formalize our specification language. Our specifications are going to look like this:

$$\begin{gathered} \langle\!| \textit{ precondition } |\!\rangle \\ \boldsymbol{r} \leftarrow f(\boldsymbol{x}) \\ \langle\!| \textit{ postcondition } |\!\rangle \end{gathered}$$

The *precondition* is a Boolean predicate that is defined over a set of variables which will be used as inputs to the neural networks we are reasoning about. We will use $\boldsymbol{x}_i$ to denote those variables. The middle portion of the specification is a number of calls to functions defined by neural networks; in this example, we only see one call to $f$, and the return value is stored in a variable $r$. Generally, our specification language allows a sequence of such assignments, e.g.:

$$\begin{gathered} \langle\!| \textit{ precondition } |\!\rangle \\ \boldsymbol{r_1} \leftarrow f(\boldsymbol{x_1}) \\ \boldsymbol{r_2} \leftarrow g(\boldsymbol{x_2}) \\ \vdots \\ \langle\!| \textit{ postcondition } |\!\rangle \end{gathered}$$

Finally, the postcondition is a Boolean predicate over the variables appearing in the precondition $\boldsymbol{x}_i$ and the assigned variables $\boldsymbol{r}_j$.

The way to read a specification, informally, is as follows:

> for any $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n$ satisfying the precondition, let $\boldsymbol{r}_1 = f(\boldsymbol{x_1}), \boldsymbol{r}_2 = g(\boldsymbol{x}_2), \ldots$, then the postcondition is true.

### Example

Recall our image brightness example from the previous section, and say $\boldsymbol{c}$ is an actual grayscale image, where each element of $\boldsymbol{c}$ is the intensity of a pixel, from 0 to 1 (black to white). Then, we can state the following specification, which informally says that the changing the brightness of $\boldsymbol{c}$ should not

change the classification:

$$
\begin{gathered}
(\!| \, |\boldsymbol{x} - \boldsymbol{c}| \leqslant \mathbf{0.1} \, |\!) \\
\boldsymbol{r}_1 \leftarrow f(\boldsymbol{x}) \\
\boldsymbol{r}_2 \leftarrow f(\boldsymbol{c}) \\
(\!| \, \mathsf{class}(\boldsymbol{r}_1) = \mathsf{class}(\boldsymbol{r}_2) \, |\!)
\end{gathered}
$$

Let us walk through this specification:

**Precondition** Take any image $\boldsymbol{x}$ where each pixel is at most 0.1 away from its counterpart in $\boldsymbol{c}$. Here, both $\boldsymbol{x}$ and $\boldsymbol{c}$ are assumed to be the same size, and the $\leqslant$ is defined pointwise.

**Assignments** Let $\boldsymbol{r}_1$ be the result of computing $f(\boldsymbol{x})$ and $\boldsymbol{r}_2$ be the result of computing $f(\boldsymbol{c})$.

**Postcondition** Then, the predicted labels in vectors $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ are the same. Recall that in a classification setting, each element of vector $\boldsymbol{r}_i$ refers to the probability of a specific label. We use class as a shorthand to extract the index of the largest element of the vector.

### Hoare logic

Our specification language looks like specifications written in *Hoare logic*. Specifications in Hoare logic are called *Hoare triples*, as they are composed of three parts, just like our specifications. Hoare logic comes equipped with deduction rules that allows one to prove the validity of such specifications. For our purposes in this book, we will not define the rules of Hoare logic, but many of them will crop up implicitly throughout the book.

## 3.3 More Examples of Properties

We will now go through a bunch of example properties and write them in our specification language.

### Equivalence of neural networks

Say you have a neural network $f$ for image recognition and you want to replace it with a new neural network $g$. Perhaps $g$ is faster and more lightweight, and since you're interested in running the network on a stream of incoming images, efficiency is very important. One thing you might want to prove is that $f$ and $g$ are equivalent; here's how to write this property:

$$\begin{gathered}
\langle\!| \ \mathsf{true} \ |\!\rangle \\
\boldsymbol{r_1} \leftarrow f(\boldsymbol{x}) \\
\boldsymbol{r_2} \leftarrow g(\boldsymbol{x}) \\
\langle\!| \ \mathsf{class}(\boldsymbol{r}_1) = \mathsf{class}(\boldsymbol{r}_2) \ |\!\rangle
\end{gathered}$$

Notice that the precondition is true, meaning that for any image $\boldsymbol{x}$, we want the predicted labels of $f$ and $g$ to be the same. The true precondition indicates that the inputs to the neural networks ($\boldsymbol{x}$ in this case) are unconstrained. This specification is very strong: the only way it can be true is if $f$ and $g$ are exactly the same function, which is highly unlikely in practice.

One possible alternative is to state that $f$ and $g$ return the same prediction on some subset of images, plus or minus some brightness, as in our above example. Say $S$ is a finite set of images, then:

$$\begin{gathered}
\langle\!| \ \boldsymbol{x}_1 \in S \wedge |\boldsymbol{x}_1 - \boldsymbol{x}_3| \leqslant \mathbf{0.1} \wedge |\boldsymbol{x}_1 - \boldsymbol{x}_2| \leqslant \mathbf{0.1} \ |\!\rangle \\
\boldsymbol{r}_1 \leftarrow f(\boldsymbol{x}_2) \\
\boldsymbol{r}_2 \leftarrow g(\boldsymbol{x}_3) \\
\langle\!| \ \mathsf{class}(\boldsymbol{r}_1) = \mathsf{class}(\boldsymbol{r}_2) \ |\!\rangle
\end{gathered}$$

This says the following: Pick an image $\boldsymbol{x}_1$ and generate two variants, $\boldsymbol{x}_2$ and $\boldsymbol{x}_3$, whose brightness differs a little bit from $\boldsymbol{x}_1$. Then, $f$ and $g$ should agree on the classification of the two images.

This is a more practical notion of equivalence than our first attempt. Our first attempt forced $f$ and $g$ to agree on all possible images, but keep in mind that most images (combinations of pixels) are noise, and therefore we don't care about their classification. This specification, instead, constrains equivalence to an infinite set of images that look like those in the set $S$.

### Collision avoidance

Our next example is one that has been a subject of study in the verification literature, beginning with the pioneering work of Katz et al. (2017). Here we have a collision avoidance system that runs on an autonomous aircraft. The system detects intruder aircrafts and decides what to do. The reason the system is run on a neural network is due to its complexity—the trained neural network is much smaller than the full set of rules.

The inputs to the system are the following:

- $v_{own}$: the aircraft's velocity
- $v_{int}$: the intruder aircraft's velocity
- $a_{int}$: the angle of the intruder with respect to the current flying direction
- $a_{own}$: the angle of the aircraft with respect to the intruder.
- $d$: the distance between the two aircrafts
- *prev*: the previous action taken.

Given the above values, the neural network decides what to do: left/right, strong left/right, or nothing. Specifically, the neural network assigns a score to every possible action, and the action with the lowest score is taken.

As you can imagine, many things can go wrong here, and if they do: disaster. Katz et al. (2017) identify a number of properties that they verify. They do not account for all possible scenarios, but they are important to check. Let us take a look at one that says if the intruder aircraft is far away, then the score for doing *nothing* should be below some threshold.

$$\{\!|\ d \geqslant 55947 \wedge v_{own} \geqslant 1145 \wedge v_{int} \leqslant 60\ |\!\}$$
$$\boldsymbol{r} \leftarrow f(d, v_{own}, v_{int}, \ldots)$$
$$\{\!|\ \text{score of nothing in } \boldsymbol{r} \text{ is below } 1500\ |\!\}$$

Notice that the precondition specifies that the distance between the two aircrafts is more than 55K feet, that the aircraft's velocity is high and the intruder's velocity is low. In which case, the postcondition specifies that doing nothing should have a low score, below some threshold. Intuitively, we should not panic if the two aircrafts are quite far apart.

Katz et al. (2017) explore a number of such properties, and also consider robustness properties in this setting. But how do we come up with such specific properties? It's not straigtforward. In this case, we really need a domain expert who knows about collision-avoidance systems, and even then, we might not cover all corner cases. It is a common sentiment in the verification community that specification is harder than verification—that is, the hard part is asking the right questions!

### Physics modeling

Here is another example the literature. We want the neural network to internalize some physical laws, like the movement of a pendulum. At any point in time, the state of the pendulum is a triple $(v, h, w)$, its vertical position $v$, its horizontal position $h$, and its angular velocity $w$. Given the state of the pendulum, the neural network is to predict the state in the next time instance, assuming that time is divided into discrete steps.

A natural property we may want to check is that the neural networks understanding of the pendulum's dynamics adheres to the law of conservation of energy. At any point in time, the energy of the pendulum is the sum of its potential energy and its kinetic energy. As it goes up, its potential energy increases and kinetic energy decreases; as it goes down, the opposite happens. The sum of kinetic and potential energies should only decrease over time. We can state this property as follows:

$$\begin{gathered} (\!| \ \mathsf{true} \ |\!) \\ v', h', w' \leftarrow f(v, h, w) \\ (\!| \ E(v', h', w') \leqslant E(v, h, w) \ |\!) \end{gathered}$$

We break the input and output vectors of the network into their three components for clarity. The expression $E(v, h, w)$ is the energy of the pendulum, which is its potential energy $mgh$, where $m$ is the mass of the pendulum and $g$ is the gravitational constant, plus its kinetic energy $0.5ml^2w^2$, where $l$ is the length of the pendulum.

### Natural language

Let us recall the natural language example from earlier in the chapter, where we wanted to classify a sentence into whether it expresses a positive or negative sentiment. We decided that we want the classification not to change if we replaced a word by a synonym. We can express this property in our language: Let $\boldsymbol{c}$ be a fixed sentence of length $n$. We assume that each element of vector $\boldsymbol{c}$ is a real number representing a word—called an *embedding* of the word. We also assume that we have a thesaurus $T$, which given a word gives us a set of equivalent words.

$$
\begin{gathered}
\{\!|\, i \in [1,n] \wedge w \in T(c_i) \wedge \boldsymbol{x} = \boldsymbol{c}[i \mapsto w] \,|\!\} \\
\boldsymbol{r}_1 \leftarrow f(\boldsymbol{x}) \\
\boldsymbol{r}_2 \leftarrow f(\boldsymbol{c}) \\
\{\!|\, \mathsf{class}(\boldsymbol{r}_1) = \mathsf{class}(\boldsymbol{r}_2) \,|\!\}
\end{gathered}
$$

The precondition specifies that variable $\boldsymbol{x}$ is just like the sentence $\boldsymbol{c}$, except that some element $i$ is replaced by a word $w$ from the thesaurus $T(c_i)$. We use the notation $\boldsymbol{c}[i \mapsto w]$ to denote $\boldsymbol{c}$ with the $i$th element replaced with $w$ and $c_i$ to denote the $i$th element of $\boldsymbol{c}$.

The above property allows 1 word to be replaced by a synonym. We can extend it to two words as follows (I know, it's very ugly, but it works):

$$
\begin{gathered}
\{\!|\, i,j \in [1,n] \ \wedge\ i \neq j \ \wedge\ w_i \in T(c_i) \ \wedge\ w_j \in T(c_j) \ \wedge\ \boldsymbol{x} = \boldsymbol{c}[i \mapsto w_i, j \mapsto w_j] \,|\!\} \\
\boldsymbol{r}_1 \leftarrow f(\boldsymbol{x}) \\
\boldsymbol{r}_2 \leftarrow f(\boldsymbol{c}) \\
\{\!|\, \mathsf{class}(\boldsymbol{r}_1) = \mathsf{class}(\boldsymbol{r}_2) \,|\!\}
\end{gathered}
$$

## Looking Ahead

We are done with the first part of the book. We have defined neural networks and how to specify their properties. In what follows, we will discuss different ways of verifying properties automatically.

Part II

# Constraint-Based Verification

Chapter 4

# Decidable Theories of First-Order Logic

In this part of the book, we will look into constraint-based techniques for verification. The idea is to take a correctness property and encode it as a set of constraints. By solving the constraints, we can decide whether the correctness property holds or not.

The constraints we will use are formulas in *first-order logic* (FOL). FOL is a very big and beautiful place, but neural networks only live in a small and cozy corner of it—the corner that we will explore in this chapter.

## 4.1 Propositional Logic

We begin with the purest of all, *propositional logic*. A formula $\varphi$ in propositional logic is over Boolean variables that are traditionally given the names $p, q, r, \ldots$. A formula $\varphi$ is defined using the following grammar:

$$
\begin{array}{lll}
\varphi :- & \mathsf{true} & \\
& \mathsf{false} & \\
& \mathit{var} & \text{Variable} \\
& \mid \varphi \wedge \varphi & \text{Conjunction (and)} \\
& \mid \varphi \vee \varphi & \text{Disjunction (or)} \\
& \mid \neg\varphi & \text{Negation (not)}
\end{array}
$$

Essentially, a formula in propositional logic defines a circuit with Boolean variables, AND gates ($\wedge$), OR gates ($\vee$), and NOR gates ($\neg$). At the end of the day, all programs can be defined as circuits, because everything is a bit on a computer and there is a finite amount of memory, and therefore a finite number of variables.

As an example, here is a formula $\varphi \triangleq (p \wedge q) \vee \neg r$. Observe the use of $\triangleq$; this is to denote that we are syntactically defining $\varphi$ to be the formula on the right of $\triangleq$, as opposed to saying that the two formulas are semantically equivalent (more on this in a bit). We will use $fv(\varphi)$ to denote the set of *free* variables appearing in the formula. For now, it is the set of all variables that are syntactically present in the formula; for example, in $fv(\varphi) = \{p, q, r\}$.

## Interpretations

Let $\varphi$ be a formula over a set of variables $fv(\varphi)$. An interpretation $I$ of $\varphi$ is a map from variables $fv(\varphi)$ to $\mathsf{true}$ or $\mathsf{false}$. For example,

$$I = \{p \mapsto \mathsf{true}, q \mapsto \mathsf{true}, r \mapsto \mathsf{false}\}$$

Given an interpretation $I$ of a formula $\varphi$, we will use $I(\varphi)$ to denote the formula where we have replaced each variable $fv(\varphi)$ with its interpretation in $I$. For example, applying $I$ above to $(p \wedge q) \vee \neg r$, we get

$$(\mathsf{true} \wedge \mathsf{true}) \vee \neg \mathsf{false}$$

## Satisfiability

We will define the following evaluation or simplification rules for a formula:

$$\begin{array}{lcl}
\mathsf{eval}(\mathsf{true}) & = & \mathsf{true} \\
\mathsf{eval}(\mathsf{false}) & = & \mathsf{false} \\
\\
\mathsf{eval}(\mathsf{true} \wedge \varphi) & = & \mathsf{eval}(\varphi) \\
\mathsf{eval}(\varphi \wedge \mathsf{true}) & = & \mathsf{eval}(\varphi) \\
\\
\mathsf{eval}(\mathsf{false} \wedge \varphi) & = & \mathsf{false} \\
\mathsf{eval}(\varphi \wedge \mathsf{false}) & = & \mathsf{false} \\
\\
\mathsf{eval}(\mathsf{false} \vee \varphi) & = & \mathsf{eval}(\varphi) \\
\mathsf{eval}(\varphi \vee \mathsf{false}) & = & \mathsf{eval}(\varphi) \\
\mathsf{eval}(\mathsf{true} \vee \varphi) & = & \mathsf{true} \\
\mathsf{eval}(\varphi \vee \mathsf{true}) & = & \mathsf{true}
\end{array}$$

$$\begin{aligned} \mathsf{eval}(\neg \mathsf{true}) &= \mathsf{false} \\ \mathsf{eval}(\neg \mathsf{false}) &= \mathsf{true} \end{aligned}$$

If a given formula has no free variables, then applying these rules repeatedly, you will get true or false. We will use $\mathsf{eval}(\varphi)$ to denote the simplest form of $\varphi$ we can get by repeatedly applying the above rules.

A formula $\varphi$ is *satisfiable* (SAT) if and only if there exists an interpretation $I$ such that

$$\mathsf{eval}(I(\varphi)) = \mathsf{true}$$

in which case we will say that $I$ is a *model* of $\varphi$ and denote it

$$I \models \varphi$$

We will also use $I \not\models \varphi$ to denote that $I$ is not a model of $\varphi$. It follows from our definitions that $I \not\models \varphi$ iff $I \models \neg\varphi$.

Equivalently, a formula $\varphi$ is *unsatisfiable* (UNSAT) if and only if for every interpretation $I$ we have $\mathsf{eval}(I(\varphi)) = \mathsf{false}$.

### Validity and equivalence

To prove properties of neural networks, we will be asking *validity* questions. A formula $\varphi$ is valid iff every possible interpretation $I$ is a model of $\varphi$. It follows that a formula $\varphi$ is valid if and only if $\neg\varphi$ is unsatisfiable.

We will say that two formulas, $\varphi_1$ and $\varphi_2$, are *equivalent* if and only if every model $I$ of $\varphi_1$ is a model of $\varphi_2$, and vice versa. We will denote equivalence as $\varphi_1 \equiv \varphi_2$.

### Implication and bi-implication

We will often use an *implication* $\varphi_1 \Rightarrow \varphi_2$ to denote the formula

$$\neg\varphi_1 \vee \varphi_2$$

Similarly, we will use a *bi-implication* $\varphi_1 \iff \varphi_2$ to denote the formula

$$(\varphi_1 \Rightarrow \varphi_2) \wedge (\varphi_2 \Rightarrow \varphi_1)$$

## 4.2 **First-Order Theories**

We can now extend propositional logic using *theories*.

Chapter 5

# Encodings of Neural Networks

Chapter 6

# Decision Procedures

Chapter 7

# Specialized Decision Procedures

Part III

# Abstraction-Based Verification

Chapter 8

# Just Enough Abstract Interpretation

Chapter 9

# Numerical Abstract Domains

Chapter 10

# Abstract Execution of Neural Networks

Chapter 11

# Abstract Deep Learning

Part IV

# Verified Reinforcement Learning

Chapter 12

# Neural Networks as Policies

Chapter 13

# Verifying RL Policies

Chapter 14

# Efficient Policy Verification

Chapter 15

# Enforcing Properties in RL

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