Formal Verification of Tree Ensembles in Safety-Critical Applications

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Formal Verification of Tree Ensembles in Safety-Critical Applications

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ABSTRACT

In the presence of data and computational resources, machine learning can be used to synthesize software automatically. For example, machines are now capable of learning complicated pattern recognition tasks and sophisticated decision policies, two key capabilities in autonomous cyber-physical systems. Unfortunately, humans find software synthesized by machine learning algorithms difficult to interpret, which currently limits their use in safety-critical applications such as medical diagnosis and avionic systems. In particular, successful deployments of safety-critical systems mandate the execution of rigorous verification activities, which often rely on human insights, e.g., to identify scenarios in which the system shall be tested.

A natural pathway towards a viable verification strategy for such systems is to leverage formal verification techniques, which, in the presence of a formal specification, can provide definitive guarantees with little human intervention. However, formal verification suffers from scalability issues with respect to system complexity. In this thesis, we investigate the limits of current formal verification techniques when applied to a class of machine learning models called tree ensembles, and identify model-specific characteristics that can be exploited to improve the performance of verification algorithms when applied specifically to tree ensembles.

To this end, we develop two formal verification techniques specifically for tree ensembles, one fast and conservative technique, and one exact but more computationally demanding. We then combine these two techniques into an abstraction-refinement approach, that we implement in a tool called VoTE (Verifier of Tree Ensembles).

Using a couple of case studies, we recognize that sets of inputs that lead to the same system behavior can be captured precisely as hyperrectangles, which enables tractable enumeration of input-output mappings when the input dimension is low. Tree ensembles with a high-dimensional input domain, however, seems generally difficult to verify. In some cases though, conservative approximations of input-output mappings can greatly improve performance. This is demonstrated in a digit recognition case study, where we assess the robustness of classifiers when confronted with additive noise.

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1 Introduction

Recent advances in machine learning (ML) marks a new milestone towards artificial intelligence (AI). In particular, machines are now capable of learning complicated pattern recognition tasks, and sophisticated decision policies. Several of these advances have contributed to new types of software that are already well-established in commercial products and services, e.g., web search engines, spam filters, and voice user interfaces. These success stories are credited to, amongst other things, rapid improvements in computing hardware, and increased access to training data.

However, ML-based systems demonstrate faulty behavior from time to time, and preventing all of these faults from occurring has proved difficult. Fortunately, developers of commercialized ML-based systems have over time managed to reduce the number of occurring faults to a point that is acceptable for many applications. Furthermore, these systems are incrementally improved over time as more data becomes available. In safety-critical applications, however, such an incremental and somewhat optimistic approach is normally not viable since the negative impact caused by errors may have irreversible effects on human lives and the environment.

1.1 Motivation

To ensure safety, design organizations in industries such as medicine and transportation rely on well-established processes, methods, and tools (PM&Ts) to ensure the absence of errors in their systems. Unfortunately,

some of these PM&Ts are incompatible with ML-based systems since machine learning models are notoriously difficult to interpret, hence rendering PM&Ts that rely on human comprehension ineffective. For example, when design organizations develop test cases, they use human insights to identify equivalence classes, i.e., sets of system inputs that cause the same system behavior. Without such insights, software testing is either ineffective due to a lack of important test cases, or intractable due to an abundance of test cases that takes too long to execute.

1.2 Aim

A natural pathway towards viable verification strategies of ML-based systems for safety-critical applications is to leverage formal analyses, which unlike tractable testing strategies, can provide definitive guarantees. However, formal verification suffer from scalability issues with respect to system complexity. Consequently, the aim of this thesis is to understand shortcomings of existing formal techniques when applied to non-trivial ML-based systems, and to address these shortcomings by tailoring verification algorithms specifically for machine learning systems. In particular, this thesis address formal verification of a class of machine learning models known as tree ensembles, e.g., random forests and gradient boosting machines.

1.3 Thesis Outline

Chapter 2 presents background information on formal verification, machine learning in general, and tree ensembles in particular. Chapter 3 presents an overview of the research conducted prior to the writing of this thesis. In particular, the research overview includes questions that guided our research, a technical overview of the three publications included in this thesis (Papers I-III), and how these contributions address the research questions. We then relate these contributions to other's work, and end the chapter by mentioning future challenges this line of research still faces. The thesis ends with copies of the three papers detailing our contributions.

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2

Background

The ability of a system to meet its stakeholder’s needs is often determined by the quality of the system specification, i.e., what the system shall do (or not do). The specification is normally derived from several different and potentially competing needs, and is foundational to verification activities. When verifying that a safety-critical system complies with its specification, extra care is given to statements that, when violated, may cause harm to humans or the environment. Here, we call these statements safety properties.

Systems can be further categorized based on our current understanding of them, both in terms of *what* the system shall do (requirements specification), and *how* the system shall do it (implementation). Here, we group systems into the following three categories; (1) well-understood systems, (2) well-specified systems, and (3) partially specified systems.

With well-understood systems, we know what the expected system behavior is in all meaningful circumstances, we know how to realize such systems, and we understand even its smallest building blocks. By using machine learning to synthesize system components, non-functional properties such as (lower) development costs and (higher) system resource utilization could potentially be improved upon compared to traditional engineering techniques. One interesting example that falls into this category is the application domain used in the work by Kraska et al. [14], where machine learning is used to synthesize efficient index structures, which can improve the runtime performance of, e.g., hash tables and databases.

With well-specified systems, we know what the system shall do, or alternatively, what the system shall *not* do. However, defining exactly how these systems should operate in order to satisfy its specification is extremely difficult. To address this issue, machine learning can be used to explore the system design space, and eventually synthesize an implementation. For example, Silver et al. [24] present a learning algorithm that can synthesize autonomous agents capable of playing complex board games, e.g., Go, chess and shogi (a Japanese variant of chess), with empirical results suggesting super-human capabilities. The rules and goal of these games are easy to specify and understand, but discovering and implementing a super-human decision policy that achieves the goal without violating the rules is extremely difficult.

Finally, with partially specified systems, we know what the system shall do in a limited number of circumstances, and extrapolating to all meaningful circumstances is difficult. For example, it is difficult to specify what all airport runways should look like (or not look like), but we can specify them by labeled examples, albeit an incomplete set of examples.

In all of these categories, formal verification is applicable, but to a varying degree. Formal verification can be used to support the construction of assurance cases, and the more complete the specification is, the more compelling the assurance cases become. Now, the concept of safety is important from an engineering perspective, and is the main motivation behind this thesis. From an algorithmic standpoint, however, the fact that properties may originate from different stakeholder needs is of less importance, be it safety, security, or functional expectations.

2.1 Formal Verification

Formal verification is an activity that proves or disproves that a realized system complies with its given specification. The term *formal* stems from the fact that desirable system properties are expressed in a formal language, and that the system subject to verification is captured by a formal model. When both the implementation and specification is formalized in an unambiguous language, verification algorithms can perform mathematical analyses that leads to verification outcomes with definitive guarantees.

It is well known that formal verification algorithms can be extremely computationally demanding, and the needed resources are believed to grow exponentially with respect to the system's complexity. In spite of that, complex real-world systems have been successfully verified using formal techniques, often by decomposing the system into smaller pieces, and leveraging conservative approximation techniques that reduce the complexity even further. As emphasized by Beckert and Hähnle [1], however, formal verification is not a silver bullet, since both decomposition and approximations comes with a price. When a system is refined into smaller and independently verifiable

components, the system specification often needs to be refined into auxiliary specifications by human domain experts, an activity that can be very time consuming, difficult, and thus a source of erroneous human assumptions. Furthermore, approximations can sometimes be too conservative, which can lead to inconclusive verification outcomes, i.e., the used verification algorithm is unable to decide between “pass” and “fail”.

In this thesis, we present an abstraction technique that turns out to be very effective (in the sense that verification outcomes are conclusive) when verifying a couple of generic properties of non-trivial tree ensembles. We only address the verification of these particular properties, namely plausibility of range and robustness against input perturbations (as defined in Section 2.3), and leave the development of more complete and domain-specific sets of properties with a fully compliant implementation to future works.

2.2 Machine Learning

As a machine learning practitioner, there are many different types of models and learning algorithms to choose from, and knowing which one to pick for a particular problem requires domain knowledge and experience. In fact, Wolpert and Macready [35] conclude that under certain settings, any two co-evolutionary algorithms used to train a model have the same performance when averaged across all possible problems, a conclusion often referred to as the no free lunch theorem. Consequently, machine learning practitioners often train several different types of models, and compare their predictive performances on a particular set of test samples. In this thesis, we address formal verification of a class of machine learning models known as tree ensembles, which use decision trees as their primary building block. Tree-based models have demonstrated great predictive performance on learning problems where the training data fits into main memory. They are currently a popular and successful choice on [kaggle.com](https://www.kaggle.com), an online community where machine learning practitioners compete against each other by training different models on publicly available datasets.

Decision Trees

A decision tree implements a prediction function $t : \mathbb{R}^n \rightarrow \mathbb{R}^m$ by partitioning its input space of n dimensions into disjoint regions, and associates each region with an output value of m dimensions, e.g., as illustrated by Figure 2.1. The tree structure is evaluated in a top-down manner, where decision functions associated with intermediate nodes determine which path to take towards the leaves, and ultimately which m -tuple to output.

In general, decision functions in decision trees may be non-linear and multivariate. Although researchers have demonstrated that decision trees with

Figure 2.1: A decision tree (to the left) partition its input space into disjoint regions (to the right), and associates each region with an output value.

non-linear [12] and multivariate [33] decision functions can be useful, state-of-the-art implementations of tree-based machine learning models normally only contain univariate and linear decision functions, e.g., the popular machine learning library named scikit-learn [18].

Tree Ensembles

Decision trees are known to suffer from a phenomenon called overfitting, i.e., the model becomes too specialized towards training data, and the prediction function generalizes poorly when confronted by previously unseen inputs. To counteract overfitting of decision trees, several types of tree ensembles have been proposed, e.g., random forests [2] and gradient boosting machines [10]. The different types of tree ensembles are normally distinguished by their learning algorithms, while their prediction functions have similar structure. Specifically, a tree ensemble implements a prediction function $f: \mathbb{R}^n \rightarrow \mathbb{R}^m$ as the sum of predictions from B different decision trees, post-processed by a function p , i.e., $f(\bar{x}) = p\left(\sum_{b=1}^B t_b(\bar{x})\right)$, where t_b is the b -th tree. Table 2.1 defines post-processing functions used by common types of tree ensembles.

Table 2.1: Examples of post-processing functions.

Name	Definition
Divisor	$p_d(y_1, \dots, y_m) = \frac{(y_1, \dots, y_m)}{B}$
Softmax	$p_s(y_1, \dots, y_m) = \frac{(e^{y_1}, \dots, e^{y_m})}{\sum_{i=1}^m e^{y_i}}$

The divisor appears in the prediction function of random forests, while the softmax function often appears in gradient boosting machines trained on classification problems.

Classification

Decision trees and tree ensembles as defined above output real-valued m -tuples, in which case they are referred to as regressors by the machine learning community. By training a regressor to predict probabilities, they can be used as classifiers. Let $f(\bar{x}) = (y_1, \dots, y_m)$ be a function trained to predict the probability y_i associated with a class i within disjoint regions in the input space, where m is the number of classes. A classifier $f_c : \mathbb{R}^n \rightarrow \{1, \dots, m\}$ is then defined as

$$f_c(\bar{x}) = \underset{i \in \{1, \dots, m\}}{\operatorname{argmax}} y_i.$$

2.3 Studied Properties

In this thesis, we focus on two generic system properties commonly used by related works; plausibility of range, and robustness against input perturbations.

Plausibility of Range

Let $f : \mathbb{R}^n \rightarrow \mathbb{R}^m$ be a function subject to verification. The function has the desired plausibility of range when its output values are within a stated boundary, i.e.,

$$\begin{aligned} \forall \bar{x} \in \mathbb{R}^n, \forall i \in \{1, \dots, m\}, \\ f(\bar{x}) &= (y_1, \dots, y_m), \\ \alpha_i &\leq y_i \leq \beta_i, \end{aligned}$$

where $\alpha_i, \beta_i \in \mathbb{R}$. In classification problems, the used function predicts probabilities, and thus $\alpha_i = 0$ and $\beta_i = 1$.

Robustness against Input Perturbations

Bruneau et al. [3] describe robustness as the ability of a system to withstand a given level of stress without suffering degradation or loss of functionality. In the context of machine learning, such a description includes a classifier's ability to maintain decisiveness in its predictions, despite noisy or adversarial input. Formally, such a relationship between inputs and outputs may be defined as follows.

Let f_c be a classifier subject to verification, $X \subset \mathbb{R}^n$ a set of input samples, $\epsilon \in \mathbb{R}_{\geq 0}$ a robustness margin, and $\Delta = \{\delta \in \mathbb{R} : -\epsilon < \delta < \epsilon\}$ perturbations. We denote by $\bar{\delta}$ a tuple of perturbations, i.e., an n -tuple of elements drawn from Δ . The classifier is robust against perturbations with respect to X and Δ iff

$$\begin{aligned} \forall \bar{x} \in X, \forall \bar{\delta} \in \Delta^n, \\ f_c(\bar{x}) &= f_c(\bar{x} + \bar{\delta}). \end{aligned}$$

In many applications, the concept of robustness may also include additional types of input perturbations, e.g., axial rotations in computer vision. Furthermore, this property relies on the set of input samples X , which is normally only partially specified.

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3

Research Overview

This chapter provides an overview of the research presented in this thesis. In particular, Section 3.1 defines research questions that guided our work, Section 3.2 provides an overview of the three papers that make up the scientific content of this thesis, and Section 3.3 provides a summary of related works. We then conclude the thesis in Section 3.4, and Section 3.5 mentions some of the future works and challenges this line of research still faces.

3.1 Research Questions

As explained in Section 1.2, the aim of this thesis is to provide an understanding of limitations with existing formal verification techniques when applied to non-trivial tree ensembles, and to explore possible algorithmic opportunities by tailoring verification algorithms specifically for tree ensembles. This section elaborates on that aim by defining two research questions: one related to the characteristics of tree ensembles, and another related to scalability.

As discussed in Section 2.1, the computational resources needed to solve verification problems are believed to grow exponentially with respect to system complexity. Consequently, at some particular complexity barrier, the computational resources needed grow so fast that problems become intractable, as illustrated by Figure 3.1.

Given the inevitable scalability barrier generally associated with formal verification, the need for more efficient verification algorithms is eminent. One way to push the scalability barrier forward is to design heuristic algorithms

Figure 3.1: Verification problems larger than a particular barrier are intractable due to a lack of computational resources.

that trade generalisation for efficiency, i.e., verification algorithms designed specifically for a particular model. This leads us to our first research question addressed by this thesis:

RQ1: are there characteristics of tree ensembles that can be exploited by formal verification algorithms?

Decades of research in computing hardware and algorithmic heuristics have managed to push this barrier forward, rendering formal verification applicable to several practical problems, e.g., formal verification of hardware circuitry, and software systems defined in languages such as Ada SPARK. However, little is known about this barrier when formal verification is applied to tree ensembles, e.g., how many trees, tree depth, and number of input and output variables can be used before the complexity barrier is encountered. This leads us to our second research question addressed by this thesis:

RQ2: is it possible to formally verify non-trivial tree ensembles with reasonable amounts of computing resources?

In this thesis, we consider a couple of days of exclusive access to a modern workstation as reasonable amount of computing resources, and we address case studies with tree ensembles that are too complex for exhaustive testing to be applicable. With a tree ensemble of 10 trees, each with a depth of 10, the rule of product yields 2^{100} ways of combining outputs from different trees, which is clearly an intractable number of combinations to test. Although highly dependent on the type of tree ensemble, application, and context, the

number of trees in a tree ensembles is typically in the range 10 – 1,000, and the tree depth is often in the range 2 – 20.

3.2 Contributions

This thesis is based upon three publications, as illustrated by Figure 3.2. Paper I was presented at the 6th International Workshop on Formal Techniques for Safety-Critical Systems (FTSCS) in November 2018, and later published in Communications in Computer and Information Science (CCIS) volume 1008, contributing with formal verification techniques designed specifically for random forests. Based on that work, we were later invited to submit an extended version of that paper to a special issue of the Science of Computer Programming journal, where we optimized and generalized principles from Paper I. Finally, Paper III was presented at the 2nd International Workshop on Artificial Intelligence Safety Engineering (WAISE), held in conjunction with the SAFECOMP conference in September 2019, and later published in Lecture Notes in Computer Science (LNCS) volume 11699. In that work, we combined techniques from Paper II to devise an abstraction-refinement approach that yields speed improvements of several orders of magnitude.

Figure 3.2: Illustration of papers in this thesis, where they were initially presented, and how the papers relate to each other.

The remainder of this section provides an overview of technical achievements of each individual paper.

Paper I: Formal Verification of Random Forests in Safety-Critical Applications by John Törnblom and Simin Nadjm-Tehrani, presented at the 6th International Workshop on Formal Techniques for Safety-Critical Systems (FTSCS), November 2018, published in Communications in Computer and Information Science (CCIS), volume 1008, Springer, February 2019.

In this paper, we present two formal verification techniques developed specifically for random forests; one fast and conservative technique that computes input-output approximations of random forests, and one exact but more computationally demanding technique that computes equivalence classes, i.e., sets of input values that all yield exactly the same output value.

We implement the verification techniques in a tool named VoRF (Verifier of Random Forests), and verify requirements placed on digit recognition classifiers and collision detection classifiers. Specifically, we use VoRF to verify that probabilities predicted in classifiers are always in the range $[0, 1]$ (the so-called range plausibility property), and that test accuracies are unaffected when test inputs are augmented by additive noise (a robustness property). As it turns out, all classifiers verified in the two case studies always compute probabilities in the range $[0, 1]$, but all classifiers are sensitive to minor additive noise. In some experiments from the digit recognition case study, changing a single pixel value by 0.5% is enough to change the classification outcome.

We also evaluate VoRF in terms of runtime performance, and conclude that the conservative technique is fast, but is often inconclusive. In such cases, we used the exact but more computationally demanding technique, which turns out to be practical for random forests trained on low-dimensional data with up to 25 decision trees, each with a tree depth of 20. To the best of our knowledge, this is the first published work that demonstrates that formal analysis of tree-based machine learning models can be computationally practical when applied to non-trivial verification problems.

Paper II: Formal Verification of Input-Output Mappings of Tree Ensembles by John Törnblom and Simin Nadjm-Tehrani, published in Science of Computer Programming, a special issue on Formal Techniques for Safety-Critical Systems, Elsevier, 2020.

This paper is an extended and significantly improved version of Paper I, where we present generalizations of the two previously published techniques to include an additional tree-based machine learning model, namely, gradient boosting machines. In particular, we show that both random forests and gradient boosting machines can be captured by a single model of additive trees, post-processed by a parameterized function p . We further prove that input-output approximations computed by the non-exact technique are in-

deed conservative, as long as p is monotonic. In the case of random forests, p is a simple constant division with the number of trees, while the addition of trees in gradient boosting machines trained on classification problems are post-processed by the softmax function, which is known to be monotonic.

Based on conclusions from Paper I, this paper also suggests an algorithmic change that improves the runtime performance of the exact verification technique. More specifically, we observed that tree ensembles normally contain infeasible path combinations which may be discarded from analysis. With the algorithmic change proposed in Paper II in place, we are able to detect these infeasible paths earlier in the analysis than before, which significantly reduces the elapsed time taken during verification, in some cases up to 10 times faster.

Paper III: An Abstraction-Refinement Approach to Formal Verification of Tree Ensembles

by John Törnblom and Simin Nadjm-Tehrani, presented at the 2nd International Workshop on Artificial Intelligence Safety Engineering (WAISE), September 2019, published in Lecture Notes in Computer Science (LNCS), volume 11699, Springer, 2019.

In this paper, we combine the two generalized techniques from Paper II into an abstraction-refinement approach to address combinatorial explosions observed while verifying the high-dimensional digit recognition case study in Paper II. We tailored the approach specifically to assess robustness against additive noise, and implemented it in the toolsuite VoTE (Verifier of Tree Ensembles). As illustrated in Figure 3.3, the approach is realized in a pipeline architecture with alternating abstraction and refinery elements, with the significant additions made to the VoTE implementation as part of this work highlighted in bold.

As mentioned earlier in this chapter, our previous works outputs equivalence classes $(X_i, \bar{y}_i)$, such that $\forall \bar{x} \in X_i, f(\bar{x}) = \bar{y}_i$, where f is the prediction function of a tree ensemble. With the algorithmic changes presented in this paper in place, the outputs produced by VoTE are conservative approximations of input-output mappings (X_i, Y_i) , such that $\forall \bar{x} \in X_i, f(\bar{x}) \in Y_i$.

It turns out that analyzing conservative approximations of input-output mappings is significantly more efficient when verifying the robustness aspects of our case studies compared to earlier works that analyze equivalence classes. In particular, the elapsed time taken during verification was reduced by several orders of magnitude, now scaling to tree ensembles with up to 50 trees with depth 10, trained on high-dimensional data.

3.3 Related Works

In this section, we summarize related works that address the verification of machine learning models using various formal techniques. The section is struc-

Figure 3.3: The abstraction-refinement approach is realized in VoTE using a pipeline architecture with alternating abstraction and refinery elements. Significant additions we made to the VoTE implementation as part of this work are highlighted in bold.

tured according to the machine learning model subject to verification, then ordered chronologically according to year of publication.

Neural Networks

Pulina and Tacchella [19] present a tool called NeVer which, to the best of our knowledge, is the earliest published work that uses formal techniques to verify a machine learning model. Specifically, Pulina and Tacchella present an abstraction-refinement technique that approximates the non-linear logistic function in neural networks by a set of intervals, which are refined into smaller pieces when the outcome of the verification result is inconclusive. They demonstrate their approach in a case study where a robotic arm is controlled by a neural network. Pulina and Tacchella then continue to improve their abstraction-refinement approach [21], and also explore the limits of SMT solvers by encoding the verification problem as one large SMT formula [20]. They conclude that formal verification of non-trivial neural networks is still an open challenge. In our works, we address similar properties as Pulina and Tacchella, i.e., plausibility of range and robustness against input perturbations.

Fast-forward to the year 2017, when deep learning appears on the Gartner hype cycle for the first time [32], an annual report produced by the research and advisory firm Gartner to explain general phenomena of interest in new technologies. State-of-the-art neural networks are now even larger in terms of size, and concerns regarding their implications on safety in applications such as autonomous vehicles accelerate the pursuit for viable verification strategies.

Around this time, the progress made in deep learning yielded significantly larger neural networks than before, but often containing simpler activation functions, e.g., the ReLU activation function which is piece-wise linear. Since then, this piece-wise linear property of many modern deep learning models have been exploited by several researchers. In particular, researchers have explored SAT- and SMT-based techniques [13, 5], various linear programming schemes [8, 11, 28], abstract interpretation [16, 25, 26], and a mixture of multiple techniques [7, 34, 17, 27]. In this thesis, we verify similar properties in similar case studies as these works, but for tree ensembles.

Tree Ensembles

Chen et al. [4] verify the robustness of tree ensembles by expressing the robustness verification problem as a max-clique graph problem, and present an approach that leads to a polynomial time algorithm when the input dimension of tree ensembles is low. These results confirm our earlier observations from Paper II, i.e., that formal verification of tree ensembles with few input variables can be practical, even for non-trivial models.

Einziger et al. [9] present a tool named VeriGB capable of verifying the robustness of gradient boosting machines. They encode the verification problem as an SMT formula, and use an off-the-shelf SMT solver to compute the verification outcome. They design the SMT formula to facilitate parallel analyses, which they leverage in three case studies executed on a machine with 36 CPU cores. Even though they experience timeouts on particularly difficult verification problems, their approach is able to quantify the robustness by treating verification problems that time out as negative outcomes. Similarly, Sato et al. [23] leverage an SMT solver, but address the plausibility of range property. When the SMT solver discovers an illegal output value, they extract the corresponding input, and construct a preprocessing filter that can prevent the violation from occurring when deployed into a production system. Current work by Devos et al. [6] also leverage an SMT solver, but aims for any tree ensemble verification problem that can be expressed as an SMT formula.

Compared to these works, we leverage conservative approximations in intermediate computations, which often reduce the elapsed time taken during verification, at the expense of precision. In Paper III, we present an abstraction-refinement approach that we implement in the tool VoTE (Verifier of Tree Ensembles). We compare empirical results from Paper II (which also uses VoTE, but without the abstraction-refinement approach), and conclude that conservative approximations decreased the elapsed time taken during verification by several orders of magnitude.

Ranzato and Zanella [22] extend on our work by formulating the abstraction-refinement approach from Paper III in an abstract interpretation framework, and implement the approach in a tool called Silva. Compared to VoTE, Silva is designed to support multiple abstract domains, and uses a

best-first tree exploration algorithm, whereas VoTE uses a depth-first algorithm. Ranzato and Zanella conclude that Silva outperforms VoTE in terms of elapsed time during verification. However, we have identified several shortcomings in their experimental setup, which could have affected the validity of their conclusions. These concerns were recently confirmed by Lundström [15]. In particular, Lundström shows that VoTE uses significantly less memory than Silva, and that VoTE is marginally better than Silva in terms in elapsed time during verification when experiments are performed in a consistent (fair) setting. In our current work (that is not part of this thesis), we leverage the small memory foot-print of VoTE to parallelize the robustness verification across multiple CPU cores, an approach which we believe may not be practical with a best-first algorithm due to memory limitations.

3.4 Conclusions

As described in Section 3.1, this thesis addresses two research question: one (RQ1) relating to characteristics of tree ensembles that can be exploited by formal verification algorithms, and another (RQ2) relating to the scalability of formal verification algorithms when are applied to non-trivial tree ensembles. In the following sections, we discuss these two questions individually.

Characteristics of Tree Ensembles

The size and complexity of tree ensembles is primarily determined by the number of trees, and the depth of each tree. These model parameters also determine the number of path combinations amongst trees, and thus the theoretical upper limit on the number of equivalence classes in a tree ensemble. In Papers I and II, we conclude that the actual number of equivalence classes in tree ensembles with a small number of input variables is significantly lower than the number of path combinations, since several combinations are infeasible. This conclusion was later confirmed by Chen et al. [4], where they prove that the robustness of gradient boosting machines against additive noise is verifiable in polynomial time, as long as the input dimension is low.

Furthermore, we recognize that state-of-the-art machine learning libraries synthesize trees with univariate and linear decision functions. Consequently, sets of inputs may be captured precisely as hyperrectangles, which facilitates efficient reasoning of input-output mappings.

Scalability

In Papers I and II, we demonstrate via a collision detection case study that non-trivial tree ensembles can be verified using a moderate workstation in less than a day, as long as the input dimension is low. This is made possible since tree ensembles with a small number of input dimensions contain

many infeasible path combinations, which can be exploited by a verification algorithm to efficiently compute and enumerate equivalence classes. As the input dimension grows, however, the number of infeasible path combinations is reduced. Tree ensembles with a high-dimensional input domain seem to be generally difficult to verify. In some cases though, conservative approximations can greatly improve performance. In Paper III, we demonstrate via a digit recognition case study that its possible to verify robustness of additive noise of tree ensembles, even when the input dimension is large.

3.5 Future Works

Modern computers are equipped with several CPU cores, most of which are unused when executing the current implementation of VoTE. When verifying robustness against input perturbations, each sample from a test set is analyzed in sequence. This sequence is trivially parallelizable across multiple CPU cores, and a near-linear speedup with respect to number of CPU cores is to be expected, assuming sufficient memory is available.

The abstraction-refinement approach currently implemented in VoTE refines conservative approximations using information from trees that appear in a fixed and predetermined order. By reordering trees dynamically before each refinement step based on how much each tree contributes to the widening of the output approximation, the number of refinement steps could potentially be reduced. Whether the dynamic reordering adds more overhead than what is gained from fewer refinement steps remains to be seen. We also plan to investigate trade-offs between the depth-first tree exploration algorithm implemented in VoTE, and the best-first tree exploration algorithm implemented in Silva, when executed concurrently on a many-core system.

Tools based on formal verification methods, in particular those that leverage conservative approximations, have demonstrated promising results in terms of run-time performance in several ML-based applications. However, formal verification assumes the presence of a formal specification, which is still incomplete in many applications of machine learning. In order to leverage formal verification in these applications, we must learn how to specify what we expect from them. Are these systems only partially specified due to insufficient engineering work, or are there fundamental issues at play that need further research? These are open questions to be studied in the future.

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