

A Review of Formal Methods applied to Machine Learning

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Abstract

We review state-of-the-art formal methods applied to the emerging field of the verification of machine learning systems. Formal methods can provide rigorous correctness guarantees on hardware and software systems. Thanks to the availability of mature tools, their use is well established in the industry, and in particular to check safety-critical applications as they undergo a stringent certification process. As machine learning is becoming more popular, machine-learned components are now considered for inclusion in critical systems. This raises the question of their safety and their verification. Yet, established formal methods are limited to classic, i.e. non machine-learned software. Applying formal methods to verify systems that include machine learning has only been considered recently and poses novel challenges in soundness, precision, and scalability.

We first recall established formal methods and their current use in an exemplar safety-critical field, avionic software, with a focus on abstract interpretation based techniques as they provide a high level of scalability. This provides a golden standard and sets high expectations for machine learning verification. We then provide a comprehensive and detailed review of the formal methods developed so far for machine learning, highlighting their strengths and limitations. The large majority of them verify trained neural networks and employ either SMT, optimization, or abstract interpretation techniques. We also discuss methods for support vector machines and decision tree ensembles, as well as methods targeting training and data preparation, which are critical but often neglected aspects of machine learning. Finally, we offer perspectives for future research directions towards the formal verification of machine learning systems.

1 Introduction

Recent advances in artificial intelligence and machine learning and the availability of vast amounts of data allow us to develop computer software that efficiently and autonomously perform complex tasks that are difficult or even impossible to design using traditional explicit programming (e.g., image classification, speech recognition, etc.). This makes machine-learned software particularly attractive even in *safety-critical applications*, as it enables performing a whole world of new functions that could not be envisioned before, e.g., autonomous driving in the automotive industry, or image-based operations (taxiing, takeoff, landing) and aircraft voice control in

the avionics industry. Another attractive aspect of machine-learned software is its ability to efficiently approximate or simulate complex processes and systems and automate decision-making, e.g., diagnosis and drug discovery processes in healthcare, or aircraft collision avoidance systems in avionics [90].

Safety-critical applications require an extremely high level of insurance that the software systems behave correctly and reliably. Today, *formal methods* are an integral part of the development process of traditional (non machine-learned) critical software system, to provide strong, mathematically-grounded guarantees on the software behavior. For instance, they are used at an industrial level in avionics [146], where the development processes of aircraft software systems have very stringent assurance and verification requirements mandated by international standards (i.e., DO-178C). This success is due to the recognition of formal methods by certification authorities and the availability of effective and efficient verification tools. Among formal verification techniques, *static analyzers* are particularly successful as they are fully automated, efficient, and correct by construction. A notable example is the Astrée static analyzer [13], used to ensure absence of run-time errors in critical avionics C code.

In contrast, research in formal methods for the development and assurance of machine learning systems remains today extremely limited. It is however rapidly gaining interest and popularity, mostly driven by the growing needs of the automotive and avionics industries. The purpose of this document is to keep up with these developments and gain a better understanding of the research ecosystem that is forming around the verification of machine learning software, and discuss further research directions. Specifically, in the following, we give an introduction to formal methods (Section 2) with a particular focus on static analysis by *abstract interpretation* [37], as it offers a unifying theory for reasoning about disparate formal verification approaches (Section 2.3). We then thoroughly overview the current state of the art in formal methods for machine learning (Section 3). We provide descriptions of the different underlying techniques and discuss and compare the scope of their application and their advantages and disadvantages. Finally, we discuss perspectives and expectations for possible worthwhile future research directions (Section 4).

2 Formal Methods

This section gives an informal overview of current formal methods for software verification, notably abstract interpretation, and selected recent examples of applications on embedded safety-critical software. We refer to [40] for another short introduction to abstract interpretation and to [114] for a tutorial.

2.1 Overview of Formal Methods

Formal methods are an array of techniques that employ logic and mathematics in order to provide rigorous guarantees about the correctness of computer software. The first principled formal methods date back from the pioneering work of Floyd [68], Hoare [83] and Naur [121] on program logic in the late 60s, although similar ideas have been attested as far back as the late 40s with a notable work by Turing [158]. Early works describe such methods through pen-and-paper proofs of tiny programs in idealized languages. Developing and checking by hand the very large proofs that are required to verify real-sized applications in realistic languages would be intractable. Hence, the last few decades have seen the development of software verification tools.

Keeping in mind the fundamental undecidability of correctness properties of programs as a consequence of Rice’s Theorem [133], it is in fact impossible to design a

tool that can decide precisely for every program whether it is correct or not. Tools must abandon either full automation (thus requiring some manual assistance), generality (handling only a subset of programs), or completeness (sometimes reporting as incorrect a correct program, which we call a false alarm, or failing to terminate). In the rest of the section, we discuss the broad categories of computer-assisted verification methods that have been subsequently proposed, and the trade-offs they make to solve these issues in practice. These approaches also vary in the set of correctness properties that can be checked and how the programmer can express them. However, a requirement of all formal methods is that they should be *sound*, that is, any correctness property established by the tool is indeed true of the actual executions of the program. In practice, tools may only be sound for subsets of programming languages (e.g., not supporting the “eval” construction), or for an idealized semantics (e.g., using reals instead of floating-point numbers), or by making implicit assumptions that must be checked by other means (e.g., no aliasing between pointers passed to functions) [107]. A formal verification tool must then make these limitations explicit and state clearly the formal guarantees that are expected despite the limitations.

Deductive Verification. Deductive methods stem directly from the work of Floyd, Hoare, and Naur [68, 83, 121]. The user provides a program and a formal specification expressed in a logic language. The specification is then propagated through the program source code, using symbolic execution as proposed by Burstall [23] or weakest preconditions as proposed by Dijkstra [51]. This generates automatically a set of verification conditions implying that the program obeys its specification. The conditions are then proved correct with the help of a solver, such as a fully automated SMT (satisfiability modulo theory) solver (e.g., z3 [49]).

One benefit of deductive verification is its ability to handle complex specifications using decidable logical theories (reasoning about, e.g., integers, floating-point numbers, pointers, arrays, recursive data-structures) and to perform modular verification by breaking down the specification into function contracts with preconditions and postconditions. However, automation is limited by the need to supplement the specification with additional annotations, notably loop variants and invariants, contracts for internal functions, and ghost variables so that the verification conditions become tractable for the prover. The progress of solvers has made deductive verification an attractive approach, but there is still the occasional need to help the solver through interactive proofs. Examples of current deductive verification platforms include Why3 [65], as well as Frama-C [45] used to check industrial C software.

Design by Refinement. Design by refinement is a related approach based on successive refinements of a sequence of state machines, from an abstract specification up to an executable implementation. Each refinement step is proven formally with the aid of an automated solver. This technique requires a large specification effort and is suited to develop formally verified software from the ground up rather than verifying existing software. A popular instance of this technique is the B method [1].

Proof Assistants. Interactive proof assistants are general-purpose tools able to produce reliable proofs of theorems, with application to mathematics, logic, and computer science. Their strength lies in the use of very expressive logic and the ability to check every proof with a small trusted core, reducing the possibilities of errors. Although they can offer some degree of automation (e.g., through tactics), they employ undecidable logics and essentially rely on a very tight interaction between the programmer and the tool, which can prove time consuming. Unlike automated SMT

solvers, the limit of what can be proved with proof assistants lies solely in the ingenuity (and time and dedication) of the user. One popular proof assistant is Coq [12], which also acts as a programming language and is able to automatically extract an executable implementation from a constructive proof. Proof assistants have been applied to prove involved correctness properties on a few complex pieces of software, such as the CompCert certified C compiler [103]. In the case of CompCert, Coq was used to prove to equivalence between a source code and its compiled version (provided that the former is free of undefined behavior), which is a very strong example of functional correctness result.

Model Checking. In the 80s, Clarke and Emerson [33] and Queille and Sifakis [128] independently invented model checking, which checks specifications on finite-state models of hardware or software systems by exhaustive exploration. It provides a sound, complete, and automatic verification method on models. Early model checking methods relied on explicit state representations, which suffer from combinatorial explosion and severely limit the size of the models considered. Symbolic model checking [111] subsequently introduced more compact representations that also permit the verification of some regular classes of infinite-state models.

The benefits of model checking are achieving both soundness and completeness, the use of temporal logic [124] to express rich specifications (including termination and other liveness properties), and the ability to check concurrent models. Model checking has been particularly successful to check hardware systems (for instance at Intel [66]) which are inherently finite. However, whenever the system to be checked is infinite-state, or is simply too large, it is the responsibility of the user to provide a simplified model. Crafting a model that is both faithful and efficiently checked is a difficult task. Even then, the soundness and completeness properties only hold with respect to the model, not the original system.

More recently, software model checking has targeted the direct verification of source code without requiring a hand-crafted model, but several trade-offs had to be made to sidestep the intractability of an exhaustive exploration of the state space. Bounded model checking [14] (e.g., the CBMC tool [35]) limits the exploration to execution traces of fixed length. The drawback of this method is that it loses soundness and completeness with respect to the full program; while it can uncover errors occurring at the beginning of the execution of the program, it cannot prove the absence of errors. Counterexample-guided abstraction refinement (CEGAR) [34] automatically extracts an abstract model from the source code based on a finite set of predicates, which is then verified using model-checking. If the correctness proof fails, the model checker extracts a counterexample which is used to refine automatically the abstract model, and the process is iterated until the proof is established. The CEGAR method has been successfully used to check the correctness of Windows device drivers at Microsoft [6]. In certain cases, however, the refinement process does not terminate.

Semantic Static Analysis. Static program analyzers perform a direct and fully automated analysis of the source code of a program without executing it. In the broad sense, the term “static analysis” also includes syntactic style checkers (so-called “linters”). We only focus here on semantic-based static analyzers that offer formal guarantees on the result of the analysis, i.e., they belong to the category of formal methods. To achieve full automation, termination, and scalability, static analyzers interpret programs at an abstract level, focusing only on the properties of interest.

A classic method for static analysis is data-flow analysis, introduced in the 70s by Kildall [94]. This technique infers program properties by propagating abstract values

from a finite-height lattice of properties along the control flow of the program. The method is popular in compilers as it features very efficient algorithms and can infer properties useful for optimization (constant propagation, live variable analysis, etc.). However, such properties are generally not expressive enough to support program verification. More general analyzers can be constructed through abstract interpretation, a theory of the approximation of program semantics introduced by Cousot and Cousot [37]. They are not limited to finite-height abstractions and can, for instance, infer variable bounds and relationships, handle dynamic memory allocation, etc. While less efficient than data-flow analyses used in compiler, they always terminate and remain relatively efficient thanks to abstractions that ignore irrelevant (or too complex) details and perform approximations. They nevertheless guarantee soundness by erring on the safe side: they over-approximate the set of possible behaviors of programs when they cannot be modeled faithfully, so that any property inferred as true on the over-approximation is also true on the original program. The benefit of static analysis by abstract interpretation is full automation, parameterized precision, and the ability to verify large programs in real languages at the source level (C, Java, etc.) or binary level. The analysis is however inherently incomplete, and can fail to verify a desired property due to over-approximations. Thus, it can output false alarms, that must be checked by other means.

Static analyzers by abstract interpretation can perform whole-program analysis to prove non-functional properties, such as absence of run-time errors, that are implicitly specified by the language and embedded in the choice of abstraction. An example is the Astrée analyzer [13] for embedded C code, discussed in the next section. They can also perform a modular proof of user-provided contracts, as in CodeContracts [64], achieving a similar goal to deductive verification but with full automation, by removing the need to annotate the program with loop invariants or contracts for private functions. In each tool, the abstractions have been tailored to the class of properties to be verified. Compared to classic model checking and deductive methods, the effort has thus shifted from the user to the analysis designer. We discuss abstract interpretation in more details in Section 2.3.

2.2 Applications in Embedded Critical Software

Formal methods have transitioned from academia to hardware and software industries, with many individual success stories (see [88] for a recent review). We present here an account, based on [146, 4], of its use on safety-critical embedded software in the avionics industry. It is a significant example as this industry is an early adopter of formal methods due to the stringent safety requirements on software, although such methods have recently made their way into less critical industries such as Facebook [52]. Nevertheless, it provides a picture of a fully realized integration of these methods and also hints at the level of maturity expected from formal methods for artificial intelligence to become usable in safety-critical applications.

As a critical aircraft component, avionic software is subject to certification by certification authorities and must obey the DO-178 international standard, which notably describes the verification process that such software must follow. Traditional methods consist in massive test campaigns and intellectual reviews, which have difficulties scaling up and maintaining a reasonable cost (which already accounts for more than half of the cost of overall software development). A shift occurred in the 2010s with the new DO-178C revision (and its DO-333 supplement) which opens the door to certification by formal methods. One key aspect of the standard is the emphasis on employing *sound formal methods*. Another key aspect is that any verification technique (formal or not) employed at the source level cannot be considered valid at the

binary level unless the compilation process is also certified, which is important in practice as some tools can only reason at the source level.

Classic certification processes combine a variety of techniques (reviews, unit tests, integration tests, etc.). Likewise, when introducing formal methods into the verification process, Atki et al. [4] present an array of different tools and techniques that are currently used (or are considered in the future) to supplement or replace legacy techniques with, as goal, to improve industrial efficiency while maintaining the requested safety and reliability level:

- Deductive verification with Frama-C [45] is used to implement unit proofs of individual C functions of some software subsets. The article reports that 95% of the proof obligations are solved automatically by the SMT solver, and the remaining part requires interactions with the prover. This activity can partially replace classic unit testing, with the additional benefit of ensuring that the properties tested are fully formalized in a contract language.
- The Astrée [13] abstract interpretation-based static analyzer is used to check for the absence of run-time errors as defined by the C standard (integer and floating-point arithmetic errors, pointer or array access errors, invalid operations, etc.) as well as assertion failures. Astrée performs a whole-program analysis at the C source level, scaling to programs of a few million lines with very few false alarms.
- The Fluctuat [48] abstract interpretation-based static analyzer is used to assess the numerical accuracy of floating-point computations in C libraries of control programs.
- The StackAnalyzer and aiT WCET abstract interpretation-based static analyzers from AbsInt (<https://www.absint.com>) are used at the binary level on the compiled code in order to compute (over-approximations of) the worst-case execution time and the worst-case stack usage, and ensure that they do not exceed the allocated resources.
- The CompCert certified compiler [103] is used to compile the C code into binary. This ensures that the compilation process does not introduce any error that was absent from the source. Note that, although the design of CompCert required a massive proof effort in Coq, its use by avionic software programmers does not require any effort at all.

These tools are complementary. For instance, the unit proof of Frama-C implicitly assumes the absence of invalid pointers, aliasing, or arithmetic overflows to optimize proof automation. Likewise, CompCert assumes that the C source has no undefined behaviors and does not offer any guarantee otherwise. These properties are ensured by the whole-program analysis performed by Astrée. In return, CompCert ensures the equivalence of the source and binary code, hence, the properties that Frama-C and Astrée validated on the C source can be assumed to hold on the binary code.

We can conclude from the choice of formal methods reported in [4] that two desirable properties for formal verification methods of safety-critical software are *soundness* (including with respect to floating-point computations) and *automation*.

2.3 Abstract Interpretation

Abstract interpretation is a general theory of the approximation of program semantics introduced in the late 70s by Cousot and Cousot [37]. It provides mathematical tools to compare different semantics and prove crucial properties, such as soundness and completeness, and formalizes the notions of approximation and abstraction.

Static Analysis by Abstract Interpretation. One important practical application of abstract interpretation is the design of static analyzers. It allows deriving, in a principled way, static analyzers from program semantics focusing on a desired program property, ensuring soundness by construction. This is achieved by applying a sequence of abstractions until the semantics becomes effectively computable.

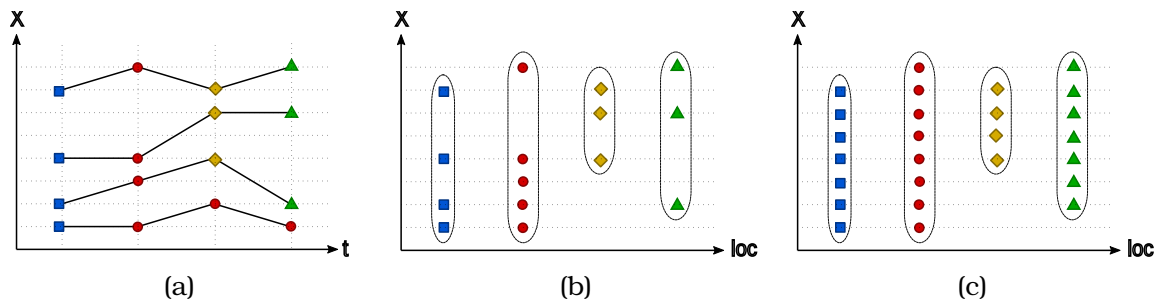


Figure 1: From Trace Semantics (a), to State Semantics (b), to Interval Semantics (c).

The method starts with a concrete semantics providing a precise mathematical expression of program behaviors. A natural idea is to model a program execution as a discrete sequence of program states. The trace semantics of a program is then the set of all its possible execution traces. Figure 1a depicts, informally, the trace semantics of a program. A state is composed of the full snapshot of the memory (depicted here simply as the value of variable X) and a control location (depicted with different shapes and colors). A first abstraction consists in collecting, at each location, the set of possible memory states, as depicted in Figure 1b. This state semantics forgets about the history of computation (i.e., which state appears before which state), and so, cannot be used to verify temporal properties. However, it is sufficient (i.e., complete for) state reachability properties, such as the absence of run-time errors. A further abstraction, the interval semantics, over-approximates the set of values of X at each control location with an interval. The benefit is that an abstract memory state can be represented in a very compact way, as a pair of a lower and upper bound for X instead of a set of values. However, we cannot tell whether the values within these bounds are actually reachable or not and, to ensure that we cover all possible program behaviors, we must assume that all these values are possible. This is represented in Figure 1c. With this abstraction, we can no longer prove that X never takes the value 4.

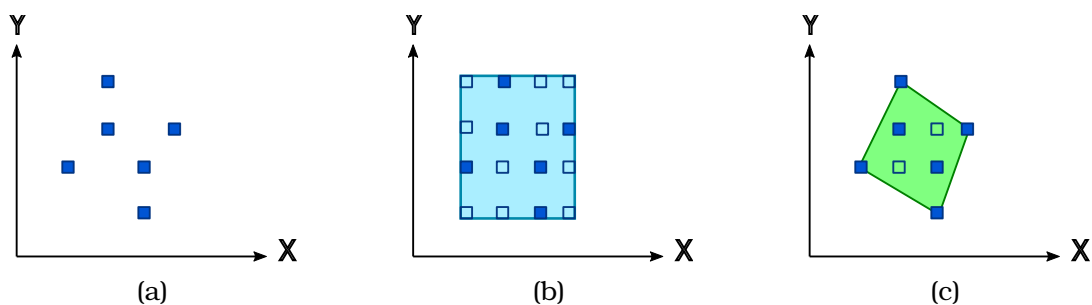


Figure 2: Concrete Set of Two-Dimensional Points (a), its Interval Abstraction (b), and its Polyhedral Abstraction (c).

Figure 2 gives another example, abstracting a set of points in two dimensions representing variables X and Y . When using the interval abstraction independently on each variable we obtain, in Figure 2b, an interval with many spurious points (shown as hollow squares in the figure). The original set-based semantics is undecidable if we assume an infinite range for variable values and, at best, extremely costly to

compute when assuming a finite but realistically large range for variables (such as $[-2^{31}, 2^{31} - 1]$). In the interval semantics, however, we can model assignments using interval arithmetic and tests as constraint programming, which feature efficient algorithms. Additionally, abstract interpretation introduces fixpoint acceleration operators, called widening, in order to approximate efficiently the limit of iterations involved in the semantics of program loops. This leads to an efficient static analyzer.

As we perform each computation step within the interval world, each step may induce some loss of precision, which can accumulate. In practice, the interval analyzer does not infer the tightest possible variable bounds. It may fail to prove the desired correctness property even when it can be expressed as an interval (such as the absence of overflow): the analysis is not complete and can lead to false alarms. To achieve the required level of precision, is thus sometimes desirable to use more expressive abstractions. Figure 2c presents the classic polyhedral abstraction [38]. On the one hand, it is more precise than intervals (it adds less spurious points) and more expressive (it can infer linear relations between variables, which are particularly useful as loop invariants). On the other hand, it is much more costly than intervals. The abstract interpretation literature proposes a large collection of abstract domains, including numeric domains such as intervals and polyhedra, but also domains for pointers, data-structures, etc., which help in finding a good balance between precision and cost. Abstract interpretation also considers abstractions as first class objects and features operators to combine them. For instance, the Astrée analyzer [13] uses over 40 distinct abstract domains, each one specialized to handle a certain semantic aspect of the proof of absence of run-time errors in embedded critical C code. This encourages the modular design of static analyzers using reusable parts.

An important benefit of static analysis by abstract interpretation is soundness by construction. Thus, only the concrete semantics must be trusted, and all subsequent abstractions, including the final computable static analysis, are sound with respect to this concrete semantics. The concrete semantics is generally a formalization of a standard describing the language (e.g., the C99 standard for Astrée [13]), possibly restricted to some implementation choices (such as integer bit-width), that the user and analyzer designer agree upon. Soundness is generally proved on pen and paper with the help of the abstract interpretation theory, which leaves the possibility of errors in the proofs and bugs in the implementation. More confidence can be achieved by performing the proofs using a proof assistant, as done for instance in the Verasco analyzer [89], but this requires a lot of effort for the analysis designer.

Unifying Theory of Formal Methods. As a general theory of semantic approximation, abstract interpretation is not only useful to derive new static analyses, but can also model other static analysis methods developed independently, such as data-flow analyses [42] or security analyses [43]. It can also reason about other formal techniques, such as strong typing [39], constraint programming [123], as well as model checking [41] and SMT solving [18]. A first benefit of this line of work is theoretical: it uncovers the abstractions that are made, often implicitly, by these techniques. It helps understanding the expressiveness and the trade-offs made by each method with respect to the most concrete semantic of the program, and provides alternate proofs of soundness and completeness. In practice, it opens the way to a principled way to combine different formal methods that would seem, at first glance, incompatible.

As we will see in the following section, a large part of the formal techniques applied to artificial intelligence employ either SMT solving, constraint solving, or abstract interpretation in a numeric abstract domain. Hence, abstract interpretation would be a reasonable choice to model, reason about, and combine these techniques. Addition-

ally, Section 2.2 reported on the industrial use of static analysis by abstract interpretation to verify current critical embedded software. As machine learning enters critical industries, it would be interesting to combine verification techniques for traditional software and for artificial intelligence using abstract interpretation as a common theory, and develop an analyzer adapted to this new generation of critical software.

3 State of the Art



Figure 3: Machine Learning Pipeline.

The main differences between machine learning software and traditional software arise from the software development process. The *machine learning pipeline* (cf. Figure 3) begins with the collection of data and its preparation for training, followed by a machine learning model training phase, and ends with the deployment of the trained model and its use to make predictions and automate tasks. The training phase is highly non-deterministic, which is in contrast with predictability and traceability requirements of traditional safety-critical software development processes. Furthermore, the trained models only give probabilistic guarantees on the prediction results, bound to the data used for training, which are not sufficient for guaranteeing an acceptable failure rate under any circumstances, as required for traditional critical software. Thus, formal verification methods need to adapt to these differences in order to ensure the safe development and deployment of machine learning software in safety-critical applications. Most formal verification methods proposed so far in the literature apply to *trained machine learning models* (Section 3.1) while only few are dedicated to the *data preparation* and *model training* phases (Section 3.2).

3.1 Formal Methods for Trained Machine Learning Models

So far, the vast majority of the research in verification of machine learning models has focused on *neural networks* [75] (Section 3.1.1), driven by their success and the interesting research challenges they bring for the formal methods community. Traditional machine learning models such as *decision trees* [117] have been initially left aside as they are much easier to verify than neural networks [9] and thus not considered interesting enough. This is not necessarily the case for decision tree ensemble models, such as *random forests* [21] and *gradient boosted decision trees* [69]. Indeed, a small but growing number of recent formal verification methods target these models as well as *support vector machines* [44] (Section 3.1.2).

3.1.1 Formal Methods for Neural Networks

Neural networks [75] are collections of connected nodes called *neurons*. Each neuron acts as a computational unit: it receives inputs or signals from other neurons, processes them, and transmits the resulting signal to other connected neurons. Connections between neurons are assigned a weight which increases or decreases the strength of the signal. Specifically, neurons apply a (non-linear) *activation function* to the (weighted) sum of their inputs to produce their output signal. Nowadays, the

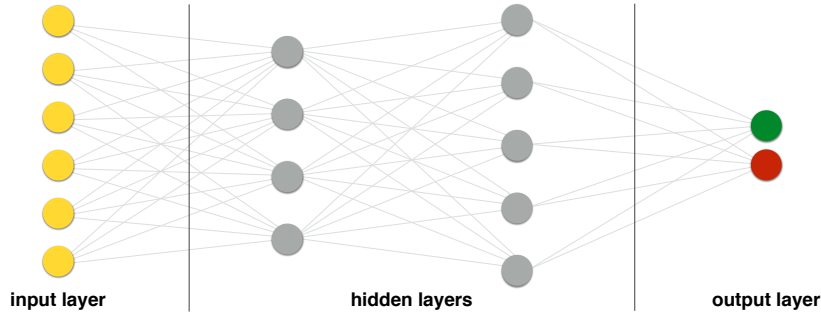


Figure 4: Feed-Forward Fully-Connected Neural Network.

most commonly used activation function is the *Rectified Linear Unit (ReLU)* [119], i.e., $ReLU(x) = \max\{0, x\}$. Other popular activations include the *sigmoid or logistic function*, i.e., $\sigma(x) = \frac{1}{1+e^{-x}}$, and the *hyperbolic tangent function (tanh)*, i.e., $\tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$.

Neurons are typically aggregated into *layers* such that neurons in one layer only connect to neurons in the (usually immediately) following layer. Multiple connection patterns are possible between layers, which define different layer types. In a *fully-connected layer* each neuron receives inputs from every neuron in the previous layer, while in a *pooling layer* or in a *convolutional layer* each neuron only receives inputs from a subset of neurons in the previous layer. Neural networks that only consist of fully-connected and pooling layers are known as *feed-forward neural networks* (cf. Figure 4), while neural networks with at least one convolutional layer are called *convolutional neural networks*. These neural networks form directed acyclic graphs in which signals travel from the input layer, through each of the hidden layers, to the output layer. Instead, *residual neural networks* use shortcuts to jump over some layers, and *recurrent neural networks* allow neurons to connect to neurons in previous layers (thus forming cycles in which signals traverse layers multiple times).

Kurd and Kelly [98] were the among the first to propose a characterizations of verification goals for neural networks used in safety-critical applications. Most existing formal methods for neural networks aim at verifying what Kurd and Kelly identify as goals G4 and G5, which respectively concern ensuring robustness to disturbances to inputs and ensuring that outputs of neural networks are not hazardous. In the following, in addition to the targeted verification goal, we also categorize methods based on the supported neural networks (i.e., architecture, activation functions, size, etc.) and the underlying technique used. We broadly distinguish between *complete verification methods* (Section 3.1.1.1) and *incomplete verification methods* (Section 3.1.1.2).

3.1.1.1 Complete Formal Methods

Complete formal verification methods generally *do not scale* to large neural network architectures (they generally require several hours for neural networks with hundreds or thousands of neurons) but are both *sound* and *complete*: they can precisely report whether or not a given property holds on a neural network, generally providing a counter-example in the later case. Note, however, that soundness is not typically guaranteed with respect to floating-point arithmetic, but only with respect to computations on reals that ignore rounding errors and may thus differ from the actual computations [122, 105]. Complete methods are often also limited to certain neural network architectures and activations (e.g., neural networks with piecewise linear layers and ReLU activations). We distinguish below between methods based on *satisfiability modulo theory (SMT) solving* [126, 60, 92, 93, 86, etc.], methods based on *mixed integer linear programming (MILP)* [29, 67, 22, 58, 149, etc.], and other complete

methods based on global optimization [134] or combinations of exact and approximate analyses [163, 164, 153, 154, 142, etc.].

SMT-based Formal Methods. SMT-based formal methods reduce the safety verification problem to a constraint satisfiability problem. Specifically, they encode a given neural network and (the negation of a) desired safety property as a set of constraints. If the constraints are satisfiable, the corresponding solution represents a counterexample to the safety property. Otherwise, the constraints are unsatisfiable, no counterexample can exist and thus the safety property holds. For instance, consider a n -layer single-output feed-forward neural network with ReLU activations after each hidden layer, and a safety property specifying a bounded input domain and requiring the output of the neural network to be a positive value. The verification of the safety property can be reduced to the following SMT problem [22]:

$$\mathbf{l} \leq \mathbf{x}_0 \leq \mathbf{u} \tag{1a}$$

$$\hat{\mathbf{x}}_{i+1} = \mathbf{W}_{i+1}\mathbf{x}_i + \mathbf{b}_{i+1} \quad \forall i \in \{0, \dots, n-1\} \tag{1b}$$

$$\mathbf{x}_i = \max\{0, \hat{\mathbf{x}}_i\} \quad \forall i \in \{1, \dots, n-1\} \tag{1c}$$

$$\mathbf{x}_n \leq 0 \tag{1d}$$

where Equation (1a) and Equation (1d) respectively represent the constraints on the inputs and (the negation of those) on the output of the neural network, while Equation (1b) encodes the affine transformations performed by the layers of the network, and Equation (1c) encodes the ReLU activation functions. Note that the presence of these non-linear ReLU constraints makes the problem NP-complete [92]. A value assignment to the problem variables that satisfies all constraints represents a valid counterexample. If the problem is unsatisfiable, the safety property is verified.

The first formal verification method for neural networks was presented by **Pulina and Tacchella** [126]. They proposed an approach for checking that the output of a feed-forward fully-connected neural network with sigmoid activations always ranges within given safety bounds. The neural network is encoded as a Boolean combination of linear constraints using a Cartesian product of intervals. Specifically, activation functions are replaced by piecewise linear approximations using p intervals (where p is a parameter of the approach). The encoding of the neural network together with the constraints encoding the desired output safety property are then fed to a black-box SMT solver. When spurious counterexamples are found, the encoding is refined to use p/r intervals (where r is the refinement rate, another parameter of the approach). The approach was implemented and evaluated on a small case study using a neural network with one hidden layer containing three neurons. The authors show that a $10x$ increase in precision corresponds to $100x$ increase in the size of the encoding, thus highlighting the difficulty in scaling-up this approach.

In follow-up work [127], Pulina and Tacchella perform a comparison of different back-end SMT solvers for their approach on various slightly larger neural networks with up to 20 hidden neurons. They conclude that the YICES SMT solver [57] seems the best candidate. Nonetheless, the scalability of the approach remains an issue.

A similar approach to that of Pulina and Tacchella is presented by Scheibler et al. [137]. It is based on bounded model checking [14] and applied to the cart-pole (or inverted pendulum) system. They also encounter scalability issues and can only handle small unrolling depths and very basic safety properties.

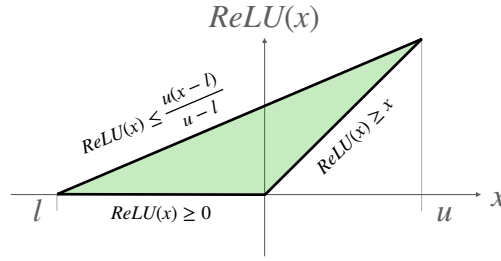


Figure 5: Convex Approximation of a ReLU Activation.

More recently, Ehlers [60] proposed an approach for proving convex input-output properties of neural networks with piecewise linear layers (i.e., fully-connected, max-pooling, and convolutional layers) and ReLU activations. The approach is implemented in a tool named **Planet** (<https://github.com/progirep/planet>). The underlying idea of the approach is to use approximations in order to reduce the search space for the SMT solver. In a first step, Planet uses interval arithmetic [82] to obtain lower and upper bound estimations for each neuron. Afterwards, Planet encodes the behavior of the neural network as a combination of linear constraints. ReLU activations are approximated using the three linear constraints shown in Figure 5, where l and u are the lower and upper bounds for a neuron x and $ReLU(x)$ is the result of the activation function. Finally, the approximation of the neural network is conjoined together with the (negation of the) desired safety property to encode the verification problem. The search for solutions is done by fixing the activation status of the ReLU activations (i.e., adding the constraint $x > 0$ to make $ReLU(x)$ always active, $ReLU(x) = x$, or adding the constraint $x \leq 0$ to make $ReLU(x)$ always inactive, $ReLU(x) = 0$) and backtracking when needed (i.e., when constraints become unsatisfiable). The approach is evaluated on a small vehicle collision avoidance use case and on a neural network with over a thousand neurons trained for digit recognition on the MNIST dataset [101]. The scalability considerably improves compared to previous works but the approach still timeouts (after four hours) for difficult verification properties (e.g., determining how much noise can be added to images to make the neural network misclassify them).

Katz et al. [92] proposed a custom SMT solver named **Reluplex** for verifying safety properties of feed-forward fully-connected neural networks with ReLU activations. The underlying approach is based on the simplex algorithm [47], extended to support ReLU constraints. Given an SMT encoding of the verification problem (cf. Equations (1a)–(1d)), Reluplex always maintains a value assignment for all variables, even if some constraints of the encoding are violated. At each step, the assignment is modified to fix some violated constraints. To ensure convergence, ReLU constraints that get fixed too often are split into two cases, each corresponding to one activation status of the ReLU. In the worst case, the problem will be split over all possible combinations of activation patterns into simple linear problems. If no valid assignment that satisfies all constraints can be found, the safety property is satisfied. The approach is applied to the verification of the ACAS Xu neural networks [90], developed as early prototype for the next-generation airborne collision avoidance system for unmanned aircraft. The neural networks take sensor data as input (i.e., speed and present course of the current aircraft and of any nearby intruder) and issue appropriate navigation advisories. They consist of six hidden layers with 300 neurons each. Reluplex requires several hours to perform the verification (over two days in one case).

Marabou [93] (<https://github.com/NeuralNetworkVerification/Marabou>) is

the successor of Reluplex. It supports neural networks with piecewise linear layers (i.e., fully-connected, max- and average-pooling, and convolutional layers) and piecewise linear activations. Unlike Reluplex, Marabou offers a divide-and-conquer solving mode, which iteratively splits the input space and thus naturally lends itself to parallel execution. Additionally, Marabou maintains symbolic lower and upper bounds for all neurons expressed as linear combinations of the input neurons [163]. This allows Marabou to determine tighter bounds and further pruning of the input space. Finally, Marabou includes several implementation improvements over Reluplex. For instance, it integrates a custom simplex solver instead of relying on an external solver. The experimental evaluation shows that Marabou (in divide-and-conquer mode running on four cores) generally outperforms both Planet [60] and Reluplex and is able to verify all ACAS Xu benchmarks within a one hour timeout per benchmark.

Bastani et al. [8] presented an approach for finding the nearest (according to the Chebyshev or L_∞ distance) adversarial example [148], i.e., the closest input that causes the neural network to produce a wrong output. They support neural networks with piecewise linear layers (i.e., fully-connected, max-pooling, and convolutional layers) and ReLU activations. For scalability, they restrict the search to a convex region around the given input in which the neural network is a linear function by fixing the activation status of the ReLU activations according to the activation status determined by the given input [116]. The problem is then encoded as a linear program and fed to a black-box linear programming solver. The approach is demonstrated on the LeNet neural network [100] (modified to use ReLU activations instead of sigmoid activations) trained on the MNIST dataset [101], and on the larger Network-in-Network neural network [106] trained on the CIFAR-10 dataset [96].

Huang et al. [86] proposed a complementary approach for proving local robustness to adversarial perturbations, i.e., proving that no adversarial example exists in a neighborhood of a given input. Their approach applies to feed-forward and convolutional neural networks and is not tailored to specific activation functions. It reduces the (infinite) neighborhood of a given input to a finite set of points and checks that all these points lead to the same neural network output. Specifically, the approach proceeds layer by layer through the neural network, propagating constraints that relate representative points between neural network layers. The approach is implemented in an open-source tool named **DLV** (<https://github.com/verideep/dlv>), which builds on the SMT solver z3 [49]. The experimental evaluation on state-of-the-art neural networks trained on the MNIST [101], CIFAR-10 [96], GTSRB [147], and ImageNet [135] datasets shows that adversarial examples can be sometimes found in seconds but the verification has prohibitive complexity for large images.

Finally, a number of approaches focus on binarized neural networks [87], which have been proposed as a memory efficient alternative to traditional feed-forward neural networks. **Narodytska et al.** [120] focus on proving local robustness to adversarial perturbations and equivalence between neural network models. Their approach reduces verification to SAT solving, starting with a simple MILP encoding which is first refined into an integer linear program and then further refined into the final SAT encoding. A counterexample-guided search procedure is then used to find property violations, or otherwise conclude that the desired safety property is satisfied. The experimental evaluation on neural networks trained on the MNIST dataset [101] shows that the approach is able to scale to neural networks with hundreds of neurons.

Another SAT-based approach for safety verification of binarized neural networks

was concurrently proposed by **Cheng et al.** [30]. Their approach first encodes the verification problem by means of a combinational miter [19], which is a hardware circuit with only one Boolean output that should always be zero. The combinational miter is then transformed into a SAT problem using standard transformation techniques. A number of optimizations are additionally proposed to speed up the SAT-solving time. The optimizations allow the approach to scale to larger binarized neural networks with thousands of neurons trained on the MNIST [101] and GTSRB [147] datasets.

MILP-based Formal Methods. MILP-based formal methods transform the safety verification problem into a mixed integer linear program. Multiple different encodings have been proposed in the literature. For instance, consider again a n -layer single-output feed-forward neural network with ReLU activations after each hidden layer, and a safety property specifying a bounded input domain and requiring the output of the neural network to be a positive value. A possible MILP encoding is [149]:

$$\mathbf{l} \leq \mathbf{x}_0 \leq \mathbf{u} \quad (2a)$$

$$\hat{\mathbf{x}}_{i+1} = \mathbf{W}_{i+1}\mathbf{x}_i + \mathbf{b}_{i+1} \quad \forall i \in \{0, \dots, n-1\} \quad (2b)$$

$$\delta_i \in \{0, 1\}^{|\mathbf{x}_i|}, \quad 0 \leq \mathbf{x}_i \leq \mathbf{u}_i \cdot \delta_i, \quad \hat{\mathbf{x}}_i \leq \mathbf{x}_i \leq \hat{\mathbf{x}}_i - \mathbf{l}_i \cdot (1 - \delta_i) \quad \forall i \in \{1, \dots, n-1\} \quad (2c)$$

$$\min \mathbf{x}_n \quad (2d)$$

where Equation (2a) represents the constraints on the inputs of the neural network, Equation (2b) encodes the affine transformations performed by the neural network layers, and Equation (2c) encodes the ReLU activation functions using binary variables to represent their activation status. Equation (2d) is the objective function, which in this case is to minimize the output of the neural network. A solution of this MILP problem with a negative neural network output \mathbf{x}_n represents a valid counterexample. Otherwise, the safety property is verified. The lower and upper bound estimations \mathbf{l}_i and \mathbf{u}_i for \mathbf{x}_i can be obtained using interval arithmetic [82] or more precise symbolic propagation methods [163, 105, 141, 164].

Cheng et al. [29] proposed an alternative MILP formulation which uses a variant of the Big M [77] encoding method for the ReLU activations:

$$\hat{\mathbf{x}}_{i+1} = \mathbf{W}_{i+1}\mathbf{x}_i + \mathbf{b}_{i+1} \quad \forall i \in \{0, \dots, n-1\} \quad (3b)$$

$$\delta_i \in \{0, 1\}^{|\mathbf{x}_i|}, \quad 0 \leq \mathbf{x}_i \leq \mathbf{M}_i \cdot \delta_i, \quad \hat{\mathbf{x}}_i \leq \mathbf{x}_i \leq \hat{\mathbf{x}}_i - \mathbf{M}_i \cdot (1 - \delta_i) \quad \forall i \in \{1, \dots, n-1\} \quad (3c)$$

where $\mathbf{M}_i = \max\{-\mathbf{l}_i, \mathbf{u}_i\}$. This encoding is fundamentally the same as the one of Equations (2b)–(2c), except that Equation (3c) uses symmetric bounds which are slightly worse than the asymmetric bounds used in Equation (2c). They address the problem of finding a lower bound on global robustness to adversarial perturbations [148] with respect to the Manhattan or L_1 distance, i.e., determining the largest neighborhood in which no adversarial example exists for any possible input of a given neural network classifier. Specifically, they reduce the problem to finding the smallest perturbation such that there exists an input classified as c and the computed probability α for c may not be among the k highest after a larger perturbation. The robustness lower bound for the neural network is the smallest among the lower bounds found for each class. They support neural networks with piecewise linear layers (i.e., fully-connected, max- and average-pooling, and convolutional layers) and ReLU and \tan^{-1} activations. The \tan^{-1} activations are approximated piecewise using results from the digital signal processing literature [130, 159]. A number of heuristics are proposed to solve the resulting MILP problem efficiently. The approach is demonstrated on neural networks

with at most 60 inputs and 70 hidden neurons. The experimental evaluation shows that the scalability of the approach relies on sometimes setting a high value for α .

Fischetti and Jo [67] focus on finding neural network inputs that maximize the activation of some hidden neurons [63] and building adversarial examples. Their approach supports neural networks with piecewise linear layers (i.e., fully-connected, max- and average-pooling, and convolutional layers) and ReLU activations. They use the MILP encoding with asymmetric bounds of Equations (2b)–(2c). In order to obtain tight lower and upper bounds l_i and u_i , they proceed layer by layer and use the MILP solver to minimize and maximize the value of each neuron in the neural network. The approach is demonstrated on neural networks with up to 70 hidden neurons trained on the MNIST dataset [101], for which adversarial examples can be found in a few minutes. For larger neural networks, the computation time becomes too large (e.g., one hour or more for neural networks with hundreds of neurons).

Bunel et al. [22] presented a unifying safety verification framework named **BaB** (Branch-and-Bound) for neural networks with piecewise-linear layers and ReLU activations. They show that their framework encompasses previous approaches such as Planet [60] and Reluplex [92]. They propose three variants of the framework: (1) BaB-relusplit, which branches over the activation status of the ReLU activations; (2) BaB-input, which branches over the inputs of the neural network, splitting in half along the largest dimension; and (3) BaBSB, which performs a smarter branching by splitting the input domain along the dimension improving the objective function the most. The experimental evaluation shows no particular difference between the BaB-relusplit and BaB-input variants, while BaBSB outperforms the other variants. Compared to Planet and Reluplex, they perform better on shallow neural networks, while on deeper neural networks such as the ACAS Xu networks [90] BaBSB reaches the same success rate as Reluplex but its runtime is two orders of magnitude smaller.

Dutta et al. [58] proposed an approach to establish ranges for the outputs of feed-forward fully-connected neural networks with ReLU activations. They discuss how to extend their approach to other activation functions by means of piecewise linear approximations. The approach reduces the problem to a MILP problem, using an encoding similar to Equations (3b)–(3c), and uses local search to speed up the MILP solver. Specifically, the approach iterates between relatively expensive MILP solver calls and inexpensive local search iterations. The MILP solver is used to find a solution that is better than the current target lower and upper bounds on the output. Local search uses gradient descent (resp. ascent) over the neural network to find another input with a lower (resp. higher) lower bound (resp. upper bound) in the input space that activates the same ReLU activations. If such an input is found, the MILP solver is invoked again with updated target lower and upper bounds, and so on until the MILP solver concludes that no better solution exists. The approach is implemented in a tool named **Sherlock** (<https://github.com/souradeep-111/sherlock>), which builds on the commercial MILP solver GUROBI [78]. The experimental evaluation on neural networks with thousands of neurons shows that Sherlock outperforms a monolithic MILP approach (but requires over three days of running time in one case). On smaller instances the monolithic approach is faster but the running time remains small (in the order of seconds) for both approaches. Moreover, both the monolithic approach and Sherlock are shown to outperform Reluplex [92].

Finally, Tjeng et al. [149] focus on finding the nearest adversarial example with

respect to a given distance metric, such as the L_1 , L_2 , or L_∞ distances. They support neural networks with piecewise linear layers and ReLU activations, encoded using the MILP formulation of Equations (2b)–(2c). They use a progressive bound tightening procedure to determine lower and upper bounds l_i and u_i for each x_i : they obtain initial coarse bounds quickly using interval arithmetic [82] and, only if these bounds are not sufficient to determine the activation status of the current ReLU activation, they resort to a more expensive procedure which uses a linear programming solver to find tighter lower and upper bounds (by minimizing and maximizing the value of the current neuron, as done by Fischetti and Jo [67]). The approach is implemented in a tool named **MIPVerify** (<https://github.com/vtjeng/MIPVerify.jl>) and is demonstrated on neural networks with thousands of neurons trained on the MNIST [101] and CIFAR-10 [96] datasets. MIPVerify is two to three orders of magnitude faster than Reluplex [92] in finding the nearest adversarial example with respect to the L_∞ distance. The experimental evaluation additionally shows that the computation time strongly correlates with the number of ReLU activations that cannot be proven to have a fixed activation status, rather than with the total number of ReLUs of a neural network.

Other Complete Formal Methods. Ruan et al. [134] presented an approach based on global optimization for verifying Lipschitz continuous neural networks [148], such as neural network with piecewise linear layers (i.e., fully-connected, max- and average-pooling, and convolutional layers) and ReLU as well as sigmoid and tanh activations. Specifically, given inputs to the neural networks and a Lipschitz continuous functions over its outputs (e.g., a function determining the confidence of the neural network in classifying an input), their approach computes lower and upper bounds on the function values. The approach is implemented in a tool named **DeepGO** (<https://github.com/trustAI/DeepGO>). Compared to Reluplex [92] and Sherlock [58], DeepGO on average is 36 times faster than Sherlock and almost 100 times faster than Reluplex. Moreover, DeepGO is shown to be able to scale to state-of-the-art neural networks with millions of neurons trained on the MNIST dataset [101].

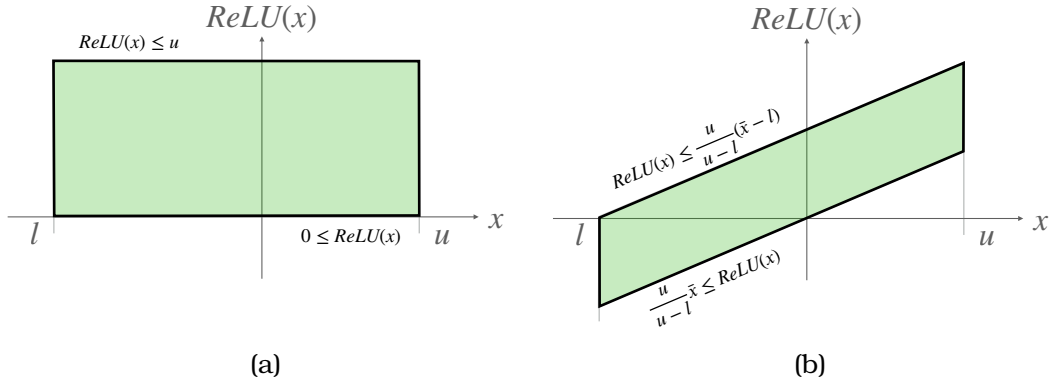


Figure 6: Naive and Symbolic Convex Approximations of a ReLU Activation.

Other complete verification methods are obtained by making incomplete methods asymptotically complete. For instance, the approach proposed by Wang et al. [163] iteratively refines the analyzed input space of a neural network when the underlying over-approximating analysis is inconclusive. They support feed-forward fully-connected neural networks with ReLU activations. More precisely, the over-approximating analysis uses symbolic intervals to track lower and upper bounds for each neuron expressed whenever possible as linear combinations of the input neurons.

When the activation status of a ReLU activation is undetermined, its range is over-approximated using the naive convex approximation shown in Figure 6a. When the estimated output range of the analyzed neural network is too large to be conclusive, the input space is split and the analysis is repeated on the resulting smaller input spaces. In particular, the input space is split in half along the dimension that influences the most the output of the neural network (i.e., the dimension with the largest output gradient). Such refinement process converges in finite steps as the Lipschitz continuity of the neural networks [148] ensures that the overestimation error of the analysis decreases as the width of the input space becomes smaller. Convergence of the approach is faster for lower values of Lipschitz constant. The approach is available and implemented in a tool named **ReluVal** (<https://github.com/tcwangshiqi-columbia/ReluVal>). The experimental evaluation shows that ReluVal is on average 200 times faster than Reluplex [92] at verifying the ACAS Xu neural networks [90]. According to the evaluation of Katz et al. [93], ReluVal also outperforms Marabou (in divide-and-conquer mode) when running on four cores, while Marabou (again in divide-and-conquer mode) on average outperforms ReluVal when running on 64 cores.

In follow-up work, Wang et al. [164] presented an improved verification tool named **Neurify** (<https://github.com/tcwangshiqi-columbia/Neurify>), which supports feed-forward and convolutional neural networks with ReLU activations. Specifically, they improve the underlying over-approximating analysis by partially retaining dependencies with the input neurons even when the activation status of a ReLU activation is undetermined. Instead of using the naive convex approximation of Figure 6a, they use the symbolic approximation shown in Figure 6b, where \bar{x} is the symbolic lower and upper bound representation of x . Additionally, Neurify iteratively minimizes the errors introduced by the approximations by splitting on the over-approximated ReLU activations with the larger output gradient. On the ACAS Xu neural networks, Neurify is on average 20 times faster than ReluVal and 5000 times faster than Reluplex. The experimental evaluation also shows that Neurify is able to verify safety properties of neural networks with over ten thousands hidden neurons such as the self-driving car convolutional neural network Dave [15].

Finally, other approaches offer combinations of exact and approximate analysis. **Tran et al.** [153] used unions of bounded convex polyhedra to compute the reachable outputs of a feed-forward fully-connected neural network with ReLU activations. The approach proceeds layer by layer, splitting polyhedra into two when ReLU activations have an undetermined activation status. Once the number of polyhedra exceeds a user-defined upper bound, the polyhedra are clustered (using k-means clustering [17] based on whether they overlap) and each cluster is then over-approximated by a hyper-rectangle. The analysis then continues by over-approximating (again with a hyper-rectangle) the output range of ReLU activations with an undetermined activation status. The precision of the approach can be improved by first partitioning the input space and then proceeding with the analysis on each partition independently. The approach is demonstrated on a few easy ACAS Xu benchmarks [90] (for which the analysis requires between four minutes and over an hour), and neural networks trained on the MNIST dataset [101] (for which local robustness can be proven in under 10 minutes for networks with hundreds of neurons).

In follow-up work, instead of polyhedra, Tran et al. [154] used **star sets** [10], which are an equivalent representation offering fast affine mapping operations and inexpensive intersections with half-spaces and emptiness checking. Their exact approach maintains a union of star sets, while their approximate analysis computes a single star set over-approximating the reachable outputs of a given neural network.

In the latter case, ReLU activations with an undetermined activation status are over-approximated as shown in Figure 5. The experimental evaluation on the ACAS Xu neural networks shows that their exact analysis is on average almost 19 times faster than Reluplex [92] and over 70 times faster than their polyhedra-based approach, while their approximate analysis is on average about 118 times faster than Reluplex.

More recently, Tran et al. [156] have proposed an extension of star sets called **image stars** to represent infinite families of images. They use image stars to prove local robustness to pixel brightening perturbations [72] of neural networks with piecewise linear layers (i.e., fully-connected, max- and average-pooling, and convolutional layers) and ReLU activations. The scalability of the approach is evaluated on state-of-the-art image classifiers such as the VGG16 and VGG19 neural networks [138]. The evaluation shows that the size of the analyzed input space, rather than the size of the neural network, is the factor that mostly affects the performance of the approach.

The polyhedra-based approach as well as the star sets-based and image star-based approaches are all implemented in an open-source tool named **NNV** [155] (<https://github.com/verivital/nnv/>) written in MATLAB. Several practical software engineering improvements have been proposed for the exact star sets-based approach by Bak et al. [11] and implemented in a tool named **NNENUM** [11] (<https://github.com/stanleybak/nenum>) written instead in PYTHON. NNENUM is able to verify all ACAS Xu benchmarks in under 10 minutes on a standard laptop.

In currently unpublished work, **Yang et al.** [172] proposed another alternative approach to the polyhedra-based approach of Tran et al. [153]. Specifically, they represent a polyhedra using its face lattice, which is a data structure containing all the faces of a polytope (i.e., its intersections with supporting hyperplanes, that is, its vertices, edges, ridges, and facets) ordered by containment. This allows performing affine transformations, intersections with hyperplanes, and projections on hyperplanes more efficiently than with polyhedra. The experimental evaluation on the ACAS Xu benchmarks shows that the face lattice-based approach outperforms Reluplex [92], Marabou [93], and the star sets-based exact approach. ReluVal [163] instead is slightly faster overall, requiring a little over 8 hours to complete all benchmarks instead of almost 9 hours needed by the face lattice-based approach.

Singh et al. [142] proposed **RefineZono**, a combination of abstract interpretation and (mixed integer) linear programming for proving local robustness to adversarial perturbations [148] of neural networks with piecewise-linear layers (i.e., fully-connected, max-pooling, and convolutional layers) and ReLU activations. Their approach uses the abstract domain of zonotopes [73] equipped with specialized transformers to over-approximate the neural network activations [140]. Specifically, each neuron of a neural network is associated with a zonotope and concrete lower and upper bounds over-approximating its possible values. In order to determine lower and upper bounds, for scalability, they use faster but less precise methods as the analysis proceeds to deeper layers of the neural networks: for the first user-defined number of layers, they rely on mixed integer linear programming as done by Fischetti and Jo [67]; for the next user-defined number of layers, they approximate ReLU activations as in Figure 5 and use a linear programming solver to find possibly coarser bounds; for the remaining layers, they simply continue the analysis with the abstract domain without additional bound tightening. When the analysis is inconclusive (i.e., the over-approximation of the neural network outputs is too large), the collected lower and upper bounds can be used to encode the robustness verification as a MILP problem (thus making the approach complete). The experimental evaluation on a neural network with 150 neurons trained on the MNIST dataset [101] shows that Refine-

Zono is faster than MIPVerify [149] for complete verification of local robustness to perturbations with respect to the L_∞ distance (up to $\epsilon = 0.03$). The approach is also demonstrated on one of the ACAS Xu benchmarks [90] known to be hard: by first uniformly splitting the input space into 6300 regions, RefineZono is able to verify the benchmark over four times faster than Neurify [164].

3.1.1.2 Incomplete Formal Methods

Incomplete formal verification methods are generally *able to scale* to large neural network architectures (they generally require at most a few minutes for neural networks with thousands of neurons) and are *sound* (often also with respect to floating-point arithmetic [140, 141, 105]) but suffer from *false positives*. Incomplete methods are also generally less limited to certain neural network architectures and activations (e.g., some also apply to recurrent neural networks [95, 175]). We distinguish below between methods based on *abstract interpretation* [72, 140, 141, 105, 161, etc.], and other incomplete methods based on simulation [169], duality [167, 59], semidefinite programming [129], or linear approximations [166].

Abstract Interpretation-based Methods. The first use of abstract interpretation for verifying neural networks was the **AI²** framework proposed by Gehr et al. [72]. They address the problem of proving local robustness to adversarial perturbations [148] for neural networks with piecewise linear layers (i.e., fully-connected, max-pooling, and convolutional layers) and ReLU activations. Their approach over-approximates the computations performed by a neural network by interpreting them in a chosen abstract domain. Thus, starting from an abstraction of the inputs of the neural network, it propagates the abstraction forward through the network layers taking affine transformations and activation functions into account, until it reaches the output layer where the abstraction represents an over-approximation of the neural network outputs. Their framework supports the abstract domains of intervals [36], zonotopes [73], and polyhedra [38], as well as their bounded powersets. In the experimental evaluation they considered pixel brightening perturbations (up to $\delta = 0.085$) against image classifiers (with up to 53000 neurons [99]) trained on the MNIST [101] and CIFAR-10 [96] datasets. The results show that the domain of zonotopes offers a good trade-off between precision and scalability of the analysis. It takes on average less than 10 seconds to verify local robustness for feed-forward neural networks with up to 18000 hidden neurons trained on MNIST. On the largest convolutional neural networks trained on CIFAR-10 however the difference in precision with respect to the less expressive domain of intervals is less significant.

In a follow-up work, Singh et al. [140] presented a custom zonotope abstract domain named **DeepZ** equipped with specially designed abstract transformers for ReLU as well as sigmoid and tanh activations. The transformers are made sound with respect to floating-point arithmetic using the methodology proposed by Miné [113]. In the experimental evaluation they consider perturbations with respect to the L_∞ distance (up to $\epsilon = 0.3$) against image classifiers (with up to 88500 hidden neurons) again trained on MNIST and CIFAR-10. The results show that DeepZ is significantly more precise and faster than AI². Moreover, DeepZ is able to verify local robustness properties of the largest convolutional neural network within a few minutes.

Another abstract domain proposed by Singh et al. [141] is the **DeepPoly** domain. DeepPoly associates to each neuron of a neural network concrete lower and upper bounds as well as symbolic bounds expressed as linear combinations of the neurons in the preceding layer of the network. It is additionally equipped with abstract trans-

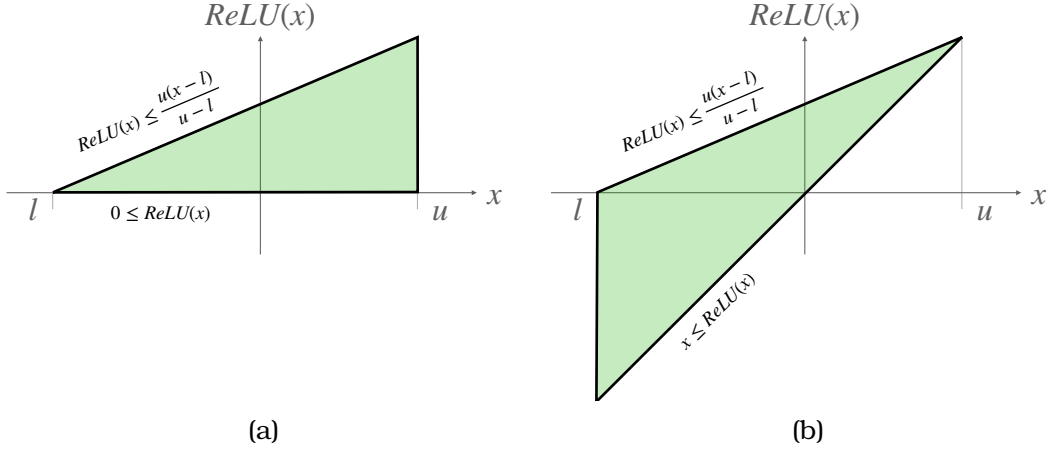


Figure 7: Alternative Convex Approximations of a ReLU Activation.

formers specifically designed for ReLU, sigmoid, and tanh activations. In particular, the ReLU abstract transformer first computes concrete lower and upper bounds l and u for a given neuron x by back-substitution of its symbolic bounds up to the input layer. Then, it chooses the tighter approximation for $ReLU(x)$ between those in Figure 7, i.e., the approximation in Figure 7a when $u \leq -l$, and that in Figure 7b otherwise. The transformers are again made sound with respect to floating-point arithmetic using the methodology proposed by Miné [113]. In the experimental evaluation they consider image classifiers (with up to 88500 hidden neurons) trained on MNIST and CIFAR-10, and perturbations with respect to the L_∞ distance (up to $\epsilon = 0.3$) as well as rotations (between -45° and 65°). The results show that DeepPoly is generally even faster and often strictly more precise than DeepZ.

Singh et al. [143] later presented the **k-ReLU** framework to jointly approximate k ReLU activations in order to produce a more precise over-approximation of a neural network layer. They instantiate the framework with the DeepPoly domain resulting in a new abstract domain called kPoly. The experimental evaluation considers perturbations with respect to the L_∞ distance (up to $\epsilon = 0.3$) against image classifiers (with up to 107496 neurons) trained on MNIST and CIFAR-10. The results show that kPoly is more precise than DeepPoly as well as RefineZono [142]. kPoly is also faster than RefineZono and has an average runtime of less than 8 minutes.

DeepZ, DeepPoly, RefineZono, and kPoly are all implemented in a tool named **ERAN** (<https://github.com/eth-sri/eran>), which builds on the ELINA abstract domain library [139] and the commercial MILP solver GUROBI [78].

In currently unpublished work, **Müller et al.** [118] have presented algorithms for running DeepPoly efficiently on a GPU. The experimental evaluation shows that this makes the analysis up to 170 times faster than DeepPoly and able to scale to neural networks with up to 967000 neurons trained on the CIFAR-10 dataset.

Li et al. [105] proposed a symbolic propagation technique to improve the precision of abstract interpretation-based verification methods for neural networks with piecewise-linear layers (i.e., fully-connected, max-pooling, and convolutional layers) and ReLU activations. Specifically, the value of each neuron in the neural network is represented symbolically as a linear combination of the input neurons and the values of the ReLU activations in previous layers. In particular, ReLU activations with an undetermined activation status are represented by fresh symbolic variables. Their approach generalizes the symbolic propagation technique used in ReluVal [163] to any abstract domain. In the experimental evaluation, they combine their symbolic

propagation technique with the abstract domains of intervals [36] and zonotopes [73], and focus on verifying local robustness to perturbations with respect to the L_∞ distance (up to $\epsilon = 0.6$) against image classifiers (with up to 89572 neurons) trained on the MNIST [101] and CIFAR-10 [96] datasets. The results show that their symbolic propagation technique significantly improves precision with a modest running time increase (it is less than two times slower in most cases and often faster).

More recently, Urban et al. [161] presented an approach for verifying fairness of feed-forward neural networks with ReLU activations used for classification of tabular data. The fairness notion that they consider is a form of global robustness, which requires that the output classification of a neural network is not affected by the values of the neural network inputs that are determined to be sensitive to bias by the user [71]. The approach combines a forward analysis with an inexpensive abstract domain (e.g., the domain of intervals [36] possibly combined with the symbolic propagation technique proposed by Li et al. [105], or the DeepPoly domain [141]) to group together the partitions of the neural network input space that share the same ReLU activation pattern, and a more expensive backward analysis with the domain of polyhedra [38], to determine the partitions that are subject to bias. The approach is implemented in an open-source tool named **Libra** (<https://github.com/caterinaurban/Libra>) and evaluated on neural networks with up to over a thousand neurons trained on the Adult [54], COMPAS [3], German Credit [55], and Japanese Credit [56] datasets. The results show that the performance of the approach correlates with the size of the analyzed input space rather than the size of the analyzed neural network (as also observed by Tran et al. [156]). The analysis might require a few days to complete on the full input space of a neural network with 20 hidden neurons, but only about three hours on a fraction of the input space of a neural network with 1280 hidden neurons.

Another complementary line of work focuses on abstracting a given neural network by computing a smaller network which over-approximates the outputs of the original network. **Prabhakar and Afzal** [125] propose an abstraction for feed-forward neural networks with ReLU activations. Their construction merges neurons layer-wise according to a partitioning strategy. The weights of the neural network are carefully replaced with intervals [36] to account for the merging, which ensures that the outputs of the abstraction soundly over-approximate the outputs of the original neural networks. The output range analysis on the resulting abstract neural network is reduced to solving a MILP problem, using an encoding similar to Equations (3b)–(3c) extended to deal with interval weights. The approach is demonstrated on the ACAS Xu neural networks [90], experimenting with abstractions with different numbers of abstract neurons (up to 32 abstract neurons). The results show that the abstraction considerably reduces the computation time needed for the analysis. On the other hand, the precision of the analysis is affected by the choice of the partitioning strategy used to guide the merging of neurons in the abstraction.

The construction of Prabhakar and Afzal was recently generalized by **Sotoudeh and Thakur** [145] to other (convex) abstract domains than the domain of intervals and other activations than ReLUs (e.g., Leaky ReLU [109] as well as sigmoid and tanh activations). They identify and formally justify sufficient and necessary conditions on the abstract domains and activations to guarantee soundness and, when these conditions are not satisfied, they propose workarounds to modify the original neural network into an equivalent one that satisfies the conditions.

Elboher et al. [62] recently presented instead an abstraction of feed-forward neu-

ral networks with ReLU activations based on counterexample-guided abstraction refinement (CEGAR) [34]. Their approach first transforms a neural network into an equivalent network in which each neuron belongs to one of four classes, determined by the weights of its outgoing connections (i.e., whether the weights are all negative or positive) and its effect on the neural network output (i.e., whether increasing its value increases or decreases the network output). A basic abstraction step then merges two neurons that belong to the same class, while a basic refinement step splits previously merged neurons. The choice of which neurons to merge or split is done heuristically and several possible heuristics are proposed. The experimental evaluation on 90 of the ACAS Xu benchmarks shows that Marabou [93] combined with their abstraction framework outperforms Marabou alone. Within a 20 hours timeout, it is able to verify 58 benchmarks, while Marabou alone can only verify 35 benchmarks. The abstraction-enhanced Marabou is also orders of magnitude faster than Marabou alone.

Finally, a couple of theoretical results on the abstract interpretation of neural networks can be found in the literature. **Baader et al.** [5] show that for any continuous function f there exists a feed-forward fully-connected neural network with ReLU activations whose abstract interpretation using the domains of intervals [36] from an input region B is an arbitrarily close approximation of f on B . In particular, their result reduces to the classical universal approximation theorem [104] when the input region B is a single input point. In practice this means that, for any neural network, there exists another arbitrarily close neural network that can be more easily verified. The result trivially holds for more expressive abstract domains than intervals.

In currently unpublished work, **Wang et al.** [165] generalize the result of Baader et al. beyond ReLU activations (e.g., including sigmoid and tanh activations).

Other Incomplete Formal Methods. Among other incomplete verification methods, **Xiang et al.** [169] proposed an approach that combines simulation and linear programming to over-approximate the outputs of feed-forward neural networks with monotonic activations (e.g., ReLU as well as sigmoid and tanh activations). The approach first discretizes the input space of the neural network into L_∞ balls centered around individual inputs. The ball radius is user-defined and determines the granularity of the discretization. Then, simulations are executed for each ball center to determine the corresponding neural network outputs. Finally, the approach proceeds layer by layer to measure the maximum deviation of the layer output with respect to the other points in each L_∞ ball by solving a finite set of convex optimization problems. At the output layer this yields an over-approximation of the neural network outputs. The finer the initial input space discretization (i.e., the smaller the user-defined ball radius), the tighter the resulting over-approximation. The approach is demonstrated on a small use case and the results show that it scales well with respect to the number of hidden layers of a neural network but poorly with respect to the size of its input space (i.e., the number of input dimensions).

Other incomplete methods focus on providing robustness guarantees to adversarial perturbations [148] with respect to a given distance metric, i.e., finding a non-trivial lower bound on the distance to the nearest adversarial example for any training input (or, equivalently, determining the largest neighborhood for any training input in which no adversarial example exists). The approach of **Wong and Kolter** [167] is based on duality and supports neural networks with piecewise linear layers (i.e., fully-connected, max-pooling, and convolutional layers) and ReLU activations, and perturbations with respect to any L_p distance. Specifically, similarly to Ehlers [60],

they reduce the problem to a linear program by approximating ReLU activations as in Figure 5. However, since the resulting formulation has a number of variables equal to the number of ReLUs in the neural network, they instead solve its dual formulation, for which any feasible solution gives a lower bound on the solution of the primal. The approach is demonstrated on relatively small neural networks (e.g., networks with two fully-connected and two convolutional layers trained on MNIST [101] and Fashion-MNIST [170]), and the authors highlight the difficulty of scaling-up the approach to larger neural network architectures such as ImageNet classifiers [135]. According to the evaluation of Tjeng et al. [149], the gap between the lower bound found by Wong and Kolter and the minimum adversarial perturbation found by MIPVerify is significant even for small neural networks, and increases for larger network architectures.

Concurrently to the work of Wong and Kolter, **Raghunathan et al.** [129] reduce the problem to solving a single semidefinite program for each pair of output labels of a neural network (rather than for each training input as Wong and Kolter). Their approach however only supports feed-forward fully-connected neural networks with one hidden layer, and perturbations with respect to the Chebyshev or L_∞ distance.

Dvijotham et al. [59] presented another approach based on duality for verifying safety properties of feed-forward neural networks with arbitrary activations. They formulate the verification problem as global optimization problem that seeks to find the largest violation to the desired safety property. If the largest violation is smaller than zero, the safety property is satisfied. To circumvent the need to solve a non-convex optimization, they reduce the problem to finding an upper bound to the largest violation, which they do by solving the dual of a Lagrangian relaxation [102] of the original optimization problem. Interestingly, for feed-forward neural networks with ReLU activations, this dual is the dual of the linear programming formulation of Ehlers [60] (but it is different from the dual derived by Wong and Kolter [167]). The approach is compared to that of Raghunathan et al. [129] and is shown to compute better bounds on robustness to L_∞ perturbations on neural networks trained on MNIST [101].

Other approaches for computing robustness lower bounds are the **Fast-Lin** and **Fast-Lip** algorithms proposed by Weng et al. [166] for feed-forward fully-connected neural networks with ReLU activations. The Fast-Lin algorithm is based on the direct computation of layer-wise lower and upper bounds for each neuron using symbolic linear approximations similarly to Neurify [164] (cf. Figure 6b), while the Fast-Lip algorithm is based on bounding the neural network local Lipschitz constant. The experimental evaluation (on neural networks with hundreds of neurons trained on MNIST [101]) shows that the lower bounds against L_∞ perturbations found by Fast-Lin and Fast-Lip are only two to three times larger than the minimum adversarial perturbation found using Reluplex [92], but Fast-Lin and Fast-Lip are over 10000 times faster. Fast-Lin and Fast-Lip are also shown to be able to scale to and find non-trivial robustness lower bounds for larger neural network with thousands of neurons.

In follow-up work, Zhang et al. [173] have proposed a generalization of Fast-Lin to feed-forward fully-connected neural networks with arbitrary activations (e.g., ReLU, sigmoid, tanh, and arctan activations). The approach is available and implemented in a tool named **CROWN** (<https://github.com/CROWN-Robustness/Crown>). The experimental evaluation (on neural networks with thousands of neurons trained on MNIST [101] and CIFAR-10 [96]) shows that CROWN finds lower bounds that are between 19% and 20% better than those found by Fast-Lin at the cost of a modest increase in computation time (CROWN being less than two times slower than Fast-Lin).

More recently, Boopathy et al. [16] presented a further generalization of CROWN named **CNN-Cert** (<https://github.com/AkhilanB/CNN-Cert>) to support convolutional neural networks, and Ko et al. [95] presented **POPQORN** (<https://github.com/ZhaoyangLyu/POPQORN>) which supports recurrent neural networks, including long short-term memory [84] and gated recurrent unit [32] architectures.

Another recent approach targeting recurrent neural networks was proposed by **Zhang et al.** [175]. They focus on proving safety properties of vanilla recurrent neural networks with ReLU activations trained for cognitive tasks [144]. Their approach consists in first training an equally performing but easier to verify neural network using idea from Xiao et al. [171], i.e., using regularization during training to encourage the stabilization of ReLU activations. Then, they unfold the trained network for the number of time steps on which the desired safety property is defined, and proceed layer by layer to compute the reachable outputs of the network using unions of polytopes. Specifically, they encode each polytope and input-output relation of a layer as a MILP problem and use a solver to partition the polytope into sub-polytopes that can each be linearly mapped to a convex polytope in the next layer. Since the number of polytopes increases with the number of layers, they propose two techniques to keep the representation tractable. A first option is a CEGAR-based [34] technique that joins polytopes when their number exceeds a user-controlled threshold, and backtraces to refine the abstraction when the resulting over-approximation is too large to be conclusive. In particular, they join polytopes that originate from the same polytope in the previous neural network layer. Another option is to attempt to find an inductive invariant, that is, a polytope such that its image through a neural network layer is contained in the polytope. This requires a fixpoint iteration with some form of widening (i.e., iteration acceleration) to ensure termination. The approach is demonstrated on the verification of a number of properties of a single use case. Their invariant generation technique overall appears to be the most precise albeit not the fastest one.

Finally, **Gopinath et al.** [76] presented an approach for inferring safety properties of feed-forward neural networks with ReLU activations. Specifically, they infer properties that correspond to activation patterns of the network ReLU activations. Input properties are convex predicates on the network input space that imply the desired output behavior, and correspond to activation patterns that constrain the activation status of some ReLUs in the neural network. Layer properties instead correspond to activation patterns that only constrain the activation status of ReLUs at some hidden layer. They thus express unions of convex regions in the input space that imply the desired output behavior. To infer input properties, they start from an input that satisfies the given postcondition and iteratively relax the corresponding activation pattern in order to constrain the activation status of the least number of ReLUs but still satisfy the given postcondition. Instead, to directly learn layer properties, they train a decision tree on input-output pairs and their corresponding activation pattern. The approach is demonstrated on one of the ACAS Xu neural networks [90] and two neural networks (with hundreds of neurons) trained on the MNIST dataset [101].

3.1.2 Formal Methods for Other Machine Learning Models

We discuss below formal verification methods for other machine learning models than neural networks. We distinguish between methods for *support vector machines* (Section 3.1.2.1) and methods for *decision tree ensembles* (Section 3.1.2.2).

3.1.2.1 Formal Methods for Support Vector Machines

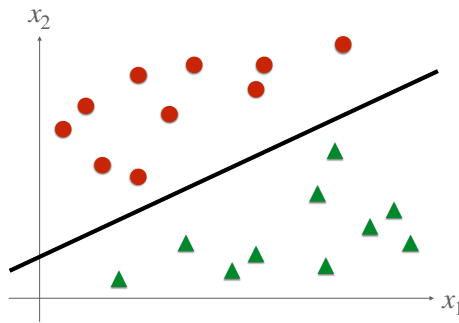


Figure 8: Linear Kernel Support Vector Machine.

Support vector machines [44] partition their input space in regions using *hyperplanes* that separate the training inputs according to their labels. They hyperplanes are chosen (i.e., learned during training) to maximize their distance (called *margin*) to their closest training inputs (called *support vectors*). Figure 8 shows a very simple support vector machine in a two-dimensional input space. When the training inputs are not linearly separable in the input space, the input space is implicitly projected, using so-called *kernel functions*, into a much higher-dimensional space in which the training inputs become linearly separable. This allows a support vector machine to also learn non-linear decision boundaries.

To the best of our knowledge, the only verification method for support vector machines was proposed by Ranzato and Zanella [131]. They focus on proving local robustness to adversarial perturbations of support vector machines based on the most commonly used kernel functions (i.e., linear, polynomial, and radial basis function kernels [44]). Their approach is based on abstract interpretation and uses the abstract domain of intervals [36] combined with reduced affine forms [112], which is a restriction of the domain of zonotopes [73] to affine forms of a given length (i.e., the dimension of the input space of the analyzed support vector machine). In particular, reduced affine forms capture dependencies between input dimensions. The approach is implemented and available in an open-source tool named **SAVer** (<https://github.com/abstract-machine-learning/saver>).

3.1.2.2 Formal Methods for Decision Tree Ensembles

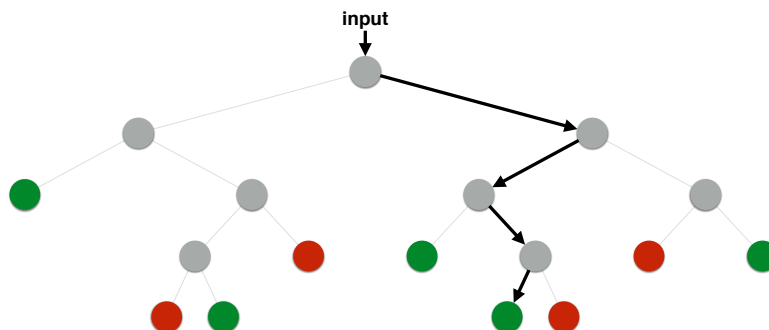


Figure 9: Decision Tree for Binary Classification.

Decision trees [20] are used for both classification and regression tasks. The leaves of *classification trees* are labeled with a class (or a probability distribution over the

classes skewed towards a particular class), while the leaves of *regression trees* can take continuous values (typically real numbers). The internal nodes of a decision tree recursively partition the input space. Each node is labeled with a Boolean split criterion over the input dimensions that decides whether to branch to the left or right subtree. Most often, decision trees employ univariate splits over a single input dimension with respect to some value. Thus, the prediction for a given input is determined starting at the root of the decision tree and recursively branching to the appropriate subtree according to the encountered split criteria, until ultimately a leaf node is reached that decides the prediction (cf. Figure 9).

Decision tree ensembles are sets of decision trees which together contribute to formulate a unique classification or regression output. One of the most used decision tree ensembles are *random forests* [21], where each tree of the ensemble is trained independently from the other trees on some random subset of the input dimensions. The final output is typically obtained through a voting mechanism (e.g., majority voting). Another popular decision tree ensemble are *gradient boosted decision trees* [69], where the ensemble is built incrementally by training each new tree on the basis of the input data samples that are misclassified by the previous trees.

Among the earliest verification methods for decision tree ensembles **Kantchelian et al.** [91] proposed an approach for finding the nearest adversarial example with respect to the L_0 , L_1 , L_2 , and L_∞ distances. They focus on sum-ensembles of regression trees with univariate split predicates (i.e., the prediction of the ensemble is the sum of all individual tree predictions) used for binary classification (i.e., by thresholding of the prediction of the ensemble). They reduce the problem to solving a MILP problem. The MILP encoding is linear in the size of the tree ensemble but the solving time can be prohibitive for ensembles that consist of a high number of trees or with a large number of input dimensions. The approach is demonstrated on decision tree ensembles trained on the MNIST dataset [101].

More recently, **Chen et al.** [28] presented a linear time algorithm for finding the nearest adversarial for a decision tree. They support decision trees with univariate split predicates and box-shaped perturbations around a given input. In particular, they focus on perturbations with respect to the L_∞ distance. Their approach consists in performing a depth-first traversal of the decision tree to compute a box for each of its leaves such that all inputs in a box fall into the corresponding leaf. Then, the minimal adversarial example corresponds to the minimal perturbation required to change a given input to be into a different box (and thus fall into a different leaf). For decision tree ensembles, they cast the problem into a max-clique searching problem in K -partite graphs, where K is the number of trees in the ensemble. In the case of large decision tree ensembles (i.e., with thousands of trees), they propose an algorithm that supports any-time termination and provides a lower bound on local robustness. The experimental evaluation compares the latter approach to that of Kantchelian et al. [91] and shows that it gives tight lower bounds with a speed-up of over 3000 times in one case (i.e., an ensemble with 300 trees trained on the HIGGS dataset [31]).

Sato et al. [136] proposed an SMT-based approach for safety verification of random forests and gradient boosted decision trees. Specifically, their approach focuses on finding inputs that lead to a violation of a given output property. They reduce the verification to solving an SMT encoding of the problem. They additionally propose a technique for generalizing a single input counterexample to a range of inputs violating the output property. The approach is demonstrated on the verification of three prop-

erties of an ensemble with 100 trees with maximum depth 3. Further experiments on scalability show a strong correlation between the size of the ensemble and the verification time. In particular, the verification time increases by 10 to 100 times when the depth of the trees is increased by one. Overall, the approach is practical for ensembles with less than 200 trees with maximum depth less than 5.

Another SMT-based approach was previously presented by **Einziger et al.** [61] for verifying local robustness to adversarial perturbations of gradient boosted decision trees used for classification. Their approach focuses on perturbations with respect to the L_∞ distance. They encode the problem as an SMT instance and rely on an off-the-shelf SMT solver for the verification. In order to speed-up the verification they propose two optimizations, i.e., pruning constraints encoding decision tree paths that are too distant from the given input, and checking local robustness with respect to each output class in parallel. The approach is implemented in a tool named VeriGB, built on top of the SMT solver Z3 [49]. The experimental evaluation on ensembles trained on the MNIST dataset [101] shows the scalability limitations of the approach (which often requires over 10 minutes for the verification of ensembles with 100 trees with depth up to 10). Interestingly, the evaluation also shows that ensembles with similar accuracy but lower tree depth tend to be more robust. Indeed, it has been observed that trees with high depth suffer more from over-fitting [79].

Other approaches for proving local robustness to adversarial perturbations are (more or less explicitly) based on abstract interpretation. Törnblom and Nadjm-Tehrani proposed an abstraction-refinement approach for random forests [150] and gradient boosted decision trees [151, 152] with univariate split predicates. The approach iteratively partitions the neighborhood of perturbations around a given input into hyper-rectangles until the analysis becomes conclusive (i.e., it is able to prove local robustness or it has found a real counterexample). It is implemented in an open-source tool named **VoTE** (<https://github.com/john-tornblom/VoTE>).

A more general framework that supports arbitrary abstract domains was presented by Ranzato and Zanella [132]. They instantiate the framework with the domain of intervals [36] and show that the approach is sound and complete for decision tree ensembles with univariate split predicates. The approach is available and implemented in an open-source tool named **Silva** (<https://github.com/abstract-machine-learning/silva>). The experimental evaluation on ensembles (with up to 150 trees with depth 10) trained on the MNIST dataset [101] shows that Silva is generally faster than VoTE [150, 151, 152] and able to scale to larger models.

Finally, very recently, **Calzavara et al.** [25] have proposed an approach that supports perturbations modeled as arbitrary imperative programs (as opposed to distance-based perturbations). Their approach consists in first performing a straight-forward conversion of a decision tree and an input perturbation into a loop-free imperative program, and then analyzing the resulting program using abstract interpretation (e.g., with the domain of polyhedra [38]). The approach generalizes to decision tree ensembles, but it is not complete (unlike VoTE [150, 151, 152] and Silva [132]).

3.2 Formal Methods for Earlier Pipeline Phases

We conclude the overview of the state of the art by discussing formal methods that apply to earlier phases in the machine learning pipeline (cf. Figure 3). We distinguish

between methods that apply to the *model training* phase (Section 3.2.1) and methods that apply to the *data preparation* phase (Section 3.2.2).

3.2.1 Formal Methods for Model Training

Formal methods for model training proposed so far in the literature have a rather narrow application scope, focusing on *robust training* to obtain machine learning models that are more robust against adversarial input perturbations. The problem of adversarial perturbations has been initially addressed in the context of spam email detection [46, 108]. For neural networks, the problem was brought up by the seminal work of Szegedy et al. [148]. Robust training aims at minimizing the worst-case loss for each given input, that is, the maximum loss (i.e., model error) over all possible perturbations of a given training input. However, since calculating the exact worst-case loss can be computationally costly in practice, robust training approaches typically minimize an estimate of the worst-case loss.

Adversarial training approaches minimize a lower bound on the worst-case loss. Specifically, they rely on fast ways to generate adversarial inputs under a considered threat model [74, 70, 85, etc.] and use them to augment the training data [74, 85, 97, etc.]. Instances of this method are typically empirically shown to be successful against known adversaries. A notable result for neural networks is the work of Madry et al. [110] against the strong adversarial attack of Carlini and Wagner [26]. Other approaches include, for instance, the work of Kantchelian et al. [91], Calzavara et al. [24], and Chen et al. [27] for decision tree ensembles. While promising, these approaches do not guarantee that models are trained to be robust against any kind of adversarial perturbation around an input under the considered threat model.

To address this lack of guarantees, *certified training* approaches instead minimize an upper bound on the worst-case loss in order to guarantee robustness on all training inputs. Among these are the approach of **Andriushchenko and Hein** [2] for decision trees, and the early approach of **Hein and Andriushchenko** [80] and the previously described concurrent approaches of **Wong and Kolter** [167] and **Raghunathan et al.** [129] for neural networks. In particular, Wong and Kolter and Raghunathan et al. essentially use their robustness lower bounds as regularizer during training to encourage robustness against all perturbations with respect to the considered distance metric. The experimental evaluation conducted by Wong and Kolter, shows that the latter approaches are complementary: Wong and Kolter achieve lower robustness test error but higher traditional test error than Raghunathan et al. The approach of Wong and Kolter has been later generalized to support neural networks with arbitrary activations [168]. However, scalability to large neural network architectures remains an issue. **Mirman et al.** [115] considerably improve in scalability by proposing a certified training approach based on abstract interpretation.

Overall, there is a trade-off between robustness and accuracy of a trained model [157]. The stronger robustness guarantees given by certified training approaches come at the cost of a significantly lower accuracy compared to models trained using adversarial training. Recently, **Balunović and Vechev** [7] addressed this problem by combining adversarial and certified training and obtained state-of-the-art robustness and accuracy results on the CIFAR-10 dataset [96] (with respect to L_∞ perturbations with $\epsilon = 2/255$) improving over the concurrent work of Zhang et al. [174].

To the best of our knowledge, addressing broader verification goals beyond robust training (e.g., what Kurd and Kelly [98] identify as goal G3) currently remains an unexplored direction in the literature.

3.2.2 Formal Methods for Data Preparation

Software employed in earlier stages of the machine learning pipeline to gather, triage, and pre-process “dirty” data is the most fragile of the entire pipeline as it generally heavily relies on implicit assumptions on the data. It is also often disregarded as single-use non-critical glue code and, for this reason, is poorly tested, let alone formally verified. However, poor choices or accidental mistakes (e.g., programming errors) made in this phase can have an important effect on the end result of the pipeline and, more dangerously, can remain completely unnoticed as a plausible end result gives no indication that something went wrong along the way [81].

Formal verification methods that address these issues are scarce in the literature. An exception is the work of **Urban and Müller** [160], which proposed an abstract interpretation framework for reasoning about data usage and a static analysis method for automatically detecting (possibly accidentally) unused input data. Other work in this space, is a currently unpublished configurable static analysis for automatically inferring assumptions on the input data [162]. Much more work is however still needed, especially in applications in which software deals with complex unstructured data and is written by domain experts which are not necessarily software engineers.

4 Research Perspectives

The overview of the state of the art shows that we are still far away from being able to verify the *entire* machine learning pipeline, which we argue is necessary to ensure the safe use of machine learning software in safety-critical applications. We conclude by discussing below a number of research directions that we have identified for each pipeline phase and that will bring us closer to this objective.

Data Preparation. For data preparation software, there is a need for further approaches for reasoning about data usage [160]. For instance, verification methods that detect (possibly accidentally) reused and duplicated data would be a valuable complement to existing approaches. More generally, approaches for tracking data provenance would provide important *traceability* guarantees. This is particularly useful when data is aggregated from different sources (which is often the case).

Another direction worthy of being pursued further is the inference of assumptions on the input data that are embedded in data preparation software [162]. Specifically, designing more sophisticated abstractions would allow inferring more informative assumptions. In turn, these assumptions could be leveraged by tools that assist in the data preparation, e.g., by automatically generating (provably safe) data cleaning code.

Model Training. In the context of model training, designing verification methods with broader application scope than robust training (cf. Section 3.2.1) is of primal importance. In particular, there is a need for approaches providing stronger formal guarantees on the training process. For instance, it would be useful to be able to verify how the behavior of the model being trained evolves on a particular input space of interest. To this end, it might be interesting to leverage the theory behind the mathematical tools used for training to design domain-specific precise abstractions.

Another interesting possibility is to develop approaches to determine constraints on the training process that enforce a desired property on the trained model. For instance, one could enforce a specific behavior for a given input range of interest, or a particular structure of the trained model that facilitates its subsequent verification [171] (or its abstraction for verification [125, 145, 62]).

Model Deployment. For trained models, future work should aim at verifying more interesting properties, beyond what exists in the literature. For instance, domain-specific robustness properties are not necessarily limited to perturbations based on distance metrics or image perturbations, but might be complex specifications over a (not necessarily convex) input space of interest. Tackling such properties will require adaptations of existing abstractions or even the design of completely new ones. Moreover, verifying *global* robustness properties rather than local robustness properties would be more adapted to safety-critical applications.

More generally, verification methods should allow verifying the behavior of trained models under *all* circumstances and not just over the expected safe input space. This is particularly useful in cases in which the trained model is part of a larger machine learning-based system [53] and is thus more susceptible to receive unexpected inputs, e.g., from malfunctioning sensors. Addressing such issues will likely require designing more sophisticated verification approaches (e.g., possibly combining forward and backward analyses [161]) and overcoming scalability challenges [156, 161] (e.g., by designing abstractions able to leverage GPUs [118]).

Another interesting case is when the trained model is approximating an existing exact reference model [90]. In this case, it would be useful to design verification methods able to relate the behavior of the inexact model to the optimal expected behavior, e.g., by determining the worst-case approximation of the trained model.

When the verification fails, having verification methods able to determine the source of the fault [50] (e.g., a particular group of nodes in a neural network) would, for instance, allow localizing and guiding any repairs. More generally, such verification methods would enhance interpretability of models such as neural networks.

Finally, there is a need for further approaches that support diverse model structures, such as recurrent neural networks [95, 175], and that can verify model implementations by taking floating-point rounding errors into account [140, 141, 105].

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