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Masters Thesis

A Framework for Formally Verifying Neural Networks in Go

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Declaration of Authorship

I, Arran Dinsmore, declare that this thesis titled, 'A Framework for Formally Verifying Neural Networks in Go' and the work presented in it is my own. I confirm that this work submitted for assessment is my own and is expressed in my own words. Any uses made within it of the works of other authors in any form (e.g., ideas, equations, figures, text, tables, programs) are properly acknowledged at any point of their use. A list of the references employed is included.

Signed: Arran Dinsmore

Date: April 2021

"Program testing can be used to show the ***presence*** *of bugs, but never to show their* ***absence****!"*

Edsger W. Dijkstra

Abstract

As machine learning for safety critical applications such as autonomous vehicles is starting to be developed beyond proof of concepts, and enter into production within society, there is a need to ensure these systems do not fail.

Traditional rigorous testing methods are not a viable approach for such black box systems, and thus there is a need for formal verification methods that can prove the robustness of a system.

Additionally, the choice of programming language used for these tasks has grown with new machine learning extensions being developed in existing languages.

This project will investigate how robust programming infrastructure can be used to enhance formal verification approaches for machine learning tasks, with the main objective of developing a formal methods framework for verifying neural networks in the Go programming language.

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Chapter 1

Introduction

1.1 Context

Machine Learning (ML) algorithms are becoming increasingly present in systems that operate within shared environments with humans, or involve direct interaction with humans themselves [Pereira and Thomas, 2020]. These systems are often defined as safety-critical, such that their failures lead to unintended and potentially harmful behaviours [Amodei et al., 2016]. Examples of these systems include autonomous automotive systems, traffic control systems, medical devices, aviation software, industrial robotics, and many more cyber-physical systems that interact with our environment. Many of these systems have so far only existed as proof of concepts, but are steadily approaching commercial use within our society.

Additionally, recent research has exposed broad vulnerabilities to adversarial attacks within data driven ML algorithms, including Neural Networks (NNs); where applying small but intentional perturbations to an input which are not noticible to humans, can lead to a model outputting an incorrect classification with high confidence [Goodfellow et al., 2014]. An example of such an attack can be seen in *Fig. 1.1*. Consequently, the testing and verification of ML for the use of controlling safety-critical systems has become a focused area of research in recent years.

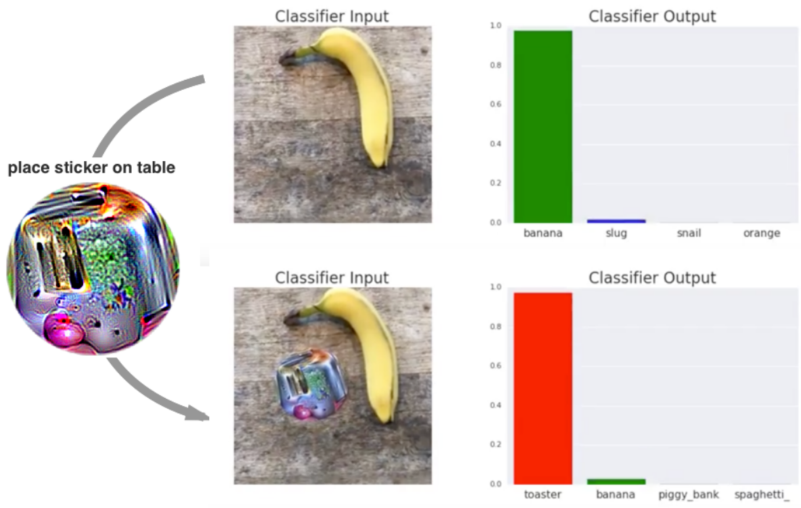

FIGURE 1.1: **Google's Adversarial Patch** – An example of a method to create targeted adversarial attacks on NNs by adding carefully designed noise via a physical patch [Brown et al., 2018].

This thesis will use the following definitions for software *testing* and *verification*. Software testing, or validation, is defined as the evaluation of a system under various conditions and observing its behaviour while looking for defects [Pereira and Thomas, 2020]. In the context of ML development, testing is used to ensure that a trained model generalises accurately to some previously unseen test data.

Verification is defined as the process of determining whether the products of a phase of the software development process fulfill the requirements established during the previous phase [Ammann and Offutt, 2008]. Formal verification in other words, formulates logical arguments that a system will not act abnormally under a wide range of circumstances, and can be used to determine not only generality, but also the robustness and correctness of a system.

The challenges regarding verification of ML models stem from the typically lower interpretability and more statistically-oriented nature of their algorithms, which lead to a lower degree of understanding than software that is explicitly programmed to perform a specific task [Bishop, 2006]. These types of systems are commonly referred to as *black box* systems, where the internal mechanisms are not revealed; in other words, it is impossible to understand a model just by looking at its parameters [Molnar, 2019].

1.2 Motivation

Public calls for *sensible* or *verifiable Artificial Intelligence (AI)* have been raised in recent years due to ever increasing development of complex and pervasive systems that are entering into our everyday lives [Russell et al., 2016].

Formal verification of software systems has seen significant progress since the early verification systems. These early systems [Boyer and Moore, 1990, Guaspari et al., 1993, Polak, 1979] often struggled to be widely adopted into industry applications. However, due to the ever increasing complexity of deployed software, new verification tools have been developed with the intent of being accessible to a wide range of industry software engineers [Fisher et al., 2017].

On the other hand, verification of ML systems has seen relatively little progress, with the exception of Multi-Agent Systems (MASs) [Kouvaros and Lomuscio, 2016, Lomuscio et al., 2017]. Indeed, due to the nature of Artificial Intelligence Verification (AIV) research, there are limited programming tools available for researchers in this area. This is especially true for work within ML, as the programming languages and tools commonly used for *traditional* verifcation are often disparate from those widely adopted by the ML communities.

Popular programming languages used for ML such as Python or Matlab currently have comparitively less formal verification tools available than those concerned with system infrastructure or embedded applications. Additionally, AIV toolkits for ML tasks in these languages are still in early stages of development, and mainly focused on the verification of NNs [Kokke, 2020].

Furthermore, the landscape of ML programming itself is forever shifting, and while there is not yet a programming language dedicated for ML tasks, huge efforts from programming language designers have been made in developing ML libraries for existing languages. This is necessary in order to handle the extremely high computational demands, and to simplify model languages to make them easier to add domain-specific optimisations and features [Innes et al., 2017].

A prime example of such development can be seen in the Go programming language, or *GoLang*. A relatively new language, which was originally developed by Google in 2009 with the intention of creating a modern general-purpose language similar to C. GoLang has seen a surge in popularity within the ML community since the release of its first extensive ML package, *Gorgonia*, in 2016, which heavily relies on the use of expression graphs [Chew, 2016]. This package allows GoLang developers to take advantage of automatic and symbolic differentiation, gradient descent optimisations, numerical stabilisation, added support for CUDA/GPGPU computation, and comparatively quicker speeds than its Python counterparts (Theano and TensorFlow) [GoLang, 2020].

A good example of a programming paradigm shift towards dedicated ML languages, is Microsoft's efforts in developing an efficient differentiable version of the Functional Programming (FP) language F [Shaikhha et al., 2019].

Consequently, as programming languages continue to develop ML capabilities, there is a need for exploring new and scalable approaches for developing AIV tools in these languages. This is especially important for programming languages which are being adopted by industry to implement ML models for the use within safety-critical or pervasive systems.

1.3 Aims & Objectives

The aim of this project is to investigate the current programming paradigms within ML development, and to explore the suitability of current formal verification toolkits available to them. Subsequently, this thesis will aim to design and implement a GoLang formal methods framework for Gorgonia NNs, providing GoLang ML developers with a set of tools which will allow them to produce safe and fair AI applications.

This framework will extend upon the work made by [Kokke, 2020], and the Sapphire library implemented in Python which successfully translates TensorFlow feed-forward NN model queries to the Z3 Satisfiability Modulo Theories (SMT) solver created by Microsoft Research [De Moura and Bjørner, 2008].

To achieve this project's aims, the following objectives should be met:

- *Objective 1* - Conduct a feasibility study with regards to developing a formal methods framework for NNs in Go.
- *Objective 2* - Implement bindings that map the parameters of a Gorgonia NN model to Z3 variables.
- *Objective 3* - Select example training data sets in order to train and verify NN models using this project's formal methods framework.
- *Objective 4* - Implement a series of NN models in Gorgonia using the data sets mentioned in *Objective 3*.

- *Objective 5* - Verify the correctness of Gorgonia NNs using the bindings developed in *Objective 2*.
- *Objective 6* - Make conclusions about the developed framework's benefits and limitations, and discuss future improvements to the methodology as described in *Objective 1*.

Chapter 2

Background & Literature Review

This chapter will provide a background understanding to the important concepts that are required by this thesis, and explore the current trends within AIV research. This includes an introduction to formal verification, both within traditional and ML software systems; an overview of the current state of NN and deep learning research, and the programming paradigms used for their development; and finally an investigation into the Go programming language infrastructure and the feasibility of using it for verifying NNs.

2.1 Neural Networks & Deep Learning

2.1.1 Overview

NNs are learning algorithms based on a loose analogy of how the human brain functions. They consist of nodes, or neurons (*see Fig. 2.1*), which act as functions that output a nonlinear combination of weighted inputs and a bias [Dreyfus, 2005]. Learning is achieved by adjusting the weights on the connections between nodes, which are analogous to synapses and neurons in nature [Sammut and Webb, 2010].

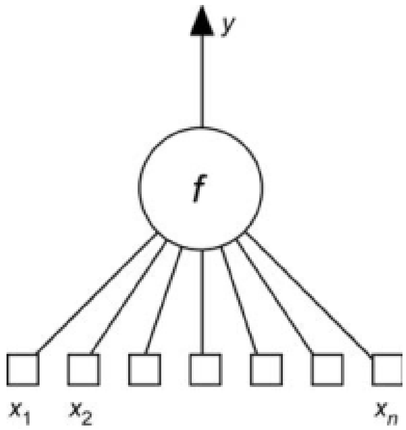

FIGURE 2.1: **Artificial Neuron** – a nonlinear bounded function $y = f(x_1, x_2, \ldots, x_n; w_2, \ldots, w_n)$ where the x_i are the input values and the w_i are the weights of the neuron [Dreyfus, 2005].

A weight is assigned to each of a neuron's inputs. They are the coefficients of a neuron's equation and therefore reflect the importance of individual inputs. A bias is a constant value assigned to each neuron. They are used to shift a neuron's activation function output in a positive or negative direction [Malik, 2019b].

A NN is made up of a series of layers; an input layer, a number of hidden layers, and an output layer. Each layer is made up of a set of neurons, where each neuron is fully connected to all neurons in the previous layer. Each neuron within a single layer does not share connections with, and operates completely independently from one another [Stanford Vision and Leaning Lab, 2012].

Using the case of Computer Vision (CV) as an example, the input layer of a NN consists of neurons encoding the values of image pixels (RGB or greyscale intensities). The encoding is typically achieved by passing the raw input value through an activation function which outputs a normalised value. Often, activation functions in modern NNs output non-linearities, an example is to use a Sigmoid Function which maps an input to a value between 0 and 1 (*see Fig. 2.2 left*) [Nielsen, 2015].

However a more common activation function found in current NN models is the Rectified Linear Unit (ReLU). Although computed as a piecewise linear function, ReLU also adds non-linearity to the output. The ReLU function maps an input to a value within the range of 0 and ∞ (*see Fig. 2.2 right*) [Malik, 2019a].

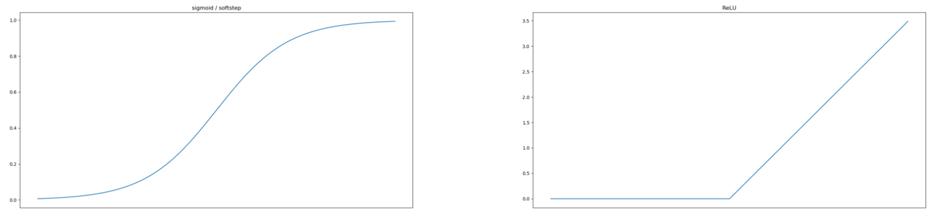

FIGURE 2.2: *Left*: The Sigmoid Function is one type of activation function. 'A bounded, differentiable, real function that is defined for all real input values and has a non negative derivative at each point' [Han and Moraga, 1995]. *Right*: An example of a ReLU activation function transforming x to a value between 0 and ∞ [Malik, 2019a].

The output layer of a CV classification network contains neurons representing the class scores of the task (*see Fig. 2.3*). For example, in a NN attempting to classify handwritten digits, the output layer would contain 10 neurons, representing the digits 0 - 9. If the first neuron fires, i.e. has an output ≈ 1, this will indicate that the network is confident the handwritten digit is 0, and so on [Nielsen, 2015].

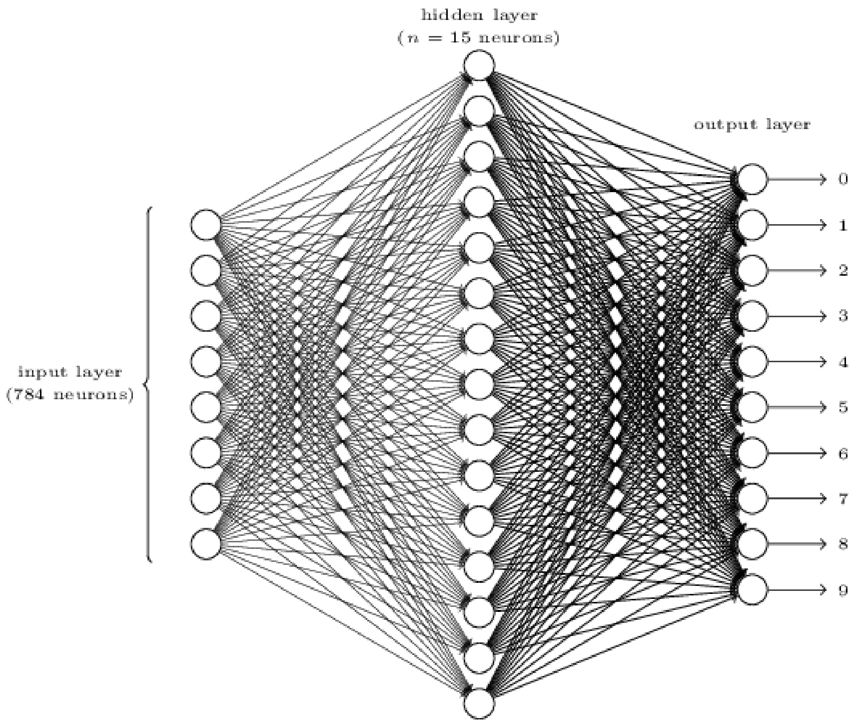

FIGURE 2.3: Neural Network. Example of a NN to classify handwritten digits. The input is a single vector of 28x28 pixels, i.e. 784 neurons, and outputs 10 neurons representing digits 0-9 [Nielsen, 2015].

NNs with a single hidden layer are able to approximate functions that contain any continuous mapping from one finite space to another, whereas with no hidden layers a NN model would only be able to represent linear functions or decision boundaries [Hornik, 1991].

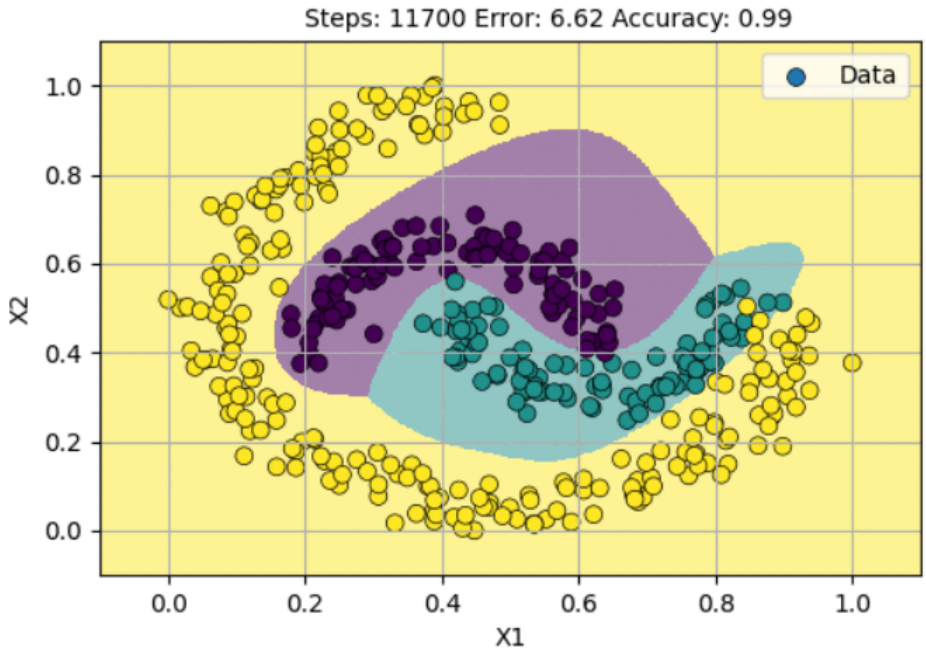

FIGURE 2.4: **Complex Decision Boundary** – Example of a decision boundary made capable by deep learning [Sapkota, 2020]

NNs are especially powerful when additional hidden layers are added to a network's architecture. By doing so, a model can not only approximate continuous functions to a high accuracy with less computational cost, but it can also represent complex composite functions [Sapkota, 2020]. An example of the complex decision boundaries that are possible from NNs with more than one hidden layer can be seen in *Fig. 2.4*.

NNs with two or more hidden layers fall under the category of deep learning, and are often referred to as Deep Neural Networks (DNNs) or Multi-Layer Perceptrons (MLPs). This subset of ML has become increasingly powerful with the rise of powerful variations of DNNs, namely Convolutional Neural Networks (CNNs) and Recurrent Neural Networks (RNNs) in recent years due to their successes within the field of CV.

2.1.2 Gradient Descent & Backpropagation

Training a NN consists of iteratively adjusting the values of weights at each neuron in order to minimise the model's output error. Although there are many algorithms available for determining the optimum values of weights, a common approach is to use some flavour of *gradient descent* together with a technique for efficiently computing partial derivatives within a directed graph called *backpropagation*.

There are three main variants of gradient descent; vanilla gradient descent or Batch Gradient Descent (BGD), Stochastic Gradient Descent (SGD), and Mini-Batch Gradient Descent (MBGD).

BGD computes the gradients of a cost function with regards to the weights within an entire training set. The cost function can take many forms depending on the architecture of the NN and the task it is concerned with, however the main principle behind it is to map the different values of each weight to a score which determines how well the model performs [Shung, 2018].

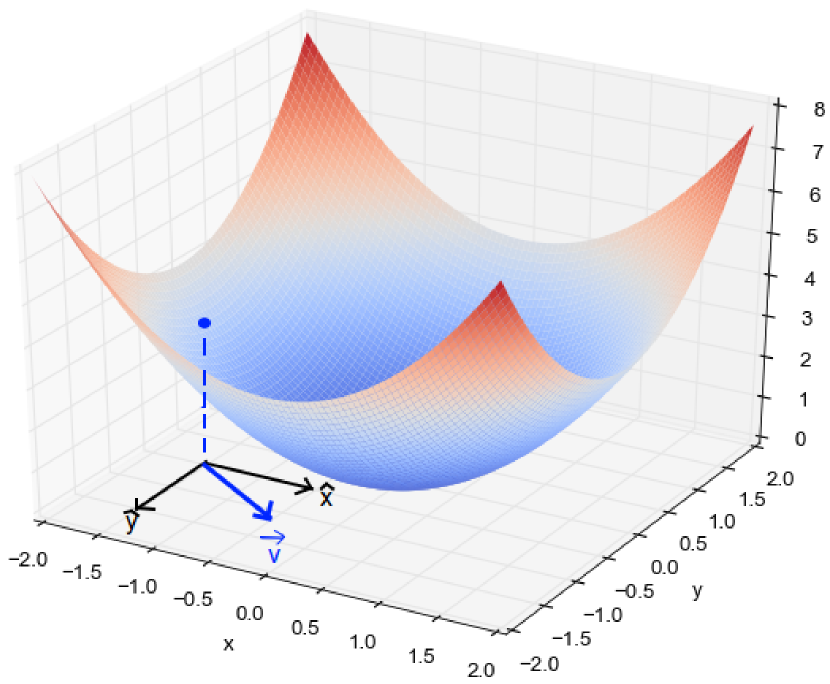

FIGURE 2.5: **Visualisation of Gradient Descent Search Space** – An example of an *ideal* search space, where the vertical z axis shows the cost function $f(x, y)$, and $\vec{v}$ represents the resulting direction of the maximum gradient applied to the parameter in question [Bendersky, 2016].

A search space can then be defined by plotting the output of a cost function against the values of the weights it is concerned with, an example of such a search space with two weights can be seen in *Fig. 2.5*. As the number of weights increases, the harder it becomes to visualise the contours of a multi-dimensional plane. BGD then computes the directional derivative of this plane given a set of weight values, and uses this value as a vector with a magnitude defined by a *learning rate* hyper-parameter to update the weights of the network [Ruder, 2017].

SGD attempts to reduce the number of computations during training by only performing updates to weights for each training example instead of recomputing gradients for similar weights at each iteration. By removing these redundant calculations, SGD typically decreases the time taken to converge to an optimum solution of weights. Additionally, due to the high variance of each update, and so long as the learning rate is steadily decreased at each iteration, SGD has an equal chance at finding the global minimum to BGD [Ruder, 2017].

MBGD on the other hand, attempts to combine the benefits from BGD and SGD by performing an update for every mini-batch of n training examples. Therefore, allowing for the precision of BGD with similar speeds as SGD.

Backpropagation is a computational technique commonly used within NN training for calculating partial derivatives used for gradient descent algorithms in linear time with respect to the number of weights being optimised. This is an important step in order to train NNs within a sensible timeframe, considering the potentially high volume of weights that are needed for complex tasks. A more detailed investigation into this technique will be discussed later in this chapter (*Section 2.4*).

2.1.3 Vulnerabilities to Adversarial Attacks

NNs and DNNs have been adopted and deployed within a wide range of industry applications for tasks such as speech recognition or facial recognition, and have shown to perform adequately for many of these tasks. However, as mentioned in *Chapter 1*, NNs have been shown to be vulnerable to adversarial attacks. Specifically, by adding small, imperceptable changes to the input features, can lead to abnormal behaviours such as missclassification in the output layer.

This observation was first made in 2014, which found properties of NNs that cause them to learn uninterpretable solutions that could have counter-intuitive properties when imperceptable non-random pertubartions are made to a test input, known as *adversarial examples* [Szegedy et al., 2014]. Interestingly, these examples were shown to be robust, such that they have the same effect across models with varying architectures, activation functions, or trained on different data sets altogether. A tentative explanation for this phenomenon was to blame the non-linear nature of NNs, and cases of poor generalisation on test data.

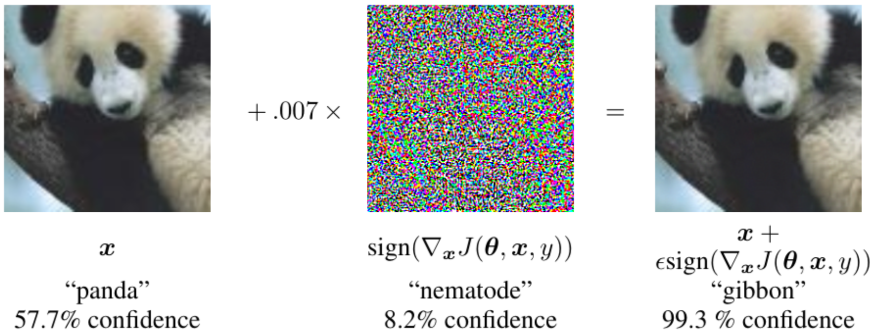

FIGURE 2.6: **Effects of Adversarial Examples** – A demonstration of the effects of adversarial examples; an input image of a panda with added noise causes the model to missclassify the image as a gibbon [Goodfellow et al., 2015].

However in 2015, further attempts to explain NN vulnerabilities to adversarial examples argued that it was not the non-linear nature, but rather the linear behaviour of NNs which is sufficient to cause adversarial examples [Goodfellow et al., 2015]. This claim was supported by the authors' demonstration that leveraging non-linear NN families such as Radial Basis Function Networks (RBFNs) can significantly reduce the vulnerabilities to adversarial examples.

FIGURE 2.7: **Effects of Adversarial Examples in Real World** – A demonstration of how adversarial examples can be used in real world situations to cause misclassification of stop signs [Eykholt et al., 2018].

Research in 2018 showed that adversarial examples can be used in real world situations in order to fool a DNN used for street sign recognition within a self-driving car's navigation system by placing black and white stickers on street signs (*see Fig. 2.7*) [Eykholt et al., 2018].

These vulnerabilities have demonstrated that NN technology has yet to reach the level of maturity necessary for applications in safety-critical systems, and have raised concerns over the robustness of NNs in general.

2.1.4 Descrimination & Neural Networks

Aside from vulnerabilities caused by intrinsic properties of NNs, there are issues which stem from the data being used to train supervised models too. That is, if the training data has inherent bias towards or against a specific class within the domain, the output of the model trained on that data will reflect these biases (*see Fig. 2.8*). Subsequently, when bias data is used to train NNs used in applications which have either a direct or indirect affect on people's lives, there is a chance that they can result in simulated descrimination of certain social groups.

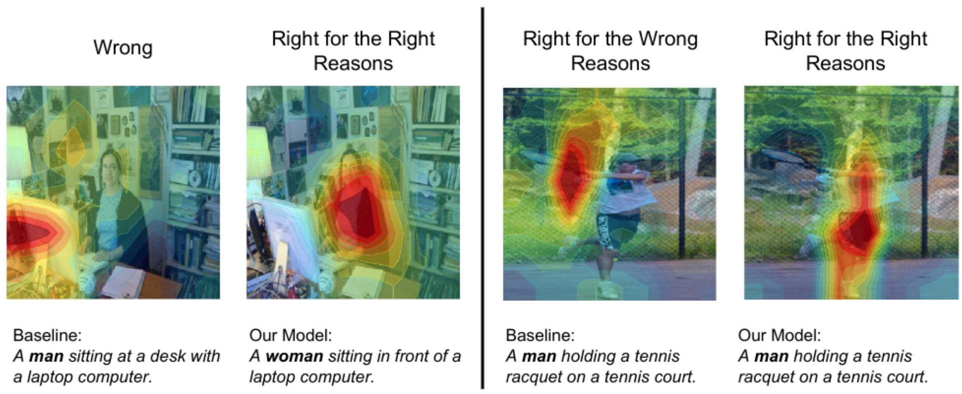

FIGURE 2.8: **Discriminating Bias in Training Data** – An example of how image captioning NNs use the features present in a bias data set to generate either incorrect captions (*left*), or use the wrong features to generate correct captions (*right*) [Burns et al., 2019].

In recent years, there have been many attempts to mitigate the effects of unwanted bias in data being fed to NNs. These include work in facial recognition, where a model is trained separately on demographic representations prior to being trained on face attribute data, thus preserving potential users' demographic privacy [Ryu et al., 2018]; or more recently, developing new regularisation techniques for Generative Adversarial Networks (GANs) which allow a model to categorise classes while ignoring bias features in the training data [Kim et al., 2019].

Although there has been significant progress in this area of research and that discussed in *Section 2.1.3*, many of the proposed solutions have not yet become ubiquitous in industry. As such, there is a need for creating formal methods which allow developers to verify the fairness and robustness of their systems in a wide range of programming environments.

2.2 Formal Verification

Formal verification is a mature and extensive discipline which has seen development in many areas of software engineering. As such, this section will attempt to provide a succinct overview of the ideas behind formal verification while keeping the focus on areas related to this thesis.

2.2.1 Background

Although formal verification stems from a long history of development within the fields of classical and first-order logic [Boole, 2009, Russell, 1937, Smith, 2011], this thesis is concerned with modern formal methods used for software engineering tasks, and thus will use the following definition.

Formal verification is defined by a set of mathematical tools used to analyse the space of possible system states both in hardware and software [Seligman et al., 2015]. In other words, checking that a system will not produce abnormal behaviours given a specific input, or to verify the correctness of hardware or software design [Grout, 2008].

Early software systems were typically verified by hand when necessary. However, as the size and complexity of software increased over time, so too did the computational cost of exhaustively verifying them. As such, huge efforts have been made over the past few decades to develop formal methods frameworks which utilise the power of computing for software engineers.

2.2.2 Theorem Provers

The earliest approach for formally verifying software, and still commonly used, is with theorem provers. Theorem provers were initially developed as interactive, or computer assisted frameworks, however over time the much harder task of automated theorem provers were introduced.

These tools allow developers to formalise theorems using some variant of mathematical logic, such as propositional logic, predicate logic, or first-order logic to name a few. Then, by using *proof checking*, one can establishes the validity of a theorem by mechanically checking the proof [Geuvers, 2009].

2.2.3 Model Checkers

Model checking is another branch of formal verification for software that came along after theorem provers. This technique consists of three main tasks, *modelling*, *specification*, and *verification*.

Modelling is the process of converting a system design into a formalism accepted by a model checking tool. Once this process has finished, a specification of the properties in which a design should satisfy must be provided before verification. Once a model and a specification have been provided, the process of verifying the system can occur. In an ideal world, the final stage can be automated, but often it is necessary to manually analyse the verification results [Clarke et al., 2018].

In other words, given a program P and a specified property ϕ, the primary goal of a model checker is to search the space of possible states of P, and ensure that ϕ holds in all scenarios [Zhang et al., 2019].

2.3 Formal Verification of Neural Networks

In recent years, there has been growing interest in using formal verification tools within the field of AI [Russell et al., 2016]. Although there have been promising advancements in areas such as MAS [Kouvaros and Lomuscio, 2016, Lomuscio et al., 2017], there is significantly less research regarding the formal verification of NNs.

The most common methods for evaluating NNs rely on testing models on previously unseen data, which can provide statistical guarantees regarding accuracy and generalisation. However this approach tends to be incomplete as it does not provide an exhaustive search of all possible inputs to the network [Akintunde et al., 2020].

Initial attempts at formally verifying NNs focused on using *reachability analysis* as a verifiable property. *Reachability analysis* is concerned with determining whether a given state is reachable in a number of steps from an initial state of a system [Akintunde et al., 2018]. The idea behind conducting such an analysis, is that it is then possible to verify that an unwanted state of a system such as those discussed in *Sections 2.1.3 & 2.1.4* is never reached during the lifecycle of the system.

Thus far, this area of research is still in its early stages, however fast progress has been made in demonstrating how it is possible to achieve real-world scalability *w.r.t* verifying NNs [Pulina and Tacchella, 2010, Xiang et al., 2018], including a handful of deep structures such as CNNs [Kouvaros and Lomuscio, 2018] and RNNs [Zhang et al., 2020].

Additionally, progress has been made in developing tools designed to utilise the many formal methods that have been worked on for decades which allow developers to analyse and verify their models easily. This includes tools such as the Maribou Framework for DNNs [Katz et al., 2019], which builds on the authors' previous work in using SMT-based techniques to verify DNNs; and the Sapphire Python library [Kokke, 2020], which translates TensorFlow feed-forward NN model queries to the Z3 SMT solver created by Microsoft Research [De Moura and Bjørner, 2008].

However, as NN development is starting to become prevalent across a wider range of programming languages and paradigms, it is important for further work to be made in developing new frameworks for formally verifying NNs, and to investigate how different programming language infrastructures can affect this development.

2.4 Programming Paradigms for Deep Learning

As NNs and DNNs become more and more ubiquitous in software applications, so to does the number of weights needed for them to perform adequately for their tasks. As such, an enormous amount of work has gone into ensuring the toolkits used by ML engineers allow for scalable and efficient development of such models.

2.4.1 Auto Differentiability

2.4.2 Computational Graphs

2.5 The Go Programming Language

2.5.1 Brief History

2.5.2 Go for ML

2.5.3 Go for Formal Verification

2.6 Conclusions

Chapter 3

Methodology

Chapter 4

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Appendix A

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