Self-Repairing Neural Networks
Provable Safety for Deep Networks via Dynamic Repair

KLAS LEINO, Carnegie Mellon University
AYMERIC FROMHERZ, Carnegie Mellon University
RAVI MANGAL, Carnegie Mellon University
MATT FREDRIKSON, Carnegie Mellon University
BRYAN PARNO, Carnegie Mellon University
CORINA PĂSĂREANU, Carnegie Mellon University and NASA Ames

Neural networks are increasingly being deployed in contexts where safety is a critical concern. In this work, we propose a way to construct neural network classifiers that dynamically repair violations of non-relational safety constraints called safe ordering properties. Safe ordering properties relate requirements on the ordering of a network’s output indices to conditions on their input, and are sufficient to express most useful notions of non-relational safety for classifiers. Our approach is based on a novel self-repairing layer, which provably yields safe outputs regardless of the characteristics of its input. We compose this layer with an existing network to construct a self-repairing network (SR-Net), and show that in addition to providing safe outputs, the SR-Net is guaranteed to preserve the accuracy of the original network. Notably, our approach is independent of the size and architecture of the network being repaired, depending only on the specified property and the dimension of the network’s output; thus it is scalable to large state-of-the-art networks. We show that our approach can be implemented using vectorized computations that execute efficiently on a GPU, introducing run-time overhead of less than one millisecond on current hardware—even on large, widely-used networks containing hundreds of thousands of neurons and millions of parameters.

Additional Key Words and Phrases: Safety, Program Repair, Machine Learning, Neural Networks, Verification

1 INTRODUCTION

Neural networks are being deployed as components in many safety- and security-critical domains, such as autonomous transport, banking, and medical diagnosis, motivating the need to provide proofs of safety for such neural components. Even well-tested, highly accurate networks may still be unsafe, leading to potentially dangerous situations. For instance, the well-studied ACAS Xu networks that implement an airborne collision avoidance system for commercial aircraft have been shown to violate key safety properties [Katz et al. 2017].

A (feed-forward) neural network $f$ is a total function of type $\mathbb{R}^n \rightarrow \mathbb{R}^m$ learned from input-output examples. In a common mode of use, neural networks are used as classifiers by taking the index of the maximum element of the output vector. Safety properties for classifiers are often expressed in terms of ordering constraints, which specify the safe sets of possible total orderings over the indices of the network’s output vector, defined by the natural order of the corresponding real components. For instance, the safety properties for ACAS Xu studied in prior work [Katz et al. 2017] specify conditions when, e.g., the first index of the network’s output should be maximal.

As the exact real values of the classifier’s output are not relevant to these properties, we may view neural networks as programs of type $\mathbb{R}^n \rightarrow T$, where $T$ contains all finite totally-ordered sets of elements $\{0 \ldots m - 1\}$. These safe ordering properties can be formalized as non-relational safety properties [Clarkson and Schneider 2008] of the logical form $P \implies Q$, where $P$ is an arbitrary decidable formula over the classifier’s input, and $Q$ is a statement in the theory of totally connected structures.

Authors’ addresses: Klas Leino, Carnegie Mellon University, kleino@cs.cmu.edu; Aymeric Fromherz, Carnegie Mellon University, fromherz@cmu.edu; Ravi Mangal, Carnegie Mellon University, rmangal@andrew.cmu.edu; Matt Fredrikson, Carnegie Mellon University, mfredrik@cmu.edu; Bryan Parno, Carnegie Mellon University, parno@cmu.edu; Corina Păsăreanu, Carnegie Mellon University, NASA Ames, pcorina@cmu.edu.
ordered sets over its output. They are a sufficiently generic formulation of non-relational safety, as the scale of each output component (also called a logit) is unconstrained, so properties that are sensitive to their values are of limited use. Some applications scale the output \( f(x) \) to produce a discrete probability distribution, thus interpreting the values as "confidence" scores. However, these are difficult to calibrate [Guo et al. 2017; Johansson and Gabrielsson 2019], and may be unreliable in practice. Safe ordering properties thus capture the relevant range of behaviors needed for non-relational safety, and we aim to construct neural networks that are provably safe according to such properties.

**Verifying Neural Network Safety.** To ensure the safety of neural networks, one strategy is to consider neural networks as programs generated by a learning routine. This casts the problem as one of normal program safety, to which techniques from the wide literature on program verification can be applied. For instance, abstract interpretation is used by Gehr et al. [2018]; Singh et al. [2019] to verify properties stated as polyhedral pre- and postconditions; combined with the appropriate use of strengthening and weakening, this leads to a strategy for producing complete Hoare-style safety proofs for neural networks. Alternatively, Katz et al. [2017] encode a network’s semantics as a system of constraints, and pose safety verification as satisfiability modulo the relevant theories.

Employing program verification methods to prove neural network safety has led to some success. However, the scalability of these techniques remains a serious challenge for the large majority of neural network applications. More importantly, post-training verification does not address the problem of constructing safe networks to begin with, and conventional training methods are unlikely to produce networks that satisfy many useful safety properties, as shown by, e.g., Lin et al. [2020]; Mirman et al. [2018]. Naively repeating training when verification fails, while supervising the correction of an observed set of counterexamples, is likely to be prohibitively expensive: training requires \( \sim 10^{10} \) floating-point operations (FLOPs) for a state-of-the-art image model [Tan and Le 2019, 2021], and \( \sim 10^{23} \) FLOPs for modern language models [Brown et al. 2020].

**Safe-by-Construction Learning.** Another strategy takes the perspective that neural networks should be safe by construction. In other words, one proves that the learning algorithm produces only safe networks, rather than verifying the networks a posteriori. Supervised learning, the most common framework for producing neural classifiers, is framed as an optimization problem:

\[
\theta^* = \arg\min_{\theta} \{ L(f_\theta, S) \}
\]

where \( f \) is a family of neural networks (referred to as the architecture) parameterized by \( \theta \in \mathbb{R}^p \), \( S \in (\mathbb{R}^n \times \{m\})^N \) is a labeled training set, and \( L \) is a real-valued loss function that measures how well \( f_\theta \) "fits" the training data. As \( S \) may be insufficient to ensure that the solution \( f_{\theta^*} \) satisfies a safety property \( \phi \), safe-by-construction methods typically modify the objective by adding a safety loss term \( L_\phi(f_\theta) \) that measures the degree to which \( f_\theta \) satisfies \( \phi \):

\[
\theta^* = \arg\min_{\theta} \{ (L(f_\theta, S) + L_\phi(f_\theta)) \}
\]

If \( L_\phi \) is carefully designed, then one may prove that when the optimization result \( \theta^* \) meets certain criteria (e.g., \( L_\phi(f_{\theta^*}) \leq 0 \)), then \( f_{\theta^*} \) is provably safe [Lin et al. 2020]. However, there is no guarantee that \( \theta^* \) will satisfy such criteria, and in those cases, one must fall back on verifying \( f_{\theta^*} \).

An alternative approach to safe learning modifies the architecture such that every network in the family is safe; in other words, one proves that \( f_\theta \) is safe for all \( \theta \). This is attractive, as safety is, in principle, decoupled from optimization, and thus not conditional on its outcome. It also ensures that learning need not be repeated for the sake of safety, and network verification is unnecessary. However, designing a provably-safe architecture that is both compatible with effective learning and
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flexible enough to support a broad set of safety properties is challenging. To date, this approach has only been employed in a few restricted settings, such as Lipschitz certification [Anil et al. 2019; Li et al. 2019b; Trockman and Kolter 2021], a relational notion of safety, and global robustness [Leino and Fredrikson 2021; Leino et al. 2021], a relaxed notion of robustness where the network is allowed to selectively abstain from prediction while maintaining safety.

Our Contributions. We present a technique for modifying neural network architectures to ensure that they satisfy safe ordering properties. In particular, we describe a transformer that, given an architecture $f$ and a set of safe ordering properties $\Phi$, produces a new architecture $f^\Phi$ such that $f^\Phi_\theta$ satisfies the conjunction of $\Phi$ for all parameters $\theta$. Viewing the neural network as a composition of layers, our transformer appends a self-repairing layer (SR-Layer) to $f$. This layer encodes a check-and-repair mechanism, so that when $f_\theta(x)$ violates $\Phi$, the SR-Layer modifies the output to ensure safety. This approach is similar in spirit to those that dynamically repair errors caused by traditional software issues like division-by-zero, null dereference, and others [Berger and Zorn 2006; Kling et al. 2012; Long et al. 2014; Perkins et al. 2009; Qin et al. 2005; Rinard et al. 2004]. Such mechanisms may be impractical for arbitrary neural network safety properties, as they may require solving arbitrarily complex constraint-satisfaction problems. We show that this is not the case for safe ordering properties, and that the solver needed for these constraints can be efficiently embedded in the repair layer.

A more pernicious issue with repair mechanisms for neural networks is that safe outputs may not be accurate, or that the steps taken to repair the network inadvertently damage its accuracy on points outside the scope of a given safety property. For example, Sotoudeh and Thakur [2021] propose a static repair method for safety properties over polyhedral pre- and postconditions, and observe non-trivial drawdown on several benchmarks, where the classifier’s previously-correct behavior on affected points is “forgotten” after repair. Thus, if not done carefully, repair may harm the model’s accuracy. We identify a key property, transparency, which ensures that the repair mechanism never has a negative impact on the network’s accuracy. Transparency requires that a prediction of the original network $f_\theta$ be retained whenever it is consistent with at least one ordering allowed by $\Phi$. However, if $\Phi$ is inconsistent with the “correct” label specified by the data, then it is impossible for the network to be safe without harming accuracy, and the repair prioritizes safety.

Beyond transparency, in some cases repair may improve classifier accuracy. This can potentially occur, for example, when the correct prediction is consistent with $\Phi$, but a suboptimal training outcome yields a model that is both unsafe and incorrect. To open the possibility for the training procedure to take repair into account during training—so that models that are more often safe and correct can be found—we design the SR-Layer, including the embedded constraint solver, to be both vectorized and differentiable. This allows the implementation of our approach within popular neural network frameworks, so that models composed with them can be efficiently trained using gradient-based optimization with hardware acceleration. Moreover, the vectorized implementation significantly reduces the run-time overhead of our check-and-repair mechanism.

Finally, while the SR-Layer achieves safety without negatively impacting accuracy, it necessarily adds computational overhead each time the network is executed. Our empirical evaluation focuses on this issue, and how the overhead is impacted by several key factors. We show that the cost of the SR-Layer depends solely on $\Phi$ and the length $m$ of the output vector, and thus importantly, is independent of the size or complexity of the underlying neural network. On three widely-used benchmark datasets (ACAS Xu [Katz et al. 2017], Collision Detection [Ehlers 2017], and CIFAR-100 [Krizhevsky and Hinton 2009]), we show that this overhead is small in real terms (0.26-0.82 ms), and does not pose an impediment to practical adoption. In fact, because the overhead is independent

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1 A classifier is accurate on an input if its prediction matches the corresponding label given in the training or test data.
of network size, its impact is less noticeable on larger networks, where the cost of evaluating the
original classifier may come to dominate that of the repair. To further characterize the role of \( \Phi \) and \( m \), we use synthetic data and random safe ordering properties to isolate the effects that the
postcondition complexity and number of classes have on network run time. Our results suggest that
while these structural traits of the specified safety property can impact run time—the satisfiability
of general ordering constraints is NP-complete [Guttmann and Maucher 2006]—this may often not
be an issue in practice.

To summarize, the main contributions of our work are as follows:

- We define a generic notion of non-relational safety for neural network classifiers, which we
call safe ordering properties,
- We present a method for transforming arbitrary neural network architectures into safe-by-
construction versions that are guaranteed to (i) satisfy a given set of safe ordering properties,
and (ii) preserve or improve the empirical accuracy of the original model.
- We show that the SR-Layer can be designed in a way that is both fully-vectorized and differ-
entiable, which enables hardware acceleration to reduce run-time overhead, and facilitates
its use during training in cases where doing so might improve the repaired model’s accuracy.
- We empirically demonstrate that the overhead introduced by the SR-Layer is small enough
for its deployment in practical settings.

The rest of the paper is organized as follows. In Section 2, we formally setup our problem. In
Section 3, we present details of the SR-Layer. In Section 4, we prove that our SR-Layer ensures
safety without loss in accuracy. In Section 5, we show how to encode the SR-Layer as a differentiable
and vectorizable computation. We describe our experimental setting and results on evaluating the
run-time overheads of the SR-Layer in Section 6. Finally, we survey the related work in Section 7
and conclude in Section 8.

2 PROBLEM SETTING

In this section, we formalize the concepts of safe ordering properties and self-repair. We begin
by presenting background on neural networks and an illustrative application of safe ordering
properties. We then formally define the problem we aim to solve, and introduce a set of desired
properties for our self-repairing transformer.

2.1 Background

Neural Networks. A neural network, \( f_\theta : \mathbb{R}^n \rightarrow \mathbb{R}^m \), is a total function defined by an architecture,
or composition of linear and non-linear transformations, and a set of weights, \( \theta \), parameterizing
its linear transformations. As neither the details of a network’s architecture nor the particular
valuation of its weights are relevant to much of this paper, we will by default omit the subscript \( \theta \),
and treat \( f \) as a black-box function. Neural networks are commonly used as classifiers, by extracting
predictions from the output \( f(x) : \mathbb{R}^m \), also called the logits of a network. Given a neural network
\( f \), we use the upper-case \( F \) to refer to the corresponding neural classifier: \( F = \lambda x. \arg\max_y \{ f(y) \} \).
For our purposes, we will assume that \( \arg\max \) returns a single index, \( i^* \in [m] \); ties may be broken
arbitrarily.

ACAS Xu: An Illustrative Example. Throughout this paper, we will use ACAS Xu as a running
example to present the problem and the solutions we propose. The Airborne Collision Avoidance
System X (ACAS X) [Kochenderfer et al. 2015] is a family of collision avoidance systems for both
manned and unmanned aircraft. ACAS Xu, the variant for unmanned aircraft, is implemented as a
large numeric lookup table (2GB) mapping sensor measurements to horizontal maneuver advisories.
The lookup table represents an optimal K-step horizon policy for a partially observable Markov
decision process formulation of the collision avoidance problem. As the table is too large for many
certified avionics systems, Julian et al. [2019] proposed the use of neural networks as a compressed,
functional representation of the lookup table.

A neural network for the ACAS Xu problem therefore is a function which, given an encoding
of the physical state of the aircraft and of a neighboring object (the intruder), outputs maneuver
advisories that the aircraft should follow to avoid collision. The physical state is comprised of six
different features: the distance (\(\rho\)) between the aircraft and the intruder, the relative angle
(\(\theta\)) from the aircraft to the intruder, the angle (\(\psi\)) from the intruder’s heading to the aircraft’s
heading, the speed of the aircraft (\(\omega_{\text{own}}\)), and of the intruder (\(\omega_{\text{inv}}\)), and the time (\(\tau\)) until loss of
vertical separation. The model outputs one of five possible advisories: either that no change is
needed, also called clear-of-conflict (COC), or that the aircraft must steer weakly to the left, weakly
to the right, strongly to the left, or strongly to the right. These advisories correspond to output
dimensions 0 through 4, respectively. The networks proposed by Julian et al. [2019] are functions
\(f : \mathbb{R}^5 \rightarrow \mathbb{R}^5\); the value \(\tau\) is discretized and 45 different neural networks are constructed, one for
each combination of the previous advisory (\(a_{\text{prev}}\)) and discretized value of \(\tau\). While Julian et al.
[2019] used the convention that the index of the minimal element of \(f(x)\) is the predicted advisory,
in this paper we will use the more common convention of the maximal value’s index. Thus, if
\(f(x) = [100, 900, 300, 140, 500]\), then \(F(x) = 1\), which corresponds to the advisory weak left.

Observing that the ACAS Xu neural networks are approximations of the original lookup table,
and could thus deviate arbitrarily from the table’s advisory on untested regions of their input space,
several researchers have proposed verifying them against a set of safety properties [Katz et al. 2017;
Lin et al. 2020; Singh et al. 2019]. Katz et al. [2017] proposed 10 such properties, which capture
requirements such as, “If the intruder is near and approaching from the left, the network advises
strong right.” Formally, this property would consist of a precondition on the network’s input that
encodes the intruder being “near,” and a postcondition that the logit corresponding to strong right
is maximal.

### 2.2 Problem Definition

Definition 1 presents the safe ordering properties that we consider throughout the rest of the paper.
Intuitively, these properties associate constraints on the relative ordering of a network’s output
values (a postcondition) with a predicate on the corresponding input (a precondition). As we will
see in later sections, the precondition does not need to belong to a particular theory, and need only
to come with an effective procedure for deciding new instances.

**Definition 1 (Safe ordering property).** Given a neural network \(f : \mathbb{R}^n \rightarrow \mathbb{R}^m\), a safe ordering
property, \(\phi = \langle P, Q \rangle\), is a precondition, \(P\), consisting of a decidable proposition over \(\mathbb{R}^n\), and a
postcondition, \(Q\), given as a Boolean combination of order relations between the real components of
\(\mathbb{R}^m\).

- **precondition** \(P\) := decidable proposition
- **ordering literal** \(q\) := \(y_i < y_j\) (\(0 \leq i, j < m\))
- **ordering constraint** \(Q\) := \(q \mid Q \land Q \mid Q \lor Q\)
- **safety property** \(\phi\) := \(\langle P, Q \rangle\)
- **set of properties** \(\Phi\) := \(\cdot \mid \phi, \Phi\)

Assuming a function, \(\text{eval} : \mathbb{R}^n \rightarrow \text{bool}\), that decides \(P\) given \(x \in \mathbb{R}^n\), notated as \(P(x)\), and a
similar \(\text{eval}\) function for \(Q\), we say \(f\) satisfies safe ordering property \(\phi\) at \(x\) iff \(P(x) \implies Q(f(x))\).
We use the shorthand \(\phi(x, f(x))\) to denote this; and given a set of properties \(\Phi\), we write \(\Phi(x, f(x))\) to
 denote \(\forall \phi \in \Phi : \phi(x, f(x))\) and \(\Phi(x)\) to denote \(\bigwedge (P_i, Q_i) \in \Phi : P_i(x) \text{true} Q_i\).
Two points about our definition of safe ordering properties bear mentioning. First, although postconditions are evaluated using the inequality relation from real arithmetic, we assume that \( \forall x . i \neq j \implies f_i(x) \neq f_j(x) \), and thus specifically exclude equality comparisons between the output components. This is a realistic assumption in nearly all practical settings, and in cases where it does not hold, can be resolved with arbitrary tie-breaking protocols that perturb \( f(x) \) to remove any equalities. Second, we omit explicit negation from our syntax, as it can be achieved by swapping the positions of the affected order relations; i.e., \( \neg(y_l < y_j) \) is just \( y_j < y_l \), as we exclude the possibility that \( y_i = y_j \).

Sections 6.3 and 6.4 provide several concrete examples of safe ordering properties. Example 2 revisits the property for ACAS Xu that was discussed in the previous section.

**Example 2 (ACAS Xu).** Recall the property described earlier: “If the intruder is near and approaching from the left, the network advises strong right.” This is a safe ordering property \((P, Q)\), where the precondition \( P \) is captured as a linear real arithmetic formula given by Katz et al. [2017]:

\[
\begin{align*}
P &\equiv 250 \leq \rho \leq 400 \land 0.2 \leq \theta \leq 0.4 \land -\pi \leq \psi \leq -\pi + 0.005 \land 100 \leq v_{\text{own}} \leq 400 \\
Q &\equiv y_0 < y_4 \land y_1 < y_4 \land y_2 < y_4 \land y_3 < y_4
\end{align*}
\]

In fact, nine of the ten properties proposed by Katz et al. [2017] are safe ordering properties. The single exception has a postcondition that places a constant lower-bound on \( y_0 \), despite the fact that the logit values of the network can be freely scaled without impacting the network’s behavior as a classifier, making the interpretation of this property unclear.

Given a set of safe ordering properties, \( \Phi \), our goal is to obtain a neural network that satisfies \( \Phi \) everywhere. In later sections, we show how to accomplish this by describing the construction of a self-repairing transformer (Definition 3) that takes an existing, possibly unsafe network, and produces a related model that satisfies \( \Phi \) at all points. While in practice, a meaningful, well-defined specification \( \Phi \) should be satisfiable for all inputs, our generic formulation of safe ordering properties in Definition 1 does not enforce this restriction; we can, for instance, let \( \Phi := (\top, y_0 < y_1), (\top, y_1 < y_0) \). To account for this, we lift predicates \( \phi \) to operate on \( \mathbb{R}^m \cup \{\bot\} \), where \( \phi(x, \bot) \) is considered valid for all \( x \).

**Definition 3 (Self-Repairing Transformer).** A self-repairing transformer, \( \text{SR} : \Phi \rightarrow (\mathbb{R}^n \rightarrow \mathbb{R}^m) \rightarrow (\mathbb{R}^n \rightarrow (\mathbb{R}^m \cup \{\bot\})) \), is a function that, given a set of safe ordering properties, \( \Phi \), and a neural network, \( f : \mathbb{R}^n \rightarrow \mathbb{R}^m \), produces a network, denoted as \( f^\Phi : \mathbb{R}^n \rightarrow (\mathbb{R}^m \cup \{\bot\}) \), that satisfies the following properties:

(i) Safety: \( \forall x . ( \exists y. \Phi(x, y) ) \implies \Phi(x, f^\Phi(x)) \)

(ii) Forewarning: \( \forall x . ( f^\Phi(x) = \bot \iff \forall y . \neg\Phi(x, y) ) \)

In other words, \( f^\Phi = \text{SR}(\Phi)(f) \) is safe with respect to \( \Phi \) and produces a non-\( \bot \) output everywhere that \( \Phi(x) \) is satisfiable. We will refer to the output of \( \text{SR} \), \( f^\Phi \), as a self-repairing network, or SR-Net.

Definition 3(i) captures the essence of the problem that we aim to solve, requiring that the self-repairing network make changes to its output according to \( \Phi \). While allowing it to abstain from prediction by outputting \( \bot \) may appear to relax the underlying problem, note that this is only allowed in cases where \( \Phi \) cannot be satisfied on \( x \): definition 3(ii) is an equivalence that precludes trivial solutions such as \( f^\Phi := \lambda x. \bot \). However, it still allows abstention in exactly the cases where it is needed for principled reasons. A set of safe ordering properties may be mutually satisfactory almost everywhere, except in some places; for example: \( \Phi := (x \leq 0.5, y_0 < y_1), (x \geq 0.5, y_1 < y_0) \). In this case, \( f^\Phi \) can abstain at \( x = 0.5 \), and everywhere else must produce outputs in \( \mathbb{R}^m \) obeying \( \Phi \).
While the properties required by Definition 3 are sufficient to ensure a non-trivial, safe-by-construction neural network, in practice, we aim to apply SR(Φ), which we will write as SRΦ, to models that already perform well on observed test cases, but that still require a safety guarantee. Thus, we wish to repair networks without interfering with the existing network behavior when possible, a property we call transparency (Property 4).

Property 4 (Transparency). Let SR : Φ → (R^n → R^m) → (R^n → (R^m ∪ {⊥})) be a self-repairing transformer. We say that SR satisfies transparency if

∀Φ : ∀f : R^n → R^m . ∀x ∈ R^n . (∃y . Φ(x,y) ∧ argmax_i y_i = F(x)) → F^Φ(x) = F(x)

In other words, SR always produces an SR-Net, f^Φ, for which the predictions derived from the safe output vectors of f^Φ agree with the predictions of the original model whenever possible.

Property 4 leads to a useful result, namely that whenever Φ is consistent with accurate predictions, then the classifier obtained from SRΦ(f) is at least as accurate as F (Theorem 5). Formally, we characterize accuracy in terms of agreement with an oracle classifier F^O that "knows" the correct label for each input, so that F is accurate on x if and only if F(x) = F^O(x). We note that accuracy is often defined with respect to a distribution of labeled points rather than an oracle; however our formulation captures the key fact that Theorem 5 holds regardless of how the data are distributed.

Theorem 5 (Accuracy Preservation). Given a neural network, f : R^n → R^m, and set of properties, Φ, let f^Φ := SRΦ(f) and let F^O : R^n → [m] be the oracle classifier. Assume that SR satisfies transparency. Further, assume that accuracy is consistent with safety, i.e.,

∀x ∈ R^n . ∃y . Φ(x,y) ∧ argmax_i y_i = F^O(x).

Then,

∀x ∈ R^n . F(x) = F^O(x) → F^Φ(x) = F^O(x)

Proof. Let x ∈ R^n such that F(x) = F^O(x). By hypothesis, we have that ∃y . Φ(x,y) ∧ argmax_i y_i = F^O(x), hence we can apply Property 4 to conclude that F^Φ(x) = F(x) = F^O(x). □

One subtle point to note is that even when Φ is consistent with accurate predictions, it is possible for a network to be accurate yet unsafe at an input. Example 6 describes such a situation. Our formulation of Property 4 is carefully designed to ensure accuracy preservation even in such scenarios.

Example 6 (Accuracy need not imply safety). Consider the property φ_2 proposed for ACAS Xu by Katz et al. [2017] which says: “Even if the intruder is distant and is significantly slower than the own ship, the score of the COC advisory should never be minimal.” This safe ordering property is applicable for all networks that correspond to a prev ≠ COC and is concretely written as follows:

P ≡ ρ ≥ 55947.691 ∧ v_own ≥ 1145 ∧ v_int ≤ 60
Q ≡ y_1 < y_0 ∨ y_2 < y_0 ∨ y_3 < y_0 ∨ y_4 < y_0

For some x such that P(x) is true, let us assume that F^O(x) = 1 and for a network f, f(x) = [100, 900, 300, 140, 500], so that F(x) = 1. Then, f is accurate at x, but the COC advisory receives the minimal score, meaning f is unsafe at x with respect to φ_2. If the transformer SR satisfies Property 4, then by Theorem 5, f^Φ_2 is guaranteed to be accurate as well as safe at x, since φ_2 is consistent with accuracy here (as φ_2 does not preclude class 1 from being maximal).
3 SELF-REPAIRING TRANSFORMER

In this section, we describe our self-repairing transformer, SR. We begin with a high-level overview of the approach (Section 3.1), and provide algorithmic details in Sections 3.2 and 3.3. In later sections, we prove that SR models Definition 3, satisfies transparency, and can be implemented as a vectorized, differentiable function.

3.1 Overview

Our self-repairing transformer, SR, leverages the fact that whenever a safe ordering property is satisfiable at a point, it is possible to bring the network to compliance. Neural networks are typically constructed by composing a sequence of layers; we thus compose an additional self-repair layer that operates on the original network’s output, and produces a result that will serve as the transformed network’s new output. This is reflected in the SR routine in Algorithm 3.1, and Figure 1 shows the resulting network. The original network, \( f \), executes normally, and the self-repair layer subsequently takes both the input \( x \) (to facilitate checking the preconditions of \( \Phi \)) and \( y := f(x) \), from which it either abstains (outputs \( \perp \)) or produces an output that is guaranteed to satisfy \( \Phi \).

The high-level workflow of the self-repair layer, SR-Layer, proceeds as follows. The layer starts by checking the input \( x \) against each of the preconditions, and derives an active postcondition. This is then passed to a solver, which attempts to find the set of orderings that are consistent with the active postcondition. If no such ordering exists, i.e., if the active postcondition is unsatisfiable, then the layer abstains with \( \perp \). Otherwise, the layer minimally permutes the indices of the original output vector in order to satisfy the active postcondition while ensuring transparency (Property 4).

3.2 Algorithmic Details of the Self-Repair Layer

The core logic of our approach is handled by a self-repair layer, or SR-Layer, that is appended to the original model, and dynamically ensures its outputs satisfy the requisite safety properties. The procedure followed by this layer, SR-Layer (shown in Algorithm 3.1), first checks if the input \( x \) and output \( y \) of the base network already satisfy \( \Phi \) (line 5). If they do, no repair is necessary and the repaired network \( f^\Phi \) can safely return \( y \). Otherwise, SR-Layer attempts to find a satisfiable ordering constraint that entails the relevant postconditions in \( \Phi \) (line 8). FindSatConstraint either returns such a term \( q \) that consists of a conjunction of ordering literals \( y_i < y_j \), or returns \( \perp \) whenever no such \( q \) exists. When FindSatConstraint returns \( \perp \), then SR-Layer does as well (lines 9-10). Otherwise, the constraint identified by FindSatConstraint is used to repair the network’s output (line 12), where Repair permutes the logit values in \( y \) to arrive at a vector that satisfies \( q \). Note that because \( q \) is satisfiable, it is always possible to find a satisfying solution by simply permuting \( y \) because the specific real values are irrelevant, and only their order matters (see Section 4).
Algorithm 3.1: Self-repairing transformer

**Inputs:** A set of safety properties, $\Phi$ and a network, $f : \mathbb{R}^n \to \mathbb{R}^m$

**Output:** A network, $f^{\Phi} : \mathbb{R}^n \to \mathbb{R}^m \cup \{\bot\}$

1. $\text{SR}(\Phi, f)$:
   1. $f^\Phi := \lambda x. \text{SR-Layer}(\Phi, x, f(x))$
   2. return $f^\Phi$

2. $\text{SR-Layer}(\Phi, x, y)$:
   1. if $\Phi(x, y)$ then return $y$
   2. else $q := \text{FindSatConstraint}(\Phi, x, y)$
   3. if $q = \bot$ then return $\bot$
   4. else $y' := \text{Repair}(q, y)$
   5. return $y'$

3.2.1 Finding Satisfiable Constraints. The FindSatConstraint procedure is shown in Algorithm 3.2. Recall that the goal is to identify a conjunction of ordering literals $q$ that implies the relevant postconditions in $\Phi$ at the given input $x$. More precisely, this means that for each precondition $P_i$ satisfied by $x$, the corresponding postcondition $Q_i$ is implied by $q$. This is sufficient to ensure that any model $y'$ of $q$ will satisfy $\Phi$ at $x$; i.e., $q(y') \implies \Phi(x, y')$.

To accomplish this, FindSatConstraint first evaluates each precondition, and obtains a disjunctive normal form (DNF), $Q_x$, of the active postcondition, defined in Equation 1 (line 9).

$$\text{Filter}(\Phi, x) := \bigwedge_{(P_i, Q_i) \in \Phi \mid P_i(x)} Q_i$$

In practice, we implement a lazy version of ToDNF that generates disjuncts as needed (see Section 5), as this step may be a bottleneck and we only need to process each clause individually. At this point, FindSatConstraint could proceed directly, checking the satisfiability of each disjunct in $Q_x$, and returning the first satisfiable one it encounters. This would be correct, but as we wish to satisfy transparency (Property 4), we first construct an ordered list of the terms in $Q_x$ which prioritizes constraints that maintain the maximal position of the original prediction, argmax($y$) (Prioritize, line 10). Property 7 formalizes the behavior required of Prioritize.

**Property 7 (Prioritize).** Given $y \in \mathbb{R}^m$ and a list of conjunctive ordering constraints $Q$, the result of $\text{Prioritize}(Q, y)$ is a reordered list $Q' = [\ldots, q_i, \ldots]$ such that:

$$\forall 0 \leq i, j < |Q|. \argmax_i y_i \in \text{Roots}(\text{OrderGraph}(q_i)) \land \argmax_i y_i \notin \text{Roots}(\text{OrderGraph}(q_j)) \implies i < j$$

where Roots($G$) denotes the set of root nodes of the directed graph $G$.

The IsSat procedure (invoked on line 12, also shown in Algorithm 3.2) determines whether a conjunctive ordering constraint is satisfiable. It is based on an encoding of $q$ as a directed graph, embodied in OrderGraph (lines 1-4), where each component index of $y$ corresponds to a node, and
Algorithm 3.2: Finding a satisfiable ordering constraint from safe-ordering properties \( \Phi \)

**Inputs:** A set of safety properties, \( \Phi \), a vector \( x : \mathbb{R}^n \), and a vector \( y : \mathbb{R}^m \)

**Output:** Satisfiable ordering constraint, \( q \)

1. OrderGraph\((q)\):
   
   \[ V := [m] \]
   
   \[ E := \{(i, j) : y_j < y_i \in q\} \]
   
   \[ \text{return } (V, E) \]

2. IsSat\((q)\):
   
   \[ g := \text{OrderGraph}(q) \]
   
   \[ \text{return } \neg \text{ContainsCycle}(V, E) \]

3. FindSatConstraint\((\Phi, x, y)\):
   
   \[ Q_x := \text{ToDNF} (\text{Filter}(\Phi, x)) \]
   
   \[ Q_p := \text{Prioritize}(Q_x, y) \]
   
   \[ \text{foreach } q_i \in Q_p \text{ do} \]
   
   \[ \quad \text{if IsSat}(q_i) \text{ then} \]
   
   \[ \quad \quad \text{return } q_i \]

4. \[ \text{return } \bot \]

3.2.2 Repairing Violations. Algorithm 3.3 describes the Repair procedure, used to ensure the outputs of the SR-Layer satisfy safety. The inputs to Repair are a satisfiable ordering constraint \( q \), and the output of the original network \( y := f(x) \). The goal is to permute \( y \) such that the result \( y' \) satisfies \( q \), without violating transparency. Our approach is based on OrderGraph, the same directed-graph encoding used by IsSat. It uses a stable topological sort of the graph encoding of \( q \) to construct a total order over the indices of \( y \) that is consistent with the partial ordering implied by \( q \) (line 2). TopologicalSort returns a permutation \( \pi \), a function that maps indices in \( y \) to their rank (or position) in the total order. Formally, TopologicalSort takes as argument a graph \( G = (V, E) \), and returns \( \pi \) such that Equation 3 holds.

\[ \forall i, j \in V . (i, j) \in E \implies \pi(i) < \pi(j) \]  

(3)
I.e., if the edge \((i, j)\) is in the graph, then \(i\) occurs before \(j\) in the ordering. In general, many total orderings may be consistent, but in order to guarantee transparency, \texttt{TopologicalSort} also needs to ensure the following invariant, captured by Property 8, capturing that the maximal index is listed first in the total order if possible.

**Property 8.** Given a graph, \(G = (V, E)\), and \(y \in \mathbb{R}^m\), the result \(\pi\) of \texttt{TopologicalSort}(G, y) satisfies

\[
\arg\max_i [y_i] \in \text{Roots}(G) \implies \pi \left( \arg\max_i [y_i] \right) = 0
\]

where \(\text{Roots}(G)\) denotes the set of root nodes of the directed graph \(G\).

In other words, the topological sort preserves the network’s original prediction when doing so is consistent with \(q\). Then, by sorting \(y\) in descending order, the sorted vector \(y^s\) can be used to construct the final output of \texttt{Repair}, \(y'\). For any index \(i\), we simply set \(y^s_i\) to the \(\pi(i)^{th}\) component of \(y^s\), since \(\pi(i)\) gives the desired rank of the \(i^{th}\) logit value and components in \(y^s\) are sorted according to the component values (line 4). An example of the complete \texttt{Repair} procedure is given by Example 9.

**Example 9 (\texttt{Repair}).** We refer again to the safety properties introduced for ACAS Xu [Katz et al. 2017]. The postcondition of property \(\phi_2\) states that the logit score for class 0 (COC) is not minimal, which can be written as the following ordering constraint:

\[ Q \equiv y_1 < y_0 \lor y_2 < y_0 \lor y_3 < y_0 \lor y_4 < y_0 \]

Suppose that for some input \(x \in \mathbb{R}^n\), the active postcondition is equivalent to \(Q\), and that \(y = [100, 900, 300, 140, 500]\). Further, suppose that \texttt{FindSatConstraint} has returned \(q := y_2 < y_0\), corresponding to the second disjunct of \(Q\) (satisfying \(q \implies Q\)). We then take the following steps according to \texttt{Repair}(q, y):

- First we let \(\pi := \text{TopologicalSort}(	ext{OrderGraph}(q), y)\). We note that all vertices of the graph representation of \(q\) are roots except for \(j = 2\), which has \(j = 0\) as its parent. We observe that \(\arg\max_i [y_i] = 1\), which corresponds to a root node; thus by Property 8, \(\pi(1) = 0\). Moreover, by our ordering constraint, we also have that \(\pi(0) = \pi(2)\). Thus, the ordering \(\pi\) where \(\pi(0) = 2\), \(\pi(1) = 0\), \(\pi(2) = 3\), \(\pi(3) = 4\), and \(\pi(4) = 1\) is a possible result of \texttt{TopologicalSort}, which we will assume for this example.
- Next we obtain by a descending sort that \(y^s = [900, 500, 300, 140, 100]\).
- Finally we obtain \(y'\) by indexing \(y^s\) by the inverse of \(\pi\), that is, \(y^s_i = y'_{\pi(i)}\). This gives us that \(y'_0 = y'_2 = 300\), \(y'_1 = y'_0 = 900\), \(y'_2 = y'_3 = 140\), \(y'_3 = y'_4 = 100\), and \(y'_4 = y'_1 = 500\), resulting in a final output of \(y' = [300, 900, 140, 100, 500]\), which we observe (i) satisfies \(Q\), and (ii) preserves the prediction of class 1.

### 3.3 Complexity

Given a neural network \(f : \mathbb{R}^n \to \mathbb{R}^m\), we define the input size as \(n\) and output size as \(m\). Also, assuming that the postconditions \(Q_i\) for all \(\langle P_i, Q_i \rangle \in \Phi\) are expressed in DNF, we define the size \(p_i\) of a property as the number of disjuncts in \(Q_i\), and define \(\alpha := |\Phi|\), i.e., the number of properties in \(\Phi\). Then, the worst-case computational complexity of \texttt{SR-Layer} is given by Equation 4, where \(O(\log(m))\) is the complexity of \texttt{ContainsCycle}, \(O(m \log(m))\) is the complexity of \texttt{TopologicalSort}, and \(\prod_{i=1}^{\alpha} p_i\) is the maximum number of disjuncts possible in \(Q_x\) if the postconditions \(Q_i\) are in DNF.

\[
O \left( \log(m) \prod_{i=1}^{\alpha} p_i + m \log(m) \right)
\]  

(4)
The complexity given by Equation 4 is with respect to a cost model that treats matrix operations—e.g., matrix multiplication, associative row/column reductions—as constant-time primitives. Crucially, note that the complexity does not depend on the size of the neural network $f$.

4 SAFETY AND ACCURACY

In this section, we present the two main theorems of our work. First, we show that the approach presented in Section 3 yields a self-repairing transformer, i.e., SR satisfies the properties from Definition 3. Second, we prove that the network transformer we propose also satisfies transparency (Property 4), ensuring a repaired network is at least as accurate as the original network (Theorem 5).

4.1 SR is a Self-Repairing Transformer

We start by proving that the transformer presented in Algorithm 3.1, SR, is self-repairing, i.e., it satisfies Properties 3(i) and 3(ii). Recall that this means that $f^k$ will either return safe outputs vectors, or in the event that $\Phi$ is inconsistent at a point, and only in that event, return $\perp$.

Let $x : \mathbb{R}^n$ be an arbitrary vector. If $\Phi(x, f(x))$ is initially satisfied, the SR-Layer does not modify the original output $y = f(x)$, and Properties 3(i) and 3(ii) are trivially satisfied. If $\Phi(x, f(x))$ does not hold, we will rely on two key properties of $\text{FindSatConstraint}$ and Repair to establish that SR is self-repairing. The first, Property 10, requires that $\text{FindSatConstraint}$ either return $\perp$, or else return ordering constraints that are sufficient to establish $\Phi$.

**Property 10 (FindSatConstraint).** Let $\Phi$ be a set of safety properties, $x : \mathbb{R}^n$ and $y : \mathbb{R}^m$ two vectors. Then $q = \text{FindSatConstraint}(\Phi, x, y)$ satisfies the following properties:

(i) $q = \perp \iff \forall y'. \neg \Phi(x, y')$
(ii) $q \neq \perp \implies (\forall y'. \ q(y') \implies \Phi(x, y'))$

**Proof.** The first observation is that the list of ordering constraints in $Q_p := \text{Prioritize}(Q_x, y)$ accurately models the initial set of properties $\Phi$, i.e.,

$$\forall y'. \Phi(x, y') \iff (\exists q \in Q_p. \ q(y')) \quad (5)$$

This stems from the definition of the disjunctive normal form, and from the fact that $\text{Prioritize}$ only performs a permutation of the disjuncts.

We also rely on the following loop invariant, stating that all disjuncts considered so far, when iterating over $\text{Prioritize}(Q_x, y)$, were unsatisfiable:

$$\forall q \in Q_p. \ \text{idx}(q, Q_p) < \text{idx}(q_i, Q_p) \implies (\forall y. \neg q(y)) \quad (6)$$

Here, $\text{idx}(q, Q_p)$ returns the index of constraint $q$ in the list $Q_p$. This invariant is trivially true when entering the loop, since the current $q_i$ is the first element of the list. Its preservation relies on $\text{IsSat}(q)$ correctly determining whether $q$ is satisfiable, i.e., $\text{IsSat}(q) \iff \exists y. \ q(y)$ [Nieuwenhuis and Rivero 2002].

Combining these two facts, we can now establish that $\text{FindSatConstraint}$ satisfies 10(i) and 10(ii). By definition, $\text{FindSatConstraint}(\Phi, x, y)$ outputs $\perp$ if and only if it traverses the entire list $Q_p$, never returning a $q_i$. From loop invariant 6, this is equivalent to $\forall q \in Q_p. \forall y'. \neg q(y')$, which finally yields property 10(i) from equation 5. Conversely, if $\text{FindSatConstraint}(\Phi, x, y)$ outputs $q \neq \perp$, then $q \in Q_p$. We directly obtain property 10(ii) as, for any $y' : \mathbb{R}^m$, $q(y')$ implies that $\Phi(x, y')$ by application of equation 5.

Next, Property 11 states that Repair correctly permutes the output of the network to satisfy the constraint that it is given. Combined with Property 10, this is sufficient to show that SR is a self-repairing transformer (Theorem 12).
We will proceed by contradiction, assuming that there do not exist vectors, and \( q \), that would otherwise have been compatible with the full set of properties \( \Phi \). (Constraint (rather than \( \perp \), TopologicalSort property, as it shows that the permutation returned by \( y \) if and only if there is no \( q \) prediction is a root of the graph encoding of \( \text{Repair} \) \( f \). Transparency trivially holds, as the repair layer does not modify the original output formalized in Property 4.

Next prove that it also preserves predictions when possible, i.e., that \( \text{SR} \) is safe-by-construction networks, we now prove that it also preserves predictions when possible, i.e., that \( \text{SR} \) satisfies transparency, as formalized in Property 4.

Let \( x : \mathbb{R}^n \) be an arbitrary vector. As in the previous section, if \( \Phi(x, f(x)) \) is initially satisfied, transparency trivially holds, as the repair layer does not modify the original output \( f(x) \). When \( \Phi(x, f(x)) \) does not hold, we will rely on several additional properties about \( \text{FindSatConstraint} \), \( \text{Repair} \), and \( \text{OrderGraph} \). The first, Property 13, states that whenever the index of the network’s prediction is a root of the graph encoding of \( q \) used by \( \text{FindSatConstraint} \) and \( \text{Repair} \), then there exists an output which satisfies \( q \) that preserves that prediction.

**Property 11 (Repair).** Let \( q \) be a satisfiable ordering constraint, and \( y : \mathbb{R}^m \) a vector. Then \( \text{Repair}(q, y) \) satisfies \( q \).

Proof. Let \( y_i < y_j \) be an atom in \( q \). Reusing notation from Algorithm 3.3, let \( y' = \text{Repair}(q, y) \), \( y^s := \text{SortDescending}(y) \), and \( \pi := \text{TopologicalSort}(\text{OrderGraph}(q), y) \). We have that \((j, i)\) is an edge in \( \text{OrderGraph}(q) \), which implies that \( \pi(j) < \pi(i) \) by Equation 3. Because the elements of \( y \) are sorted in descending order, and assumed to be distinct (Definition 1), we obtain that \( y^s_{\pi(i)} < y^s_{\pi(j)} \), i.e., that \( y'_i < y'_j \).

**Theorem 12 (SR is a Self-Repairing Transformer).** \( \text{SR} \) (Algorithm 3.1) satisfies conditions (i) and (ii) of Definition 3.

Proof. By definition of Algorithm 3.1, \( \text{FindSatConstraint}(\Phi, x, y) = \perp \) if and only if \( f^a(x) = \text{SR}(\Phi)(f)(x) \) outputs \( \perp \). We derive from Property 10(i) that this is equivalent to \( \forall y'. \neg \Phi(x, y') \), which corresponds exactly to Property 3(ii). Conversely, if \( \Phi \) is satisfiable for input \( x \), i.e., \( \exists y' \). \( \Phi(x, y') \), then \( \text{FindSatConstraint}(\Phi, x, y) \) outputs \( q \neq \perp \). By definition, we have \( f^a(x) = \text{Repair}(q, y) \), which satisfies \( q \) by application of Property 11, which in turn implies that \( \Phi(x, f^a(x)) \) by application of Property 10(ii).

### 4.2 SR is Transparent

Now that we have demonstrated that our approach produces safe-by-construction networks, we next prove that it also preserves predictions when possible, i.e., that \( \text{SR} \) satisfies transparency, as formalized in Property 4.

Let \( x : \mathbb{R}^n \) be an arbitrary vector. As in the previous section, if \( \Phi(x, f(x)) \) is initially satisfied, transparency trivially holds, as the repair layer does not modify the original output \( f(x) \). When \( \Phi(x, f(x)) \) does not hold, we will rely on several additional properties about \( \text{FindSatConstraint} \), \( \text{Repair} \), and \( \text{OrderGraph} \). The first, Property 13, states that whenever the index of the network’s prediction is a root of the graph encoding of \( q \) used by \( \text{FindSatConstraint} \) and \( \text{Repair} \), then there exists an output which satisfies \( q \) that preserves that prediction.

**Property 13 (OrderGraph).** Let \( q \) be a satisfiable, disjunction-free ordering constraint, and \( y : \mathbb{R}^m \) a vector. Then,

\[
\arg\max_i \{y_i\} \in \text{Roots}((\text{OrderGraph}(q))) \iff \exists y'. q(y') \land \arg\max_i \{y_i\} = \arg\max_i \{y'_i\}
\]

The intuition behind this property is that \( i^* := \arg\max_i \{y_i\} \) belongs to the roots of \( \text{OrderGraph}(q) \) if and only if there is no \( y_{i^*} < y_j \) constraint in \( q \); hence since \( q \) is satisfiable, we can always permute indices in a solution \( y' \) to have \( \arg\max_i \{y'_i\} = i^* \). Formally, Lemma 17 in Section 5.1.2 entails this property, as it shows that the permutation returned by \( \text{TopologicalSort} \) satisfies it.

Next, Property 14 formalizes the requirement that whenever \( \text{FindSatConstraint} \) returns a constraint (rather than \( \perp \)), then that constraint will not eliminate any prediction-preserving solutions that would otherwise have been compatible with the full set of properties \( \Phi \).

**Property 14 (FindSatConstraint).** Let \( \Phi \) be a set of safety properties, \( x : \mathbb{R}^n \) and \( y : \mathbb{R}^m \) two vectors, and \( q = \text{FindSatConstraint}(\Phi, x, y) \). Then,

\[
q \neq \perp \land \left( \exists y'. \Phi(x, y') \land \arg\max_i \{y_i\} = \arg\max_i \{y'_i\} \right) \implies \exists y'. q(y') \land \arg\max_i \{y_i\} = \arg\max_i \{y'_i\}
\]

Proof. Let us assume that \( q \neq \perp \), and that \( \exists y'. \Phi(x, y') \land \arg\max_i \{y_i\} = \arg\max_i \{y'_i\} \).

We will proceed by contradiction, assuming that there does not exist \( y'' \) such that \( q(y'') \) and
argmax\(i\{y_i\} = \arg\max\{y_i\}\), which entails that argmax\(i\{y_i\} \neq \text{Roots(Order}\text{Graph}(q))\) by application of Property 13. In combination with the specification of Prioritize (Property 7), this implies that any \(q' \in Q_p\) such that \(\exists y'. q'(y') \land \text{argmax}_i\{y_i\} = \text{argmax}_i\{y_i'\}\) occurs before \(q\) in Prioritize\((Q_x, y)\), i.e., \(\text{idx}(q', Q_p) < \text{idx}(q, Q_p)\). From loop invariant 6, we therefore conclude that there does not exist such a \(q' \in Q_p\), which contradicts the hypothesis \(\Phi(x, y')\) by application of Equation 5. \(\square\)

Lastly, Property 15 states that Repair (Algorithm 3.3) will always find an output that preserves the original prediction, whenever the constraint returned by FindSatConstraint allows it. This is the final piece needed to prove Theorem 16, the desired result about the self-repairing transformer.

**Property 15 (Repair).** Let \(q\) be a satisfiable term, and \(y : \mathbb{R}^m\) a vector. Then,

\[
( \exists y'. q(y') \land \text{argmax}_i\{y_i\} = \text{argmax}_i\{y_i'\} ) \implies \text{argmax}_i\{\text{Repair}(q, y)_i\} = \text{argmax}_i\{y_i\}
\]

Proof. Assume that there exists \(y'\) such that \(q(y')\) and \(\text{argmax}_i\{y_i\} = \text{argmax}_i\{y_i'\}\). This entails that \(\text{argmax}_i\{y_i\} \in \text{Roots(Order}\text{Graph}(q))\) (Property 13), which in turn implies that \(\pi(\text{argmax}_i\{y_i\}) = 0\) (Property 8). By definition of a descending sort, we have that \(\text{argmax}_i\{\text{Repair}(q, y)_i\} = j\), such that \(\pi(j) = 0\), hence concluding that \(j = \text{argmax}_i\{y_i\}\) by injectivity of \(\pi\). \(\square\)

**Theorem 16 (Transparency of SR).** SR, the self-repairing transformer described in Algorithm 3.1 satisfies Property 4.

Proof. That the SR transformer satisfies transparency is straightforward given Properties 13-15. Let us assume that there exists \(y'\) such that \(\Phi(x, y')\) and \(\text{argmax}_i\{y_i'\} = F(x)\). By application of Property 10(i), this implies that \(\text{FindSatConstraint}(\Phi, x, f(x))\) outputs \(q \neq \bot\), and therefore that there exists \(y'\) such that \(q(y')\) and \(\text{argmax}_i\{y_i'\} = F(x)\) by application of Property 14, since \(F(x)\) is defined as \(\text{argmax}_i\{f_i(x)\}\). Composing this fact with Property 15, we obtain that \(F^\Phi(x) = F(x)\), since \(F^\Phi(x) = \text{argmax}_i\{f^\Phi(x)\}\) by definition. \(\square\)

5 **VECTORIZING SELF-REPAIR**

Widely-used machine learning libraries, such as TensorFlow [Abadi et al. 2016], simplify the implementation of parallelized, hardware-accelerated code by providing a collection of operations on multi-dimensional arrays of uniform type, called tensors. One can view such libraries as domain-specific languages that operate primarily over tensors, providing embarrassingly parallel operations like matrix multiplication and associative reduction, as well as non-parallel operations like iterative loops and sorting routines. In this section, we present matrix-based algorithms implementing the core procedures used by SR-Layer described in Section 3. As we will later see in Section 6, taking advantage of these frameworks allows our implementation to introduce minimal overhead, typically fractions of milliseconds. Additionally, it means that SR-Layer can be automatically differentiated, making it fully compatible with training and fine-tuning.

Several of the subroutines of FindSatConstraint and Repair (Algorithms 3.2 and 3.3 presented in Section 3) operate on an OrderGraph, which represents a conjunction of ordering literals, \(q\). An OrderGraph contains a vertex set, \(V\), and edge set, \(E\), where \(V\) contains a vertex, \(i\), for each class in \(\{0, \ldots, m - 1\}\), and \(E\) contains an edge, \((i, j)\), from vertex \(i\) to vertex \(j\) if the literal \(y_j < y_i\) is in \(q\). We represent an OrderGraph as an \(m \times m\) adjacency matrix, \(M\), defined according to Equation 7.

\[
M_{ij} := \begin{cases} 
1 & \text{if } (i, j) \in E; \text{i.e., } y_j < y_i \in q \\
0 & \text{otherwise}
\end{cases}
\]
Algorithm 5.1: Stable Topological Sort

Inputs: A graph, $G$, represented as an $m \times m$ adjacency matrix, and a vector, $y : \mathbb{R}^m$
Result: A permutation, $\pi : [m] \rightarrow [m]$

1 TopologicalSort($G, y$):
2 \[
P := \text{all_pairs_longest_paths}(G)
\]
3 \[
\forall i, j \in [m]. P'_{ij} := \begin{cases} y_i & \text{if } P_{ij} \geq 0 \\
\infty & \text{otherwise}
\end{cases}
\]
4 \[
\forall j \in [m]. v_j := \min \{ P'_{ij} \} \quad // \text{set the value of each vertex to the smallest value among its ancestors}
\]
5 \[
\forall j \in [m]. d_j := \max \{ P_{ij} \} \quad // \text{calculate the depth of each vertex in the graph}
\]
6 \[
\text{return argsort([ } \forall j \in [m] . (-v_j, d_j) ] ) \quad // \text{break ties in favor of minimum depth}
\]

Section 5.1 describes the matrix-based algorithm that we use to conduct the stable topological sort that Repair (Algorithm 3.3) depends on. It is based on a classic parallel algorithm due to Dekel et al. [1981], which we modify to ensure that SR satisfies transparency (Property 4). Section 5.2 describes our approach to cycle detection, which is able to share much of the work with the topological sort. Finally, Section 5.3 discusses efficiently prioritizing ordering constraints, needed to ensure that SR satisfies transparency.

5.1 Stable Topological Sort

Our approach builds on a parallel topological sort algorithm given by Dekel et al. [1981], which is based on constructing an all pairs longest paths (APLP) matrix. However, Dekel et al.'s algorithm is not stable in the sense that the resulting order depends only on the graph, and not on the original order of the sequence, even when multiple orderings are possible. While for our purposes this is sufficient for ensuring safety, it is not for transparency. We begin with background on constructing the APLP matrix, showing that it is compatible with a vectorized implementation, and then describe how it is used to perform a stable topological sort.

5.1.1 All Pairs Longest Paths. The primary foundation underpinning many of the graph algorithms in this section is the all pairs longest paths (APLP) matrix, which we will denote by $P$. On acyclic graphs, $P_{ij}$ for $i, j \in [m]$ is defined to be the length of the longest path from vertex $i$ to vertex $j$. Absent the presence of cycles, the distance from a vertex to itself, $P_{ii}$, is defined to be 0. For vertices $i$ and $j$ for which there is no path from $i$ to $j$, we let $P_{ij} = -\infty$.

We compute $P$ from $M$ using a matrix-based algorithm from Dekel et al. [1981], which requires taking $O(\log m)$ matrix max-distance products, where the max-distance product is equivalent to a matrix multiplication where element-wise multiplications have been replaced by additions and element-wise additions have been replaced by the pairwise maximum. That is, a matrix product can be abstractly written with respect to operations $\otimes$ and $\oplus$ according to Equation 8, and the max-distance product corresponds to the case where $x \otimes y := x + y$ and $x \oplus y := \max\{x, y\}$.

\[
(AB)_{ij} := (A_{i1} \otimes B_{1j}) \oplus \ldots \oplus (A_{ik} \otimes B_{kj})
\]

(8)
Using this matrix product, \( P = P^{2^\left\lfloor \log_2 (m) \right\rfloor} \) can be computed recursively from \( M \) by performing a fast matrix exponentiation, as described in Equations 9 and 10.

\[
p^k = p^{b/2}p^{b/2} \tag{9}
\]

\[
P_{ij}^1 = \begin{cases} 
1 & \text{if } M_{ij} = 1 \\
0 & \text{if } M_{ij} = 0 \land i = j \\
-\infty & \text{otherwise}
\end{cases} \tag{10}
\]

5.1.2 Stable Sort. We propose a stable variant of the Dekel et al. [1981] topological sort, shown in Algorithm 5.1. Crucially, this variant satisfies Property 8 (Lemma 17), which Section 3.2.2 identifies as sufficient for ensuring transparency. Essentially, the value of each logit \( y_j \) is adjusted so that it is at least as small as the smallest logit value corresponding to vertices that are parents of vertex \( j \), including \( j \) itself. A vertex, \( i \), is a parent of vertex \( j \) if \( P_{ij} \geq 0 \), meaning that there is some path from vertex \( i \) to vertex \( j \) or \( i = j \). The logits are then sorted in descending order, with ties being broken in favor of minimum depth in the dependency graph. The depth of vertex \( j \) is the maximum of the \( j \)th column of \( P_{ij} \), i.e., the length of the longest path from any vertex to \( j \). An example trace of Algorithm 5.1 is given in Figure 2. By adjusting \( y_j \) into \( v_j \) such that for all ancestors, \( i \), of \( j \), \( v_i \geq v_j \), we ensure each child vertex appears after each of its parents in the returned ordering—once ties have been broken by depth—as the child’s depth will always be strictly larger than that of any of its parents since a path of length \( d \) to an immediate parent of vertex \( j \) implies the existence of a path of length \( d + 1 \) to vertex \( j \).

**Lemma 17.** TopologicalSort satisfies Property 8.

**Proof.** Note that the adjusted logit values, \( v \), are chosen according to Equation 11.

\[
v_j := \min_{i \mid i \text{ is an ancestor of } j \lor i = j} \{ y_i \} \tag{11}
\]

We observe that (i) for all root vertices, \( i, v_i = y_i \), and (ii) the root vertex with the highest original logit value will appear first in the topological ordering. The former follows from the fact that the root vertices have no ancestors. The latter subsequently follows from the fact that the first element in a valid topological ordering must correspond to a root vertex. Thus if \( \operatorname{argmax}_i \{ y_i \} = i^* \in \text{Roots}(g) \), then \( i^* \) is the vertex with the highest logit value, and so by (ii), it will appear first in the topological ordering produced by TopologicalSort, establishing Property 8. \( \square \)

5.2 Cycle Detection

\( \text{IsSat} \), a subroutine of \( \text{FindSatConstraint} \) (Algorithm 3.2) checks to see if an ordering constraint, \( q \), is satisfiable by observing if there are any cycles in the corresponding dependency graph, \( \text{OrderGraph}(q) \). Here we observe that the existence of a cycle can easily be decided from examining \( P \), according to Algorithm 5.2—by checking if \( P_{ii} > 0 \) for some \( i \in [m] \); i.e., if there exists a non-zero-length path from any vertex to itself. Since \( P_{ii} \geq 0 \), this is equivalent to \( \text{Trace}(P) > 0 \). While strictly speaking, \( P_{ij} \), as constructed by Dekel et al. [1981], only correctly reflects the longest path from \( i \) to \( j \) in acyclic graphs, it can nonetheless be used to detect cycles in this way, as for any \( k \leq m, P_{ij} \) is guaranteed to be at least \( k \) if there exists a path of length \( k \) from \( i \) to \( j \), and any cycle is guaranteed to have length at most \( m \).

5.3 Prioritizing Root Vertices

As specified in Property 7, in order to satisfy transparency, the search for a satisfiable ordering constraint performed by \( \text{FindSatConstraint} \) must prioritize constraints, \( q \), in which the original
Fig. 2. Example trace of Algorithm 5.1. (a): The dependency graph and original logit values, \( y \). The values of each logit are provided; the non-bracketed number indicates the logit index and the number in brackets is the logit value, e.g., \( y_0 = 2 \). Arrows indicate a directed edge in the dependency graph; e.g., we require \( y_4 < y_0 \).
(b): updated values passed into \texttt{argsort} as a tuple. For example, \( y_4 \) is assigned \((2, 1)\), as its smallest ancestor \((y_0)\) has logit value 2 in (a) and its depth is 1; and \( y_2 \) is assigned value \((1, 2)\) because its logit value in (a), 1, is already smaller than that of any of its parents, and its depth is 2. The values are sorted by \textit{decreasing} value and \textit{increasing} depth, thus the final order is \( \langle y_1, y_3, y_0, y_4, y_2 \rangle \), corresponding to the permutation \( \pi \), where \( \pi(0) = 2, \pi(1) = 0, \pi(2) = 4, \pi(3) = 1, \) and \( \pi(4) = 3 \).

\begin{algorithm}
\caption{Matrix-Based Cycle Detection}
\begin{algorithmic}[1]
\State \textbf{Inputs:} A graph, \( G \), represented as an \( m \times m \) adjacency matrix
\State \textbf{Result:} A boolean
\Procedure{ContainsCycle}{$G$} \Comment{a boolean function that returns true if \( G \) contains a cycle.}
\State \( P := \texttt{all_pairs_longest_paths}(G) \)
\State \Return Trace\( (P) > 0 \)
\EndProcedure
\end{algorithmic}
\end{algorithm}

predicted class, \( F(x) \), is a root vertex in \( q \)'s corresponding dependency graph. We observe that root vertices can be easily identified using the dependency matrix \( M \). The in-degree, \( d^{in}_j \), of vertex \( j \) is simply the sum of the \( j \)th column of \( M \), given by Equation 12. Meanwhile, the root vertices are precisely those vertices with no ancestors, that is, those vertices \( j \) satisfying Equation 12.

\[ d^{in}_j = \sum_{i \in [m]} M_{ij} = 0 \tag{12} \]

In the context of \texttt{FindSatConstraint}, the subroutine \texttt{Prioritize} lists ordering constraints \( q \) for which \( d^{in}_{F(x)} = 0 \) in \texttt{OrderGraph}(\( q \)) before any other ordering constraints. To save memory, we do not explicitly list and sort all the disjuncts of \( Q_x \) (the DNF form of the active postconditions for \( x \)); rather we iterate through them one at a time. This can be done by, e.g., iterating through each disjunct twice, initially skipping any disjunct in which \( F(x) \) is not a root vertex, and subsequently skipping those in which \( F(x) \) is a root vertex.

6 EVALUATION

We have shown that self-repairing networks (SR-Nets) provide safety to an existing network without affecting accuracy as long as safety and accuracy are mutually consistent. This comes with no additional training cost, suggesting that the only potential downside of SR-Nets is the
run-time overhead introduced by the SR-Layer. In this section, we present an empirical evaluation of our approach to demonstrate its scalability, and find that the run-time performance is not an issue in practice—overheads range from 0.2-0.8 milliseconds, and scale favorably with the size and complexity of properties.

We explore the capability of our approach on a variety of domains, demonstrating its ability to solve previously studied safety-verification problems (Sections 6.1 and 6.2), and its ability to efficiently scale both (i) to large convolutional networks (Section 6.3) and (ii) to arbitrary, complex safety properties containing disjunctions and overlapping preconditions (Section 6.4).

We implemented our approach in Python, using TensorFlow to vectorize our SR-Layer (Section 5). All experiments were run on an NVIDIA TITAN RTX GPU with 24 GB of RAM, and a 4.2GHz Intel Core i7-7700K with 32 GB of RAM.

### 6.1 ACAS Xu

ACAS Xu [Kochenderfer et al. 2015] is a collision avoidance system for unmanned aircraft that has been frequently studied in the context of neural network safety verification [Julian et al. 2019; Katz et al. 2017; Lin et al. 2020; Singh et al. 2019]. While the system was originally implemented as a large numeric lookup table mapping sensor measurements to horizontal maneuver advisories, Julian et al. [2019] proposed the use of a family of 45 neural networks to operate as a compressed, functional approximation of the lookup table. Katz et al. [2017] proposed 10 safety properties for this family of networks, which have become standard for research on this problem. We consider 9 of these properties, which can be expressed as safe ordering properties (Section 2.2). The remaining property, \( \phi_1 \), requires in its postcondition that the logit output corresponding to the “clear-of-conflict” (COC) advisory is less than 1,500, an arbitrary numerical value; we argue that this is not a compelling property, since the scale of logit outputs is not meaningful, thus \( \phi \) can be trivially satisfied by scaling the network’s output.

Each of the 45 networks consists of six hidden dense layers of 50 neurons each. Each network needs to satisfy some subset of the 10 safety properties; that is, more than one safety property may apply to each model, but not all safety properties apply to each model. A network is considered safe if it satisfies all of the relevant safety properties. Among the 45 networks, Katz et al. [2017] reported that 9 networks were already safe after standard training, while 36 were unsafe, exhibiting safety property violations.

The data used to train the 45 networks is not publicly available; however, Lin et al. [2020] provide a synthetic test set for each network, consisting of 5,000 points uniformly sampled from the specified state space and labeled using the respective network as an oracle. We note that because this test set is labeled using the original models, the accuracy of each original model on this test set is necessarily 100%.

Table 1a presents the results of applying our SR transformer to each of the 45 provided networks. In particular, we consider the number of networks for which safety can be guaranteed, and the accuracy of the resulting SR-Net. We compare our results to those using ART [Lin et al. 2020], a recent approach to safe-by-construction learning. ART aims to learn neural networks that satisfy non-relational safety properties expressed using linear real arithmetic constraints. It updates the loss function to be minimized during learning by adding a term, referred to as the correctness loss, that measures the degree to which a neural network satisfies or violates the safety property. A value of zero for the correctness loss ensures that the network is safe. However, there is no guarantee that learning will converge to zero correctness loss, and the resulting model may not be as accurate as one trained with conventional methods.

Because the safety properties for each network are satisfiable on all points, Definition 3 tells us that safety is guaranteed for all 45 SR-Nets. In this case, we see that ART also manages to produce
45 safe networks after training; however we see that it comes at a cost of nearly 6 percentage points in accuracy, even on the networks that were already safe. Meanwhile, transparency (Property 4) tells us that SR-Nets will only see a decrease in accuracy relative to the original network when accuracy is in direct conflict with safety. On the 9 original networks that were reported as safe, clearly no such conflict exists, and accordingly, we see that the corresponding SR-Nets achieve the same accuracy as the original networks (100%). On the 36 unsafe networks, we find again that the SR-Nets achieved 100% accuracy. In this case, it would have been possible that the SR-Nets would have achieved lower accuracy than the original networks, as some of the safety properties have the potential to conflict with accuracy. For example, the postcondition of the property $\phi_8$ requires that the predicted maneuver advisory is either to continue straight (COC) or to turn weakly to the left. Thus, correcting $\phi_8$ on inputs for which it is violated would necessarily change the network’s prediction on those inputs; and, since the labels are derived from the original networks’ predictions, this would lead to a drop in accuracy. However, we find that none of the test points include violations of such properties (even though such violations exist in the space generally [Katz et al. 2017]), as evidenced by the fact that the SR-Net accuracy remained unchanged.

Table 2 shows the average overhead introduced by applying SR to each of the ACAS Xu networks. We see that the absolute overhead is only approximately a quarter of a millisecond per instance on average, accounting for less than an 8× increase in prediction time.

### 6.2 Collision Detection

The Collision Detection dataset [Ehlers 2017] provides another instance of a safety verification task that has been studied in the prior literature. In this setting, a neural network controller is trained to predict whether two vehicles following curved paths at different speeds will collide. As this is a binary decision task, the network contains two outputs, corresponding to the case of a collision and the case of no collision. Ehlers proposes 500 safety properties for this task, corresponding to $\ell_\infty$ robustness regions around 500 particular inputs. That is, property $\phi_i$ for $i \in \{1, \ldots, 500\}$ corresponds to a point, $x_i$, and radius, $\epsilon_i$, and is defined according to Equation 13.

$$\phi_i(x, y) := ||x_i - x||_\infty \leq \epsilon_i \implies y = F(x_i) \quad (13)$$

Such properties can be represented as safe ordering properties, where the postcondition of $\phi_i$ is defined to be $y_0 > y_1$ if $F(x_i) = 0$ and $y_0 < y_1$ if $F(x_i) = 1$. 

| method   | safe networks | mean accuracy (%) |
|----------|---------------|-------------------|
| 36 unsafe nets | original | 0 / 36 | 100.0 |
| ART | 36 / 36 | 94.4 |
| SR-Net | 36 / 36 | 100.0 |
| 9 safe nets | original | 9 / 9 | 100.0 |
| ART | 9 / 9 | 94.3 |
| SR-Net | 9 / 9 | 100.0 |

| method   | properties certified | accuracy (%) |
|----------|----------------------|--------------|
| original | 328 / 500 | 99.9 |
| ART | 481 / 500 | 96.8 |
| SR-Net | 500 / 500 | 99.9 |

Table 1. Safety certification results on the (a) ACAS Xu [Julian et al. 2019] and (b) Collision Detection [Ehlers 2017] datasets, which have been studied in the prior literature. We compare the success rate and accuracy to that of ART [Lin et al. 2020], a recent safe-by-construction approach. The original network is provided as a baseline. Best results are shown in bold.
Table 2 presents the results of applying our SR transformer to the original network provided by Ehlers. Similarly to before, we consider the number of properties with respect to which safety can be guaranteed, and the accuracy of the resulting SR-Net, comparing our results to those of ART.

We see in this case that ART was unable to guarantee safety for all 500 properties. Meanwhile, it resulted in a drop in accuracy of approximately 3 percentage points. On the other hand, it is simple to check that the conjunction of all 500 safety properties is satisfiable for all inputs; thus, Definition 3 tells us that safety is guaranteed with respect to all properties. Meanwhile SR-Nets impose no penalty on accuracy, as none of the test points themselves violate the properties.

Table 2 shows the overhead introduced by applying SR to the collision detection model. In absolute terms, we see that the overhead is approximately half a millisecond per instance, accounting for less than a 3× increase in prediction time.

### 6.3 Scaling to Larger Domains

One major challenge for many approaches that attempt to verify network safety—particularly post-learning methods—is scalability to very large neural networks. Such networks pose a problem for several reasons. Many approaches analyze the parameters or intermediate neuron activations using algorithms that do not scale polynomially with the network size. This is a problem not only in theory, with large networks used in practice containing numbers of parameters in the hundreds of millions. Furthermore, abstractions of the behavior of large networks may see compounding imprecision in large, deep networks.

Our approach, on the other hand, treats the network as a black-box and is therefore not sensitive to its specifics. In this section we demonstrate that this is borne out in practice; namely the absolute overhead introduced by our SR-Layer remains relatively stable even on very large networks.

For this, we consider a novel set of safety properties for the CIFAR-100 image dataset [Krizhevsky and Hinton 2009], a standard benchmark for object recognition tasks. The CIFAR-100 dataset is comprised of 60,000 32 × 32 RGB images categorized into 100 different classes of objects, which are grouped into 20 superclasses of 5 classes each. We propose a set of safe ordering constraints that are reminiscent of a variant of top-\(k\) accuracy restricted to members of the same superclass, which has been studied recently in the context of certifying relational safety properties of neural networks [Leino and Fredrikson 2021]. More specifically, we require that if the network’s prediction belongs to superclass \(C_k\) then the top 5 logit outputs of the network must all belong to \(C_k\). Formally, there are 20 properties, one for each superclass, where the property, \(\phi_k\) for superclass \(C_k\), for \(k = \{1, \ldots, 20\}\), is defined according to Equation 14. Notice that with respect to these properties, a standardly trained network can be accurate, yet unsafe, at a point, even without accuracy and safety being mutually inconsistent.

\[
\phi_k(x, y) := F(x) \in C_k \implies \bigwedge_{i,j \mid i \in C_k, j \notin C_k} y_j < y_i
\]

Table 2 shows the overhead introduced by applying SR, with respect to these properties, to two different networks trained on CIFAR-100. The first is a convolutional neural network (CNN) that is much smaller than is typically used for vision tasks, containing approximately 1 million parameters. The second is a standard residual network architecture, ResNet-50 [He et al. 2016], with approximately 24 million parameters.

|                      | ACAS Xu Collision Detection | CIFAR-100 (small CNN) | CIFAR-100 (ResNet-50) | Synthetic |
|----------------------|-----------------------------|-----------------------|-----------------------|-----------|
| absolute overhead (ms)| 0.26                        | 0.58                  | 0.77                  | 0.82      | 0.27      |

Table 2. Absolute overhead introduced by the SR-Layer per input.
In absolute terms, we see that both networks incur less than 1ms of overhead per instance relative to the original model (0.77ms and 0.82ms, respectively), making SR a practical option for providing safety in both networks. Moreover, the absolute overhead varies only by about 5% between the two networks, suggesting that the overhead is not sensitive to the size of the network. This overhead accounts for approximately a $12 \times$ increase in prediction time on the CNN. Meanwhile, the overhead on the ResNet-50 accounts for only a $6 \times$ increase in prediction time relative to the original model. The ResNet-50 is a much larger and deeper network; thus its baseline prediction time is longer, so the overhead introduced by the SR-Layer accounts for a smaller fraction of the total computation time. In this sense, our SR transformer becomes relatively less expensive on larger networks.

Interestingly, we found that the original network violated the safety properties on approximately 98% of its inputs, suggesting that obtaining a violation-free network without SR might prove particularly challenging. Meanwhile, the SR-Net eliminated all violations, with no cost to accuracy, and less than 1ms in overhead per instance.

### 6.4 Handling Arbitrary, Complex Safety Properties

Safe ordering properties are capable of expressing a wide range of compelling non-relational safety properties. Moreover, our SR transformer is a powerful, general tool for ensuring safety with respect to arbitrarily complex safe ordering properties, comprised of many conjunctive and disjunctive clauses. Notwithstanding, the properties presented in our evaluation thus far have been relatively simple. In this section we explore more complex safe ordering properties, and describe experiments that lend insight as to which factors most impact the scalability of our approach.
To this end, we designed a synthetic dataset with associated safety properties that are randomly generated according to several specified parameters, allowing us to assess how aspects such as the number of properties (\(\alpha\)), the number of disjunctions per property (\(\beta\)), and the dimension of the output vector (\(m\)) impact the run-time overhead. In our experiments, we fix the input dimension, \(n\), to be 10. The synthetic data, which we will denote by \(D(\alpha, \beta, m)\), are generated according to the following procedure.

(i) First, we generate \(\alpha\) random properties. The preconditions take the form \(b_l \leq x \leq b_u\), where \(b_l\) is drawn uniformly at random from \([0, 1.0 - \epsilon]\) and \(b_u := b_l + \epsilon\). We choose \(\epsilon = 0.4\) in our experiments; as a result, the probability that any two preconditions overlap is approximately 30%. The ordering constraints are disjunctions of \(\beta\) randomly-generated cycle-free ordering graphs of \(m\) vertices, i.e., \(\beta\) disjuncts. Specifically, in each graph, we include each edge, \((i, j)\), for \(i \neq j\) with equal probability, and require further that at least one edge is included, and the expected number of edges is \(\gamma\) (we use \(\gamma = 3\) in all of our experiments). Graphs with cycles are resampled until a graph with no cycles is drawn.

(ii) Next, for each property, \(\phi\), we sample \(N/\alpha\) random inputs, \(x\), uniformly from the range specified by the precondition of \(\phi\). In all of our experiments we let \(N = 2,000\). For each \(x\), we select a random disjunct from the postcondition of \(\phi\), and find the roots of the corresponding ordering graph. We select a label, \(y^*\) for \(x\) uniformly at random from this set of roots, i.e., we pick a random label for each point that is consistent with the property for that point.

(iii) Finally, we generate \(N\) random points that do not satisfy any of the preconditions of the \(\alpha\) properties. We label these points via a classifier trained on the \(N\) labeled points already generated in (ii). This results in a dataset of \(2N\) labeled points, where 50% of the points are captured by at least one safety property.

We use a dense network with six hidden layers of 1,000 neurons each as a baseline, trained on \(D(4, 4, 8)\). Table 2 shows the overhead introduced by applying SR to our baseline network. We see that the average overhead is approximately a quarter of a millisecond per instance, accounting for a 10× increase in prediction time. Figure 3 provides a more complete picture of the overhead as we vary the number of properties (\(\alpha\)), the number of disjuncts per property (\(\beta\)), the number of classes (\(m\)), or the depth of the network (\(\delta\)).

We observe that among these parameters, the overhead is sensitive only to the number of classes. This is to be expected, as the complexity of the SR-Layer scales directly with \(m\) (see Section 3.3), requiring a topological sort of the \(m\) elements of the network’s output vector. On the other hand, perhaps surprisingly, increasing the complexity of the safety constraints through either additional safe ordering properties or larger disjunctive clauses in the ordering constraints had little effect on the overhead. While in the worst case the complexity of the SR-Layer is also dependent on these parameters (Section 3.3), if \(\text{FindSatConstraint}\) finds a satisfiable disjunct quickly, it will short-circuit. The average-case complexity of \(\text{FindSatConstraint}\) is therefore more nuanced, depending to a greater extent on the specifics of the constraints rather than simply their size. Altogether, these observations suggest that the topological sort in SR-Layer tends to account for the majority of the overhead.

Finally, the results in Figure 3 regarding the depth of the network concur with what we observed in Section 6.3 previously; namely that the overhead does not depend on the size of the network.

7 RELATED WORK
We have already discussed the relationship of our work to the most closely related safe-by-construction learning approaches (Section 1). Section 7.1 presents a broader survey of techniques for verifying neural networks and establishing safety guarantees by-construction. Section 7.2 discusses
the relationship of our approach to dynamic repair methods for traditional software issues, as well as safety in control systems.

7.1 Neural Network Verification

**Static Verification and Repair.** A number of approaches for verification of already-trained neural networks have been presented in recent years. These approaches largely treat neural networks as programs that are, incidentally, generated by a learning routine. These verification efforts have focused on verifying non-relational safety properties similar to our safe ordering properties, as well as **local robustness** which requires that in some local region centered at an input $x_0$, the prediction of a classifier remains invariant, and certain fairness properties which impose non-interference between specified input features and the network’s output.

The abstract interpretation approaches from [Gehr et al. 2018; Singh et al. 2019] verify properties that associate polyhedra with pre- and postconditions. This enables non-relational safety verification, and, by propagating an appropriate abstract domain through the network, local robustness certification. Reluplex [Katz et al. 2017] encodes a network’s semantics as a system of constraints, and poses safety and local robustness verification as constraint satisfiability for the relevant theories. These approaches can encode safe ordering constraints, which are a special case of polyhedral postconditions, but as discussed in the introduction, do not provide effective means to constructing safe networks. The verification approach from [Huang et al. 2017] addresses local robustness using a forward symbolic analysis in combination with SMT-based queries. Another approach [Urban et al. 2020] verifies fairness using an algorithm based on abstract interpretation. While all these approaches provide useful guarantees, they cannot verify safe ordering properties directly.

A number of techniques formulate local robustness verification as an optimization problem, solved by an off-the-shelf optimizer [Bastani et al. 2016; Dvijotham et al. 2018; Raghunathan et al. 2018; Tjeng et al. 2019; Wong and Kolter 2018]. Some techniques [Anderson et al. 2019] use an optimizer together with an abstract interpreter in an interactive loop for verifying local robustness. The scalability issues encountered with these approaches are addressed by making them compatible with hardware acceleration in Müller et al. [2021], by parallelizing constraint solving [Wu et al. 2020], and by designing verifiers that are carefully tuned for the property under consideration, particularly in the case of local robustness certification [Fromherz et al. 2021; Weng et al. 2018]. Section 5 takes this approach with our implementation of the SR-Layer, enabling hardware acceleration and compatibility with gradient-based optimization methods.

Many of the above approaches can provide counterexamples when the network is unsafe, but none of them are capable of repairing the network. A repair approach is proposed in [Sotoudeh and Thakur 2021] that can provably repair neural networks using piecewise-linear activations with respect to non-relational safety specifications expressed using polyhedral pre- and postconditions. In case the specifications are over a finite set of points, neural networks using any activation function can be repaired. The approach is restricted to repairs that can be brought about by updating the parameters of a single layer. This is because the repair problem is formulated as a series of linear programs, one per layer in the network, over the parameters of the model, aiming to find a set of safe parameters that is closest in norm distance to those of the original model. While the closeness objective is a heuristic intended to favor accuracy preservation, our repair satisfies transparency (Property 4), which guarantees that accuracy will be preserved when the safety property allows it.

**Safe-by-Construction Learning.** A number of recent efforts aim to learn neural networks that are correct by construction. Many approaches [Fischer et al. 2019; Li et al. 2019a; Madry et al. 2018] modify the learning objective by adding a penalty for unsafe or incorrect behavior, but do not provide a guarantee when the loss meets certain criteria. In all such cases, static verifiers are needed...
to achieve guarantees, and balancing accuracy against the modified learning objective is a concern. Here we focus on techniques that provide guarantees without requiring external verifiers.

ART [Lin et al. 2020] aims to learn neural networks that satisfy non-relational safety properties expressed using linear real arithmetic constraints. It updates the loss function to be minimized during learning by adding a term, referred to as the correctness loss, that measures the degree to which a neural network satisfies or violates the safety property. A value of zero for the correctness loss ensures that the network is safe. Given a precondition over the network inputs, correctness loss is calculated by first computing an over-approximation of the reachable set of network outputs and then, if this over-approximate set does not imply the desired safety postcondition, computing the worst-case distance between a point in the over-approximate set and it’s projection on the desired postcondition. The over-approximate set is computed via a differentiable abstract interpreter, and is thus compatible with training. To balance the precision-efficiency tradeoff typically faced by abstract interpreters, this approach integrates an abstraction refinement loop in the learning process. However, there is no guarantee that learning will converge to zero correctness loss, and the resulting model may not be as accurate as one trained with conventional methods. In contrast, our transformer is guaranteed to produce a safe network that preserves accuracy.

A similar approach is presented in Mirman et al. [2018] to enforce local robustness for all input samples in the training dataset. This technique also updates the learning objective and uses a differentiable abstract interpreter for over-approximating the set of reachable outputs. A negative value for the modified loss guarantees that the corresponding network is locally robust on all training samples, but cannot extend this guarantee to unseen examples, so static verification must also be used to achieve guarantees in deployed networks. For both this approach and that of Lin et al. [2020], the run time of the differentiable abstract interpreter depends heavily on the size and complexity of the network, and it may be difficult or expensive to scale them to many architectures.

As discussed in Section 1, an alternative way to achieve correct-by-construction learning is to modify the architecture. This approach has been successfully employed to construct networks that have a fixed Lipschitz constant [Anil et al. 2019; Li et al. 2019b; Trockman and Kolter 2021], a relational property that is useful for certifying robustness and ensuring good training behavior in certain settings. Recently, it was shown by Leino and Fredrikson [2021]; Leino et al. [2021] how to modify the architecture to achieve several relaxed notions of global robustness, where the modified network is allowed to selectively abstain from prediction at inputs where local robustness cannot be certified. Donti et al. [2021] used optimization layers to enforce stability properties of neural network controllers. These techniques are closest to ours in spirit, although we focus on non-relational safety properties for classifiers, and more specifically safe ordering properties, which have not been addressed previously in the literature.

7.2 Dynamic Repair In Other Domains

Shielding Control Systems. Control systems interact with their environment in a tight loop; based on the state of the environment, the controller picks an action to perform, and in turn, this action updates the environment state. Agents learned via reinforcement learning, reactive systems, and hybrid systems are examples of such systems. Safety specifications for controllers are typically expressed in terms of environment states that should never be reached by the system. In order to ensure safety, the controller has to plan ahead: it can never allow the system to visit an environment state that leads to an unsafe state in the future. Recent approaches have proposed ensuring safety of these systems by constructing run-time check-and-repair mechanisms, also referred to as shields [Alshiekh et al. 2018; Bloem et al. 2015; Zhu et al. 2019]. Shields check at run time if the system is headed towards an unsafe state and provide corrections for potentially unsafe actions when necessary. However, in order to conduct these run-time checks, shields need access to
a model of the environment that describes the environment dynamics, i.e., the effect of controller actions on environment states. Though shields and our proposed SR-Layer share the run-time check-and-repair philosophy, they are designed for different problem settings.

*Recovering from Program Errors.* Embedding run-time checks into a program to ensure safety is a familiar technique in the program verification literature. Contract checking [Findler and Felleisen 2002; Meyer 1992], run-time verification [Havelund and Rosu 2001], and dynamic type checking are all instances of such run-time checks. If a run-time check fails, the program exits with a special error value. A large body of work also exists on gracefully recovering from errors caused by traditional software issues such as divide-by-zero, null-dereference, memory corruption, and infinite loops [Berger and Zorn 2006; Kling et al. 2012; Long et al. 2014; Perkins et al. 2009; Qin et al. 2005; Rinard et al. 2004]. These approaches are particularly relevant in the context of long-running programs. Typically, the goal is to repair the program state just enough so that computation can continue.

8 CONCLUSION AND FUTURE DIRECTIONS

Our primary contribution in this work is a method for transforming an arbitrary neural network into a safe-by-construction self-repairing network, termed SR-Net, which is guaranteed to satisfy a given set of safe ordering properties without harming the accuracy of the original network. This serves as a powerful tool for providing safety with respect to a broad class of non-relational safety properties that we characterize in this work; the importance of which is underscored by the increasing use of neural networks in safety- and security-critical systems.

Unlike many prior approaches, our technique avoids several common shortcomings. First, it does not place the burden on the practitioner to obtain a safe model. Many approaches to neural network safety certification simply label a network as safe or unsafe post-learning. If the network is declared unsafe (or cannot be definitively proven safe, e.g., if the certification fails to terminate), the practitioner is forced to seek a new model. By contrast, our approach repairs any supplied model, eliminating this issue altogether. Second, the success of our technique is not dependent on training dynamics or the parameters of the network being repaired—it guarantees safety without further training or modifications to the network’s parameters. Finally, the scalability of our approach is not fundamentally limited by the size or architecture of the model being repaired. This allows it to be applied to large, state-of-the-art models, which is impractical for most other existing approaches.

Primarily then, the potential downside to our approach is the run-time overhead introduced by the SR-Layer. Nonetheless, we demonstrate in our evaluation (Section 6) that our approach is in fact practical as presented, maintaining overheads of less than one millisecond per instance on a wide variety of applications. Issues related to overhead are mitigated to some extent by our vectorized implementation, which allows us to leverage GPUs to reap the benefits of large-scale parallelism. Still, the concern over the computational cost of the SR-Layer highlights performance optimizations as a potential avenue for further broadening the applicability of our repair method.

One interesting facet of our approach that remains largely unexplored is the differentiability of the SR-Layer. In principle, this opens the door to benefits that could be obtained by training against the repairs made by the SR-Layer. Though we found that a “vanilla” attempt to training with the SR-Layer did not provide clear advantages over appending it to a model post-learning, we believe this remains an interesting future direction to explore. It is conceivable that a careful approach to training SR-Nets could lead to superior accuracy, as the network could learn to use the modifications made by the SR-Layer to its advantage. Furthermore, aspects of the algorithm, including, e.g., the heuristic used to prioritize the search for a satisfiable graph (see Section 3.2.1), could be parameterized and learned, potentially leading to both accuracy and performance benefits.
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