Bringing Engineering Rigor to Deep Learning

Kexin Pei
kpei@cs.columbia.edu
Columbia University

Shiqi Wang
tcwangshiqi@cs.columbia.edu
Columbia University

Yuchi Tian
yuchi.tian@columbia.edu
Columbia University

Justin Whitehouse
jaw2228@cs.columbia.edu
Columbia University

Carl Vondrick
vondrick@cs.columbia.edu
Columbia University

Yinzhi Cao
yinzhi.cao@jhu.edu
Johns Hopkins University

Baishakhi Ray
rayb@cs.columbia.edu
Columbia University

Suman Jana
suman@cs.columbia.edu
Columbia University

Junfeng Yang
junfeng@cs.columbia.edu
Columbia University

ABSTRACT

Deep learning (DL) systems are increasingly deployed in safety- and security-critical domains including autonomous driving, robotics, and malware detection, where the correctness and predictability of a system on corner-case inputs are of great importance. Unfortunately, the common practice to validating a deep neural network (DNN) – measuring overall accuracy on a randomly selected test set – is not designed to surface corner-case errors. As recent work shows, even DNNs with state-of-the-art accuracy are easily fooled by human-imperceptible, adversarial perturbations to the inputs. Questions such as how to test corner-case behaviors more thoroughly and whether all adversarial samples have been found remain unanswered.

In the last few years, we have been working on bringing more engineering rigor into deep learning. Towards this goal, we have built five systems to test DNNs more thoroughly and verify the absence of adversarial samples for given datasets. These systems check a broad spectrum of properties (e.g., rotating an image should never change its classification) and find thousands of error-inducing samples for popular DNNs in critical domains (e.g., ImageNet, autonomous driving, and malware detection). Our DNN verifiers are also orders of magnitude (e.g., 5,000×) faster than similar tools. This article overviews our systems and discusses three open research challenges to hopefully inspire more future research towards testing and verifying DNNs.

1 INTRODUCTION

Deep Learning (DL) has made tremendous progress over the past few years, achieving or surpassing human-level performance for a diverse set of tasks including visual recognition [37, 46, 69], speech recognition [39, 90], and playing games [59, 68]. These advances have led to widespread adoption and deployment of DL in security- and safety-critical systems such as self-driving cars [6, 13, 15], malware detection [65, 92], and aircraft collision avoidance systems [43].

This wide adoption of DL presents new challenges as the predictability and correctness of such systems are of crucial importance. Unfortunately, DL systems, despite their impressive capabilities, often demonstrate unexpected or incorrect behaviors for several reasons such as biased training data, overfitting, and underfitting of the models. In safety- and security-critical settings, such incorrect behaviors can lead to disastrous consequences such as a fatal collision of a self-driving car. For example, a Google self-driving car recently crashed into a bus partly because it expected the bus to yield under a set of rare conditions, but the bus did not [33]. In 2016, a Tesla car in autopilot crashed into a trailer partly because the autopilot system failed to recognize the trailer as an obstacle due to its “white color against a brightly lit sky” and the “high ride height” [78]. A similar incident happened in 2019 [79]. These disasters call for more thorough validation of DL systems against corner cases.

Unfortunately, prior approaches to validating DL systems are not designed to thoroughly surface corner-case errors. A common practice is to measure a DL system’s prediction accuracy on a randomly selected test set, which often covers few or none corner cases. One can gather and label as much real-world data as possible [1, 5], but given the enormous input space, such blind gathering risks at once wasting much manual effort and missing many corner cases. Unsurprisingly, recent work on adversarial DL [32, 56, 77] showed that human-imperceptible perturbations easily fooled today’s most accurate DL systems to the inputs. Adversarial DL itself, however, is designed to find only the most effortless adversarial samples quickly. It limits the perturbations to minimal noise, not realistic transformations such as light condition change [62]. Nor does it try to find as many adversarial samples as possible. Questions such as how to find more corner cases under diverse transformations and whether all corner cases for a given dataset have been found remain open.

This challenge of thoroughly checking DL systems sounds extremely familiar as researchers have been working towards the same goal for traditional software. Unfortunately, the plethora of testing and verification tools created for traditional software cannot directly apply to DL because the two programming paradigms are drastically different. In traditional software engineering, developers translate the decision logic in their brains into program statements, each of which gradually progresses toward a final goal. In DL engineering, the decision logic is automatically extracted from a vast dataset and embedded in millions of opaque weight parameters. Consider statement coverage, the predominant empirical metric to quantify testing thoroughness of traditional software. Such traditional software testing metric is meaningless in a DL system as any single input can exercise all statements executed by DL inference.

In the last three years, we have been building new testing and verification tools to bring more rigor to DL engineering. Given the challenges in specifying a full functional spec of a deep neural network (DNN) as it would amount to specifying that for human brains, we design our tools to check transformation-invariant properties such as "slight light condition change must not change the image class." They explore design tradeoffs between scalability (whether the tool can scale to large DNNs), completeness (whether the tool can find all property violations for a given dataset), and domain knowledge needed (whether the tool requires access to the DNN internals). We briefly describe each system below.

- DeepXplore is a whitebox testing tool that defines the first test coverage metric for DNNs we call *neuron coverage* – the percentage of activated neurons by a test set, and uses this metric to guide the generation of new inputs to increase coverage [61].
- DeepTest leverages neuron coverage to test autonomous-driving systems by adding fogs or rains to road scenes [80].
- VeriVis is a blackbox verification tool that exhaustively checks a computer vision system correctly handles certain transformations of an image (e.g., all rotations within five degrees have the same correct image label) [62].
- ReluVal is a whitebox verification tool that, given an input range, leverages interval arithmetic and symbolic analysis to compute rigorous DNN output bounds for property verification [86]. It can prove the absence of adversarial examples or find all input sub-intervals that may contain adversarial examples.
- Neurify improves upon ReluVal and leverages what we call linear relaxation to tighten the DNN output bounds further and reduce false positives [85].

A key additional benefit of exhaustive testing and verification is that our tools can serve as an objective, rigorous benchmark for many DNN techniques. For instance, any technique purporting to make DNNs robust against adversarial attacks should not be evaluated only on the attacks designed to find adversarial samples quickly. Instead, they should be evaluated on the exhaustive set of attack samples that our tools, especially the verifiers, generate. Experiments using tools did reveal such issues in prior robustness training techniques.

Our tools have found thousands of corner-case errors over a broad spectrum of DL systems including ImageNet-scale image classifiers, object detectors, malware detectors, self-driving car systems, and cloud computer vision systems built by Google, Amazon, IBM, and Microsoft. They also verified some of these DL systems on popular datasets.

Our verification tools outperform other tools of the same kind by orders of magnitude (5,000× on average). We are encouraged to see that the concepts and algorithms in our tools start to gain adoption by other research groups and the industry [14, 27, 35, 49–52, 58, 74, 89, 93, 94].

This article overviews our tools because we are most familiar with them; we are by no means the only group in this emerging area of testing and verifying DL. In fact, multiple groups have also begun working in this area [28, 31, 44, 55, 70, 71, 81, 88]. We hope our article will help inspire more researchers to join us in tackling this important and exciting challenge of robust DL.

2 THE PROPERTIES TO CHECK

We design our tools to check *transformation-invariant* properties: given input x and transformation $\mathcal{T}$ such as lighting condition change, a DNN's prediction on the transformed sample $\mathcal{T}(x)$ should be similar to that on the original sample x, in most cases the same label. (It is conceivable to relax the property and include a set of related labels, though our systems did not use this relaxed form.) If the DNN outputs a real number such as the driving angle in autonomous driving, the difference between the predictions on the two samples should be smaller than a given threshold.

Our rationale behind this design choice is that the decision logic contained in a DNN is often opaque even to its designers. For instance, creating a complete specification for the correct behavior of a self-driving car under different driving conditions essentially equals recreating the logic of a human driver, computationally infeasible and not practical. In addition, the nature of optimization means that there are multiple acceptable ways through different internal states for satisfying the final goal. For instance, a car can be safely driven on the road with many slightly different but similar steering

Table 1: Transformations supported by our tools to check safety properties. The ✓mark indicates that the tool supports the transformation, and ✗otherwise.

Transformation $\mathcal{T}$	DeepXplore	DeepTest	VeriVis	ReluVal	Neurify
L-norm	✗	✗	✗	✓	✓
Smoothing	✗	✓	✓	✗	✗
Contrast	✗	✓	✓	✗	✓
Brightening	✓	✓	✓	✗	✓
Occlusion	✓	✓	✓	✗	✗
Affine	✓	✓	✓	✗	✓
Weather	✗	✓	✓	✗	✗

angles. Therefore, we conjecture that DL testing and verification should focus on partial, input-output correctness rather than complete functional correctness.

Although simple, transformation-invariant properties can express crucial safety requirements of a wide range of DL systems. For example, they can ensure that the recognized phrases/sentences of a speech recognition system will not change under different background noises. Malware detection systems should not change their classifications from malware to benign due to varying types of code obfuscation/transformation techniques that do not affect malicious functionality [91].

One caveat is that, like all other DL testing and verification tools, our tools check properties on the individual, not all possible, inputs. A fundamental assumption in DL (and machine learning in general) is that the decision logic learned from a representative dataset will generalize to all data produced by the same underlying distribution as the dataset. Therefore, the guarantees achieved on individual inputs should hopefully also generalize.

Table 1 summarizes the transformations supported by our tools to check safety properties. We consider seven general categories of transformation functions, much more complete and realistic than adding slight noise as in prior adversarial DL. Many of these transformations are widely used by computer vision researchers to emulate the naturally occurring distortions and deformations and motivate the new design of model architectures to be invariant against such transformations [17, 23, 87]. The first category of transformation is more general that computer vision. It covers domains such as malware detection or aircraft collision avoidance. For instance, changing the number of authors of a malicious PDF file should not change its classification. We describe each transformation category in the following.

L-norm bounded perturbation. Testing and verifying L-norm based properties includes perturbing the input x into $x' = \mathcal{T}(x)$ so that $L_p(x' - x)$, the distance between x and x', is bounded a user-defined value. Our tools support L_1-norm or L_∞-norm. This property category is widely used in adversarial testing of image classifiers [32], malware detectors [61], self-driving cars [61, 62, 80, 85] and aircraft collision avoidance systems [44, 85, 86].

Smoothing. This transformation emulates the blurring effect that may be encountered in different scenarios, such as autonomous driving or face authentication. It is part of the convolution-based transformations which apply a convolution kernel on the input image and produce the output images such that each pixel values are determined by its local neighbors and the corresponding kernel weights. In particular, the smoothing transformations we consider include the average blurring, median blurring, erosion, and dilation, which compute the average, median, minimum, and maximum of the pixel values within the kernel, respectively, and replace the center pixel value of the kernel with the result of the computation.

Contrast, Brightening, and Occlusion. These transformations emulate the lighting effect, variations of camera configurations (in rendering visual inputs), and occlusions by unexpected objects in front of the camera. Specifically, changing the contrast or brightness of a visual input involves multiplying or adding the same constant c for each pixel values. Adding occlusions is straightforward: defining a patch using another image with a smaller size and overlaying it in the original image.

Affine transformation. Affine transformations emulate the potential distortions of the image that may happen in the real world. They operate on the coordinates of pixels. In particular, this category includes five operations: rotation, shear, scale, translation, and reflection. All the operations include multiplying with the matrix of the pixel coordinates with a 3-by-3 affine transformation matrix. We refer interested readers to [62, 80] for a detailed description of such transformations.

Weather. Finally, it is important to check whether a model, especially those working with visual inputs in the wild (e.g., autonomous driving and collision avoidance), is robust against different weather conditions. However, it is challenging to mathematically represent weather conditions without making strong assumptions. To emulate such transformations, we employ a simple patch image such as rain or fog effect and directly overlay it on the original image. There exist more advanced techniques using the generative adversarial network (GAN) [48]. We discuss this in our future research problem in Section 5.

3 THE TOOLS

This section overviews the five tools we have built, discussing each's key techniques and related work. All are open sourced.

3.1 DeepXplore

DeepXplore is the first (to the best of our knowledge) systematic white-box testing system for DNNs. It has two key techniques. First, it defines *neuron coverage* as a new metric to measure the test coverage of DNNs. The intuition is that the neurons in a DNN are for recognizing features in input, with earlier layers recognizing lower-level features and later layers higher-level features. Thus, the neurons activated by a test input serves as a good indicator of the decision logic exercised by the test. Neuron coverage is analogous to statement coverage, the empirical test coverage metric for traditional software.

Second, given an input, DeepXplore uses neuron coverage to guide the generation of new inputs that (1) increase neuron coverage and (2) are realistic transformations of the given input. The basic idea works as follows. To increase neuron coverage, DeepXplore computes a change to the input that maximizes a particular neuron's activation. Since DNNs are differentiable, DeepXplore leverages gradient descent to compute this input change. However, this greedily computed change is not necessarily a realistic transformation of the input. For instance, it may alter the pixel values by different amounts when the transformation we wanted is brightening, which requires that all pixel values change by the same amount. DeepXplore thus revises the greedy change based on these constraints, computing a new input that can indeed be a realistic transformation of the given input.

Many follow-up projects improved different aspects of DeepXplore, such as the coverage metric [14, 49, 58, 89], the application domains and properties [27, 52, 80, 93, 94], the test generation algorithm [35, 50, 51, 74].

3.2 DeepTest

DeepTest extends the coverage guided training developed in DeepXplore in testing autonomous driving DNNs. It supports a much broader set of transformations, including different weather conditions. Some of them are not differentiable, so gradient descent is not directly applicable. DeepTest proposes neuron coverage guided greedy search to generate error-inducing inputs and maximize neuron coverage. In this greedy algorithm, different transformations are combined, and those transformations that can successfully increase the neuron coverage will be recorded and prioritized while more images are synthesized.

DeepTest also leverages metamorphic relations to identify erroneous behaviours. Intuitively, the steering angle of a self-driving cars on synthesized inputs should not differ much from the steering angle on original inputs. However, there is no one true steering angle given each input for an autonomous car. For examples, small variations of steering angles can still be tolerated by cars. Therefore, a tighter metamorphic relation will result in more false positives. To strike a balance between false positives and false negatives, the following metamorphic relations are defined. The predicted labels of original images are $\{\theta_{o1}, \theta_{o2}, ..., \theta_{on}\}$. The predicted labels of synthesized images are $\{\theta_{t1}, \theta_{t2}, ..., \theta_{tn}\}$. The respective manual labels are $(\{\hat{\theta}_1, \hat{\theta}_2, ..., \hat{\theta}_n\})$. The metamorphic relation are defined as $(\hat{\theta}_i - \theta_{ti})^2 \leq \lambda \, MSE_{orig}$. while $MSE_{orig} = \frac{1}{n}\sum_{i=1}^{n}(\hat{\theta}_i - \theta_{oi})^2$. λ is a parameter used for making trade-off between false positives and false negatives.

3.3 VeriVis

Despite finding thousands of corner-case errors, our testing tools cannot guarantee that all errors are found or there are no errors for a given input and transformation. This limitation is analogous to the testing of traditional software.

To provider stronger guarantees, we build VeriVis, a black-box verification tool for computer vision systems that can fully verify a DNN against a given image and a supported transformation (Section 2). For instance, it can verify however one rotates an image within five degrees, the resultant images all have the same label as the given image.

A difficult challenge is that the parameter of a transformation is often continuous and can be an arbitrary real number, such as the rotation degree which can be 1, 0.1, 0.01, etc. How to exhaustively verify a model against the infinitely many possible transformed inputs? Fortunately, our key insight is that the image space itself is discrete because the pixel values are integers from 0–255 and coordinates are integers bounded by the image size. Leveraging this insight, VeriVis reduces the continuous, infinite transformation parameter space into a finite number – polynomial to the image size – of parameter values. For instance, up to n^3 ($n = w \cdot h$ is the image size) number of rotation degrees can provably cover all possible rotated images. This technique is analogous to the state-space reduction in model checking [12, 20, 30] and helps DeepXplore avoid redundantly checking many equivalent inputs.

3.4 ReluVal

There are two challenges of whichVeriVis falls short. First, many safety-critical DNNs work in continuous input and output space. For instance, the unmanned aircraft collision avoidance system X (ACAS Xu), which uses DNNs to predict the best actions such as "90-degree left" according to the distance, speed, and approaching angle of an intruder plane in the vicinity. NASA and FAA [2, 53] successfully tested it and is on schedule to install it in over 30,000 passengers and cargo aircraft worldwide [57] and US Navy's fleets [7]. It is thus paramount to guarantee that ACAS Xu predicts robust actions for given input ranges. Second, a discrete space can still be too large to check exhaustively. For instance, a 28-by-28 MNIST hand-written digit data [47] with $L_\infty = 1$ bounded perturbation can have up to 2^{784} number of concrete images to check.

We build ReluVal to address these difficult challenges. It focuses on verifying properties of the following form: a DNN never violates any safety property (e.g., , no collisions) for any (maliciously fed) values in an input range (e.g., , between 0 and 500 mph for the intruder speed). Mechanically, given an input range X, ReluVal propagates it through the layers of a DNN and computes a sound overapproximation of the output bound Y leveraging a classic static analysis technique called abstraction interpretation [25]. It does so by executing every operator of the DNN abstractly in the interval domain leveraging interval arithmetic [63]. If Y contains no property violations, ReluVal has soundly verified that the DNN has no violations on X.

A key challenge in ReluVal is the inherent overestimation caused by input dependencies [26, 63, 86] when interval arithmetic is applied to complex functions. Specifically, the operands of each hidden neuron depend on the same input to the DNN, but interval arithmetic assumes that they are independent and may thus compute an output range much larger than the true range. For instance, consider a simplified neural network in which input x is fed to two neurons that compute $2x$ and $-x$ respectively, and the intermediate outputs are summed to generate the final output $f(x) = 2x - x$. If the input range of x is $[0, 1]$, the true output range of $f(x)$ is $[0, 1]$. However, naive interval arithmetic will compute the range of $f(x)$ as $[0, 2] - [0, 1] = [-1, 2]$, introducing a huge overestimation error.

Much of our research effort in ReluVal focuses on mitigating this challenge; here we describe two effective techniques to tighten output bounds. The first is *symbolic interval*, similar to symbolic execution for traditional software [16, 45, 66, 67]. In particular, ReluVal tracks the intermediate computations using not only the intervals but also the symbolic values whenever possible. In the preceding example, ReluVal tracks the intermediate outputs symbolically ($[2x, 2x]$ and $[-x, -x]$ respectively) to compute the range of the final output as $[x, x]$. When propagating symbolic bound constraints across a DNN, ReluVal correctly handles non-linear functions such as ReLU ($max(x, 0)$), one of the most common neuron activation functions, and calculates proper symbolic upper and lower bounds.

The second is *iterative interval refinement*. When the output range of the DNN is too large to be conclusive, ReluVal iteratively bisects the input range and repeats the range propagation on the smaller input ranges. This technique is in a spirit similar to abstraction refinement [11, 38]. Mathematically, we prove that interval refinement on practical DNNs always converges in finite steps.

Compared to the state-of-art DNN verifier Reluplex which leverages SMT and linear programming solvers, ReluVal is on average over 200× faster. In addition, ReluVal is amenable to massive parallelization so that the speedup could be much bigger compared hard-to-parallelize SMT solvers. Concurrent to ReluVal, other DNN verifiers [28, 81, 88] have also been developed. To the best of our knowledge, ReluVal is the only one that scales to DNNs with tens of thousands of neurons.

3.5 Neurify

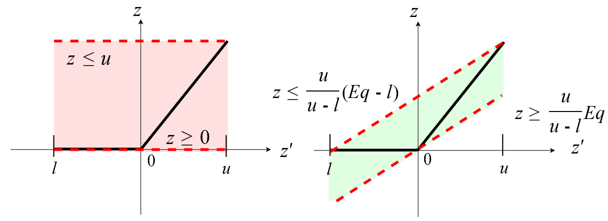
We build Neurify to address two challenges in ReluVal. Consider $ReLU(x) = max(x, 0)$. When the symbolic input interval may span 0, ReluVal concertizes the output interval to $[0, u]$ where u is the concrete upper bound of x, shown in Figure 1(a). It does so to avoid symbolic reasoning of both linear pieces of the ReLU, which may easily explode considering the large number of ReLU nodes in a DNN. However, this concretization method eliminates any symbolic dependencies tracked. Second, ReluVal bisects the DNN input interval to refine the DNN output bound, but doing so at the DNN input is not efficient or direct because overestimation happens actually at internal ReLU nodes.

Neurify solves these challenges using two techniques. First, instead of concretizing the output interval of an overestimated node to $[0, u)$, Neurify uses *symbolic interval relaxation* to bound the output as shown in Figure 1(b), simultaneously simplifying the symbolic constraints to avoid explosion while retaining more accurate dependencies. This technique is similar to linear relaxation in [88], but Neurify adapts it to represent the bounds symbolically. Second, Neurify splits directly at an overestimated node and produces two sets of linear equations, one covering the case when the node input is smaller than or equal to 0, the other the node input is greater than 0. Each set of linear equations is then solved efficiently using off-the-shell LP solvers.

These techniques cut down overestimation errors by up to 59.64% compared to ReluVal. As a result, Neurify is over 20× faster than ReluVal and 5,000× faster than Reluplex.

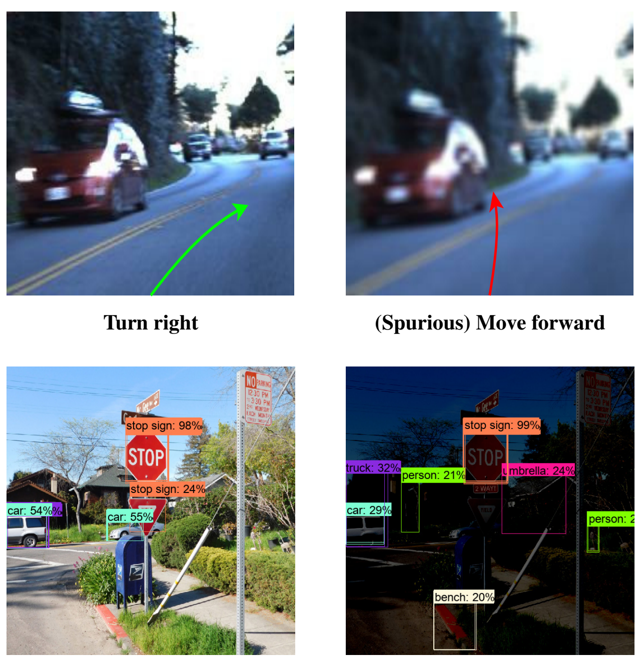
4 A TASTE OF THE RESULTS

We evaluate our comprehensive toolset on a wide range of applications including the safety-critical domains as well as common benchmarks. These include (1) 12 ImageNet classification models [18, 37, 40, 41, 69, 75, 76, 95]; (2) 6 self-driving systems such as Nvidia's DAVE2 [3, 4, 10, 15, 21, 22, 83]; (3) 5 online commercial vision APIs [8, 19, 34, 42, 54] built by the largest companies including Google, Microsoft, Amazon, and IBM; (4) 4 handwritten digit classification models [47];



(a) Naive concretizaion (b) Symbolic linear relaxation

Figure 1: Subfigure (a) shows how ReluVal concretizes the output interval of a ReLU when its input spans 0, and (b) how Neurify uses symbolic linear relaxation to simplify constraints while retaining dependencies.



Turn right (Spurious) Move forward

No pedestrian (Spurious) Pedestrian detected

Figure 2: The right shows error-inducing inputs generated from the original inputs (left). The properties and models under test are (from top to bottom): blurring on Rambo, brightening on Faster-RCNN Inception-V2.

(5) 42 models in aircraft collision avoidance systems (ACAX XU) [44]; and (6) 6 malware detectors for Android and PDF files [9, 24, 36, 60, 72, 73, 82, 84].

As our extensive evaluation on these datasets and systems shows, our tools effectively found thousands of error-inducing inputs even for models with state-of-the-art accuracy. They also verified the absence of errors for up to 32% of the images ImageNet dataset are robust against transformations described in Section 2. Figure 2 presents some interesting errors found. The upper row shows that Rambo [22], Top-ranked self-driving models in Udacity challenge [3, 4, 22] is not robust against blurring effect. The lower row shows that state-of-the-art object detection model – faster RCNN [64] detects spurious pedestrian when the lighting condition changes. Besides images, our tools also found errors in non-visual DNNs such as malware detectors [60, 72]. For instance, changing three attributes of a malicious PDF file – size from 1 to 34, number of actions from 0 to 21, and number of font objects from 1 to 20 – causes the malware detector to classify it as benign.

5 CONCLUSIONS AND OPEN CHALLENGES

In this article, we reviewed the tools and core techniques we have developed in the last three years towards rigorous testing and verification of DL systems. Although the initial results are auspicious, several difficult open challenges remain to be addressed.

First, as discussed in Section 2, all current DNN verification tools focus on verifying properties on a limited set of samples with the hope that the guarantees achieved on individual samples generalize to unseen samples. We believe this fundamental question requires making certain probabilistic assumptions on the distributions of the dataset (i.e., the distribution of available data is the same with those unseen) – the same underlying assumption for why machine learning generalizes. The next concrete research question is how we can adapt existing specific testing and verification techniques (e.g., interval analysis, mixed-integer programming) on reasoning distributions of inputs.

Second, the properties and specifications considered so far are largely “syntactic" such as changing the lighting effect should not change an image’s semantics. How can we support verification of richer properties and semantic transformations such as "changing the season from summer to winter?"

Third, although our tools support many operations (e.g., convolutions and ReLUs) in DNNs, they cannot handle batch normalization or other activation functions such as Sigmoid [29]. How to define reasonable coverage metric or compute intervals or sound overapproximation for these operations?

These open research questions are by no means a complete list in this exciting new research area. For instance, robust training is another exciting direction that leverages the errors found to train more robust DNNs. We hope our initial research findings and insights introduced in this article helps shed light on these important topics and inspire more research effort towards reliable DL.

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