Bridging LTL$_f$ Inference to GNN Inference for Learning LTL$_f$ Formulae

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Motivation

Problem. Learning *linear temporal logic on finite traces* (LTL$_f$) formulae in *arbitrary form* to characterize the high-level behavior of a system from observation traces with *noise*.

Challenge.

1. *huge search space* of the target formula in arbitrary form
2. *wrong search bias* resulting from noisy data

Contributions

1. We theoretically bridge LTL$_f$ inference to GNN inference, which provides a new method for learning arbitrary LTL$_f$ formulae from noisy data.
2. Based on the theoretical result, we design a GNN-based approach, named as `GLTLf`.
3. Experimental results demonstrate that our approach is stronger robustness for noisy data and better scalability in data size.

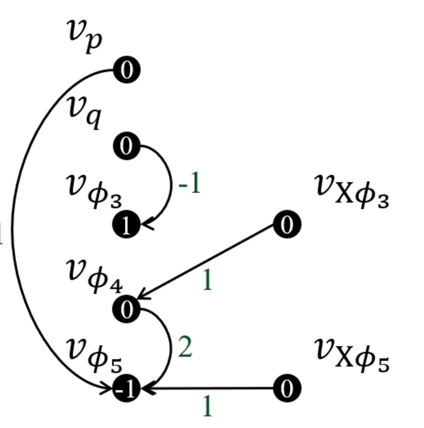
LTL$_f$ Graph

Definition 1 (simplified). *Let ϕ be an LTL$_f$ formula. Its* LTL$_f$ graph *G_ϕ is a four-tuple $(V_\phi, E_\phi, \mathsf{W}_\phi, \mathsf{b}_\phi)$ defined as follows,*

- *if* $\mathsf{unfold}(\phi_i) = p$, *then* $V_\phi = V_\phi \cup \{v_p\}$ *and* $\mathsf{b}_\phi(v_p) = 0$;
- *if* $\mathsf{unfold}(\phi_i) = \neg\phi_j$, *then* $V_\phi = V_\phi \cup \{v_{\phi_j}\}$, $E_\phi = E_\phi \cup \{\langle v_{\phi_j}, v_{\phi_i}\rangle\}$, $\mathsf{W}_\phi(\langle v_{\phi_j}, v_{\phi_i}\rangle) = -1$, *and* $\mathsf{b}_\phi(v_{\phi_i}) = 1$;
- *if* $\mathsf{unfold}(\phi_i) = \phi_j \wedge \phi_k$, *then* $V_\phi = V_\phi \cup \{v_{\phi_j}, v_{\phi_k}\}$, $E_\phi = E_\phi \cup \{\langle v_{\phi_j}, v_{\phi_i}\rangle, \langle v_{\phi_k}, v_{\phi_i}\rangle\}$, $\mathsf{W}_\phi(\langle v_{\phi_j}, v_{\phi_i}\rangle) = 1$, $\mathsf{W}_\phi(\langle v_{\phi_k}, v_{\phi_i}\rangle) = 1$, *and* $\mathsf{b}_\phi(v_{\phi_i}) = -1$;
- *if* $\mathsf{unfold}(\phi_i) = \mathsf{X}\phi_j$, *then* $V_\phi = V_\phi \cup \{v_{\mathsf{X}\phi_j}\}$, $E_\phi = E_\phi \cup \{\langle v_{\mathsf{X}\phi_j}, v_{\phi_i}\rangle\}$, $\mathsf{W}_\phi(\langle v_{\mathsf{X}\phi_j}, v_{\phi_i}\rangle) = 1$, *and* $\mathsf{b}_\phi(v_{\phi_i}) = \mathsf{b}_\phi(v_{\mathsf{X}\phi_j}) = 0$;
- *if* $\mathsf{unfold}(\phi_i) = \phi_k \vee (\phi_j \wedge \mathsf{X}\phi_i)$, *then* $V_\phi = V_\phi \cup \{v_{\phi_k}, v_{\phi_j}, v_{\mathsf{X}\phi_i}\}$, $E_\phi = E_\phi \cup \{\langle v_{\phi_k}, v_{\phi_i}\rangle, \langle v_{\phi_j}, v_{\phi_i}\rangle, \langle v_{\mathsf{X}\phi_i}, v_{\phi_i}\rangle\}$, $\mathsf{W}_\phi(\langle v_{\phi_k}, v_{\phi_i}\rangle) = 2$, $\mathsf{W}_\phi(\langle v_{\phi_j}, v_{\phi_i}\rangle) = 1$, $\mathsf{W}_\phi(\langle v_{\mathsf{X}\phi_i}, v_{\phi_i}\rangle) = 1$, $\mathsf{b}_\phi(v_{\phi_i}) = -1$, *and* $\mathsf{b}_\phi(v_{\mathsf{X}\phi_i}) = 0$,

where $p \in \mathbb{P} \cup \{\top, \bot\}$ and ϕ_j, ϕ_k are LTL$_f$ formulae.

Example 1. *Let $\phi = p\mathsf{U}(\mathsf{X}\neg q)$ be an LTL$_f$ formula.* $\mathsf{sub}(\phi) = \{p, q, \phi_3, \phi_4, \phi_5\}$, *where $\phi_3 = \neg q$, $\phi_4 = \mathsf{X}\phi_3$, and $\phi_5 = p\mathsf{U}\phi_4$.*



- $\phi_5 = \phi_4 \vee (p \wedge \mathsf{X}\phi_5)$
- *Relation of satisfaction of p, ϕ_4, $\mathsf{X}\phi_5$, and ϕ_5:*
  - *if p is $\bot$, ϕ_4 is $\bot$, and $\mathsf{X}\phi_5$ is $\bot$, then ϕ_5 is $\bot$;*
  - *if p is $\bot$, ϕ_4 is $\bot$, and $\mathsf{X}\phi_5$ is $\top$, then ϕ_5 is $\bot$;*
  - *if p is $\bot$, ϕ_4 is $\top$, and $\mathsf{X}\phi_5$ is $\bot$, then ϕ_5 is $\top$;*
  - ...
- **Boolean → real**: $\bot \to \leq 0$ *and* $\top \to \geq 1$

State Classifier

Definition 2 (simplified). *Let ϕ be an LTL$_f$ formula such that $|\mathsf{sub}(\phi)| = L$, $(V_\phi, E_\phi, \mathsf{W}_\phi, \mathsf{b}_\phi)$ an LTL$_f$ graph of ϕ, and $\pi = s_0, s_1, \ldots, s_n$ a trace. $(\mathbf{x}^{(0)}_{s_i})_j = 1$ if $\phi_j \in s_i$ or $(\mathbf{x}^{(0)}_{s_i})_j = 0$ otherwise. $\mathbf{x}^{(t)}_{s_i}$ is defined as follows:*

$$\mathbf{x}^{(t)}_{s_i} = \sigma(\mathbf{C}_\phi \mathbf{x}^{(t-1)}_{s_i} + \mathbf{A}_\phi \mathbf{x}_{s_{i+1}} + \mathbf{b}_\phi), \tag{1}$$

$$(\mathbf{C}_\phi)_{ij} = \begin{cases} \mathsf{W}_\phi(\langle v_{\phi_j}, v_{\phi_i}\rangle), & \text{if } \langle v_{\phi_j}, v_{\phi_i}\rangle \in E_\phi \text{ and } \phi_j \in \mathsf{sub}(\phi) \\ 0, & \text{otherwise,} \end{cases}$$

$$(\mathbf{A}_\phi)_{ij} = \begin{cases} \mathsf{W}_\phi(\langle v_{\phi_j}, v_{\phi_i}\rangle), & \text{if } \langle v_{\phi_j}, v_{\phi_i}\rangle \in E_\phi \text{ and } \phi_j \in \{\mathsf{X}\phi_k \mid \phi_k \in \mathsf{sub}(\phi)\} \\ 0, & \text{otherwise,} \end{cases}$$

$$(\mathbf{b}_\phi)_i = \mathsf{b}_\phi(v_{\phi_i}), \quad \text{for all } v_{\phi_i} \in V_\phi \text{ and } \phi_i \in \mathsf{sub}(\phi).$$

By $\mathcal{S}_\phi$ we denote the state classifier *$\mathcal{S}_\phi$, i.e., $\mathbf{x}^{(T)}_{s_i} = \mathcal{S}_\phi(\mathbf{x}^{(0)}_{s_i}, \mathbf{x}_{s_{i+1}}, T)$.*

Trace Classifier

Definition 3. *Let ϕ be an LTL$_f$ formula such that $|\mathsf{sub}(\phi)| = L$, and $\pi = s_0, s_1, \ldots, s_n$ a trace. By $\mathcal{T}_\phi$ we denote the* trace classifier *which takes a vector $\mathbf{x}^{(0)}_{s_i}$ and a number of iterations $T \in \mathbb{N}$ as input and $\mathbf{x}^{(T)}_{s_i}$ as output; i.e., $\mathbf{x}^{(T)}_{s_i} = \mathcal{T}_\phi(\mathbf{x}^{(0)}_{s_i}, T)$, where*

$$\mathcal{T}_\phi(\mathbf{x}^{(0)}_{s_i}, T) = \begin{cases} \mathcal{S}_\phi(\mathbf{x}^{(0)}_{s_i}, \mathcal{T}_\phi(\mathbf{x}^{(0)}_{s_{i+1}}, T), T), & 0 \leq i < n \\ \mathcal{S}_\phi(\mathbf{x}^{(0)}_{s_i}, \mathbf{0}, T), & i = n \end{cases} \tag{2}$$

Relationship between GNNs and LTL$_f$

Theorem 1. *Let ϕ be an LTL$_f$ formula such that $|\mathsf{sub}(\phi)| = L$. For every trace $\pi = s_0, s_1, \ldots, s_n$, $(\mathcal{T}_\phi(\mathbf{x}^{(0)}_{s_0}, L))_L = 1$ if and only if $\pi \models \phi$.*

GLTLf: GNN-based Learning Approach

Framework. The framework of `GLTLf` is summarized as follows.

1. First train a simple homogeneous AC-GNN model $\mathcal{S}$ to distinguish positive and negative traces.
2. Then interpret the parameters of $\mathcal{S}$ to obtain an LTL$_f$ formula ϕ_A.

Converting Traces to Graphs. Let $\pi = s_0, s_1, \ldots, s_n$ be a trace. Its *directed path graph* $G_\pi = (V_\pi, E_\pi)$:

- each vertex v_i in V_π corresponds to a state s_i in π;
- for each pair of states s_i, s_{i+1} in π, there is an edge $\langle v_{i+1}, v_i\rangle$ in E_π.

Training GNNs as Classifiers. Each vertex $v_i \in V_\pi$ has a feature vector $\mathbf{x}_{v_i}$ ($[x_1, \ldots, x_{|\mathbb{P}|}, x_\top, x_{|\mathbb{P}|+2}, \ldots, x_L]$).

- State classifier $\mathcal{S}$ follows Definition 2, but $\mathbf{C}$, $\mathbf{A}$, and $\mathbf{b}$ need to be trained.
- Trace classifier $\mathcal{T}$ is defined by Definition 3.
  - $(\mathcal{T}(\mathbf{x}^{(0)}_{v_i}, L))_j$ indicates whether $\pi_i \models \phi_j$, where $\phi_j \in \mathsf{sub}(\phi)$.

GLTLf: GNN-based Learning Approach

Interpreting. Interpret a sub-formula from $(\mathbf{C})_i$, $(\mathbf{A})_i$, and $(\mathbf{b})_i$.

1. First recommend a set of candidate formulae based on the *interpretation similarity*.
2. Then select the best formula based on the *discrimination effect for the traces*.

Result Analysis

Competitor.

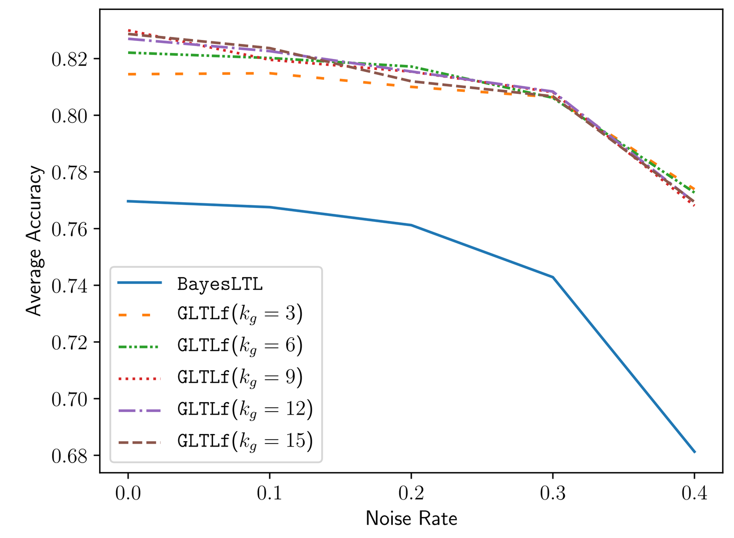
approach	noisy data	arbitrary formulae
`C.&M.` (Camacho and McIlraith 2019)	×	✓
`BayesLTL` (Kim et al. 2019)	✓	×
`MaxSAT-DT` (Gaglione et al. 2021)	✓	✓
`GLTLf` (Ours)	✓	✓

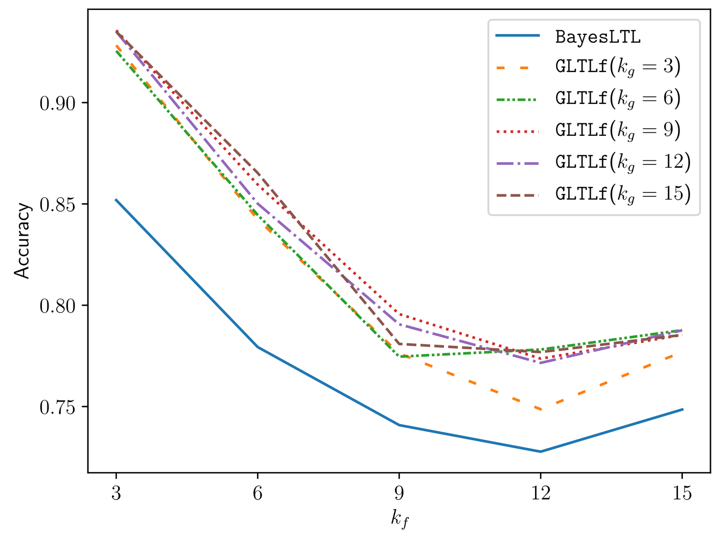
Comparisons on Noise-free Data.

	$k_f = 3$			$k_f = 6$			$k_f = 9$			$k_f = 12$			$k_f = 15$		
	Acc(%)	F$_1$(%)	N_s	Acc(%)	F$_1$(%)	N_s	Acc(%)	F$_1$(%)	N_s	Acc(%)	F$_1$(%)	N_s	Acc(%)	F$_1$(%)	N_s
`MaxSAT-DT`	100	100	49	100	100	19	100	100	8	100	100	5	100	100	5
`C.&M.`	99.77	99.77	50	97.93	96.79	47	97.14	95.55	35	95.10	91.91	20	93.74	87.49	8
`BayesLTL`	85.19	85.96	50	77.94	76.78	50	74.08	75.73	50	72.77	73.47	50	74.85	77.32	50
`GLTLf`	93.50	93.09	50	86.53	86.28	50	78.09	78.66	50	77.69	78.63	50	78.53	79.34	50

- `GLTLf` significantly surpasses `BayesLTL`.
- Although `MaxSAT-DT` and `C.&M.` are in the lead, they cannot solve long formulae.

Comparisons on Noise Data, Scalability, and Robustness.





- `GLTLf` is proven to be more noise-tolerated then other approaches.
- `GLTLf` can handle long formulae with higher performance compared to other approaches.
- `GLTLf` is able to solve formulae in various sizes and is rather robust.
  - Larger networks achieve better accuracies, even when solving short formulae.
  - Small networks can also get good performance on long formulae.

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