Learning to Check LTL Satisfiability and to Generate Traces via Differentiable Trace Checking

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Content

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Motivation

Linear temporal logic (LTL) satisfiability checking

- *e.g.*, input: $p_1 \, \mathcal{U} \bigcirc p_2$, output: SAT
- important applications, *e.g.*, model checking[6], goal-conflict analysis[5,18], and business process[21]
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- *logical approaches*: *e.g.*, based on logical reasoning mechanisms, such as model checking [23,24], tableau [1,11,27,29], temporal resolution [8,26], anti-chain [30], and Boolean satisfiability (SAT) problem [12–17]
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- promising approximators for checking LTL satisfiability *in polynomial time*[19]

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Learning-based approaches

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- Is it enough to answer the SAT or UNSAT enough?

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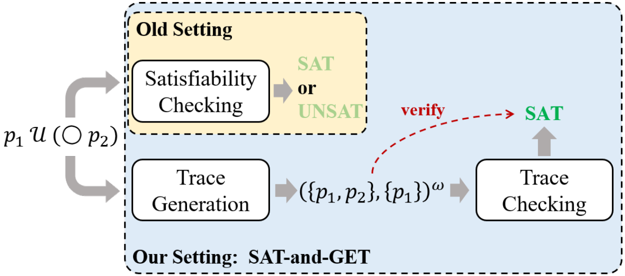
LTL satisfiability checking and trace generation (*SAT-and-GET*)

- *e.g.*, input: $p_1 \,\mathcal{U}\, \bigcirc p_2$, output: SAT because $(\{p_1, p_2\}, \{p_1\})^\omega \models p_1 \,\mathcal{U}\, \bigcirc p_2$



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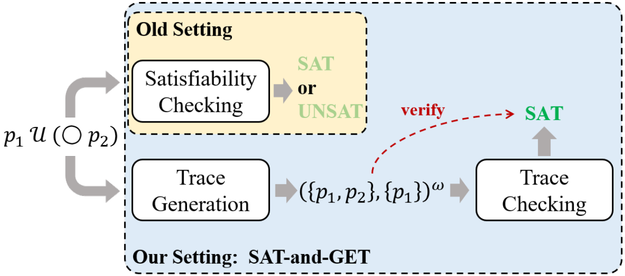

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Challenges

- bridging the gap between the *continuous domain* and the *discrete domain*

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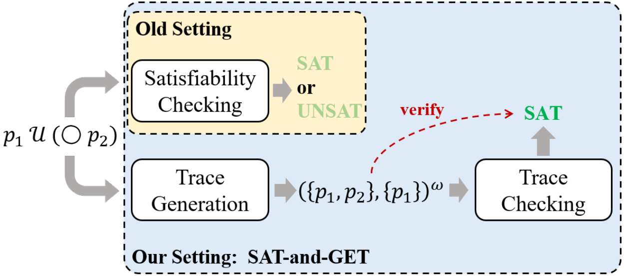

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Challenges

- bridging the gap between the *continuous domain* and the *discrete domain*
- *supervision confusion* from multiple satisfiable traces

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Deep reinforcement learning-based approach (OSUG)[20]

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Our contributions

- an *LTL encoding method* to parameterize a neural network and theoretically prove that its inference process (*neural trace checking*) is able to simulate LTL trace checking
- a novel approach *jointly* trains a neural network for LTL satisfiability checking and a neural network for trace generation guided by neural trace checking

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LTL Encoding

Definition 1 (LTL Encoding)

Let $\mathbb{P}$ be a set of atom propositions, ϕ an LTL formula over $\mathbb{P}$, $(V, E, v_1, \mathtt{lab}_V, \mathtt{lab}_E) = \mathtt{tree}(\phi)$, and $\langle v_1, \ldots, v_{|\phi|} \rangle = \mathtt{pretravel}(\mathtt{tree}(\phi))$. The *LTL encoding* η of ϕ is a 6-tuple

$$(\boldsymbol{\eta}_{right}, \boldsymbol{\eta}_{atom}, \boldsymbol{\eta}_{\neg}, \boldsymbol{\eta}_{\wedge}, \boldsymbol{\eta}_{\bigcirc}, \boldsymbol{\eta}_{\mathcal{U}}),$$

where $\boldsymbol{\eta}_{right} \in \{0,1\}^{|\phi| \times |\phi|}$, $\boldsymbol{\eta}_{atom} \in \{0,1\}^{|\phi| \times |\mathbb{P}|}$, and $\boldsymbol{\eta}_{\neg}, \boldsymbol{\eta}_{\wedge}, \boldsymbol{\eta}_{\bigcirc}, \boldsymbol{\eta}_{\mathcal{U}} \in \{0,1\}^{|\phi|}$; moreover, for all subscripts i and j, $(\boldsymbol{\eta}_{right})_{i,j} = 1$ if $\mathtt{lab}_E((v_i, v_j)) = R$ and $(\boldsymbol{\eta}_{right})_{i,j} = 0$ otherwise, $(\boldsymbol{\eta}_{atom})_{i,j} = 1$ if $\mathtt{lab}_V(v_i) = p_j$ and $(\boldsymbol{\eta}_{atom})_{i,j} = 0$ otherwise, $(\boldsymbol{\eta}_{\circ})_i = 1$ if $\mathtt{lab}_V(v_i) = \circ$ and $(\boldsymbol{\eta}_{\circ})_i = 0$ otherwise, where $\circ \in \{\neg, \wedge, \bigcirc, \mathcal{U}\}$.

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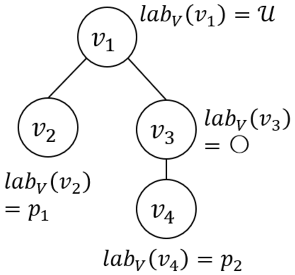
Let $\phi = p_1 \,\mathcal{U}\, \bigcirc p_2$ be an LTL formula. $\texttt{pretravel}(\texttt{tree}(\phi)) = \langle v_1, v_2, v_3, v_4 \rangle$. The LTL encoding η of ϕ is



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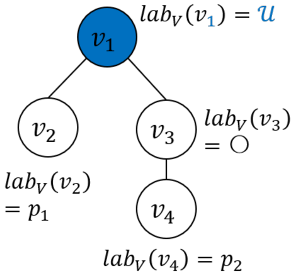

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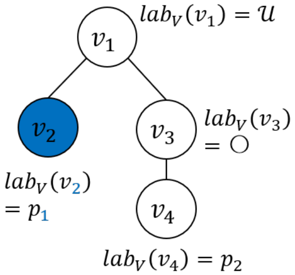

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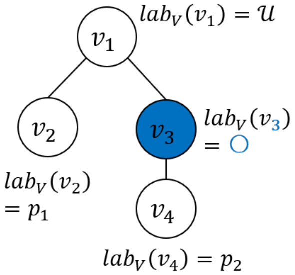

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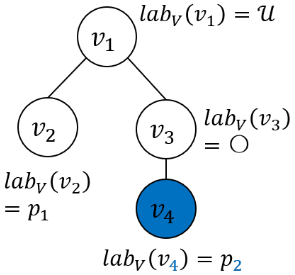

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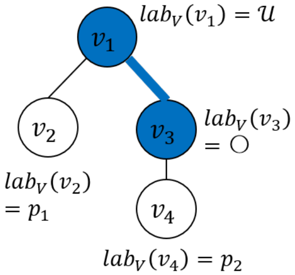

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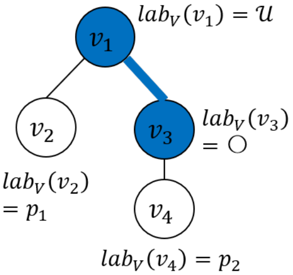

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Neural Modeling of Trace Checking

Definition 2 (Tensorized Trace)

Let $\mathbb{P}$ be a set of atom propositions and π a trace over $\mathbb{P}$. The *tensorized trace* of π is a 2-tuple $(\boldsymbol{s}, \boldsymbol{l})$ computed by Algorithm 2, where $\boldsymbol{s} \in \mathbb{R}_{[0,1]}^{|\pi| \times |\mathbb{P}|}$ and $\boldsymbol{l} \in \mathbb{R}_{[0,1]}^{|\pi|}$, and where $\mathbb{R}_{[0,1]}$ denotes the real value range from 0 to 1.

Algorithm 2: TENSORIZE

Input: A trace π over a set of atomic propositions $\mathbb{P}$.
Output: The tensorized trace $(\boldsymbol{s}, \boldsymbol{l})$ of π.

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s ← 0 where s ∈ {0,1}^{|π|×|P|}, l ← 0 where l ∈ {0,1}^{|π|}
for each state π[i] of π do
    for each atomic proposition p_j ∈ P do
        if p_j ∈ π[i] then
            (s)_{i,j} ← 1
    if i is loop-start time then
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$$\boldsymbol{s} = \begin{bmatrix} 1 & 1 \\ 1 & 0 \end{bmatrix}, \quad \boldsymbol{l} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}.$$

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- `NTCNet` is parameterized by $\theta = \eta$.
- The satisfaction vectors $\boldsymbol{x}_i \in \mathbb{R}^{|\phi|}$ where $i \in [1, |\pi|]$ are initialized by $\mathbf{0}$.

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Table 1: Converting logical operations to soften forms.

formal logic	$a \wedge b$	$a \vee b$	$\neg a$
soften logic	$\sigma(a+b-1)$	$\sigma(a+b)$	$1-a$

$$(\boldsymbol{p}_i)_j = \sum_{k=1}^{|\mathbb{P}|} (\boldsymbol{\theta}_{atom})_{j,k} (\boldsymbol{s})_{i,k}. \tag{2}$$

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soften logic	$\sigma(a+b-1)$	$\sigma(a+b)$	$1-a$

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Neural Modeling of Trace Checking

Neural network parameterized by LTL encoding (NTCNet)

- NTCNet is parameterized by $\theta = \eta$.
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- NTCNet$((\boldsymbol{s}, \boldsymbol{l})\,|\eta) = (\boldsymbol{x}_1)_1$ denotes the result of *neural trace checking* of the satisfaction relation between π and ϕ.

Neural Modeling of Trace Checking

Theorem 1 (Correctness of Neural Trace Checking)

Let ϕ be an LTL formula and η its LTL encoding. For any trace π, $\texttt{NTCNet}(\textsc{Tensorize}(\pi)|\eta) = 1$ if and only if $\pi \models \phi$.

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- Important step: the computation of $(\boldsymbol{u}_1)_j^{(|\pi|)}$ suffices to check whether $\pi \models \phi_j$.
- Lemma 2 shows that $(\boldsymbol{u}_i)_j^{(t)} = 1$, if there exists a time i' where $0 \leq i' - i < t$ such that $\pi_{i'} \models \phi_k$ and $\pi_{i''} \models \phi_{j+1}$ for all $i'' \in [i, i')$.

Neural Modeling of Trace Checking

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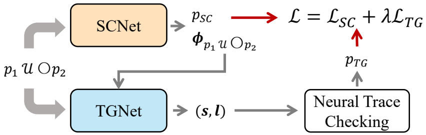
- Important step: the computation of $(\boldsymbol{u}_1)_j^{(|\pi|)}$ suffices to check whether $\pi \models \phi_j$.
- Lemma 2 shows that $(\boldsymbol{u}_i)_j^{(t)} = 1$, if there exists a time i' where $0 \leq i' - i < t$ such that $\pi_{i'} \models \phi_k$ and $\pi_{i''} \models \phi_{j+1}$ for all $i'' \in [i, i')$.
- Lemma 3 shows that $\boldsymbol{u}$ is monotonically increasing with time points.
- NTCNet is *differentiable*.

Overview of VSCNet

Train VSCNet

- SCNet extracts the formula representation ϕ and predicts the satisfiable probability p_{SC}.
- TGNet exploits ϕ to generate a tensorized trace $(\boldsymbol{s}, \boldsymbol{l})$.
- jointly training of SCNet and TGNet with NTCNet:

$$\mathcal{L} = \mathcal{L}_{SC} + \lambda \mathcal{L}_{TG} \qquad (5)$$



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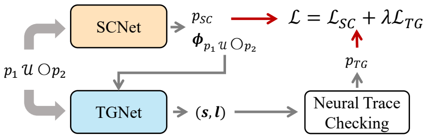

Figure 3: The overview of training VSCNet.

Apply VSCNet to solve SAT-and-GET

Algorithm 3: Solving the SAT-and-GET problem

Input: An LTL formula ϕ, and two threshold hyperparameters β_{T} for finding tensorized traces and β_{SAT} for determining the satisfiability of ϕ.

Output: Whether ϕ is satisfiable or not and a satisfiable trace π of ϕ if it is satisfiable.

$(p_{SC}, \boldsymbol{\phi}) \leftarrow \mathtt{SCNet}(\phi)$
$(\boldsymbol{s}, \boldsymbol{l}) \leftarrow \mathtt{TGNet}(\boldsymbol{\phi})$
$\pi \leftarrow \textsc{round}((\boldsymbol{s}, \boldsymbol{l}), \beta_{\mathrm{T}})$
if $\pi \models \phi$ *or* $p_{SC} > \beta_{SAT}$ **then**
  return *SAT*, π
else
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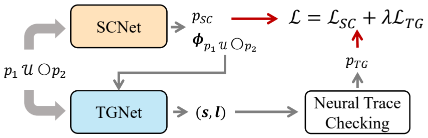

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Apply VSCNet to solve SAT-and-GET

1. obtain the p_{SC} and a *soften* tensorized trace $(\boldsymbol{s}, \boldsymbol{l})$

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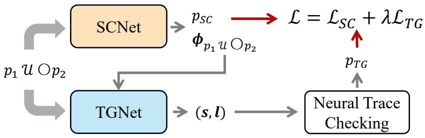

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Apply VSCNet to solve SAT-and-GET

1. obtain the p_{SC} and a *soften* tensorized trace $(\boldsymbol{s}, \boldsymbol{l})$
2. round probabilistic $(\boldsymbol{s}, \boldsymbol{l})$ to π

Algorithm 3: Solving the SAT-and-GET problem

Input: An LTL formula ϕ, and two threshold hyperparameters $\beta_{\top}$ for finding tensorized traces and β_{SAT} for determining the satisfiability of ϕ.

Output: Whether ϕ is satisfiable or not and a satisfiable trace π of ϕ if it is satisfiable.

```
(p_SC, φ) ← SCNet(φ)
(s, l) ← TGNet(φ)
π ← ROUND((s, l), β_⊤)
if π ⊨ φ or p_SC > β_SAT then
    return SAT, π
else
    return UNSAT
```

```
π[i] ← ∅ for each (s)_i
for each (s)_{i,j} ∈ s do
    if (s)_{i,j} > β_⊤ then
        π[i] ← π[i] ∪ {p_j}
k ← arg max_i((l)_i)
π ← π[1], ..., (π[k], ..., π[m])^ω
```

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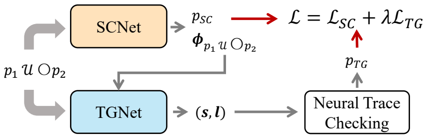

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Apply VSCNet to solve SAT-and-GET

1. obtain the p_{SC} and a *soften* tensorized trace $(\boldsymbol{s}, \boldsymbol{l})$
2. round probabilistic $(\boldsymbol{s}, \boldsymbol{l})$ to π
3. check whether $\pi \models \phi$ by a classical trace checking algorithm [22]

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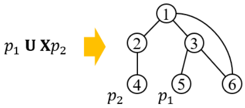
SCNet and TGNet



- construct the one-step unfolded graph (OSUG)[20]

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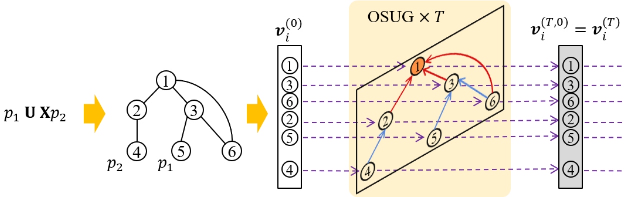

$$v_g^{(T)} = \text{MEAN}(v_1^{(T)}, \dots, v_6^{(T)})$$

$$p_{SC} = \text{MLP}(v_g^{(T)})$$

- construct the one-step unfolded graph (OSUG) [20]
- compute the graph embedding $v_g^{(T)} \in \mathbb{R}^{d_h}$ and vertex embeddings $v_i^{(T)} \in \mathbb{R}^{d_h}$ using a 10-layer OSUG-based extractor

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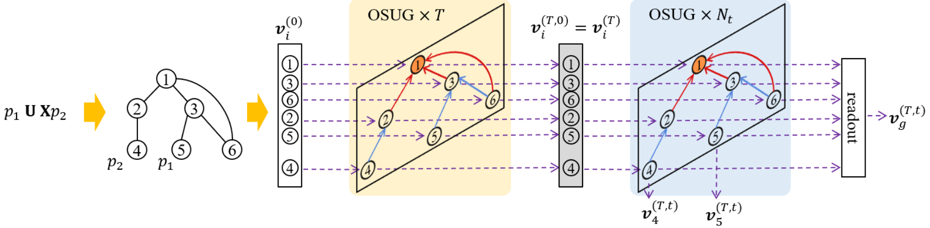

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$$\boldsymbol{l} = \mathrm{softmax}([x_1, \dots, x_{N_t}]),$$

$$\text{where } x_i = \mathrm{MLP}(\boldsymbol{v}_g^{(T,i)}) \text{ for } i \in [1, N_t]$$

$$(\boldsymbol{s})_{i,j} = \left(\mathrm{softmax}\left(\mathrm{MLP}(\boldsymbol{v}_j^{(T,i)})\right)\right)_2$$

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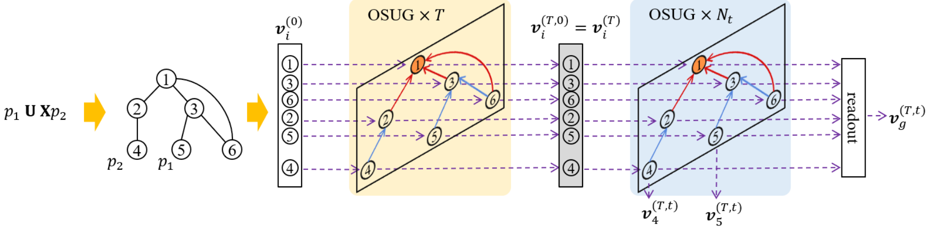

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- iteratively generate a trace state by state

Highlights of `VSCNet`

`VSCNet` ensures the soundness in $1/2$ of cases.

- Given an LTL formula ϕ, `SCNet` returns a satisfiability conclusion and `TGNet` returns a trace π.
- $\pi \models \phi$ and `SCNet` answers that ϕ is *satisfiable*: π confirms the answer of `SCNet`.
- $\pi \models \phi$ and `SCNet` answers that ϕ is *unsatisfiable*: π is able to correct the answer of `SCNet`.

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`VSCNet` are able to check the satisfiability of an LTL formula in polynomial time.

- The inference time of both `SCNet` and `TGNet` is polynomial in terms of the size of the input formula.
- Although the inference time does not include the training time, model training can be done offline and once.

Content

Competitors and Datasets

Competitors: a random approach, two logic-based approaches, and seven neural network-based approaches

Table 2: Overview of Competitors

Approach	SC	TG
random	✓	✓
Aalta [14,17]	✓	✓
nuXmv [3]	✓	✓
TreeNN-inv [19]	✓	×
TreeNN-MP [19]	✓	×
TreeNN-con [19]	✓	×
Transformer-SC [19]	✓	×
Transformer-TG [10]	×	✓
Transformer	✓	✓
OSUG [20]	✓	✓
VSCNet-T (our)	✓	✓
VSCNet-G (our)	✓	✓

Competitors and Datasets

Competitors: a random approach, two logic-based approaches, and seven neural network-based approaches
Datasets: *SPOT* and large-scale datasets [17,19]

- *LTL-as-LTL$_f$* [25]: some coming from industrial scenes
- *LTL$_f$-Specific* [4,12]: generated by common patterns
- *NASA-Boeing* [2,9]: real-world specifications
- *DECLARE* [7]: widely used in the business process management

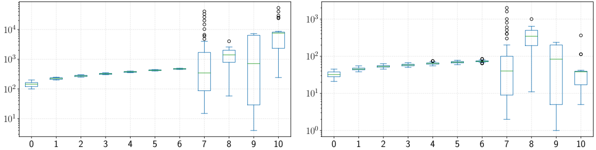

Figure 4: The boxplots of the formula size and the number of atomic propositions

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`Transformer-TG` [10]	×	✓
`Transformer`	✓	✓
`OSUG` [20]	✓	✓
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Setups

Training and testing

- train all neural networks on the training set of *SPOT*-$[100, 200)$ with hyperparameters optimized on the validation set of *SPOT*-$[100, 200)$
- *directly* evaluate all neural networks on the test set of *SPOT*-$[100, 200)$ to demonstrate their performance on in-distribution datasets
- *directly* evaluate all neural networks on the *SPOT* test sets with larger formulae and on the large-scale datasets to test the generalizability of neural networks on out-of-distribution datasets

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Metrics

- LTL satisfiability checking: accuracy (acc.), precision (pre.), recall (rec.), and F1 score
- semantic accuracy (sacc.)[10], where D is a set of satisfiable formulae and π is the trace generated by approaches:

$$\text{sacc.} = \frac{|\{\phi \in D | \pi \models \phi\}|}{|D|}, \tag{6}$$

Comparison on Synthetic Datasets

Table 3: Evaluation results on the test set of *SPOT*-$[100, 200)$

approach	acc.	pre.	rec.	F1	sacc.	time
random	50.01	50.01	49.28	49.64	51.88	0
Aalta	100.00	100.00	100.00	100.00	100.00	12,784,302
nuXmv	100.00	100.00	100.00	100.00	100.00	6,848
TreeNN-inv	93.27	97.75	88.58	92.94	-	434
TreeNN-MP	86.54	90.74	81.40	85.82	-	455
TreeNN-con	89.38	95.96	82.22	88.56	-	459
Transformer-SC	72.56	74.24	69.10	71.58	-	**104**
Transformer-TG	-	-	-	-	47.67	5,484
Transformer	59.30	62.79	45.64	52.86	45.09	10,601
OSUG	98.47	99.15	97.79	98.46	55.22	2,816
VSCNet-T (our)	93.45	97.47	89.22	93.16	71.86	364
VSCNet-G (our)	**99.15**	**99.47**	**98.83**	**99.15**	**91.01**	**156**

- On in-distribution datasets, compared with neural network-based approaches, VSCNet achieves SOTA performance on SAT-and-GET.

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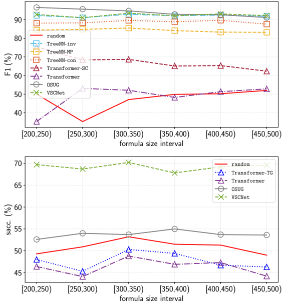

Figure 5: Evaluation results on other *SPOT* test sets.

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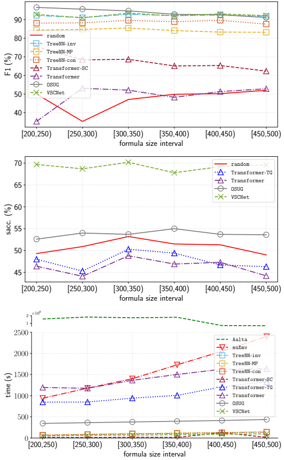
- Good generalizability of VSCNet against different formula sizes.
- VSCNet is significantly more efficient than logic-based SOTA approaches while achieving comparable performance.



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Comparison on Large-Scale Datasets

Table 4: Evaluation results on the large-scale datasets.

approach	*LTL-as-LTL$_f$* acc.	F1	sacc.	time	*LTL$_f$-Specific* acc.	F1	sacc.	time	*NASA-Boeing* acc.	F1	sacc.	time	*DECLARE* acc.	F1	sacc.	time
random	50.75	65.46	54.96	0	51.59	47.88	92.96	0	62.90	77.23	24.19	0	53.21	69.46	0.00	0
`Aalta`	100.00	100.00	100.00	122,682	100.00	100.00	100.00	36,027	100.00	100.00	100.00	3,601	100.00	100.00	100.00	61,220
`nuXmv`	100.00	100.00	100.00	6,804	100.00	100.00	100.00	766	100.00	100.00	100.00	41	100.00	100.00	100.00	3,743
`TreeNN-inv`	88.05	93.53	-	453	**98.53**	**98.37**	-	305	83.87	91.23	-	33	78.38	87.88	-	176
`TreeNN-MP`	82.18	90.03	-	480	96.29	95.98	-	234	70.97	83.02	-	25	95.50	97.70	-	129
`TreeNN-con`	84.61	91.10	-	475	98.35	98.11	-	230	51.61	68.09	-	25	0.00	0.00	-	129
`Transformer-SC`	72.99	82.64	-	**161**	83.12	75.45	-	**55**	71.05	83.08	-	**3**	0.00	0.00	-	**3**
`OSUG`	8.62	15.87	55.26	11,444	55.71	71.55	93.09	5,173	3.23	6.25	**46.77**	341	10.09	18.33	0.00	15,730
`VSCNet-T` (our)	88.35	**93.71**	**81.46**	368	90.76	90.56	83.80	177	**90.32**	**94.92**	**46.77**	21	95.41	97.65	0.00	94
`VSCNet-G` (our)	**88.85**	94.03	51.68	**91**	45.94	61.66	**93.36**	**25**	83.87	91.23	43.55	**3**	**100.00**	**100.00**	0.00	**6**

- All neural network-based approaches exhibit varying degrees of performance fluctuations on the large-scale datasets.

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- `VSCNet` is comparable with the logic-based approaches in LTL satisfiability checking.
- `VSCNet` is significantly more efficient than the logic-based approaches.

Ablation Study

Table 5: Ablation results of VSCNet-T and its variants on all *SPOT* test sets.

variants	[100, 200)			[200, 250)			[250, 300)			[300, 350)			[350, 400)			[400, 450)			[450, 500)		
	acc.	F1	sacc.	acc.	F1	sacc.	acc.	F1	sacc.	acc.	F1	sacc.	acc.	F1	sacc.	acc.	F1	sacc.	acc.	F1	sacc.
VSCNet-T	93.45	93.16	**71.86**	93.10	92.78	**69.70**	91.60	91.05	**68.70**	93.80	93.47	**70.20**	92.55	92.08	**67.80**	**93.45**	**93.09**	**69.20**	**92.60**	**92.16**	**69.60**
- w/o SS	77.75	71.39	55.51	75.95	68.33	51.90	77.00	70.13	54.00	76.50	69.28	53.00	77.20	70.47	54.40	75.55	67.64	51.10	75.80	68.07	51.60
- w STS	93.66	**93.37**	54.53	**93.15**	**92.81**	51.30	**92.00**	**91.50**	52.10	**94.35**	**94.07**	53.60	**93.30**	**92.90**	52.30	93.35	92.97	51.10	92.45	91.97	48.60
- w/o NTC & w STS	**93.74**	93.44	55.10	92.85	92.44	52.30	91.85	91.28	53.60	93.60	93.22	54.20	**93.30**	92.87	54.60	92.85	92.41	53.70	92.55	92.04	53.90

- VSCNet-T vs. VSCNet-T w STS:
  - The supervision of satisfiable traces is harmful to generating satisfiable traces.
- VSCNet-T vs. VSCNet-T w/o NTC & w STS:
  - NTCNet guides trace generation better than directly using a satisfiable trace for supervision.

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	acc.	F1	sacc.	acc.	F1	sacc.	acc.	F1	sacc.	acc.	F1	sacc.	acc.	F1	sacc.	acc.	F1	sacc.	acc.	F1	sacc.
VSCNet-T	93.45	93.16	**71.86**	93.10	92.78	**69.70**	91.60	91.05	**68.70**	93.80	93.47	**70.20**	92.55	92.08	**67.80**	**93.45**	**93.09**	**69.20**	**92.60**	**92.16**	**69.60**
- w/o SS	77.75	71.39	55.51	75.95	68.33	51.90	77.00	70.13	54.00	76.50	69.28	53.00	77.20	70.47	54.40	75.55	67.64	51.10	75.80	68.07	51.60
- w STS	93.66	**93.37**	54.53	**93.15**	**92.81**	51.30	**92.00**	**91.50**	52.10	**94.35**	**94.07**	53.60	**93.30**	**92.90**	52.30	93.35	92.97	51.10	92.45	91.97	48.60
- w/o NTC & w STS	**93.74**	93.44	55.10	92.85	92.44	52.30	91.85	91.28	53.60	93.60	93.22	54.20	**93.30**	92.87	54.60	92.85	92.41	53.70	92.55	92.04	53.90

- VSCNet-T vs. VSCNet-T w STS:
  - The supervision of satisfiable traces is harmful to generating satisfiable traces.
- VSCNet-T vs. VSCNet-T w/o NTC & w STS:
  - NTCNet guides trace generation better than directly using a satisfiable trace for supervision.
- VSCNet-T vs. VSCNet-T w/o SS:
  - The joint learning of the module for trace generation and the module for satisfiability checking is mutually reinforcing.
- The ablation study on VSCNet-G exhibits similar results.

Content

Conclusion and Discussion

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1. Bridge between LTL trace checking and neural trace checking.
2. Design a joint approach of LTL satisfiability checking and trace generation, which can be realized by a neural network trainable with classical gradient descent.
3. Theoretically prove the correctness of the bridge and empirically confirmed the effectiveness of the joint approach.

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Discussion

1. Out-of-distribution datasets: plan to explore parameter-efficient fine-tuning to improve the generalizability in future work.
2. Fixed trace size: in practice, it may be sufficient to set N_t to a small constant for most cases and our approach also works for every LTL formula that has satisfiable traces whose sizes are smaller than N_t.
3. Verifiable unsatisfiable results: future work will also study how to explore neural network technology to generate unsatisfiable cores.

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