NeVer 2.0: Learning, Verification and Repair of Deep Neural Networks

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Abstract. In this work we present an early prototype of NeVer 2.0, a new system for automated synthesis and analysis of deep neural networks. NeVer 2.0 borrows its design philosophy from NeVer, the first package that integrated learning, automated verification and repair of (shallow) neural networks in a single tool. The goal of NeVer 2.0 is to provide a similar integration for deep networks by leveraging a selection of state-of-the-art learning frameworks and integrating them with verification algorithms to ease the scalability challenge and make repair of faulty networks possible.

Keywords: Deep Neural Networks · Network Pruning · Network Verification.

1 Introduction

Adoption and successful application of deep neural networks (DNNs) in various domains have made them one of the most popular machine-learned models to date — see, e.g., [27] on image classification, [35] on speech recognition, and [15] for the general principles and a catalog of success stories. Despite the impressive progress that the learning community has made with the adoption of DNNs, it is well known that their application in safety- or security-sensitive contexts is not yet hassle-free. From their well-known sensitivity to adversarial perturbations [26,6,25], i.e., minimal changes to correctly classified input data that cause a network to respond in unexpected and incorrect ways, to other less-investigated, but possibly significant properties — see, e.g., [18] for a catalog — the need for tools to analyze and possibly repair DNNs is strong.

As witnessed by an extensive survey [10] of more than 200 recent papers, the response from the scientific community has been equally strong. As a result, many algorithms have been proposed for verification of neural networks and tools implementing them have been made available. Some examples of well-known and fairly mature verification tools are Marabou [13], an SMT-based tool that answers queries regarding the properties of a DNN by transforming the queries into constraint satisfiability problems; ERAN [25], a robustness analyzer based on abstract interpretation and MIPVerify [28], another robustness analyzer based
on mixed integer programming (MIP). Other widely-known verification tools are Neurify [31], a robustness analyzer based on symbolic interval analysis and linear relaxation, NNV [30], a tool implementing different methods for reachability analysis, Sherlock [31], an output range analysis tool and NSVerify [2], also for reachability analysis. A number of verification methodologies — without a corresponding tool — is also available like [32], a game based methodology for evaluating pointwise robustness of neural networks in safety-critical applications. Most of the above-mentioned tools and methodologies work only for feedforward fully-connected neural networks with ReLU activation functions, with some of them featuring verification algorithms for convolutional neural networks with different kinds of activation function. To the best of our knowledge, current state-of-the-art tools are restricted to verification/analysis tasks, in some cases they are limited to specific network architectures and they might prove difficult to use for the non-initiated.

In this work we present an early prototype of NeVer 2.0, a new system that aims to bridge the gap between learning and verification of DNNs and solve some of the above mentioned issues. NeVer 2.0 borrows its design philosophy from NeVer [22], the first tool for automated learning, analysis and repair of neural networks. NeVer was designed to deal with multilayer perceptrons (MLPs) and its core was an abstraction-refinement mechanism described in [21,23]. As a system, one peculiar aspect of NeVer was that it included learning capabilities through the shark [11] library. Concerning the verification part, NeVer could utilize any solver integrating Boolean reasoning and linear arithmetic constraint solving — HYSAT [5] at the time. A further peculiarity of the approach was that NeVer could leverage abstract counterexamples to (try to) repair the MLP, i.e., retrain it to eliminate the causes of misbehaviour.

Our goal for NeVer 2.0 is to provide the same features of NeVer, but in an updated package that has the following features:

- Loading of datasets, trained and untrained models provided in a variety of formats; currently NeVer 2.0 supports directly popular datasets, e.g., MNIST [16] and Fashion MNIST [33], but support for further datasets can be added through a common interface; models (either trained or not) can be supplied to NeVer 2.0 using ONNX [3] and PyTorch [4] formats — TensorFlow [5] support is under development.
- Training of DNNs through state-of-the-art frameworks; currently NeVer 2.0 is based on PyTorch, but further extensions are planned to handle different kinds of learning models (e.g., kernel-based machines) that are not handled natively by PyTorch, or to leverage specific capabilities of other learning frameworks.
- Manipulation of DNNs including, but not limited to, pruning [24], quantization [34], and transfer learning [29]; currently NeVer 2.0 builds on Py-

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3 https://onnx.ai/
4 https://pytorch.org/
5 https://www.tensorflow.org/
TORCH to manipulate DNNs, and only two mainstream pruning techniques are implemented, namely network slimming \cite{24} and weight pruning \cite{17}.

- Verification of DNNs: currently, NeVer 2.0 leverages external tools as backends to provide verification capabilities; connectors to Marabou \cite{13}, ERAN \cite{25} and MIPVerify \cite{28} are currently implemented; we plan to add abstraction-refinement algorithms that improve on and extend those available in NeVer, but their development is still underway.

- Repair of DNNs should enable the results of verification to improve on the results of learning; currently, NeVer 2.0 features the same mechanism of NeVer, i.e., it relies on the capability of the embedded learning algorithms to exploit counterexamples and retrain the network in a better way — a sort of adversarial training guided by verification; we expect to reach tighter integration of verification and learning once our custom verification algorithms are implemented.

The version of NeVer 2.0 corresponding to this work is available online \cite{8} under the Commons Clause (GNU GPL v3.0) license.

The rest of the paper is structured as follows. In Section 2 we introduce some basic notations and definition to be used through the paper. In Section 3 we describe the architecture and the current implementation of NeVer 2.0. In Section 4 we show some early results obtained with NeVer 2.0 prototype using MNIST datasets to learn and verify fully-connected ReLU networks. We conclude the paper with and our future research agenda in Section 5.

2 Preliminaries

A neural network is a system of interconnected computing units called neurons. In fully connected feed-forward networks, neurons are arranged in disjoint layers, with each layer being fully connected only with the next one, and without connection between neurons in the same layer. Given a feed-forward neural network $N$ with $n$ layers, we denote the $i$-th layer of $N$ as $h^{(i)}$. We call a layer without incoming connections input layer $h^{(1)}$, a layer without outgoing connections output layer $h^{(n)}$, while all other layers are referred to as hidden layers. Each hidden layer performs specific transformations on the inputs it receives. In this work we consider hidden layers that make use of linear and batch normalization modules.

Given an input vector $x$, a linear module computes a linear combination of its values as follows:

$$L^{(i)} = W^{(i)} \cdot x + b^{(i)}$$  \hspace{1cm} (1)

where $W^{(i)}$ is the matrix of weights and $b^{(i)}$ is the vector of the biases associated with the linear module in the $i$-th layer and $L^{(i)}$ is the corresponding output. Entries of both $W^{(i)}$ and $b^{(i)}$ are learned parameters. In our target architectures, each linear module is followed by a batch normalization module. This is done to address the so-called internal covariate shift problem, i.e., the change
of the distribution of each layer’s input during training \[12\]. The mathematical formulation of batch normalization layers can be expressed as

$$
BN^{(i)} = \frac{\gamma^{(i)}}{\sqrt{\sigma^{(i)} + \epsilon^{(i)}}} \odot (L^{(i)} - \mu^{(i)}) + \beta^{(i)}
$$

(2)

All the operators in this equation are element-wise operators: in particular \(\odot\) and the fractional symbol represent respectively the Hadamard product and division. \(BN^{(i)}\) and \(L^{(i)}\) are the output and the input vectors of the module, respectively. \(\gamma^{(i)}, \mu^{(i)}, \sigma^{(i)}, \beta^{(i)}\) are vectors, whereas \(\epsilon^{(i)}\) is a scalar value. These are learned parameters of the batch normalization layer. In particular \(\mu^{(i)}\) and \(\sigma^{(i)}\) are the estimated mean and variance of the inputs computed during training.

Finally, the output of hidden layer \(i\) is computed as \(h^{(i)} = \Phi^{(i)}(BN^{(i)})\), where \(\Phi^{(i)}\) is the activation function associated to the neurons in the layer. We consider only networks utilizing Rectified Linear Unit (ReLU) activation functions, i.e., \(\Phi^{(i)} = \max(0, BN^{(i)})\). Given an input vector \(x\), the network \(N\) computes an output vector \(y\) by means of the following computations

$$
\begin{align*}
    h^{(1)} &= x \\
    h^{(i)} &= \Phi^{(i)}(BN^{(i)}(L^{(i)}(h^{(i-1)})))) \quad i = 2, \ldots, n-1 \\
    y &= h^{(n)} = L(h^{(n-1)})
\end{align*}
$$

(3)

A neural network can be considered as a non-linear function \(f_w: \mathcal{X} \rightarrow \mathcal{Y}\), where \(\mathcal{X}\) is the input space of the network, \(\mathcal{Y}\) is the output space and \(w\) is the vector representing the weights of all the connections. We consider neural network applied to classification of \(d\)-dimensional vectors of real numbers, i.e., \(\mathcal{X} \subseteq \mathbb{R}^d\) and \(\mathcal{Y} \subseteq \mathbb{R}^m\), where \(d\) is the dimension of the input vector and \(m\) is the dimension of the output vector and thus also the number of possible classes of interest. We assume that given an input sample \(x\) the output vector \(f_w(x)\) contains the likelihood that \(x\) belongs to one of the \(m\) classes. The specific class can be computed as

$$
\arg \max_{c \in \{1, \ldots, m\}} (f_w(x))_c
$$

where \((f_w(x))_c\) denotes the \(c\)-th element of \(f_w\). Training of (deep) neural networks poses substantial computational challenges since for state-of-the-art models the size of \(w\) can be in the order of millions. As in any machine learning task, training must select weights to maximize the likelihood that the network responds correctly, i.e., if the input \(x\) is of class \(k\), the chance of misclassification should be as small as possible, where misclassification occurs whenever the following holds

$$
\arg \max_{c \in \{1, \ldots, m\}} (f_w(x))_c \neq k
$$

Training can be achieved through minimization of some kind of loss function whose value is low when the chance of misclassification is also low. While there
are many different kinds of loss functions, in general they are structured in the following way:

\[ J(w) = \frac{1}{n} \sum_{k=0}^{n} Err(y_k, \text{arg max}_{c \in \{1, \ldots, m\}} (f_w(x_k))_c) + \lambda \cdot Reg(w) \] (4)

where \( n \) is the number of training pairs \((x_k, y_k)\), \( y_k \) is the correct class label of \( x_k \), \( Err \) represents the loss caused by misclassification, \( Reg \) is a regularization function, and \( \lambda \) is the parameter controlling the effect of \( Reg \) on \( J \). The regularization function is needed to avoid overfitting, i.e., the high variance of the training results with respect to the training data. The regularization function usually penalizes models with high complexity by smoothing out sharp variations induced in the trained network by the \(Err\) function. A common regularization function is, for example, the L2 norm:

\[ Reg(w) = \frac{1}{2n}||w||_2 \] (5)

### 3 System architecture and implementation

**NeVer 2.0** is conceived as a modular API to manage DNNs, from training to verification and repair. In Figure 1 we present an overview of the architecture divided in six main packages. The main elements we consider in this work are training, pruning and verification: these packages are organized mostly around Strategy patterns that define general interfaces to perform network operations, and specialized subclasses that actually support those operations. Additionally, to have full control of the internal model and to separate the main elements from implementation details, we designed our own network representation structured as a graph whose nodes correspond to disjoint layers. To leverage the capabilities of current learning frameworks, we designed a set of conversion strategies to/from our internal representation and the representations whereon learning frameworks are based. The aims and the internal structures of the packages shown in Figure 1 are described in detail in the remainder of this Section.
3.1 Internal Representation

The classes supporting the internal representation are shown in Figure 2. There are two abstract base classes, namely `NeuralNetwork` and `LayerNode`. Conceptually, `NeuralNetwork` is a container of `LayerNode` objects organized inside as a graph. A list of `ModelRepresentation` objects is kept for internal usage — see subsection 3.2 for details. In the current prototype the only concrete subclass of `NeuralNetwork` is `SequentialNetwork` which represents networks whose corresponding graph is a list, i.e., each layer is connected only to the next one. More complex topologies for concrete architectures can be implemented, should the need arise. The concrete subclasses of `LayerNode` are the building blocks that we currently support: `BatchNorm1DNode`, `FullyConnectedNode` and `ReLUNode`, i.e., batch normalization layers, fully connected layers and ReLU layers, respectively. These building blocks are sufficient to encode the DNNs that we introduced in Section 2. It should be noted that our representation is not an “executable” representation, i.e., it does not provide the capability to compute the output of a DNN given the input, therefore our nodes contain only enough information to create the corresponding executable representations in different learning frameworks and/or support the encoding for verification purposes. The class `Tensor` is our utility class for tensorial data. Currently it is simply an alias for the `ndarray` class in `numpy`, but we have added it as a wrapper to isolate NEVer 2.0 classes from implementation details.

3.2 Converters and Representations

The design of a model representation to generalize those used in different learning frameworks is based on the Adapter design pattern, as shown in Figure 3. We have defined the abstract class `ModelRepresentation`, which is then specialized by `PyTorchNetwork` and `ONNXNetwork` to encode PyTorch and ONNX models, respectively. The concrete subclasses wrap the actual network model in the corresponding learning framework or interchange format, as in the case of ONNX. Conversion between our internal representation and the concrete subclasses of...
ModelRepresentation are provided by subclasses of ConversionStrategy — we may consider this also as a Builder pattern implementation. ConversionStrategy defines an interface with two functions: one for converting from our internal representation to a specific model representation, and the other for performing the inverse task. The concrete subclasses of ConversionStrategy implement the functions for the corresponding concrete subclasses of ModelRepresentation. As new type of learning frameworks/model are added to NeVer 2.0, new concrete subclasses of ModelRepresentation should be added to support conversion.

### 3.3 Training

In Figure 4 we show the internal design of the Training package whose main element is the abstract class TrainingStrategy. The current abstraction of a training strategy features a single function which requires a NeuralNetwork and a Dataset and returns a (trained) NeuralNetwork. The concrete subclasses of TrainingStrategy provide the actual training procedures. Currently, we have designed and implemented a single training procedure based on the Adam optimizer [14] and adapted to the concrete pruning procedures we have implemented. Our implementation requires a PyTorch representation to train the network, but this is handled transparently by NeVer 2.0 architecture. The class Dataset is meant to represent a generic dataset. As such it features four functions: one for loading the training set — the set of data considered to train the network — one for loading the test set — the set of data considered to assess the accuracy of the
network and two for adding a data sample to the training set and to the test set respectively. The actual datasets are represented by concrete subclasses of Dataset. Currently, we have implemented the corresponding concrete class for the MNIST dataset MNISTDataset and for the FMNIST dataset FMNISTDataset.

### 3.4 Pruning

As mentioned in our paper [7], we believe that pruning can be one of the keys to ease the verification of DNNs, therefore we decided to include abstractions and concrete classes to support pruning in the current realization of NeVER 2.0. In Figure 5 we show the architecture, where the abstract class PruningStrategy is meant to represent a generic pruning methodology, and consists of a single function which requires a NeuralNetwork and a Dataset and returns the pruned NeuralNetwork. Concrete subclasses implement the actual pruning procedures: currently we have designed and implemented two concrete strategies, namely WeightPruning and NetworkSlimming — both based on PyTorch representations. In particular, the former strategy selects all the weights which are smaller than a certain threshold and sets them to 0. The latter strategy leverages the weights of the batch normalization layers to identify low-importance neurons and remove them from the network — more details can be found in [9] and [19]. The distinctive parameters of the pruning strategies are provided as attributes in the concrete classes. In particular, if pre-training and/or fine-tuning are required for the pruning procedure then a suitable training strategy must be provided to the pruning strategy as an attribute.

### 3.5 Verification

As shown in Figure 6 we have designed the abstract class VerificationStrategy to represent a generic verification methodology. This abstract class defines an interface consisting of a single function which requires a NeuralNetwork and a Property and returns a Boolean value depending on whether the property is verified or not and a counterexample (if available). The abstract class Property represents a generic property that should be verified. Currently we have two
Fig. 6. UML diagram of the classes related to the verification strategies.

concrete classes: SMTLIBProperty and LocalRobustnessProperty. SMTLIBProperty represent a generic property which NeVer 2.0 reads from a file formatted according to SMTLIB\textsuperscript{6} syntax \cite{3}. LocalRobustnessProperty is a “pre-cooked” property encoding the search of an adversarial example corresponding to a specific data sample. The concrete subclasses of VerificationStrategy that we have implemented so far are EranVerification, MarabouVerification and MIPVerifyVerification which leverage, respectively, ERAN \cite{25}, Marabou \cite{13} and MIPVerify to verify the property.

4 Preliminary experimental analysis

We test the current capabilities of NeVer 2.0 by replicating the setup of the experiment reported in \cite{7}. In this experiment we analyze how the integration of pruning and verification can ease analysis of DNNs — currently, a distinctive capability that NeVer 2.0 offers. We test two different network architectures and two different pruning methods considering all three verification backends available in NeVer 2.0. The DNNs we consider are both fully connected networks with three hidden layers: one with 64, 32, 16 hidden neurons, and the other with 128, 64, 32 hidden neurons. In both networks the activation function is the ReLU. We experimented with weight pruning (based on \cite{9}) and network slimming (based on \cite{19}). To analyze the performances of the different pruning methods we test them with three different sets of pruning parameters which correspond to increasing magnitudes of pruning. The results of our experiment are summarized in Table 1. We consider three versions of each DNN: the version before pruning (baseline), the one obtained after a specialized training for network slimming (sparse), the version after the application of weight pruning (WP) and the one obtained after network slimming (NS). The results of our experiment prove that NeVer 2.0 — albeit still at the prototypical stage — is ready to verify networks of some practical interest, and its combination of pruning and verification may offer some advantage over the straight usage of its backends.

\textsuperscript{6} http://smtlib.cs.uiowa.edu/
Table 1. Results — originally reported in [7] — obtained by running NeVer 2.0 with Marabou, ERAN and MIPVerify. The values reported represent the number of problems which were solved successfully within the timeout of 600 CPU seconds. The column Base represent the base architecture, Param represent the set of parameters used for increasing magnitude of pruning and Network represent the kind of network considered. Marabou, MIPVerify, and ERAN represent the number of problems solved by Marabou, MIPVerify and ERAN, respectively.

5 Planned extensions

NeVer 2.0 is an ongoing project and we have already planned various extensions. First, we aim to increase the variety of networks that can be represented by adding more concrete subclasses to LayerNode. In particular, we expect to be able to design and implement convolutional layers, the related batch normalization layers, different kinds of pooling layers and different kinds of activation functions. With these extensions, that should be matched by corresponding training, pruning and verification enhancements, NeVer 2.0 should be able to represent all the main kinds of DNNs which current state-of-the-art verification methodologies can deal with.

The second addition that we have already planned, relates to the addition of converters to/from other major learning frameworks, starting from TensorFlow. This addition should include also the capability of visualizing and modifying the network architecture through a graphical user interface, in the hope that NeVer 2.0 becomes more easily accessible also to the non-initiated.

Further additions that we wish to add include quantization, which we believe would create interesting synergies with pruning, and repair, i.e, the capability to modify a neural network to make it compliant to the property of interest. In particular, besides basic form of repair that are already supported by NeVer 2.0, i.e., verification-based adversarial learning, we expect to provide tighter integration between learning and verification.
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