Teaching Temporal Logics to Neural Networks

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Abstract. We show that a deep neural network can learn the semantics of linear-time temporal logic (LTL). As a challenging task that requires deep understanding of the LTL semantics, we show that our network can solve the trace generation problem for LTL: given a satisfiable LTL formula, find a trace that satisfies the formula. We frame the trace generation problem for LTL as a translation task, i.e., to translate from formulas to satisfying traces, and train an off-the-shelf implementation of the Transformer, a recently introduced deep learning architecture proposed for solving natural language processing tasks. We provide a detailed analysis of our experimental results, comparing multiple hyperparameter settings and formula representations. After training for several hours on a single GPU the results were surprising: the Transformer returns the syntactically equivalent trace in 89\% of the cases on a held-out test set. Most of the “mispredictions”, however, (and overall more than 99\% of the predicted traces) still satisfy the given LTL formula. In other words, the Transformer generalized from imperfect training data to the semantics of LTL.

Keywords: Machine Learning · Verification · Logic

1 Introduction

In recent years, machine learning, especially deep learning, has revolutionized several areas of computer science and achieved human-level performance in tasks such as image recognition [15], face recognition [44], translation [49,46], or board games [27,12]. In the area of computer-aided verification, however, deep learning techniques are often being considered as insufficient. Mostly, due to two reasons: 1) the perception that deep neural networks are unable to solve complex logical reasoning tasks reliably, and 2) the gap of technologies used in formal methods and machine learning. Applications of machine learning in logical reasoning problems are therefore few, and mostly restricted to sub-problems within larger logical frameworks, such as resolving heuristics in solvers [20,338].

In this paper, we attempt to bridge the technology gap by explaining recent advances in deep learning research and show that off-the-shelf implementations of state-of-the-art machine learning architectures can be trained for a classical
problem in computer-aided verification: the satisfiability problem of linear-time temporal logic (LTL). LTL is a modal logic with temporal modalities for describing the possibly infinite behavior of a reactive system [31]. For example, \( \neg \text{grant} \rightarrow \text{request} \), states that grants can only be given after a request is observed (i.e. an arbiter may not give spurious grants). LTL satisfiability is a PSPACE-complete problem that has been studied extensively, e.g., [32, 36, 23]. It can be used to analyze specifications, e.g., checking whether specifications are vacuously true or unsatisfiable. This is of great interest because specifications can contain as much errors as code. Furthermore, solvers for LTL satisfiability can be used to enhance other verification algorithms by performing symmetry checks or analyze implications between different formulations of a specification.

On the machine learning side, we picked Transformers [46], a deep learning architecture that can read and write sequences of characters or words (i.e. it is a sequence-to-sequence architecture). Transformers are surprisingly versatile and quickly became state-of-the art in many natural language processing tasks [7]. Transformers have also been used to analyze code [10, 16].

We consider LTL satisfiability as a translation task: to “translate” a given LTL formula into a satisfying trace. This allows us to directly apply the deep learning methodology and simply learn the semantics of LTL from a large set of examples. For that purpose we generated a dataset consisting of pairs of an LTL formula and an arbitrarily chosen satisfying trace. We train an off-the-shelf implementation of the Transformer on this data set and observe that after a couple of hours of training, they achieve an accuracy of more than 89% on held-out test data. The most surprising finding of this work is that most of the “mispredictions” of the Transformer actually satisfy the given LTL formula - these mispredictions just do not exactly match the arbitrarily chosen example trace. This means that the Transformer architecture generalized from imperfect data to the semantics of LTL. We also provide an in-depth analysis of how transformers process temporal logic formulas by visualizing what parts of the formula were most influential in the decisions of the Transformer. Finally, we show that the choice of representation of the formulas has an impact on the final performance. We hope that these contributions will lead to enhanced automation of verification techniques through the integration of deep learning.

The remainder of this paper is structured as follows: We continue with the definition of the LTL trace generation problem in Section 2 and will then explain the Transformer architecture in detail in Section 3. In Section 4, we describe our data set of LTL formulas. The experiments are described and analyzed in Section 5. We give a detailed overview of related work in Section 6 and conclude in Section 7.

2 Linear-Time Temporal Logic

Let \( AP \) be a set of atomic propositions. A (explicit) trace \( t \) is an infinite sequence over subsets of the atomic propositions. We define the set of traces \( TR := (2^AP)^\omega \). We use the following notation to manipulate traces: Let \( t \in TR \)
be a trace and \( i \in \mathbb{N} \) be a natural number. With \( t[i] \) we denote the set of propositions at \( i \)-th position of \( t \). Therefore, \( t[0] \) represents the starting element of the trace. Let \( j \in \mathbb{N} \) and \( j \geq i \). Then \( t[i, j] \) denotes the sequence \( t[i] t[i + 1] \ldots t[j - 1] t[j] \) and \( t[i, \infty] \) denotes the infinite suffix of \( t \) starting at position \( i \).

**Linear-time temporal Logic.** Linear-time temporal logic (LTL) \([31]\) combines the usual Boolean connectives with temporal modalities such as the Next operator \( \circ \) and the Until operator \( \mathcal{U} \). The syntax of LTL is given by the following grammar:

\[
\varphi ::= p \mid \neg \varphi \mid \varphi \land \varphi \mid \circ \varphi \mid \varphi \mathcal{U} \varphi
\]

where \( p \in \text{AP} \) is an atomic proposition. \( \circ \varphi \) means that \( \varphi \) holds in the next position of a trace; \( \varphi \mathcal{U} \varphi_2 \) means that \( \varphi_1 \) holds until \( \varphi_2 \) holds. There are several derived operators, such as \( \Diamond \varphi \equiv \text{true} \lor \varphi \), \( \square \varphi \equiv \neg \Diamond \neg \varphi \), and \( \varphi_1 \mathcal{W} \varphi_2 \equiv (\varphi_1 \mathcal{U} \varphi_2) \lor \square \varphi_1 \). \( \Diamond \varphi \) states that \( \varphi \) will eventually hold in the future and \( \square \varphi \) states that \( \varphi \) holds globally; \( \mathcal{W} \) is the weak version of the until operator.

Let \( p \in \text{AP} \) and \( t \in \text{Traces} \). The semantics of an LTL formula is defined as the smallest relation \( \models \) that satisfies the following conditions:

- \( t \models p \) iff \( p \in t[0] \)
- \( t \models \neg \varphi \) iff \( t \not\models \varphi \)
- \( t \models \varphi_1 \land \varphi_2 \) iff \( t \models \varphi_1 \) and \( t \models \varphi_2 \)
- \( t \models \circ \varphi \) iff \( t[1, \infty] \models \varphi \)
- \( t \models \varphi_1 \mathcal{U} \varphi_2 \) iff there exists \( i \geq 0 : t[i, \infty] \models \varphi_2 \)
  and for all \( 0 \leq j < i \) we have \( t[j, \infty] \models \varphi_1 \)

**Satisfiability of LTL.** The satisfiability problem of LTL is to decide, given an LTL formula \( \varphi \), whether there exists a trace \( t \in \text{Traces} \) such that \( t \models \varphi \). We define the trace generation problem of LTL as the following sub problem: Given a satisfiable LTL formula \( \varphi_{\text{sat}} \), construct a trace \( t \) such that \( t \models \varphi_{\text{sat}} \).

**Symbolic Traces.** Let \( \text{Prop}_{\Sigma} \) be the set of all well-formed propositional formulas over \( \Sigma \). We define a symbolic trace as a sequence in \( \text{Prop}_{\Sigma}^\omega \). A symbolic trace \( t_s \) defines the set \( \text{Traces}(t_s) \) of traces \( t \) where \( t[i] \) satisfies \( t_s[i] \) for all \( i \). We also say an explicit trace \( t \) is an instance of a symbolic trace \( t_s \) if \( t \in \text{Traces}(t_s) \).

**Example 1.** Given \( \text{AP} = \{a, b, c\} \), the symbolic trace \( (a \land b)^\omega \) defines the infinite set of traces \( \{a^\omega \mid \forall i : a \in a[i]\} \). Traces \( t_c = \{a, b, c\}^\omega \) and \( t_{ac} = \{a, b\}^\omega \) are two of infinite many instances of the symbolic trace \( (a \land b)^\omega \), i.e., \( t_c, t_{ac} \in \{a \land b\}^\omega \).

Analogously to the satisfiability with explicit traces, the symbolic satisfiability problem of LTL is to decide, given an LTL formula \( \varphi \), whether there exists a symbolic trace \( t_s \in \text{Prop}_{\Sigma}^\omega \). Given a satisfiable LTL formula \( \varphi_{\text{sat}} \), the symbolic trace generation problem of LTL asks for a construction of a symbolic trace \( t_s \) such that every instance of \( t_s \) satisfies the formula, i.e., \( \forall t \in t_s : t \models \varphi_{\text{sat}} \).
Fig. 1. A high-level overview of the Transformer architecture: The input sequence is processed in one go by multiple encoding layers. The intermediate result is then given to each decoder layer. The decoder takes the already computed output and computes the next output step-by-step.

Neither problem has necessarily an unambiguous solution and every explicit trace that satisfies an LTL formula is also a solution for the symbolic satisfiability problem. Note that for each satisfiable LTL formula there exists both, an explicit and a symbolic satisfying trace that can be finitely represented as a lasso, i.e., a finite prefix $u$ followed by a period $v$ that is repeated infinitely often.

3 The Transformer

In this section, we give an overview of the Transformer [46], which is a deep neural network architecture initially proposed for solving natural language processing tasks. Transformers have recently become the state-of-the-art architecture for many natural language processing tasks, such as translation or summarization, replacing, e.g., recurrent neural networks (RNNs) such as long short-term memories (LSTMs) [17]. Transformers are designed to handle sequences of input elements by computing hidden embeddings for each element in parallel. They make use of the so-called attention mechanism that enables the Transformer to relate arbitrary input elements to each other and to process the input sequence all at once.

We will explain this mechanism in detail further below. There are several benefits to this approach: First, the training can be massively parallelized, and can thus effectively exploit modern hardware. Second, the processing of the input data in the neural network is very flexible, i.e., the input elements do not have to be processed one after another. Third, the number of steps information has to flow through the neural network is significantly decreased, alleviating problems with computing gradients through many operations.
There are publicly available implementations of the Transformer, e.g., [6, 45], which can handle a wide range of tasks. This makes this approach highly accessible for users outside the machine learning domain. We begin by describing an overview of the architecture before zooming into the details of the architecture, i.e., the encoder, decoder, and attention mechanisms.

**Architecture Overview.** A Transformer follows a basic encoder-decoder structure (see Figure 1). The encoder constructs a hidden embedding $z_i$ for each input embedding $x_i$ of the input sequence $x = (x_0, \ldots, x_n)$ in one go. An embedding is a mapping from plain input, for example words or characters, to a high-dimensional vector, for which learning algorithms and toolkits exist, e.g., word2vec [26]. Given the encoder’s output $z = (z_0, \ldots, z_k)$, the decoder generates a sequence of output embeddings $y = (y_0, \ldots, y_m)$ step-by-step. Note that the length of the input and output sequences does not have to be the same. Since the transformer architecture contains no recurrence nor any convolution, a positional encoding is added to the input and output embeddings that allows to distinguish between different orderings. The transformer architecture is well-suited for the trace generation problem as we specifically ask for a witness instead of a binary classification.

**Encoder.** The encoder consists of multiple layers where each layer is composed of the following two components: a so-called self-attention mechanism and a fully connected feed-forward neural network (see Figure 2). Each component is followed by a layer-normalization [2] step, which significantly reduces the training time by normalizing the activities of the neurons. The feed-forward neural network $FFNN$ consists of two linear transformations with a ReLU activation in
between, i.e., \( FFNN(x) = \max(0, xW_1 + b_1)W_2 + b_2 \). Instead of maintaining a hidden state, e.g. in a recurrent neural network architecture, the self-attention mechanism allows the neural network to incorporate the hidden embedding of other important input elements into the hidden embedding of the current element under consideration.

We begin by describing the notion of attention intuitively. Consider a Transformer trained for translation and the input sentence “The animal didn’t cross the street because it was too tired”. Figure 3 (left) depicts the attention that the neural network pays to the other words in the sentence when encoding the word “it”. The most attention is focused on the phrase “The animal”. Computing the attention is parallelized in multiple attention-heads that potentially pay attention to different parts of the input. Figure 3 (right) shows one attention head during the encoding of the formula \((a U b) \land (a U \neg b)\). When encoding the second until-operator this particular attention head pays very close attention to the \(b\) of the first until-operator. Intuitively, it pays attention that the second until-operator has to take the first conjunct into the account as well. This means the Transformer cannot simply satisfy the formula by outputting \(\neg b\) and \(b\) on the first position of the trace as this would lead to a contradiction. As we will see in our experimental results, the transformer constructs the following trace instead: \(a \land \neg b ; b ; true\omega\), where \(\omega\) denotes the beginning of the next position. I.e., it delays the satisfaction of the first until to the second position.

We describe the attention mechanism in more technical detail. To compute the hidden embedding for the \(i\)-th character of the formula we fist add the aforementioned positional encoding to the input embeddings \(x_i\). Then, the self-attention is computed as follows. For each input embedding \(x_i\), we compute 1) a query vector \(q_i\), 2) a key vector \(k_i\), and 3) a value vector \(v_i\) by multiplying \(x_i\) with weight matrices \(W_k\), \(W_v\), and \(W_q\), which are learned during the training process.

The main idea of the self-attention mechanism is to compute a score for each pair \((x_i, x_j)\) representing which positions in the sequence should be considered
the most when computing the embedding of \( x_i \). In our visualizations, for example in Figure 3, stronger colored edges correspond to a higher attention value [47]. This mechanism is especially suited for our LTL trace generation problem as the whole context of the formula has impact on the choice of the decoder.

This is implemented by the so-called Scaled Dot-Product Attention: For example, consider a self-attention computation of \( x = (x_0, x_1, x_2) \). To compute the hidden embedding of \( x_0 \) we first take the dot products of the query vector \( q_0 \) and key vectors \( k_0, k_1, \) and \( k_2 \). Intuitively, the query vector asks for a “selection” of different keys that it wants to know more about. Those scores are then divided by a constant \( \sqrt{d_k} \), where \( d_k \) is the key dimension, to obtain more stable gradients. Taking the softmax results in three attention scores \( s_0, s_1, \) and \( s_2 \), which are the attentions for \( (x_0, x_0), (x_0, x_1), \) and \( (x_0, x_2) \) respectively. Note that each \( s_i \) is between 0 and 1 and \( s_0 + s_1 + s_2 = 1 \). The hidden embedding of \( x_0 \) is then obtained by the linear combination of \( v_0, v_1, \) and \( v_2 \) where \( v_i \) is scaled with score \( s_i \). This maps the queried keys to their values, where keys with higher attention scores contribute more to the embedding. Intuitively, this mechanism can be seen as an indexing scheme over a multi-dimensional vector space.

The hidden embeddings can be calculated all at once using matrix operations [46]. Let \( Q, K, V \) be the matrices obtained by multiplying the input vector \( X \) consisting of all \( x_i \) with the weight matrices \( W_k, W_v, \) and \( W_q \):

\[
\text{Attention}(Q, K, V) = \text{softmax} \left( \frac{QK^T}{\sqrt{d_k}} \right) V.
\]

**Decoder.** In contrast to the encoder, which processes the input sequence at once, the output sequences are computed step-by-step until the end of string (\(<\text{EOS}>\)) element is chosen (see Figure 4). The decoder is again a layered architecture where each layer consists in addition to a self-attention layer, which processes already decoded elements, and feed-forward neural network of a layer that computes the attention between the output and input sequences. This is the key concept of the Transformer architecture: In contrast to the self-attention mechanism, the weight matrix \( W_q \) of the encoder-decoder attention layer is learned during the decoding process. The key and value matrices \( W_k \) and \( W_v \) are the ones learned during the encoding process. Intuitively, this represents queries from the decoder \( Q_{\text{dec}} \) asking for the values \( V_{\text{enc}} \) of the keys \( K_{\text{enc}} \) it is the most interested in while decoding a position of the output sequence, i.e., the \( \text{Attention}(Q_{\text{dec}}, K_{\text{enc}}, V_{\text{enc}}) \) is computed. Figure 5 shows an encoder-decoder attention head between the input formula \((a \cup b) \land (a \cup \neg b)\) and the symbolic trace \( a \land \neg b ; b ; \text{true}^\omega \). This head focuses on matching the atomic proposition \( b \) of the second until operator to the first position of the trace and, thus, distinguishes between the same atomic propositions in the formula.

### 4 Data Set

Our data consists of pairs of an LTL formula and a satisfying trace. We randomly generated 1 million unique, satisfiable LTL formulas, where the size of \( AP \) was
fixed to 5 and the maximum size of the formula’s syntax tree, was set to 25. The LTL formulas contain an arbitrary amount of equally distributed \( \neg, \land, \lor \) and \( \mathcal{U} \) operators. The data set was split into a training set of 800K formulas, a validation set of 100K formulas, and a test set of 100K formulas.

We consider two representations of these formulas - in regular LTL syntax and in Polish notation. For example, the LTL formula \((a \land b) \mathcal{U} c\) in Polish notation is: \(\mathcal{U} \land a \land b \land c\). Note that the implicit encoding of the tree structure in Polish notation allows us to drop the parentheses. We will see in the evaluation that the choice of the representation has an impact on the performance of the Transformer.

The traces described by LTL formulas are infinitely long, but we know that they are ultimately periodic and can hence be represented as lassos \(uv^{\omega}\), where \(u\) and \(v\) are finite sequences of sets of atomic propositions. We use a compact, symbolic representation of ultimately periodic traces as follows: Each position in the trace is separated by the delimited “;” and the beginning of the period \(v\) is signaled by the character “{” and analogously its end by “}”. True and False are represented by “1” and “0”, respectively. For example given two atomic propositions \(a\) and \(b\), the trace \(\{a\}\{a\}\{a\}\{b\}\omega\) is represented by \(a \land \neg b; a \land \neg b; a \land \neg b; b \land \neg a\). Note that each step of the trace is specified by a logical formula. This allows us to underspecify the propositions when they do not matter. For
example the LTL formula $Qa$ is satisfied by the symbolic trace: $1;\{a\}$, which leaves open whether $a$ holds on the first position as well.

For constructing a satisfying symbolic trace, we implemented an LTL trace generator as follows. Given a satisfiable LTL formula $\varphi$, our base-line trace generator constructs a Büchi automaton $A_\varphi$ that accepts exactly the language defined by the LTL formula, i.e., $L(A_\varphi) = L(\varphi)$. From this automaton, we construct an arbitrary accepted symbolic trace, by searching for an accepting run in $A_\varphi$. We used Spot [9] for the manipulation of LTL formulas and automata. Since we generated the data with an existing LTL satisfiability tool, it consists mostly of examples that are easy for current automata-based algorithms. This bias towards the automata-base algorithms is not a problem in this work, as we do not aim for a performance comparison with these algorithms.

To give the interested reader an idea of the level of difficulty of the data set, we here present three randomly chosen examples from our training sets, where the first line shows the LTL formula and the trace in mathematical notation and the second line shows the representation of the data (in Polish notation):

| LTL formula | satisfying symbolic trace |
|-------------|---------------------------|
| $((dUc)U(c\land d)) \land (b \land \neg(dUc))$ | $true ; b \land \neg c \land \neg d ; \neg c \land d ; d ; true^\omega$ $1;\&\&!c!d;!c!d;d\{1\}$ |
| $\neg(O((c \land (trueUc) \land O(c))Uc))$ | $true ; \neg b \land \neg c ; (\neg b)^\omega$ $1;\&!c!d;\{1\}$ |
| $O((\neg(c \land d))U(c))$ | $true ; c \lor \neg d ; \neg d ; true^\omega$ $1;\&!c!d;d\{1\}$ |

5 Experimental Results and Analysis

The experiments were implemented using the tensor2tensor library that provides an implementation of the Transformer architecture [15]. Our implementation
processes the input and output sequences character-by-character by computing an embedding of the ascii values. We trained all Transformers on a single NVIDIA T4 GPU with different hyperparameters. For every choice of hyperparameters the training of the Transformer took less than 7 hours.

Our experimental findings are structured as follows. We describe our evaluation metrics in Subsection 5.1. In Subsection 5.2, we present the performance of the Transformer with different hyperparameters. As an important optimization, we show in Section 5.3 that providing the LTL formulas in Polish notation results in a gain in performance compared to an infix notation. In the last subsection, we will analyze successfully and failed translations of the neural network in more detail by zooming into the attention mechanism. Based on those observations, we find an interesting class of LTL formulas that appear to be particularly hard for a neural network to translate.

### 5.1 Evaluation Method

In our evaluation we have to distinguish syntactic and semantic accuracy, since the trace generation problem of LTL is an ambiguous problem. The fraction of formulas that is translated into a trace that is syntactically equivalent to the trace in our data set is referred to as the syntactic accuracy. Traces that are not syntactically equivalent to the trace chosen in the data can still satisfy the given formula. We therefore also define semantic accuracy, which is the fraction of traces that satisfy the given formula. For the output decoding, we utilized beam search, which is a heuristic best-first search algorithm that solely keeps track of a predetermined number of best partial solutions. For every Transformer, we used a beam size of 4 and an $\alpha$ of 0.6 \cite{49}.

### 5.2 Experimental Results

The Transformer architecture leaves many parameter choices. In Table 1 we show the effect of the most significant parameters on the performance of Transformers. It is evident that performance benefits from an increase in the number

| Layers | Layer Size | Heads | Batch Size | Train Steps | Syn Acc | Sem Acc |
|--------|------------|-------|------------|-------------|---------|---------|
| tiny   | 2          | 128   | 4          | 4096 100K   | 80.4%   | 97.5%   |
| tiny-l4| 4          | 128   | 4          | 4096 100K   | 84.7%   | 98.8%   |
| tiny-l8| 8          | 128   | 4          | 4096 100K   | 89.2%   | 99.4%   |
| tiny-l12| 8        | 128   | 4         | 4096 100K   | 89.8%   | 99.5%   |
| tiny-h8| 2          | 128   | 8          | 4096 100K   | 79.8%   | 98.0%   |
| tiny-h16| 2         | 128   | 16         | 4096 100K   | 81.2%   | 98.0%   |
| small  | 2          | 256   | 4          | 4096 100K   | 82.3%   | 98.2%   |
| small-l4| 4         | 256   | 4          | 4096 100K   | 87.4%   | 99.1%   |
| medium | 2          | 512   | 4          | 4096 100K   | 85.9%   | 98.6%   |
of hidden layers. In fact, we identified the number of hidden layers having the most significant effect on performance. Increasing the size of hidden layers or the number of attention heads has a positive effect on performance as well.

In Figure 6 we show the evolution of both the syntactic accuracy and the semantic accuracy during the training process. Note the significant difference between the syntactic and semantic accuracy. This demonstrates the importance of a suitable performance measure when evaluating machine learning algorithms on formal methods tasks.

5.3 Impact of Notation

We found that the notation of formulas has an impact on the performance of Transformers. We compared infix notation with Polish notation for Transformers with 8 hidden layers of size 128 and 4 attention heads that we trained for 100K steps with a batch size of 4096. For Polish notation we achieved a 3% higher syntactic accuracy of 89.2% and a semantic accuracy of 99.4% that is less than 1% higher on our test set.

We believe that mainly two aspects contribute to the performance gain. In contrast to the infix notation, the Polish notation is a parenthesis-free notation. In addition, the outermost operator of the formula receives always the same positional encoding making it easier to identify it.

5.4 Example Predictions

To evaluate and inspect the results, we ran the Transformer with hyperparameter configuration tiny-l8 on several handcrafted examples. The Transformer has never seen these example inputs during training. The evaluation on our
handcrafted examples examines to what extend the training on random input formulas transfers to “typical” LTL formulas.

The first formula combines the temporal modalities “globally” and “eventually”, which is a common pattern in specifications for reactive systems. It requires that the atomic proposition $a$ appears infinitely often on a trace. The Transformer outputs a trace with an empty prefix and a period containing $a$, i.e., every trace that contains $a$ infinitely often.

For this example, we visualized the attention mechanism in Fig. 7. When trying to satisfy $\Diamond a$, both heads pay close attention to the negation of the first three positions, which would lead to a contradiction if the Transformer decides to place an $a$ before the fourth position.

The third example shows that the Transformer avoids such contradictions even in association with temporal operators. The formula requires that eventually an $a$ has to hold as well as a position where $a$ is not allowed to hold. The
Fig. 8. All self-attention heads of the formula $a U b \land a U \neg b$. Each color corresponds to a different attention head.

Transformer avoids a contradiction by first fulfilling the first conjunct $\diamond a$ on the first position and then the second conjunct $\diamond \neg a$ on the second position.

$$\diamond a \land \diamond \neg a \; ; \; a ; \neg a ; \text{true}^\omega$$

$\& U a U ! a \; a ; ! a ; \{1\}$

5.5 Example of a Misprediction

Our last two examples describe formulas with multiple until statements that describe overlapping intervals. We know that these formulas are hard as they are the source of PSPACE-hardness of LTL.

The first formula overlaps two until intervals by requiring that $a$ has to hold until $b$ holds, as well as $\neg b$ holds. Here, the Transformer still predicts a correct trace: The predicted trace first satisfies $\neg b$ at the first position while delaying the satisfaction of the first until to the second position by requiring $a$ at the first position as well. Figure 8 shows the self-attention heads for this formula. While processing the second until operator, the blue attention head pays attention to its top level operator, the conjunction.

$$a U b \land a U \neg b \; a \land \neg b ; b ; \text{true}^\omega$$

$\& U a U ! b \; \& a ! b ; b ; \{1\}$

We scaled this formula to three overlapping until intervals, and observe that the Transformer fails: It predicts the trace $a \land \neg b ; b \land c ; \text{true}^\omega$, which does not satisfy the LTL formula.

$$\langle a U b \land c \rangle \land \langle a U \neg b \land c \rangle \land \langle a U b \land \neg c \rangle \; a \land \neg b ; b \land c ; \text{true}^\omega$$

$\& U a \& b U ! a \& b c U a \& b ! c \; \& a ! b ; b c ; \{1\}$

Since the Transformer can solve this hard logical reasoning task for two until statements, we expect it to scale very well when being trained with more GPUs on larger formulas. Especially because the architecture of the Transformer allows for heavy parallelization of the learning task.
6 Related Work

The goal of this work is not to compete against existing work on LTL satisfiability [32,36,23,22,37], but to study how recent advances in deep learning can be applied to core problems of computer-aided verification.

Closely related to our work is NeuroSAT [39], which is a deep neural network for solving the Boolean satisfiability problem. A simplified NeuroSAT architecture was trained for unsat-core predictions [38], improving the performance of, for example, Z3 [28] by 6%. They use (message passing) graph neural networks [34,24,13,50] instead of Transformers. Similar learning techniques have been used to learn better heuristics for 2QBF solvers [20]. In contrast to NeuroSAT, we applied off-the-shelf techniques from deep learning.

Deep learning has recently been proposed for automating mathematical reasoning in (interactive) theorem provers [11,25,4,29,21] and other mathematical domains [33,35]. Transformers were used to solve differential equations [19].

Transformers have also been considered for the analysis of code [10]. Earlier works applying Transformers studied natural language-like prediction tasks, such as summarizing code [10] or variable naming and misuse [16]. Other works focused on recurrent neural networks or graph neural networks for code analysis, e.g. [30,14,5,48,1]. Another area in the intersection of formal methods and machine learning is the verification of neural networks [41,40,43,12,18,8].

7 Conclusion

We showed that deep neural networks can generalize from randomly generated examples to the semantics of complex modal logics such as linear-time temporal logic (LTL). By formulating the satisfiability problem of LTL as a translation task, off-the-shelf Transformers were able to predict correct traces over 99% of the time. We identified and addressed two major challenges of bridging the gap between formal methods and deep learning.

The key challenge from the formal methods point of view is the acquisition of data. In our experiments we found that training neural networks randomly generated data generalized surprisingly well to simple handcrafted examples. However, this will likely not hold in general and the generation or acquisition of representative training data will be an important research problem in its own right.

The key challenge from the machine learning point of view is the design of rigorous evaluation methods. For LTL satisfiability, we showed that evaluating only the (syntactic) accuracy on the given data, can be misleading: syntactic “mispredictions” were mostly still correct traces for the given LTL formula. A big question from the machine learning point of view is whether new neural architectures and learning frameworks need to be designed to process symbolic input, or whether it will pay off to reuse existing neural architectures.

The potential that arises from the advent of deep learning in formal methods is immense. Deep learning will allow us to abstract from minor implementation
details and make bigger jumps in the development of new automated verification methods. It also challenges us to rethink how we ask research questions, as deep learning tends to be good at human-level tasks, but many problem representations and research questions in formal methods are not formulated in human-readable ways (e.g., SAT encodings). Deep learning thus offers and at the same time forces us to move closer to applications.

References

1. Allamanis, M., Brockschmidt, M., Khademi, M.: Learning to represent programs with graphs. arXiv preprint arXiv:1711.00740 (2017)
2. Ba, L.J., Kiros, J.R., Hinton, G.E.: Layer normalization. CoRR abs/1607.06450 (2016), http://arxiv.org/abs/1607.06450
3. Balunovic, M., Bielik, P., Vechev, M.: Learning to solve smt formulas. In: Bengio, S., Wallach, H., Larochelle, H., Grauman, K., Cesare-Bianchi, N., Garnett, R. (eds.) Advances in Neural Information Processing Systems 31. pp. 10317–10328. Curran Associates, Inc. (2018). http://papers.nips.cc/paper/8233-learning-to-solve-smt-formulas.pdf
4. Bansal, K., Loos, S.M., Rabe, M.N., Szegedy, C., Wilcox, S.: HOList: An environment for machine learning of higher-order theorem proving. In: arXiv preprint arXiv:1904.03241 (2019)
5. Bhatia, S., Kohli, P., Singh, R.: Neuro-symbolic program corrector for introductory programming assignments. In: 2018 IEEE/ACM 40th International Conference on Software Engineering (ICSE). pp. 60–70 (May 2018). https://doi.org/10.1145/3180155.3180219
6. Britz, D., Goldie, A., Luong, T., Le, Q.: Massive Exploration of Neural Machine Translation Architectures. ArXiv e-prints (Mar 2017)
7. Devlin, J., Chang, M., Lee, K., Toutanova, K.: BERT: pre-training of deep bidirectional transformers for language understanding. CoRR abs/1810.04805 (2018), http://arxiv.org/abs/1810.04805
8. Dreossi, T., Donzé, A., Seshia, S.A.: Compositional falsification of cyber-physical systems with machine learning components. Journal of Automated Reasoning 63(4), 1031–1053 (2019)
9. Duret-Lutz, A., Lewkowicz, A., Fauchille, A., Michaud, T., Renault, E., Xu, L.: Spot 2.0a framework for ltl and ω-automata manipulation. In: International Symposium on Automated Technology for Verification and Analysis. pp. 122–129. Springer (2016)
10. Fernandes, P., Allamanis, M., Brockschmidt, M.: Structured neural summarization. arXiv preprint arXiv:1811.01824 (2018)
11. Gauthier, T., Kaliszyk, C., Urban, J.: Tactictoe: Learning to reason with hol4 tactics. arXiv preprint arXiv:1804.00595 (2018)
12. Gehr, T., Mirman, M., Drachsler-Cohen, D., Tsankov, P., Chaudhuri, S., Vechev, M.: Ai2: Safety and robustness certification of neural networks with abstract interpretation. In: 2018 IEEE Symposium on Security and Privacy (SP). pp. 3–18. IEEE (2018)
13. Gilmer, J., Schoenholz, S.S., Riley, P.F., Vinyals, O., Dahl, G.E.: Neural message passing for quantum chemistry. In: Proceedings of the 34th International Conference on Machine Learning-Volume 70. pp. 1263–1272. JMLR. org (2017)
14. Gupta, R., Pal, S., Kanade, A., Shevade, S.: Deepfix: Fixing common C language errors by deep learning. In: Thirty-First AAAI Conference on Artificial Intelligence (2017)

15. He, K., Zhang, X., Ren, S., Sun, J.: Delving deep into rectifiers: Surpassing human-level performance on imagenet classification. In: 2015 IEEE International Conference on Computer Vision, ICCV 2015, Santiago, Chile, December 7-13, 2015. pp. 1026–1034 (2015), https://doi.org/10.1109/ICCV.2015.123, https://doi.org/10.1109/ICCV.2015.123

16. Hellendoorn, V.J., Sutton, C., Singh, R., Maniatis, P.: Global relational models of source code. In: International Conference on Learning Representations (2020), https://openreview.net/forum?id=BJlnbRTnwr

17. Hochreiter, S., Schmidhuber, J.: Long short-term memory. Neural computation 9(8), 1735–1780 (1997)

18. Huang, X., Kwiatkowska, M., Wang, S., Wu, M.: Safety verification of deep neural networks. In: International Conference on Computer Aided Verification. pp. 3–29. Springer (2017)

19. Lample, G., Charton, F.: Deep learning for symbolic mathematics. arXiv preprint arXiv:1912.01412 (2019)

20. Lederman, G., Rabe, M.N., Lee, E.A., Seshia, S.A.: Learning heuristics for quantified boolean formulas through deep reinforcement learning (2020), http://arxiv.org/abs/1807.08058

21. Lee, D., Szegedy, C., Rabe, M.N., Loos, S.M., Bansal, K.: Mathematical reasoning in latent space. CoRR abs/1909.11851 (2019), http://arxiv.org/abs/1909.11851

22. Li, J., Yao, Y., Pu, G., Zhang, L., He, J.: Aalta: an ltl satisfiability checker over infinite/finite traces. In: Proceedings of the 22nd ACM SIGSOFT international symposium on foundations of software engineering. pp. 731–734 (2014)

23. Li, J., Zhang, L., Pu, G., Vardi, M.Y., He, J.: Ltl satisfiability checking revisited. In: 2013 20th International Symposium on Temporal Representation and Reasoning. pp. 91–98. IEEE (2013)

24. Li, Y., Yu, R., Shahabi, C., Liu, Y.: Diffusion convolutional recurrent neural network: Data-driven traffic forecasting. arXiv preprint arXiv:1707.01926 (2017)

25. Loos, S., Irving, G., Szegedy, C., Kaliszyk, C.: Deep network guided proof search. In: LPAR (2017)

26. Mikolov, T., Chen, K., Corrado, G., Dean, J.: Efficient estimation of word representations in vector space. In: 1st International Conference on Learning Representations, ICLR 2013, Scottsdale, Arizona, USA, May 2-4, 2013, Workshop Track Proceedings (2013), http://arxiv.org/abs/1301.3781

27. Moravčík, M., Schmidt, M., Burch, N., Lisý, V., Morrill, D., Bard, N., Davis, T., Waugh, K., Johanson, M., Bowling, M.H.: Deepstack: Expert-level artificial intelligence in no-limit poker. CoRR abs/1701.01724 (2017), http://arxiv.org/abs/1701.01724

28. de Moura, L.M., Bjørner, N.: Z3: an efficient SMT solver. In: Tools and Algorithms for the Construction and Analysis of Systems, 14th International Conference, TACAS 2008, Held as Part of the Joint European Conferences on Theory and Practice of Software, ETAPS 2008, Budapest, Hungary, March 29-April 6, 2008. Proceedings. pp. 337–340 (2008), https://doi.org/10.1007/978-3-540-78800-3_24, https://doi.org/10.1007/978-3-540-78800-3_24

29. Paliwal, A., Loos, S.M., Rabe, M.N., Bansal, K., Szegedy, C.: Graph representations for higher-order logic and theorem proving. CoRR abs/1905.10006 (2019), http://arxiv.org/abs/1905.10006
30. Piech, C., Huang, J., Nguyen, A., Phulsuksombati, M., Sahami, M., Guibas, L.: Learning program embeddings to propagate feedback on student code. In: International Conference on Machine Learning. pp. 1093–1102 (2015)
31. Pnueli, A.: The temporal logic of programs. In: 18th Annual Symposium on Foundations of Computer Science, Providence, Rhode Island, USA, 31 October - 1 November 1977. pp. 46–57 (1977). https://doi.org/10.1109/SFCS.1977.32
32. Rozier, K.Y., Vardi, M.Y.: Ltl satisfiability checking. In: International SPIN Workshop on Model Checking of Software. pp. 149–167. Springer (2007)
33. Saxton, D., Grefenstette, E., Hill, F., Kohli, P.: Analysing mathematical reasoning abilities of neural models. CoRR abs/1904.01557 (2019), http://arxiv.org/abs/1904.01557
34. Scarselli, F., Gori, M., Tsoi, A.C., Hagenbuchner, M., Monfardini, G.: The graph neural network model. IEEE Transactions on Neural Networks 20(1), 61–80 (2008)
35. Schlag, I., Smolensky, P., Fernandez, R., Jojic, N., Schmidhuber, J., Gao, J.: Enhancing the transformer with explicit relational encoding for math problem solving. arXiv preprint arXiv:1910.06611 (2019)
36. Schuppan, V., Darnawan, L.: Evaluating ltl satisfiability solvers. In: International Symposium on Automated Technology for Verification and Analysis. pp. 397–413. Springer (2011)
37. Schwendimann, S.: A new one-pass tableau calculus for pltl. In: International Conference on Automated Reasoning with Analytic Tableaux and Related Methods. pp. 277–291. Springer (1998)
38. Selsam, D., Bjørner, N.: Guiding high-performance SAT solvers with unsat-core predictions. In: Theory and Applications of Satisfiability Testing - SAT 2019 - 22nd International Conference, SAT 2019, Lisbon, Portugal, July 9-12, 2019, Proceedings. pp. 336–353 (2019). https://doi.org/10.1007/978-3-030-24258-9_24
39. Selsam, D., Lamm, M., Bünz, B., Liang, P., de Moura, L., Dill, D.L.: Learning a SAT solver from single-bit supervision. In: 7th International Conference on Learning Representations, ICLR 2019, New Orleans, LA, USA, May 6-9, 2019 (2019), https://openreview.net/forum?id=HJMC_iA5tm
40. Seshia, S.A., Desai, A., Dreossi, T., Fremont, D.J., Ghosh, S., Kim, E., Shivakumar, S., Vazquez- Chanlatte, M., Yue, X.: Formal specification for deep neural networks. In: International Symposium on Automated Technology for Verification and Analysis. pp. 20–34. Springer (2018)
41. Seshia, S.A., Sadigh, D.: Towards verified artificial intelligence. CoRR abs/1606.08514 (2016), http://arxiv.org/abs/1606.08514
42. Silver, D., Schrittwieser, J., Simonyan, K., Antonoglou, I., Huang, A., Guez, A., Hubert, T., Baker, L., Lai, M., Bolton, A., et al.: Mastering the game of go without human knowledge. Nature 550(7676), 354–359 (2017)
43. Singh, G., Gehr, T., Püschel, M., Vechev, M.: An abstract domain for certifying neural networks. Proceedings of the ACM on Programming Languages 3(POPL), 1–30 (2019)
44. Taigman, Y., Yang, M., Ranzato, M., Wolf, L.: Deepface: Closing the gap to human-level performance in face verification. In: 2014 IEEE Conference on Computer Vision and Pattern Recognition, CVPR 2014, Columbus, OH, USA, June 23-28, 2014. pp. 1701–1708 (2014). https://doi.org/10.1109/CVPR.2014.220 https://doi.org/10.1109/CVPR.2014.220
45. Vaswani, A., Bengio, S., Brevdo, E., Chollet, F., Gomez, A.N., Gouws, S., Jones, L., Kaiser, L., Kalchbrenner, N., Parmar, N., Seppassi, R., Shazeer, N., Uszkoreit, J.: Tensor2tensor for neural machine translation. CoRR abs/1803.07416 (2018), http://arxiv.org/abs/1803.07416

46. Vaswani, A., Shazeer, N., Parmar, N., Uszkoreit, J., Jones, L., Gomez, A.N., Kaiser, L., Polosukhin, I.: Attention is all you need. In: Advances in Neural Information Processing Systems 30: Annual Conference on Neural Information Processing Systems 2017, 4-9 December 2017, Long Beach, CA, USA. pp. 5998–6008 (2017), http://papers.nips.cc/paper/7181-attention-is-all-you-need

47. Vig, J.: A multiscale visualization of attention in the transformer model. In: Proceedings of the 57th Conference of the Association for Computational Linguistics, ACL 2019, Florence, Italy. July 28 - August 2, 2019, Volume 3: System Demonstrations. pp. 37–42 (2019), https://www.aclweb.org/anthology/P19-3007/

48. Wang, K., Singh, R., Su, Z.: Dynamic neural program embedding for program repair. In: ICLR (2018)

49. Wu, Y., Schuster, M., Chen, Z., Le, Q.V., Norouzi, M., Macherey, W., Krikun, M., Cao, Y., Gao, Q., Macherey, K., et al.: Google’s neural machine translation system: Bridging the gap between human and machine translation. arXiv preprint arXiv:1609.08144 (2016)

50. Wu, Z., Pan, S., Chen, F., Long, G., Zhang, C., Yu, P.S.: A comprehensive survey on graph neural networks. arXiv preprint arXiv:1901.00596 (2019)