End-to-End Learning of LTL_f Formulae by Faithful LTL_f Encoding

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Abstract

It is important to automatically discover the underlying treestructured formulae from large amounts of data. In this paper, we examine learning linear temporal logic on finite traces (LTL_f) formulae, which is a tree structure syntactically and characterizes temporal properties semantically. Its core challenge is to bridge the gap between the concise tree-structured syntax and the complex LTL f semantics. Besides, the learning quality is endangered by explosion of the search space and wrong search bias guided by imperfect data. We tackle these challenges by proposing an LTLf encoding method to parameterize a neural network so that the neural computation is able to simulate the inference of LTL_f formulae. We first identify *faithful* LTL_f *encoding*, a subclass of LTL_f encoding, which has a one-to-one correspondence to LTL_f formulae. Faithful encoding guarantees that the learned parameter assignment of the neural network can directly be interpreted to an LTL_{f} formula. With such an encoding method, we then propose an end-to-end approach, TLTLf, to learn LTL_f formulae through neural networks parameterized by our LTL_f encoding method. Experimental results demonstrate that our approach achieves state-of-the-art performance with up to 7% improvement in accuracy, highlighting the benefits of introducing the faithful LTL_f encoding.

Introduction

Formulae with tree structures widely exist in data mining and knowledge management, e.g., linear temporal logic (LTL) (Luo et al. 2022) and regular expression (Ye et al. 2023). Therefore, it is important to automatically discover the underlying tree structured formulae from large amounts of data. In this paper, we focus on linear temporal logic on finite traces (LTL_f) formulae (Baier and McIlraith 2006; Giacomo and Vardi 2013), which are tree-structured formulae characterizing temporal properties. LTL f has been successfully used in many applications, typically, characterizing the high-level behaviors of a system based on observed traces in planning (Neider and Gavran 2018). For example, LTL_f can specify that an agent keeps walking forward until (U) it encounters a block $(p_1 \cup p_2)$, where p_1 and p_2 express "agent walking forward" and "agent encountering a block", respectively. Besides planning, learning LTL_f formulae can also be

applied in apprenticeship learning (Kasenberg and Scheutz 2017), behavior classification (Camacho and McIlraith 2019), and explainable artificial intelligence (Kim et al. 2019).

Learning LTL_f formulae is a challenging problem. The core challenge is to bridge the gap between the concise treestructured syntax and the complex LTL_f semantics. Besides, a formula with *arbitrary form* has only semantic constraints and no syntactic constraints. Finding such a formula probably leads to explosion of the search space. On the other hand, *imperfect data*, *e.g.*, incorrect labels (Kim et al. 2019), tend to introduce wrong search bias far away from the target formula.

To tackle the above challenges, some approaches (Camacho and McIlraith 2019; Luo et al. 2022) modeled the relation between syntax and semantics by introducing an intermediate representation, but they need to pay additional costs from learning the over-expressive intermediate representation. There are also some approaches (Neider and Gavran 2018; Gaglione et al. 2021) that uniformly encoded syntactic and semantic constraints as Boolean satisfiability problem (SAT) or maximum satisfiability problem (MaxSAT), but they suffer from the high computational complexity of SAT or MaxSAT. Other approaches (Lemieux, Park, and Beschastnikh 2015; Shah et al. 2018; Kim et al. 2019) directly encoded syntactic constraints, exploiting well-designed heuristics to search for formulae satisfying semantic constraints. However, the heuristics are limited in scope and are time-consuming. In confront of imperfect data, some approaches (Neider and Gavran 2018; Camacho and McIlraith 2019) directly ignored them, and others (Lemieux, Park, and Beschastnikh 2015; Shah et al. 2018; Kim et al. 2019) limited the hypothesis space by templates.

In this paper, we propose an LTL_f encoding method for faithfully bridging the neural network inference and the LTL_f inference. An LTL_f encoding is a parameter assignment of the target neural network ensuring that, under certain simple conditions, an LTL_f formula is able to be directly interpreted from the neural network. We identify the conditions where LTL_f encodings and LTL_f formulae are one-to-one corresponding, and refer to the encoding under these conditions as *faithful LTL_f encoding*, which provides a compact encoding of the LTL_f syntax. We model the LTL_f semantics via designing an inference process with LTL_f encoding; in other words, inference with LTL_f encoding simulates the inference of LTL_f formulae. Based on this theoretical re-

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sult, we propose an end-to-end approach, TLTLf, to learn LTL_f formulae. Specifically, TLTLf learns a neural network that is parameterized by the LTL_f encoding method, and subsequently interprets an LTL_f formula from the learned parameter assignment of the neural network.

Following the assessment of the state-of-the-art (SOTA) approach (Luo et al. 2022), we evaluate TLTLf across datasets with and without imperfect data. Experimental results show that TLTLf achieves SOTA performance and improves the accuracy by up to 7% compared with the SOTA approach. Besides, the LTL_f formula learnt by TLTLf is highly faithful to the network from which it is extracted, giving the same satisfiability results over 95% traces. Following the work (Kim et al. 2019; Luo et al. 2022), we also evaluate TLTLf on imperfect data generated by assigning incorrect labels to a subset of the original data. Results demonstrate that TLTLf still outperforms other approaches on imperfect data.

Related Work

Learning LTL formulae from positive and negative traces. Neider and Gavran (2018) provided two methods to learn LTL formulae, one based on SAT and the other based on the decision tree. Besides, Camacho and McIlraith (2019) designed a SAT-based method to learn formulae from the symbolic state representation of LTL formulae. However, both studies are limited by an assumption that the training data are precise. Kim et al. (2019) handled imperfect data based on Bayesian inference. Their use of templates limits the hypothetical space of formulae. Overall, these approaches cannot handle imperfect data and learn arbitrary formulae simultaneously.

Recently, several studies have realized the importance of learning arbitrary LTL_f formulae from imperfect data. Gaglione et al. (2021) proposed a MaxSAT-based approach to tolerate imperfect data, but the scalability is limited by the computational complexity of the MaxSAT solver. The work (Luo et al. 2022) is the closest to this work. Based on a theoretical result that the graph neural network (GNN) inference is able to simulate the LTL_f inference in checking if a trace is satisfied, Luo et al. (2022) first trained a GNN classifier for the trace satisfiability problem and then interpreted LTL_f formulae from the model parameters. However, they do not guarantee the faithfulness between the GNN inference and the LTL_f inference, *i.e.*, the result of the interpreted LTL_f formula is probably different from that of the GNN classifier in checking if a trace is satisfied. This is because they only proved that, given a formula, a GNN classifier can always be constructed to simulate LTL_f inference, but not vice versa, which means that the expressive power of a GNN classifier is stronger than an LTL_f formula. It results in additional costs from learning the over-expressive GNN classifier. In contrast, the interpreted LTL_f formula in this work is more faithful with the learnt neural network.

Learning temporal logic formulae from other forms of data. Some work learns temporal logic formulae from other forms of data, such as Markov decision process (Kasenberg and Scheutz 2017) and only positive traces (la Rosa and McIlraith 2011; Lemieux, Park, and Beschastnikh 2015; Le and

Lo 2015; Shah et al. 2018; Cao et al. 2018). In the business process modeling, some studies (Maggi, Bose, and van der Aalst 2012; Ciccio, Mecella, and Mendling 2013; Maggi et al. 2018; Leno et al. 2020) use temporal logic to model the declarative process model learned from the event log, which is viewed as a kind of positive traces.

Learning other formal languages. Our work is also relevant to learning logical representations, such as regular language (Angluin 1987; Giantamidis and Tripakis 2016; Bollig et al. 2009; Angluin, Eisenstat, and Fisman 2015; Fiterau-Brostean et al. 2017; Gabel and Su 2008, 2010; Ye et al. 2023) and other forms of temporal formulae (Asarin et al. 2011; Jin et al. 2015; Bombara et al. 2016; Xu et al. 2016; Xu and Julius 2016; Kong, Jones, and Belta 2016; Arif et al. 2020; Brunello, Sciavicco, and Stan 2020; Roy, Fisman, and Neider 2020; Xu et al. 2019; Maggi, Montali, and Peñaloza 2020). Although the expressive power of temporal formulae is weaker than that of regular languages, learning temporal formulae is more compact and easy to understand (Camacho and McIlraith 2019). Our approach will potentially be extended to learn formulae in other formal languages.

Learning tree structure. There have been various studies on learning tree structure. They can be divided into two main categories. One is to extract a latent tree structure for each example to improve the performance. For example, in nature language processing (NLP), the syntactic dependency tree of the sentence is extracted to improve the performance on tasks like semantic role labeling (Shi, Malioutov, and Irsoy 2020; Zhang et al. 2022) and sentiment analysis (Li et al. 2021; Hou et al. 2021). Syntactic dependency parsing is a classical problem in NLP and there have been some mature tools like the natural language toolkit (Bird, Klein, and Loper 2009). For the neural approach, Chen and Manning (2014) used three types of operations of a stack and a queue to construct the syntactic dependency tree and used a neural network to predict the operation in each construction step. The other category is to design an approach to learning the tree structure of specific semantics. Fargier, Gimenez, and Mengin (2018) proposed a greedy learning algorithm to learn lexicographic preference trees from positive examples. Sun et al. (2020) and Xie et al. (2021) used a tree-structured decoder to generate the abstract syntax tree of code from the natural language description. Ye et al. (2023) used a differentiable approach to learn the syntax tree of regular expressions from both positive and negative examples. Compared with the above studies, our approach learns the tree-structured LTL_f formulae with a completely different tree structure from both positive and negative examples.

Preliminaries

Linear temporal logic. *Linear temporal logic (LTL)* (Pnueli 1977) is a modal logic typically used to express temporally extended constraints over state trajectories. Derived from LTL, LTL interpreted over finite traces (Baier and McIlraith 2006; Giacomo and Vardi 2013) is referred to as *finite LTL*_f. The syntax of LTL_f for a finite set of atomic propositions \mathbb{P} is built up of \top (true) and \bot (false), standard logical operators (\land and \neg), and temporal logical operators *next* (X) and *until*

(U), described as follows:

$$\phi := p \mid \neg \varphi \mid \varphi_1 \land \varphi_2 \mid \mathsf{X}\varphi \mid \varphi_1 \mathsf{U}\varphi_2,$$

where $p \in \mathbb{P} \cup \{\top, \bot\}$ and φ, φ_1 , and φ_2 are LTL_f formulae.

The other operators or (\lor) , weak next (N), release (R), eventually (F), and always (G) are commonly used, but they can be defined using the above fundamental operators, *i.e.*, $\varphi_1 \lor \varphi_2 := \neg(\neg \varphi_1 \land \neg \varphi_2)$, $N\varphi := \neg X \top \lor X\varphi$, $\varphi_1 R\varphi_2 :=$ $\neg(\neg \varphi_1 U \neg \varphi_2)$, $F\varphi := \top U\varphi$, and $G\varphi := \neg(\top U \neg \varphi)$. For brevity, we only consider the fundamental operators in this paper, but our approach can be extended to handle all operators of LTL_f.

The prefix form of an LTL_f formula ϕ , denoted by pre(ϕ), is defined recursively as follows:

$$\operatorname{pre}(\phi) = \begin{cases} p, & \phi = p \in \mathbb{P}, \\ \alpha \operatorname{pre}(\phi_1), & \phi = \alpha \phi_1, \alpha \in \{\neg, \mathsf{X}\}, \\ \beta \operatorname{pre}(\phi_1) \operatorname{pre}(\phi_2), & \phi = \phi_1 \beta \phi_2, \beta \in \{\land, \mathsf{U}\}. \end{cases}$$
(1)

The syntax tree of an LTL_f formula ϕ , denoted by $T(\phi)$, is defined as follows:

- if $\phi = p$, then $T(\phi)$ is a tree with a single node v_p .
- if $\phi = \beta \phi_i$, where $\beta \in \{\neg, X\}$, then the root node of $T(\phi)$ is v_β and it has a unique subtree $T(\phi_i)$.
- if $\phi = \phi_i \beta \phi_j$, where $\beta \in \{\land, \mathsf{U}\}$, then the root node of $T(\phi)$ is v_β and it has two subtrees, where the left subtree is $T(\phi_i)$ and the right subtree is $T(\phi_j)$.

The node sequence obtained by preorder traversal of all nodes in an LTL_f syntax tree $T(\phi)$, denoted by $pretravel(T(\phi))$, is defined as follows:

$$pretravel(T(\phi)) = \begin{cases} v_p, & \phi = p \in \mathbb{P}. \\ v_{\alpha}, pretravel(T(\phi_1)), & \phi = \alpha\phi_1, \alpha \in \{\neg, \mathsf{X}\}. \\ v_{\beta}, pretravel(T(\phi_1)), \\ pretravel(T(\phi_2)), & \phi = \phi_1\beta\phi_2, \beta \in \{\land, \mathsf{U}\}. \end{cases}$$

$$(2)$$

LTL_f formulae are interpreted over finite *traces* of propositional states. A finite trace is represented by $\pi = s_0, s_1, \ldots, s_n$, where $s_t \in 2^{\mathbb{P}}$ is a state at time t. For every state s_i of π and every $p \in \mathbb{P}$, p holds if $p \in s_i$ or $\neg p$ holds otherwise. The traces mentioned in this paper are finite. The size of π is the number of states of π , denoted by $|\pi|$. By π_i we denote a *sub-trace* of π beginning from the state s_i . Let π be a trace and $|\pi| = n$. The *satisfaction relation* \models is defined as follows:

$$\begin{array}{ll} \pi_i \models p & \text{iff} \quad p \in s_i, \\ \pi_i \models \neg \phi & \text{iff} \quad \pi_i \not\models \phi, \\ \pi_i \models \phi_1 \land \phi_2 & \text{iff} \quad \pi_i \models \phi_1 \text{ and } \pi_i \models \phi_2, \\ \pi_i \models X\phi & \text{iff} \quad i < n \text{ and } \pi_{i+1} \models \phi, \\ \pi_i \models \phi_1 \mathsf{U}\phi_2 & \text{iff} \quad \exists i \le k \le n, \pi_k \models \phi_2 \text{ and} \\ \forall i \le j < k, \pi_j \models \phi_1. \end{array}$$

where ϕ , ϕ_1 , ϕ_2 are LTL_f formulae, and $p \in \mathbb{P} \cup \{\top, \bot\}$. Learning LTL_f formulae. We focus on the problem of learning a *target LTL_f formula* to characterize the behaviors observed in a set of *positive traces* (Π^+), while to exclude behaviors observed in a set of *negative traces* (Π^-). The target formula is an *LTL_f classifier over traces* aiming to separate the provided positive and negative traces. We denote $\Pi = \Pi^+ \cup \Pi^-$. We define lab: $\Pi \to \{0, 1\}$: for any $e \in \Pi$, lab(e) = 1 if $e \in \Pi^+$, or lab(e) = 0 if $e \in \Pi^-$. The *accuracy* of an LTL_f formula ϕ for Π is defined as:

$$\operatorname{acc}(\phi, \Pi) = \frac{|\{\pi \in \Pi^+ | \pi \models \phi\}| + |\{\pi \in \Pi^- | \pi \not\models \phi\}|}{|\Pi|}.$$
(3)

LTL_f Encoding and Inference

The key part of TLTLf is a neural network parameterized by the LTL_f encoding method. So in this section, we first show the definition of LTL_f encoding to parameterize TLTLf, as well as the model structure of TLTLf for inference of the satisfaction relation over traces. Afterwards, we introduce a subclass of LTL_f encoding, namely *faithful LTL_f encoding*, and show a one-to-one correspondence between LTL_f formulae and faithful LTL_f encodings.

Model Structure of TLTLf

The input of TLTLf is a trace and its output is the satisfaction relation between TLTLf and a trace. The trainable parameters of TLTLf are given by Definition 1.

Definition 1 Let \mathbb{P} be a set of atomic propositions and $L \in \mathbb{N}$. The parameter set of TLTLf of size L is defined as $\Gamma = \{(\Gamma_{right})_{i,j} \in \mathbb{R} | 1 \leq i \leq L-2, i+2 \leq j \leq L\} \cup \{(\Gamma_{atom})_{i,j} \in \mathbb{R} | 1 \leq i \leq L, 1 \leq j \leq |\mathbb{P}|\} \cup \{(\Gamma_{\neg})_i, (\Gamma_{\wedge})_i, (\Gamma_{\nabla})_i, (\Gamma_{\text{none}})_i \in \mathbb{R} | 1 \leq i \leq L\}.$ For brevity, we also reuse Γ to denote an assignment of the parameter set Γ of TLTLf.

To establish a relationship between parameters of TLTLf and an LTL_f syntax tree, we confine that every parameter in Γ be assigned a value between 0 and 1. We call a parameter assignment with this restriction an LTL_f encoding, formally defined below.

Definition 2 An LTL_f encoding of TLTLf of size L is defined as $\theta = \{(\theta_{right})_{i,j} \in \mathbb{R}^{(0,1)} | 1 \le i \le L-2, i+2 \le j \le L\} \cup \{(\theta_{atom})_{i,j} \in \mathbb{R}^{(0,1)} | 1 \le i \le L, 1 \le j \le |\mathbb{P}|\} \cup \{(\theta_{\neg})_i, (\theta_{\wedge})_i, (\theta_{\nabla})_i, (\theta_{0none})_i \in \mathbb{R}^{(0,1)} | 1 \le i \le L\},$ where $\mathbb{R}^{(0,1)}$ denotes the real value range from 0 to 1.

An LTL_f encoding is able to represent an LTL_f syntax tree. Let $T(\phi)$ be an LTL_f syntax tree and pretravel $(T(\phi)) = v_1, v_2, ..., v_L$. For all $i \in [1, L]$, the parameters $\theta_{\neg}, \theta_{\wedge}, \theta_{\mathsf{X}}, \theta_{\mathsf{U}}$ and θ_{atom} determine whether v_i is $v_{\neg}, v_{\wedge}, v_{\mathsf{X}}, v_{\mathsf{U}}$ and v_p for $p \in \mathbb{P}$, respectively. We introduce θ_{none} to encode a null node so as to represent a smaller syntax tree using an LTL_f encoding of a greater size. For example, if we want to use an LTL_f encoding of size L+1 to represent $T(\phi)$, we should set $(\theta_{\mathsf{none}})_{L+1}$ to 1. The parameter $(\theta_{\mathsf{right}})_{i,j}$ is used to represent whether the right child of v_i is v_j . Since pretravel $(T(\phi))$ is the prefix form of ϕ , the left or the only child of v_i should be v_{i+1} if v_i has children. We use the following Example 1 to illustrate an LTL_f encoding.

Example 1 Let $\mathbb{P} = \{p_1, p_2\}$ and θ be an LTL_f encoding of TLTLf of size 3 where $(\theta_{\neg})_1 = 0.8, (\theta_X)_1 = 0.3, (\theta_{atom})_{2,1} = (\theta_{none})_3 = 1$ and other parameters are

assigned 0. The LTL_f formula that θ represents is the most likely to be $\neg p_1$ while it may also be Xp₁ since $(\theta_X)_1 = 0.3$.

In fact, an arbitrary parameter assignment of TLTLf can be converted to an LTL_f encoding of TLTLf of the same size, as shown in the following equation.

$$\begin{aligned} &(\theta_{\text{right}})_{i,j} = \frac{e^{(\Gamma_{\text{right}})_{i,j}}}{(\eta_{\text{right}})_i}, (\theta_{\text{atom}})_{i,j} = \frac{e^{(\Gamma_{\text{atom}})_{i,j}}}{(\eta_{\text{op}})_i}, \\ &(\theta_{\neg})_i = \frac{e^{(\Gamma_{\neg})_i}}{(\eta_{\text{op}})_i}, (\theta_{\wedge})_i = \frac{e^{(\Gamma_{\wedge})_i}}{(\eta_{\text{op}})_i}, \\ &(\theta_{\mathsf{X}})_i = \frac{e^{(\Gamma_{\mathsf{X}})_i}}{(\eta_{\text{op}})_i}, (\theta_{\mathsf{U}})_i = \frac{e^{(\Gamma_{\mathsf{U}})_i}}{(\eta_{\text{op}})_i}, (\theta_{\text{none}})_i = \frac{e^{(\Gamma_{\text{none}})_i}}{(\eta_{\text{op}})_i}, \end{aligned}$$

where

$$\begin{aligned} (\eta_{\text{right}})_{i} &= \sum_{j=i+2}^{L} e^{(\Gamma_{\text{right}})_{i,j}} + \sum_{j=1}^{|\mathbb{P}|} e^{(\Gamma_{\text{atom}})_{i,j}} \\ &+ e^{(\Gamma_{\text{none}})_{i}} + e^{(\Gamma_{\text{n}})_{i}} + e^{(\Gamma_{\text{X}})_{i}}, \\ (\eta_{\text{op}})_{i} &= \sum_{j=1}^{|\mathbb{P}|} e^{(\Gamma_{\text{atom}})_{i,j}} + e^{(\Gamma_{\text{none}})_{i}} \\ &+ e^{(\Gamma_{\text{n}})_{i}} + e^{(\Gamma_{\text{n}})_{i}} + e^{(\Gamma_{\text{X}})_{i}} + e^{(\Gamma_{\text{U}})_{i}}. \end{aligned}$$

$$(5)$$

Thus, TLTLf is defined as a neural network parameterized by Definition 1, which is then transformed to an LTL_f encoding by Equation (4). Given a trace π , TLTLf computes a satisfaction relation between the LTL_f encoding of TLTLf and the trace. Such an inference process of TLTLf is formalized in Definition 3.

Definition 3 Let \mathbb{P} be a set of atomic propositions and Γ a parameter assignment of TLTLf of size $L \in \mathbb{N}$. θ is constructed from Γ by Equation (4). Given a trace $\pi = s_0, s_1, ..., s_n$ over \mathbb{P} , TLTLf computes satisfaction vectors $x_i \in \mathbb{R}^L$ (where $0 \le i \le n$) defined as follows:

$$\begin{aligned} &(x_i)_j = \sigma(\sum_{k=1}^{|\mathbb{P}|} (\theta_{\text{atom}})_{j,k} I(p_k \in s_i) + (\theta_{\mathsf{X}})_j (x_{i+1})_{j+1} \\ &+ (\theta_{\neg})_j \sigma(1 - (x_i)_{j+1}) + (\theta_{\wedge})_j \sigma((x_i)_{j+1} + (r_i)_j - 1) \\ &+ (\theta_{\mathsf{U}})_j ((r_i)_j + \sigma((x_i)_{j+1} + (x_{i+1})_j - 1))), \end{aligned}$$

$$(6)$$

where

$$\begin{aligned} &(r_i)_j &= \sum_{k=L}^{j+2} (\theta_{\text{right}})_{j,k}(x_i)_k, \\ &\sigma(x) &= \min(1, \max(0, x)), \end{aligned}$$

and $(x_i)_{L+1} = 0$, $(x_{n+1})_k = 0$ for all $1 \le k \le L+1$, and I(C) returns 1 if C is satisfied or 0 otherwise. By $\text{ESat}(\theta, \pi)$ we denote the satisfaction relation between θ and π . Finally TLTLf outputs $\text{ESat}(\theta, \pi)$ as $(x_0)_1$.

Intuitively, $(x_i)_j$ represents whether $\pi_i = s_i, s_{i+1}, ..., s_n$ satisfies the *j*-th sub-formula of the formula that θ represents. The computation of $(x_i)_j$ is based on the definition of the satisfaction relation of LTL_f . Specifically, we first calculate $(r_i)_j$, which denotes whether the right sub-formula of the *j*-th sub-formula satisfies π_i . Here θ_{right} plays a role of right-child selection. In Equation (6), $\theta_{\neg}, \theta_{\wedge}, \theta_{\chi}, \theta_{\cup}$ are used to select operators while θ_{atom} is used to select atomic propositions. For example, if the *j*-th sub-formula is of the form of $\neg \phi_{j+1}$, then the equation can be simplified to $(x_i)_j = \sigma(1-(x_i)_{j+1})$, which means that the *j*-th sub-formula satisfies π_i if its only child sub-formula does not satisfy π_i . We use the following Example 2 to illustrate Definition 3.

Example 2 Let $\pi = \{p_1, p_2\}, \{p_2\}$ and θ be the LTL_f encoding of TLTLf given in Example 1. Then the satisfaction vector is $x_0 = [0, 1, 0], x_1 = [0.8, 0, 0]$. The inference output is $\text{ESat}(\theta, \pi) = (x_0)_1 = 0$.

The Faithful Subclass of LTL_f Encoding

As shown in Example 1, not every LTL_f encoding corresponds to an LTL_f formula. So in the following we introduce the notion of *faithful LTL_f* encoding by adding additional constraints to ensure the correspondence.

Definition 4 Let θ be an LTL_f encoding of TLTLf of size L. θ is said to be faithful if it satisfies the following conditions:

- $1. \ \forall \gamma \in \theta : \gamma = 0 \lor \gamma = 1.$
- 2. $\forall i \in [1, L] : (\theta_{\text{none}})_i + \sum_{j=1}^{|\mathbb{P}|} (\theta_{\text{atom}})_{i,j} + (\theta_{\neg})_i + (\theta_{\wedge})_i + (\theta_{X})_i + (\theta_{U})_i = 1.$
- 3. $\sum_{j=1}^{|\mathbb{P}|} (\theta_{\text{atom}})_{L,j} + (\theta_{\text{none}})_L = 1 \land \forall i \in [1, L-1] :$ $\sum_{j=i+2}^{L} (\theta_{\text{right}})_{i,j} + (\theta_{\text{none}})_i + \sum_{j=1}^{|\mathbb{P}|} (\theta_{\text{atom}})_{i,j} + (\theta_{\neg})_i + (\theta_{\mathsf{X}})_i = 1.$
- 4. $(\theta_{\text{none}})_1 = 0 \land \forall i \in [2, L] : \sum_{j=1}^{i-2} (\theta_{\text{right}})_{j,i} + (\theta_{\neg})_{i-1} + (\theta_{\land})_{i-1} + (\theta_{\lor})_{i-1} + (\theta_{U})_{i-1} + (\theta_{\text{none}})_i = 1.$
- 5. $\forall i \in [1, L-1] : (\theta_{\text{none}})_{i+1} \ge (\theta_{\text{none}})_i.$

Intuitively, Condition 1 ensures all the parameters are assigned Boolean values. Condition 2 forces each node on the syntax tree to represent only one operator or one atomic proposition. Condition 3 restricts the number of children of a node according to the operator. If this node represents a binary operator, it will not represent other operators or atomic propositions because of Condition 2. Thus this node will have exactly one right child according to Condition 3. Besides, the node v_L has no child node so it must represent an atomic proposition or must not be used. Condition 4 restricts the number of fathers of a node. Except for the root node that has no father, every valid node v_i (where $(\theta_{none})_i = 0$) has exactly one father node. Condition 5 is used to restrict that null nodes v_i (where $(\theta_{none})_i = 1$) are placed continuously at the end of the node sequence obtained by preorder traversal of all nodes. Condition 6 restricts that, if v_i is the right child of v_i , then every node v_t between them does not have a right child v'_t such that t' > j.

The faithful LTL_f encoding ensures the LTL_f formula that it represents to be unique, as shown in the following example.

Example 3 Consider the LTL_f encoding θ of TLTLf given in Example 1 again. A faithful LTL_f encoding closed to θ is $\hat{\theta}$, where $(\hat{\theta}_{\neg})_1 = 1, (\hat{\theta}_X)_1 = 0, (\hat{\theta}_{atom})_{2,1} = 1, (\hat{\theta}_{none})_3 = 1$ and other parameters are assigned 0. The LTL_f formula that $\hat{\theta}$ represents is unique, which is $\neg p_1$.

Faithful LTL_f Encoding vs LTL_f Formula

For an arbitrary LTL_f formula ϕ , we introduce a function to encode ϕ into a parameter assignment of TLTLf of an equal or greater size, formalized in the following Definition 5.

Definition 5 Let ϕ be an LTL_f formula, $T(\phi)$ its syntax tree, and pretravel $(T(\phi)) = v_1, v_2, ..., v_L$. The function for encoding ϕ into a parameter assignment of TLTLf of size $L' \geq L$, denoted by $\theta_{\phi(L')}$, is defined as follows:

• $\forall 1 \leq i \leq L : (\theta_{\text{right}})_{i,j} = 1 \text{ if } v_j \text{ is the right child of } v_i and (\theta_{\text{right}})_{i,j} = 0 \text{ otherwise.}$

- $\forall 1 \leq i \leq L : (\theta_{\text{atom}})_{i,j} = 1 \text{ if } v_i = v_{p_j} \text{ and } (\theta_{\text{atom}})_{i,j} = 0 \text{ otherwise.}$
- $\forall 1 \leq i \leq L : (\theta_{\beta})_i = 1 \text{ if } v_i = v_{\beta} \text{ and } (\theta_{\beta})_i = 0$ otherwise, where $\beta \in \{\neg, \land, \mathsf{X}, \mathsf{U}\}.$
- $\forall L < i \leq L'$: $(\theta_{\text{none}})_i = 1, (\theta_{\text{right}})_{i,j} = 0, (\theta_{\beta})_i = 0, where \beta \in \{\neg, \land, X, U\}.$

Example 4 Let ϕ be $p_1 \bigcup X p_2$. We have $\operatorname{pretravel}(T(\phi)) = v_{\bigcup}, v_{p_1}, v_{X}, v_{p_2}$. Then in the encoding $\theta_{\phi(5)}$, we have $(\theta_{\bigcup})_1 = 1$, $(\theta_{\operatorname{atom}})_{2,1} = 1$, $(\theta_{X})_3 = 1$, $(\theta_{\operatorname{atom}})_{4,2} = 1$, $(\theta_{\operatorname{right}})_{1,3} = 1$, $(\theta_{\operatorname{none}})_5 = 1$, and other parameters are assigned 0.

The following lemma shows that the parameter assignment of TLTLf encoded from an LTL_f formula must be a faithful LTL_f encoding.¹

Lemma 1 Let ϕ be an LTL_f formula, then $\theta_{\phi(L')}$ is a faithful LTL_f encoding of TLTLf of size L'.

The following Definition 6 shows how to decode a faithful LTL_f encoding to a symbol sequence. Then Example 5 illustrates the decoding method.

Definition 6 Let θ be a faithful LTL_f encoding of TLTLfof size L. The decoding function $decode(\theta) = o_1 \dots o_L$ is defined as follows:

$$o_{i} = \begin{cases} p_{j}, & (\theta_{\text{atom}})_{i,j} = 1, \\ \beta, & (\theta_{\beta})_{i} = 1, \beta \in \{\neg, \land, \mathsf{X}, \mathsf{U}\}, \\ \epsilon, & (\theta_{\text{none}})_{i} = 1. \end{cases}$$
(8)

Example 5 Consider ϕ and $\theta_{\phi(5)}$ in Example 4 again. Since $(\theta_U)_1 = 1, (\theta_{atom})_{2,1} = 1, (\theta_X)_3 = 1, (\theta_{atom})_{4,2} = 1$ and $(\theta_{none})_5 = 1$, We have decode $(\theta_{\phi(5)}) = Up_1Xp_2$, which is exactly the prefix form of ϕ .

The following Theorem 1 shows that the decoding method always results in the prefix form of an LTL_f formula.

Theorem 1 For every faithful LTL_f encoding θ of TLTLf, decode(θ) is the prefix form of a certain LTL_f formula.

Now we can prove that faithful LTL_f encodings and the prefix forms of LTL_f formulae have one-to-one correspondence, by showing that the decoding method is both subjective (Theorem 2) and injective (Theorem 3).

Theorem 2 For any LTL_f formula ϕ with $pretravel(T(\phi)) = v_1, v_2, ..., v_L$ and any $L' \ge L$, there exists a faithful LTL_f encoding θ of size L' such that $decode(\theta) = pre(\phi)$.

Theorem 3 Given two different faithful LTL_f encodings of the same size, namely θ_1 and θ_2 , decode $(\theta_1) \neq$ decode (θ_2) .

Inference for the Satisfaction Relation

Now we achieve Theorem 4 to guarantee an equivalence between the inference of TLTLf and the inference of LTL_f .

Theorem 4 For any LTL_f formula ϕ with $\operatorname{pretravel}(T(\phi)) = v_1, v_2, ..., v_L$, any $L' \geq L$ and any trace $\pi = s_0, s_1, ..., s_n$, it holds that $\operatorname{ESat}(\theta_{\phi(L')}, \pi) = 1$ if $\pi \models \phi$, or $\operatorname{ESat}(\theta_{\phi(L')}, \pi) = 0$ otherwise.

Learning LTL_f Formulae by LTL_f Encoding

For learning LTL_f formulae, we first build TLTLf parameterized by an LTL_f encoding and then train it to distinguish positive traces from negative traces. Afterwards, we give an algorithm to extract the formula from TLTLf.

The faithful conditions are used in both the network structure and the optimization objective. The construction process of θ is similar to using the softmax function. We use it to make θ satisfy Condition 2 and Condition 3 as much as possible. Notice that θ satisfies Condition 2 because $\forall i \in [1, L](\theta_{\text{none}})_i + \sum_{j=1}^{|\mathbb{P}|} (\theta_{\text{atom}})_{i,j} + (\theta_{\neg})_i + (\theta_{\wedge})_i +$ $(\theta_{\lambda})_i + (\theta_{\cup})_i = \frac{e^{(\Gamma_{\text{none}})_i}}{(\eta_{\text{op}})_i} + \sum_{j=1}^{|\mathbb{P}|} \frac{e^{(\Gamma_{\text{atom}})_{i,j}}}{(\eta_{\text{op}})_i} + \frac{e^{(\Gamma_{\neg})_i}}{(\eta_{\text{op}})_i} + \frac{e^{(\Gamma_{\neg})_i}}{(\eta_{\text{op}})_i} = 1$. Similarly, Condition 3 in Definition 4 is approximately satisfied.

For each trace π in the set of positive traces Π^+ and the set of negative traces Π^- , we use the LTL_f encoding θ to infer the satisfaction relation. The classification objective is:

$$\zeta_1 = \sum_{\pi \in \Pi} (\operatorname{ESat}(\theta, \pi) - \mathsf{lab}(\pi))^2, \tag{9}$$

where $\forall \pi \in \Pi^+$, $\mathsf{lab}(\pi) = 1$ and $\forall \pi \in \Pi^-$, $\mathsf{lab}(\pi) = 0$.

We additionally use regularization loss to make θ approximately satisfy Condition 4, 5, and 6 in Definition 4. The regularization terms are formulated as:

$$\begin{aligned} \zeta_{2} &= \sum_{i=2}^{L} (\sum_{j=1}^{i-2} (\theta_{\text{right}})_{j,i} + (\theta_{\neg})_{i-1} + (\theta_{\wedge})_{i-1} + (\theta_{X})_{i-1} \\ &+ (\theta_{U})_{i-1} + (\theta_{\text{none}})_{i} - 1)^{2}, \\ \zeta_{3} &= \sum_{i=1}^{L-1} \text{Relu}((\theta_{\text{none}})_{i} - (\theta_{\text{none}})_{i+1}), \\ \zeta_{4} &= \sum_{i=1}^{L-2} \sum_{j=i+2}^{L} \sum_{t=i+1}^{j-1} \sum_{t'=j+1}^{L} \text{Relu}((\theta_{\text{right}})_{i,j} \\ &+ (\theta_{\text{right}})_{t,t'} - 1). \end{aligned}$$
(10)

They are obtained from the corresponding conditions by converting constraints like x = y to $(x - y)^2$ and x > y to Relu(y - x). The final objective to be minimized is:

$$\zeta = \zeta_1 + \alpha_1 \zeta_2 + \alpha_2 \zeta_3 + \alpha_3 \zeta_4, \tag{11}$$

where $\alpha_1, \alpha_2, \alpha_3$ are coefficients for regularization terms.

LTL_f Encoding Interpretation

We interpret an LTL_f formula from an LTL_f encoding by Algorithm 1. The algorithm interprets the LTL_f encoding from bottom to top and calculates the score of the interpretations for each sub-formula (s_j in line 12) according to the LTL_f encoding. The score of an interpretation is obtained by multiplying all related parameters in the LTL_f encoding. The following Example 6 illustrates how Algorithm 1 works.

Example 6 Suppose an LTL_f encoding θ of size 3 shown in Table 1 and the beam width 2 are input to Algorithm 1. The outcomes of execution steps of Algorithm 1 are shown in

¹All the proofs of lemmas/theorems are provided in the technical report available at https://github.com/a79461378945/TLTLf.git.

Algorithm 1: Interpreting LTL_f Formula

	8 · · · · · · · · · · · · · · · · · · ·							
	Input :LTL _f encoding θ of size L, the beam width							
	ω , the training set Π							
	Output : An LTL _f formula ϕ interpreted from θ							
1	$\theta_{\text{right}}, \theta_{\text{none}}, \theta_{\text{atom}}, \text{ and } \theta_{\text{op}} \leftarrow \text{computed by}$							
	Equation (7) on θ , where $op \in \{\neg, \land, X, U\}$;							
2	$i \leftarrow L;$							
3	3 while $i > 1$ do							
4	$f_i \leftarrow \emptyset;$							
5	for $p_k \in \mathbb{P}$ do							
6	$ \begin{bmatrix} f_i \leftarrow f_i \cup \{(p_k, (\theta_{\text{atom}})_{i,k})\}; \end{bmatrix}$							
7	for $(\phi_k, s_k) \in f_{i+1}$ do							
8	$ f_i \leftarrow$							
	$\int_{i} \bigcup \{ ((\neg, \phi_k), (\theta_{\neg})_i s_k), ((X, \phi_k), (\theta_{X})_i s_k) \};$							
9	for $i+2 \leq j \leq L$ do							
10	for $((\phi_l, s_l), (\phi_r, s_r)) \in f_{i+1} \times f_j$ do							
11	$f_i \leftarrow f_i \cup$							
	$\{((\wedge,\phi_l,\phi_r),(\theta_{\wedge})_i(\theta_{\mathrm{right}})_{i,r}s_ls_r)\} \cup$							
	$\left\{ ((U,\phi_l,\phi_r),(\theta_{U})_i(\theta_{\mathrm{right}})_{i,r}s_ls_r) \right\};$							
12	Sort $f_i = \{(\phi_j, s_j)\}$ according to s_j , keep top ω							
	elements and remove the others;							
13	$\lfloor i \leftarrow i - 1;$							
14	$\phi \leftarrow$ the best formula obtained from f_1 according to							
	the classification accuracy on Π :							

15 return ϕ ;

Table 2, where the top 2 interpretations and their scores for each f_i are displayed in bold. For i = 3, the interpretations of f_3 can only be an atomic proposition. The score of $f_3 = p_1$ is $(\theta_{\text{atom}})_{3,1}$ according to Algorithm 1 (line 5). We keep p_1 and p_2 as the top 2 interpretations for f_3 . The score of $f_2 = Xp_1$ is obtained by multiplying $(\theta_X)_2$ and the score of $f_3 = p_1$. Continuing this way we finally obtain the top 2 interpretations for f_1 , namely p_2 and $p_1 \wedge p_2$.

Evaluation

Competitors. We compared TLTLf with four SOTA approaches, including C. &M. (Camacho and McIlraith 2019), BayesLTL (Kim et al. 2019), MaxSAT-DT (Gaglione et al. 2021) and GLTLf (Luo et al. 2022). C. &M. cannot learn from imperfect data but can learn arbitrary formulae. BayesLTL can learn from imperfect data but cannot learn arbitrary formulae. MaxSAT-DT, GLTLf and our proposed TLTLf can learn arbitrary formulae from imperfect data.

Datasets. We reused the datasets that are provided by (Luo et al. 2022). There are 5 domains for $k_f \in \{3, 6, 9, 12, 15\}$ and each domain has 50 datasets. For each dataset, there is a formula with k_f operators, and there are 250/250 positive/negative traces for this formula constituting the training set and 500/500 positive/negative traces for this formula constituting the test set. For generating the imperfect data, a portion of traces from the original data were randomly chosen to reverse labels; *i.e.*, original positive labels are turned to be negative, and vice versa. The percentage δ of traces with wrong labels is determined by the imperfect rate drawn from

i	$(\theta_{\rm none})_i$	$ (\theta_{\neg})_i$	$ (heta_\wedge)_i$	$ (\theta_{X})_i$
1	0	0	0.8	0
2	0	0	0	0.1
3	0	0	0	0
i	$(heta_{U})_i$	$(\theta_{\mathrm{atom}})_{i,1}$	$ (heta_{ ext{atom}})_{i,2} $	$ (\theta_{\mathrm{right}})_{i,3} $
i 1	$(heta_{U})_i$	$\mid (heta_{ ext{atom}})_{i,1} \mid 0$	$ (heta_{ ext{atom}})_{i,2} 0.2$	$ \begin{vmatrix} (\theta_{\text{right}})_{i,3} \\ 1 \end{vmatrix}$
i 1 2	$\frac{(\theta_{U})_i}{0}$	$ \begin{array}{ } (\theta_{\mathrm{atom}})_{i,1} \\ \hline 0 \\ \hline 0.3 \end{array} $	$ \begin{array}{c c} (\theta_{\rm atom})_{i,2} \\ \hline 0.2 \\ \hline 0.6 \\ \end{array} $	

Table 1: The parameters in Example 6.

i	ϕ_i	related parameter	f_i	score
	p_1	$(\theta_{\rm atom})_{3,1} = 0.7$	p_1	0.7
3	p_2	$(\theta_{\rm atom})_{3,2}=0.3$	p_2	0.3
	p_1	$(\theta_{\rm atom})_{2,1} = 0.3$	p_1	0.3
2	p_2	$(\theta_{\rm atom})_{2,2} = 0.6$	p_2	0.6
2			Xp_1	0.07
	$X\phi_3$	$(\theta_{X})_3 = 0.1$	Xp_2	0.03
	p_2	$(\theta_{\rm atom})_{1,2} = 0.2$	p_2	0.2
			$p_1 \wedge p_1$	0.168
		$(\theta_{\wedge})_1 = 0.8$	$p_1 \wedge p_2$	0.336
1	$\phi_2 \wedge \phi_3$	$(\theta_{\rm right})_{1,3} = 1$	$p_2 \wedge p_1$	0.072
			$p_2 \wedge p_2$	0.144

Table 2: Executing Algorithm 1 for Example 6.

$\{10\%, 20\%, 30\%, 40\%\}.$

Settings. All experiments were conducted on a Linux system equipped with an Intel(R) Xeon(R) Gold 6248R processor with 3.0 GHz and 126 GB RAM. The time limit is set to 1 hour and the memory limit set to 10 GB for each instance. We used grid search to find optimal hyperparameters of TLTLf. We used Adam (Kingma and Ba 2015) to optimize the parameters in our model. Detailed settings for all approaches can be found in our technical report. In our experiments, all approaches first learn an LTL_f formula and then are evaluated to estimate the classification performance on the test set.

Comparison across datasets. As shown in Table 3, TLTLf obviously outperforms BayesLTL and GLTLf. Although MaxSAT-DT and C. &M. seem to have the best performance, they run out of time in more cases when k_f increases; in contrast, TLTLf keeps successful in all cases and it keeps a high accuracy when k_f increases. If we treat the accuracy of failed cases as 0, then the accuracies of MaxSAT-DT and C. &M. on datasets with $k_f = 9$ drop to 16% and 68%, respectively, obviously lower than that of TLTLf.

Comparison on imperfect data. TLTLf also outperforms other approaches on imperfect data, as shown in Figure 1(a). MaxSAT-DT and C. &M. fail to solve any formula on imper-



Figure 1: (a) Accuracy achieved by different imperfect rates. The results are averaged by 5 datasets with $k_f \in \{3, 6, 9, 12, 15\}$. (b) Network accuracy and the accuracy of formula interpreted from the network. (c) Consistency. (d) Accuracy achieved by different encoding sizes L. (e) Accuracy achieved by different beam widths ω for Algorithm 1.

	1	$k_f = 3$			$k_f = 6$			$k_f = 9$		k	$c_f = 12$		<i>k</i>	$c_f = 15$	
	Acc	\mathbf{F}_{1}	$N_{\rm s}$	Acc	\mathbf{F}_{1}	$N_{\rm s}$	Acc	\mathbf{F}_{1}	$N_{\rm s}$	Acc	F_1	$N_{\rm s}$	Acc	F_1	$N_{\rm s}$
MaxSAT-DT	100	100	49	100	100	19	100	100	8	100	100	5	100	100	5
С.&М.	99.7	99.7	50	97.9	96.7	47	97.1	95.5	35	95.1	91.9	20	93.7	87.4	8
BayesLTL	85.1	85.9	50	77.9	76.7	50	74.0	75.7	50	72.7	73.4	50	74.8	77.3	50
GLTLf	94.3	94.2	50	90.0	90.3	50	84.0	83.2	50	83.0	83.2	50	83.0	83.5	50
TLTLf	98.0	97.9	50	95.3	95.4	50	91.9	91.3	50	89.5	88.9	50	90.4	90.2	50

Table 3: Experimental results for L = 10 across different approaches. Acc stands for the average accuracy (%) for successful cases. F₁ stands for the average F₁ score (%) for successful cases. N_s stands for the number of cases out of total 50 cases that are successfully solved within the time limit.

fect training data. In contrast, TLTLf still has a high average accuracy 88.47% even when being trained on datasets with a moderately high imperfect rate $\delta = 0.3$.

Comparison on the performance of interpreting. Both TLTLf and GLTLf involve network training and interpreting, so we compare the performance gap between the two parts for TLTLf with that for GLTLf. Figure 1(b) shows that TLTLf has a smaller performance gap than GLTLf. This result suggests that the neural model underpinned TLTLf is more interpretable. We further assess consistency between the inference of neural model and that of the interpreted formula, indicating their agreement on the test set. For example, if the neural model and the interpreted formula give the same classification results on 95 out of 100 test traces, then the consistency between them is 95%. TLTLf achieves higher consistency, aligning with its reduced performance gap between the neural network and interpreted formula.

Hyper-parameters analysis. To analyze the impact of different hyper-parameters, we conducted experiments with various sizes of encoding and beam widths, on the datasets with $k_f = 9$. During the analysis of one hyper-parameter, the other hyper-parameter was set as default. From Figure 1(d),

it can be seen that with the increase of the size of encoding, the accuracy increases to a certain extent until L = 8. This may be caused by that k_f was set to 9 for all experimental datasets. Figure 1(e) shows that the accuracy first increases rapidly as the beam width increases and then remains stable. This implies that $\omega = 100$ is sufficient to guarantee a high accuracy for the formula interpreted by Algorithm 1.

Conclusion and Future Work

Learning tree-structured LTL_f formulae from imperfect data is important and challenging. In this paper we have proposed TLTLf parameterized by the LTL_f encoding to simulate LTL_f inference. TLTLf bridges the gap between the concise tree-structured syntax and the complex LTL_f semantics. Besides, we have identified the faithful LTL_f encoding, which has a one-to-one correspondence to the prefix form of LTL_f formulae. Experiment results demonstrate that TLTLfachieves the SOTA performance and yields LTL_f formulae more consistent with the learnt neural network than existing approaches do. Future work will extend our approach to LTLor other formal languages.

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