eNNcode: Optimization-Based Analysis of Neural Networks

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Abstract

The increasing use of neural networks (NNs) in high-stakes decision-making requires rigorous analysis to ensure safety, fairness, and explainability. Formal verification tools for neural networks typically focus on determining the *satisfiability* of properties such as safety or fairness. However, many fairness and explainability tasks go beyond satisfiability and instead rely on arbitrary *optimization* objectives. To address such problems, neural networks are often encoded as mixed-integer linear optimization (MILO) problems with linear objectives. In practice, these encodings are usually implemented in an ad-hoc manner, limiting comparability across works, reducing transparency, and increasing implementation effort. We address this gap by introducing eNNcode, a user-friendly PyPI library that converts any neural network with piecewise-linear activation function in Open Neural Network Exchange (ONNX) format into a MILO instance. The library supports arbitrary linear constraints on input and output nodes, as well as user-defined optimization objectives. Our experiments show that eNNcode achieves performance comparable to existing libraries, despite its simplicity and ease of use. Overall, eNNcode facilitates reproducible and standardized optimization-based analysis of neural networks.

1 Introduction

Deep neural networks have achieved remarkable success in domains such as computer vision and natural language processing, leading to their widespread adoption in numerous real-world AI applications, including safety-critical areas such as healthcare and autonomous driving. Despite these achievements, neural networks often operate as black-box models, making their internal reasoning difficult to interpret. Moreover, several types of vulnerabilities have been identified in modern architectures, one of the most prominent being *adversarial fragility* [Szegedy *et al.*, 2014]. This term refers to the tendency of models to produce drastically different predictions when their inputs are modified by small, carefully crafted perturbations. The growing awareness of such reliability issues has even led to the establishment of specialized databases to track AI-related incidents and prevent recurring failures [McGregor, 2021].[1]

To address these challenges, formal verification techniques for neural networks have emerged as a powerful tool to ensure the safety and reliability of neural networks. Unlike statistical methods such as cross-validation that evaluate model behavior on finite datasets, formal verification aims to mathematically prove whether certain properties, such as safety or robustness, hold for all possible inputs. These approaches typically check the *satisfiability* of logical specifications [Demarchi *et al.*, 2023], which is sufficient to determine whether a given property is guaranteed by the network.

However, tasks related to explainability or fairness often go beyond satisfiability and instead require solving optimization problems, for example, determining the minimal change a loan applicant must make for their application to be accepted. While user-friendly tools for formal verification exist already, such as the CAISAR platform [Girard-Satabin *et al.*, 2022], there is still no widely adopted framework that supports optimization-based analysis of neural networks. In fact, encoding a neural network into MILO is usually implemented in an ad-hoc manner, limiting comparability across works, reducing transparency, and increasing implementation effort. To bridge this gap, we introduce eNNcode, a lightweight and user-friendly library that converts any neural network with piecewise-linear activation functions into a MILO instance. In contrast to existing tools such as Gurobi-ML [Gurobi Optimization, LLC, 2024b], eNNcode accepts models in the standardized ONNX fformat, making it independent of underlying machine-learning libraries, and supports convolutional layers that Gurobi-ML does not handle. Moreover, unlike OMLT [Ceccon *et al.*, 2022], eNNcode remains lightweight, easy to install, and designed for maximum usability. Our experiments demonstrate that eNNcode achieves runtime and memory performance comparable to existing libraries while overcoming their practical limitations in usability and model compatibility. A demonstration of our PyPI-library[2] is available as a video.[3]

[1]https://incidentdatabase.ai/
[2]https://pypi.org/project/enncode/
[3]https://doi.org/10.5281/zenodo.20427178

2 Related Work

Constrained optimization in machine learning is an active research area.[4] In particular, mathematical optimization over neural networks is a central theme in research on counterfactual explanations and various other topics [Jiang *et al.*, 2023b; Marzari *et al.*, 2024; Jiang *et al.*, 2024; Benussi *et al.*, 2022; Jiang *et al.*, 2023a; Wu *et al.*, 2020; ElAraby *et al.*, 2023; Ovalle *et al.*, 2025; Dong *et al.*, 2025; Stinchfield *et al.*, 2025; Grimstad and Andersson, 2019; Papalexopoulos *et al.*, 2022; Lorenz *et al.*, 2025]. Despite this relevance, there is no widely adopted tool for encoding neural networks into optimization models. Many of the above works implement custom formulations rather than relying on a shared library—hindering comparability and increasing prototyping effort. We therefore review existing libraries for encoding neural networks as constraints and discuss limitations that may impede broader adoption. The most prominent tool is Gurobi Machine Learning (GurobiML) [Gurobi Optimization, LLC, 2024b], which converts trained models directly into constraints within a Gurobi model. While reliable, GurobiML supports only linear layers with ReLU activations and lacks compatibility with the standardized ONNX format; it instead requires access to source code from frameworks such as PyTorch or Keras. Other tools build upon algebraic modeling languages such as Pyomo [Bynum *et al.*, 2021]. For instance, ReluMIP [Lueg *et al.*, 2021] translates ReLU-based networks into MILO formulations via Pyomo or Gurobi interfaces. Similarly, the Optimization & Machine Learning Toolkit (OMLT) [Ceccon *et al.*, 2022] embeds trained ML models into optimization problems using Pyomo to express network architectures as constraints. Although this promotes solver independence, significant additional effort emerges during model instantiation. Finally, verification frameworks such as DNNV [Shriver *et al.*, 2021] offer unified interfaces for verifiers like MIPVerify [Tjeng *et al.*, 2019] and Marabou [Wu *et al.*, 2024]. However, these tools only support verification tasks rather than optimization, placing them outside of our scope.

3 Overview

We visualize the workflow of eNNcode in Figure 1. Consider a user who has trained a neural network and exported it in the standardized Open Neural Network Exchange (ONNX) format. The goal is to perform rigorous mathematically grounded analysis, such as optimization or verification, on the network. To enable this, eNNcode converts the ONNX model into a MILO instance, where the input nodes of the neural network become free decision variables and all intermediate and output nodes are defined as linear constraints that faithfully encode the network's behavior. This transformation allows users to express arbitrary linear objectives or additional constraints on inputs and outputs while preserving exact functional equivalence with the original neural network.

On a technical level, eNNcode begins by parsing the provided ONNX file into an internal representation of the neural network. The parser follows a factory-pattern architecture, instantiating specialized parsers for each

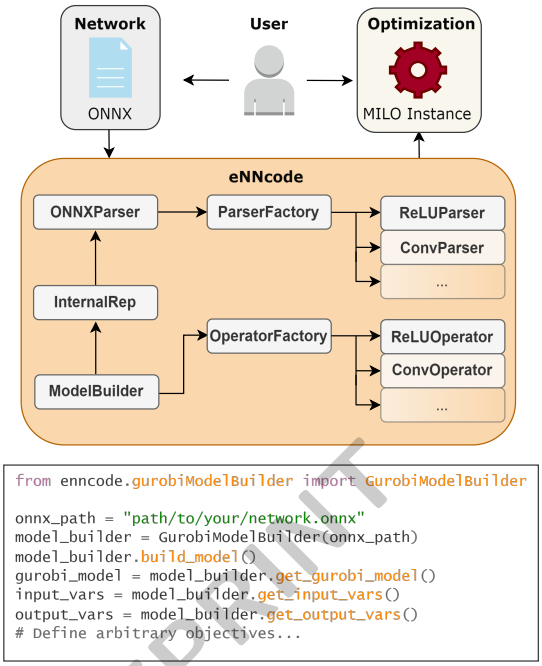

Figure 1: Workflow with eNNcode

supported node operation to ensure modularity and extensibility. Currently, eNNcode supports all piecewise linear operators defined in the Verification of Neural Networks Competition [Demarchi *et al.*, 2023], including `Add`, `Sub`, `Mul`, `Div`, `MatMul`, `AveragePool`, `MaxPool`, `Conv`, `ReLU`, `Concat`, `Reshape`, `Flatten`, `Unsqueeze`, `BatchNormalization`, `Dropout`, `Gemm`, and `Identity`. In practice, these operations can represent architectures that are powerful enough for image-based tasks [Redmon *et al.*, 2016; Krizhevsky *et al.*, 2012; Simonyan and Zisserman, 2015].

Once parsed, the internal representation contains all information required to encode the network as a MILO instance. Similarly to parsing, encoding also adopts a factory pattern in which each operation type has a dedicated implementation that converts the operation into linear constraints. After successful initialization, the resulting MILO model is returned to the user, who can then define additional constraints or optimization objectives directly on this instance. To facilitate usability, metadata such as variable names corresponding to input and output nodes are exposed through the interface. The lower half of Figure 1 illustrates, from a user-perspective, how simple it is to obtain the Gurobi instance from an ONNX-formatted network with eNNcode.

Compatibility ONNX files represent the computational graph of a neural network. The set of supported operators, their attributes and expected semantics are defined by the Operator Set (Opset) [The ONNX Community, 2026]. Because newer Opset versions may introduce additional operators or modify existing ones, the current implementation of eNNcode is based on the specifications of the Opset version 11 but remains compatible with other versions, provided that they do not alter the definitions of node types supported

[4] See NeurIPS'25 Workshop: Constrained Optimization for ML

	Time (Sec.)				**Storage** (MByte)			
Variant	MNIST	MNIST *(CNN)*	Concrete	Wine	MNIST	MNIST *(CNN)*	Concrete	Wine
eNNCode	10.686 ± 5.147	13.901 ± 09.291	0.0256 ± 0.0013	0.0335 ± 0.0014	01.299 ± 0.0852	01.712 ± 0.085	0.0451 ± 0.0107	0.0534 ± 0.0110
OMLT	08.057 ± 1.706	14.077 ± 23.281	0.0405 ± 0.0136	0.0474 ± 0.0140	21.770 ± 0.1271	13.919 ± 0.356	0.2911 ± 0.2662	0.3451 ± 0.2670
Gurobi-ML	05.919 ± 4.657	-	0.0223 ± 0.0005	0.0241 ± 0.0009	00.818 ± 0.0006	-	0.0521 ± 0.0008	0.0559 ± 0.0006

Table 1: Overview on the time and memory consumption.

by eNNcode. To ensure correct translation, compatibility of the ONNX model with the GurobiPy instance is automatically verified. When incompatibilities are detected, detailed and precise error messages are returned to the user. Upon successful conversion, eNNcode performs an automatic correctness validation to ensure that the MILO encoding faithfully represents the original neural network. This validation compares the outputs produced by the encoded optimization model with those computed by the ONNX Runtime [Microsoft and ONNX Runtime Contributors, 2024]. Specifically, MILO input variables are fixed to random values, and the optimizer's output is compared against ONNX Runtime references. If discrepancies occur, eNNcode iteratively analyzes subgraphs to isolate faulty nodes and provide precise user feedback.

4 Experiments

Although the main contribution of our library is qualitative, namely providing a user-friendly interface with broad support for neural layer types, we also present a quantitative comparison in terms of runtime and memory usage.

Baselines We compare eNNcode with two existing libraries: OMLT [Ceccon *et al.*, 2022] and Gurobi Machine Learning [Gurobi Optimization, LLC, 2024b]. OMLT is an optimizer-agnostic framework built on top of Pyomo [Bynum *et al.*, 2021], offering support for encoding neural networks in ONNX models as optimization models. Gurobi Machine Learning is an open-source library developed by Gurobi that supports relatively simple architectures, excluding convolutional layers, for several major machine-learning frameworks such as TensorFlow and PyTorch. We exclude ReLU-MIP [Lueg *et al.*, 2021] from our comparison because it only supports sequential TensorFlow models, which we consider too restrictive for general applicability. Verification frameworks are also omitted, as they are restricted to property checking rather than optimization tasks, which is the focus of our work. To the best of our knowledge, OMLT and Gurobi-ML represent the only publicly available libraries capable of translating neural networks into MILO instances without imposing strong restrictions.

Benchmark In our experiments, we search for counterfactual explanations (CXs) across various neural network classifiers. For a given input $x \in \mathbb{R}^n$ to a (binary) classifier $h : \mathbb{R}^n \to \{0, 1\}$, a CX is an instance $x' \in \mathbb{R}^n$ that induces an alternative classification, i.e., $h(x') \neq h(x)$, while remaining as close as possible to the original input according to the distance $d_{\ell_1}(x, x')$ [Wachter *et al.*, 2017]. This definition extends naturally to multi-class classifiers.

Our benchmark includes four networks. Two of them are taken from the example notebooks of OMLT [Cecrle *et al.*, 2024] and trained on the MNIST dataset [Deng, 2012]. The remaining two are binary classifiers for tabular datasets commonly used in counterfactual explanation research: one trained on the *Concrete Compressive Strength Dataset* [Yeh, 1998], and the other on the *Wine Quality Dataset* [Cortez *et al.*, 2009]. All four models exclusively use ReLU activation functions. We evaluate runtime and memory consumption over multiple iterations. In each iteration, a network receives an original data point from its corresponding dataset along with a randomly selected target class that differs from the ground-truth label. We measure all steps required for model initialization and subsequent optimization. Additionally, we impose a time limit of 240 seconds for each optimization call.

Results & Discussion The results are summarized in Table 1. We first discuss the runtime performance. In general, no clear winner can be identified across all benchmarks. For the fully connected MNIST network, Gurobi-ML achieves the best average runtime, but this advantage is limited since it does not support convolutional layers and cannot be applied to the MNIST CNN benchmark [Gurobi Optimization, LLC, 2024a]. In contrast, both *eNNCode* and OMLT support fully connected as well as convolutional networks and achieve comparable runtimes, with a slight advantage of *eNNCode* over OMLT on the tabular classifiers. Within the specified time limit, all variants find counterfactual explanations except for OMLT on the MNIST CNN, where approximately 40% of the runs reach time out (excluded from the reported results). Regarding memory consumption, OMLT consistently exhibits by far the highest storage requirements in all test cases, likely due to its more complex internal workflow. In comparison, *eNNCode* requires significantly less memory and remains comparable to Gurobi-ML across the benchmarks.

Key Takeaways Overall, eNNcode achieves competitive runtime performance across all benchmarks while also supporting convolutional architectures. Moreover, it consistently requires low memory and remains comparable to Gurobi-ML, making it a robust and broadly applicable encoding approach.

5 Conclusion & Future Work

We presented eNNcode, a user-friendly PyPi library for encoding neural networks in ONNX format into MILO instances. In future work, we plan to extend eNNcode to support encodings for the Z3 optimizer [de Moura and Bjørner, 2008]. Moreover, integrating our library into the CAISAR platform could facilitate a wider adoption and a seamless switching between verification and optimization tasks.

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