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Foundations and Trends® in Programming Languages

Published, sold and distributed by:
now Publishers Inc.
PO Box 1024
Hanover, MA 02339
United States
Tel. +1-781-985-4510
www.nowpublishers.com
sales@nowpublishers.com

Outside North America:
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PO Box 179
2600 AD Delft
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The preferred citation for this publication is

G. Singh *et al.*. *Safety and Trust in Artificial Intelligence with Abstract Interpretation.* Foundations and Trends® in Programming Languages, vol. 8, no. 3-4, pp. 250–408, 2025.

ISBN: 978-1-63828-587-8

Foundations and Trends® in Programming Languages
Volume 8, Issue 3-4, 2025

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Foundations and Trends® in Programming Languages, 2025, Volume 8, 4 issues. ISSN paper version 2325-1107. ISSN online version 2325-1131. Also available as a combined paper and online subscription.

Contents

Safety and Trust in Artificial Intelligence with Abstract Interpretation

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ABSTRACT

Deep neural networks (DNNs) now dominate the AI landscape and have shown impressive performance in diverse application domains, including vision, natural language processing (NLP), and healthcare. However, both public and private entities have been increasingly expressing significant concern about the potential of state-of-the-art AI models to cause societal and financial harm. This lack of trust arises from their black-box construction and vulnerability against natural and adversarial noise.

As a result, researchers have spent considerable time developing automated methods for building safe and trustworthy DNNs. Abstract interpretation has emerged as the most popular framework for efficiently analyzing realistic DNNs among the various approaches. However, due to fundamental differences in the computational structure (e.g., high

Gagandeep Singh, Jacob Laurel, Sasa Misailovic, Debangshu Banerjee, Avaljot Singh, Changming Xu, Shubham Ugare and Huan Zhang (2025), "Safety and Trust in Artificial Intelligence with Abstract Interpretation", Foundations and Trends® in Programming Languages: Vol. 8, No. 3-4, pp 250–408. DOI: 10.1561/2500000062.

nonlinearity) of DNNs compared to traditional programs, developing efficient DNN analyzers has required tackling significantly different research challenges than encountered for programs.

In this monograph, we describe state-of-the-art approaches based on abstract interpretation for analyzing DNNs. These approaches include the design of new abstract domains, synthesis of novel abstract transformers, abstraction refinement, and incremental analysis. We will discuss how the analysis results can be used to: (i) formally check whether a trained DNN satisfies desired output and gradient-based safety properties, (ii) guide the model updates during training towards satisfying safety properties, and (iii) reliably explain and interpret the black-box workings of DNNs.

1

Introduction

Deep neural networks (DNNs) are currently the dominant technology in artificial intelligence (AI) and have shown impressive performance in diverse applications, including autonomous driving, medical diagnosis, text generation, and logical reasoning. However, they lack transparency due to their black-box construction and are vulnerable to environmental and adversarial noise. These issues have caused concerns about their safety and trust when deployed in the real world. Although standard training optimizes the model's accuracy, it does not take into account desirable safety properties such as *robustness* (the DNN should behave similarly for similar inputs), *fairness* (the DNN output should not depend too much on some legally protected attribute, such as gender or race), and *monotonicity* (if the inputs are partially ordered, so should be the outputs). As a result, state-of-the-art models remain untrustworthy. Building trust in DNNs is essential to realizing their vast potential to positively transform society and the economy and is one of the grand challenges in computer science today.

1.1 Safety-informed DNN Deployment Cycle

Figure 1.1 presents a general safety-informed pipeline for DNN development, applicable to any application domain. Safety, accuracy, and efficiency can often conflict with each other. DNN accuracy improves with model size but that increases the inference cost. Similarly, models maximizing safety can have reduced accuracy. For example, a DNN classifier that always predicts the same class for all inputs is robust but has very low accuracy. As a result, it may not be possible to obtain DNNs that optimize all three objectives simultaneously. Depending on the target application, a developer may prioritize accuracy over trust or vice-versa. The goal of safety-informed DNN development is to ensure a sufficient balance between accuracy, safety, and efficiency.

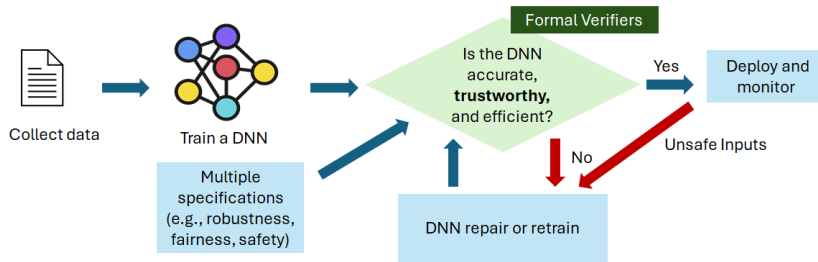


Figure 1.1: Development pipeline for building accurate, trustworthy, and efficient DNNs. Verification is used for testing model trustworthiness (green diamond).

In this pipeline, first, representative training data for the target application is collected and a DNN is trained to maximize its accuracy on test inputs from the training distribution. Next, a domain expert creates (manually or algorithmically) a set of formal safety specifications (e.g., robustness, fairness) characterizing the expected DNN behavior in different real-world scenarios. The set of inputs covered by these specifications can be infinite.

The expert then checks whether the model meets the safety standards. Since DNNs may not satisfy all the specifications, the standards can require that at least a significant fraction of all specifications be satisfied for trustworthiness. If the model meets the criteria, then the DNN is considered fit for deployment. Otherwise, it is iteratively re-

paired (e.g., by fine-tuning) until we obtain the desired balance between accuracy, safety, and efficiency.

During deployment, the DNN inputs are monitored for distribution shifts, i.e., the inputs are not from the training distribution. If the runtime system detects a distribution shift, it reports representative samples to the domain experts. They then design new specifications, and the model undergoes another round of repair (or full retraining).

How formal methods can help. For checking that the model satisfies safety specifications, the standard practice is to evaluate the DNN behavior on a finite set of inputs satisfying the specifications. However, this cannot guarantee safe and trustworthy DNN behavior on all specification inputs. The unseen set can be huge and contain inputs often seen during real-world deployment. To address these limitations, there is growing work on checking the safety of DNN models and interpreting their behavior, on an infinite set of unseen inputs from safety specifications using formal methods, which provides a more reliable metric for measuring a model's safety than standard empirical methods. For example, a repaired DNN preserving the original test set accuracy and efficiency but satisfying the trustworthy specifications more often is a better model than the unrepaired one as it is less likely to show undesirable behavior during real-world deployment. Formal methods can also be used during training to guide the model to satisfy desirable safety and trustworthiness properties. The models trained this way are more likely to satisfy safety specifications than those without.

This monograph presents a comprehensive treatment of the techniques that guarantee the safety of DNNs by formally modeling the behavior of modern DNNs and efficiently computing with abstractions that represent those behaviors. Our main focus will be on approaches that leverage a general framework for automated analysis of programming languages called abstract interpretation, the most successful formal methods for automatically reasoning about DNNs. We emphasize that the knowledge of the topics covered in this monograph is necessary not only for computer scientists but for practitioners from all areas building DNN-based applications, e.g., natural sciences, aerospace, finance, etc.

Next, we describe how safety and trustworthy properties can be formally specified for DNNs, then we will discuss the key ideas and design

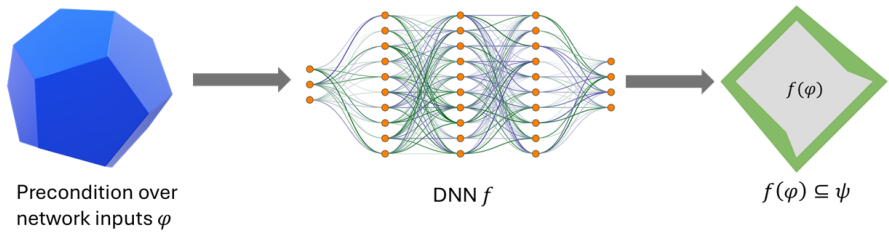
considerations in developing abstract interpretation based methods for the formal verification and training of DNNs. We will also discuss how abstract interpretation enables reliable explanations and interpretations of DNNs as well as analysis of differentiable programs.

1.2 Formal Specifications for DNNs

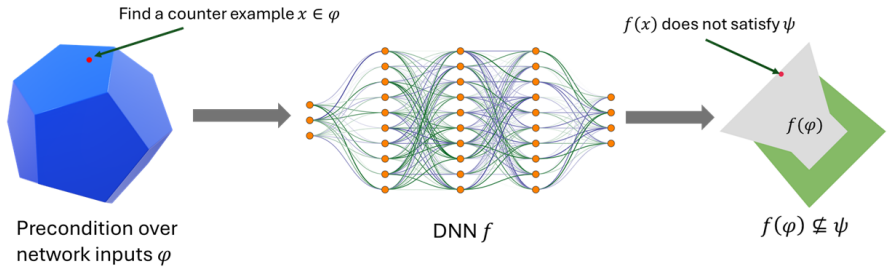
Mathematically, we model a trained DNN as a pure function f. Its input x can be images, text, videos, sensor measurements, or other data. We denote the output of the DNN as $f(x)$, which can be a classification of the input into one of the predefined classes, the regression that estimates a continuous value, or the set of tokens generated by a language model. We denote gradients of f as $f'(x)$.

For a trained DNN f, a developer specifies the property of interest using two formulas: (1) *the precondition* φ, which specifies the set of inputs on which the DNN should not misbehave and (2) *the postcondition* ψ, which specifies safe and trustworthy behaviors of the DNN for the given inputs. These behaviors are typically constraints on the DNN's outputs or its gradients. The preconditions and postconditions are domain-dependent and usually designed by DNN developers.A tool for DNN verification (*a verifier*) aims to automatically check if the postcondition on the DNN's outputs and/or gradients is satisfied for all inputs specified by the precondition.

A property specification is a tuple (φ, ψ), where φ is the precondition and ψ is the postcondition. Both formulas φ and ψ typically represent *an infinite number of inputs/outputs.* We denote the set of the results of the evaluations of the DNN on all inputs described by the precondition φ as $f(\varphi) = \{f(x) \mid x \in \varphi\}$. Similarly, we denote the set of all gradients as $f'(\varphi)$. The verifier then checks for the inclusion of the set of possible executions of the DNN into the set of outputs that satisfy the postcondition, i.e., $f(\phi) \subseteq \psi$ (or $f'(\phi) \subseteq \psi$) holds. *Single execution* specifications, as shown in Figure 1.2, require that each DNN output $f(x)$ where $x \in \varphi$ must independently satisfy ψ. *Relational* specifications require reasoning about multiple related executions of the same or different DNNs. As we will show in Section 3, a general way to represent and compute with φ and ψ in these settings is as disjunctions



(a) Verified



(b) Counterexample

Figure 1.2: Single execution specifications require that the DNN output for each input from φ must independently satisfy ψ.

of convex polyhedra within the framework of abstract interpretation. φ and ψ can also define distributions leading to *probabilistic* specifications.

Local and global properties. The set of specifications for DNNs can be broadly classified as *local* or *global*. The precondition φ for local properties defines a local neighborhood around a sample input from the test set. For example, given a test image correctly classified as a car by a DNN, the commonly used *local robustness property* specifies that if the original image was classified as a car, then all images generated by rotating the original image within $\pm d$ degrees are also classified as a car. We present many local properties in Sections 3.1 and 3.2.

In contrast, global properties are not defined with respect to a specific test input. Verifying global properties yields stronger safety guarantees compared to local properties, however, global properties are difficult to formulate for popular domains, such as vision and NLP, where the individual features processed by the DNN have no clear semantic meaning. While verifying local properties is not ideal, the local

verification results enable testing the safety of the model on an infinite set of unseen inputs, not possible with standard methods. We present several concrete global properties in Section 3.1.

1.3 Verifying Specifications over DNNs

DNN verification can be seen as an instance of program verification, since one can write a DNN as a program, i.e., there is a direct translation from the mathematical representation of the DNN as a function f into a side-effect free program. However, since it is well-known that program verification is *undecidable* (one cannot prove the correctness of an arbitrary program with respect to an arbitrary property of interest), DNN verification is also undecidable in general. Certain DNN verification problems, such as robustness verification of feedforward networks with ReLU activations, are decidable but still NP-complete in general (Katz *et al.*, 2017).

State-of-the-art verifiers are therefore incomplete in general, i.e., they can fail to prove a specification when it holds. However, when they succeed, the DNN will satisfy the specification. In this monograph, we focus on *white-box* verifiers that require access to the model parameters. Verification of closed-source models requires *black-box* verifiers. We refer the interested readers to the relevant material in this direction in Section 1.7. The white-box verifiers can be formulated using the elegant framework of abstract interpretation. The verifier is parameterized by the choice of an *abstract domain* with two main components: abstract elements and abstract transformers. Abstract elements are mathematical objects symbolically representing an infinite set of numerical points over which the verifier operates. Abstract transformers overapproximate the effect of applying the transformations inside the DNN program (e.g., affine or ReLU assignments) on abstract elements.

There is a tradeoff between the cost and overapproximation error (also known as precision) of an incomplete verifier: expensive verifiers are more precise while cheap verifiers are imprecise. Both are determined by the design of the abstract domain and transformers. The key consideration in designing an efficient verifier applicable to real-world DNNs is managing this tradeoff. The classical domains, such as Polyhe-

dra and Octagons, used for analyzing programs are not well suited for DNN verification. This is because the DNNs have a different structure compared to traditional programs. For example, DNNs have a large number of non-linear assignments but typically do not have loops. For efficient verification, researchers have developed numerous new abstract domains and transformers tailored for DNN verification. These abstract domains can scale to realistic DNNs with millions of neurons, or more than 100 layers, verifying diverse safety properties in different real-world applications. We will present them in Section 3. We will also discuss how verification can be done incrementally to improve efficiency when verifying a large number of similar DNNs and specifications as needed for the developement pipeline in Figure 1.1.

1.4 Training Provably Safe DNNs

DNNs trained with standard training often do not satisfy safety specifications as safety satisfaction is not part of their training objective. Adversarial or counter-example guided training augment the training data with violating examples during training, however the trained models still cannot be proven to be safe in most cases. To overcome these limitations, certified training methods have been developed in recent years which directly incorporate the verifier computations within the training loop and generate models with a high degree of provability, i.e., they are more likely to satisfy specifications and are relatively easier to prove than DNNs obtained with competing methods.

In certified training, if the model f does not satisfy the specification, as checked by a verifier, its weights are updated to increase the provability. The gradient updates are derived by formulating a differentiable property loss on the verifier output, which measures how far the model is from satisfying the property. Since gradient updates are derived from the verifier code, its computations must be expressible as a differentiable function of model weights and parallelizable on GPUs for scalability. Overall, certified training can be seen as training f where the model updates are derived by differentiating the surrogate approximation of the DNN within φ, computed by the verifier.

While certified training improves the provability, safety specifications can be in conflict with accuracy. Using an imprecise verifier during training can result in overregularization and a significant reduction in the standard accuracy. However, precise verifiers often have complicated code which makes the optimization problem too complicated to solve during training, yielding suboptimal results. Also, employing a verifier during training is more expensive than when used for checking specifications on an already trained DNN, as now the verifier is called during every training iteration. Balancing the provability, accuracy, and cost is therefore the main challenge when developing state-of-the-art methods. Researchers have developed a variety of abstractions, refinements, and loss formulations to enable efficient training. We will cover these methods in detail in Section 4.

1.5 Explaining and Interpreting DNNs

Popular methods for explaining DNN predictions identify relevant input features that influence the DNN output the most. However, they do not give guarantees about the robustness of the generated explanations. Relying on non-robust explanations can lead to a false sense of confidence in an untrustworthy model. We will discuss how abstract interpretation can be leveraged to generate explanations with robustness guarantees in Section 5, reliably improving DNN transparency.

Abstract interpretation-based DNN verifiers generate high-dimensional abstract elements at different layers capturing complex relationships between neurons and DNN inputs to prove DNN safety. However, the individual neurons and inputs in the DNN do not have any semantic meaning, unlike the variables in programs, therefore it is not clear whether the safety proofs are based on any meaningful features learned by the DNN. If the DNN is proven to be safe but the proof is based on meaningless features not aligned with human intuition, then the DNN behavior cannot be considered trustworthy. While there has been a lot of work on interpreting black-box DNNs, standard methods can only explain the DNN behavior on individual inputs and cannot interpret the complex invariants encoded by the abstract elements capturing DNN behavior on an infinite set of inputs.

The main challenge in interpreting DNN proofs is mapping the complex abstract elements to human-understandable interpretations.

Section 5 presents ProFIt, the first method for interpreting robustness proofs computed by DNN verifiers. The technique can interpret proofs computed by different verifiers. It builds upon the novel concept of *proof features* computed by projecting the high-dimensional abstract elements onto individual neurons. The proof features can be analyzed independently by generating the corresponding interpretations. Since certain proof features can be more important for the proof than others, a priority function over the proof features that signifies the importance of each proof feature in the complete proof is defined. The method extracts a set of proof features by retaining only the more important parts of the proof that preserve the property.

A comparison of proof interpretations for DNNs trained with standard and robust training methods shows that the proof features corresponding to the standard networks rely on spurious input features that are not aligned with human intuition. The proofs of adversarially trained DNNs filter out some of these spurious features. In contrast, the networks trained with certifiable training produce proofs that do not rely on any spurious features but they also miss out on some meaningful features. Proofs for training methods that combine both empirical and certified robustness not only preserve meaningful features but also selectively filter out spurious ones. These insights suggest that DNNs can satisfy safety properties but their behavior can still be untrustworthy.

1.6 Analyzing and Verifying Differentiable Programs

Differentiable programming, which includes automatic differentiation (AD), is the backbone of machine learning. AD computes the gradients alongside the values of the program's output variables. AD computations generalize many machine learning and signal processing applications. Thus, generalized abstractions for AD analysis can be deployed across applications: a neural network, an image filter, and a differential equation solver can be expressed and analyzed in the same language, even when combined in complex programs. Despite AD's ubiquity, automated formal reasoning of derivatives that AD computes has lagged.

Analyzing gradient properties is important for today's trustworthy AI: for instance, the sensitivity of DNN's output to input noise can be expressed as finding bound for the absolute gradients values. The same bounds can help with selecting low precision data types in machine learning algorithms to prevent overflows. Fairness can be formalized as a monotonicity property on a specific attribute, which is satisfied when all derivatives are strictly positive.

To answer these questions, it is not sufficient to reason about the output of a function (e.g., DNN) f for all inputs in φ. Instead one has to reason about f', the derivative of f. For instance, to prove the monotonicity of f, one should ensure that its derivative f' is strictly positive or negative for all inputs in φ. Figure 1.3 presents an intuition of this workflow.

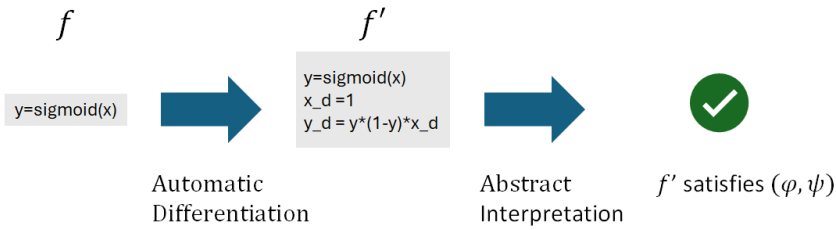


Figure 1.3: Verifying derivative properties requires first computing the derivative of a function f (given as a piece of code) using automatic differentiation. The derivative program is then analyzed with abstract interpretation to prove the desired property (φ, ψ) holds for the derivative f' instead of f itself.

Section 6 will present a general framework for precise analysis of AD computations. This approach leverages ideas from abstract interpretation of DNNs and generalizes them to find precise abstract transformers of gradient computation. It overcomes the limitation of standard program analysis, which treats the gradient computation as any other code, and leads to significant imprecision, and is in some cases ill-defined. We will present the advantage of the AD-specific abstract transformers on the case study for monotonicity analysis for a decision-making DNN.

1.7 Sources and Further Reading

Many recent studies demonstrate the power of modern DNNs, e.g., Bojarski *et al.* (2016) for autonomous driving, Amato *et al.* (2013) for medical diagnosis, Brown *et al.* (2020) for text generation, and Pan *et al.* (2023) for logical reasoning. Many domains have standard datasets for training and inference, e.g., in vision MNIST (LeCun *et al.*, 1989), CIFAR10 (Krizhevsky, 2009), and ImageNet (Deng *et al.*, 2009).

At the same time, recent research also points out key concerns: Ribeiro *et al.* (2016) discusses the issues of black-box model construction and non-interpretability; Szegedy *et al.* (2014) and Kurakin *et al.* (2017) discuss vulnerability against environmental and adversarial noise. Works that pointed out problems with standard training include Shafique *et al.* (2020) for robustness, Dwork *et al.* (2012) for fairness, and Sill (1997) for monotonicity. Tsipras *et al.* (2019) and Wong *et al.* (2021) point out problems with using a finite set of test inputs to ensure DNN safety during deployment. Many recent works, identify classes of slight adversarial perturbations that impact the DNN decisions (Madry *et al.*, 2017; Goodfellow *et al.*, 2014; Heo *et al.*, 2019).

For examples of local robustness to image rotations and its classification see, e.g., Balunovic *et al.* (2019). For examples of global properties in air traffic collision avoidance systems see, e.g., Katz *et al.* (2017), and in security vulnerability classification see, e.g., Chen *et al.* (2021). Beyond manual design, there is a growing line of work on automatically generating formal specifications for DNNs. These include Geng *et al.* (2022), Chaudhary *et al.* (2024b), Geng *et al.* (2024), and Jin *et al.* (2024).

Checking the safety of DNNs has been a very active area of research with many publications, primarily during inference and relying on white-box access to the model, such as Balunovic *et al.* (2019), Singh *et al.* (2019b), Zhang *et al.* (2018a), Singh *et al.* (2018), Singh *et al.* (2019d), Paulsen *et al.* (2020), Xu *et al.* (2021), Tran *et al.* (2019b), Wu *et al.* (2022b), Anderson *et al.* (2019), Katz *et al.* (2019), Singh *et al.* (2019a), Wong and Kolter (2018), Lan *et al.* (2022), Wang *et al.* (2018), Bunel *et al.* (2020), Wang *et al.* (2021), Ugare *et al.* (2022), Kabaha and Drachsler-Cohen (2022), Palma *et al.* (2021a), Dathathri *et al.* (2020),

Munakata *et al.* (2023), Ranzato *et al.* (2021), Banerjee *et al.* (2024b), Banerjee *et al.* (2024a), and Zhou *et al.* (2024). Black-box DNN verifiers are based on collecting DNN output for inputs from φ and providing probabilistic guarantees. These include Baluta *et al.* (2021), Webb *et al.* (2019), Chaudhary *et al.* (2024a), and Chaudhary *et al.* (2025).

Certified training leverages DNN verifiers during training obtaining models that have higher provability than those with standard training. Examples include Gowal *et al.* (2019), Mirman *et al.* (2018), Xu *et al.* (2020), Zhang *et al.* (2020), Shi *et al.* (2021), Yang *et al.* (2023), Müller *et al.* (2023a), Balunovic and Vechev (2020), and Hu *et al.* (2023b).

Numerous methods aim to provide transparency of DNNs. Standard methods include Ribeiro *et al.* (2016) and Wu *et al.* (2023) and Wong *et al.* (2021). Marques-Silva and Ignatiev (2022), Malfa *et al.* (2021), Ignatiev *et al.* (2019), Darwiche and Hirth (2020), and Wu *et al.* (2023) generate explanations with formal guarantees. The work of Banerjee *et al.* (2024a) presents ProFIt, the first method for interpreting robustness proofs computed by DNN verifiers.

Various uses of automatic differentiation are presented (Hückelheim *et al.*, 2018). Static analysis of AD computations is introduced by Laurel *et al.* (2022a), Laurel *et al.* (2022b), and Laurel *et al.* (2023). Verification of properties involving gradients and Jacobians are discussed by Zhang *et al.* (2019), Fazlyab *et al.* (2019b), and Shi *et al.* (2022)

Abstract interpretation was introduced in the seminal work by Cousot and Cousot (1977). Over the past almost 50 years, this approach to program analysis has flourished and demonstrated many uses. There are numerous books, monographs, and tutorials describing the foundations of abstract interpretations, for instance Cousot (2021), Nielson *et al.* (2005), Miné (2017), and Rival and Yi (2020).

Examples of abstract domains for neural networks include DeepPoly/CROWN (Singh *et al.*, 2019b; Zhang *et al.*, 2018a), DeepZ/FastLin (Singh *et al.*, 2018; Weng *et al.*, 2018), Star sets (Tran *et al.*, 2019b), and DeepJ (Laurel *et al.*, 2022a). These custom solutions can scale to realistic DNNs with up to a million neurons (Müller *et al.*, 2021a), or more than 100 layers (Wu *et al.*, 2022b), verifying diverse safety properties in different real-world applications. Examples include autonomous driving (Yang *et al.*, 2023), job-scheduling (Wu *et al.*, 2022b), data

center management (Chakravarthy *et al.*, 2022), biology (Mohr *et al.*, 2021), aerospace (Cohen *et al.*, 2024), and financial modeling (Laurel *et al.*, 2023). For examples of refinements of abstract domains used in machine learning see e.g., Wang *et al.* (2018), Singh *et al.* (2019d), Müller *et al.* (2021b), Ryou *et al.* (2021), Wang *et al.* (2021), Wu *et al.* (2022b), and Yang *et al.* (2021).

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