Learning Temporal Logic Formulas from Time-series Data

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Joint work with L. Bortolussi, E. Medvet, J. V. Deshmukh, S. Silvetti, F. Pigozzi, P. Indri, S. Mohammadinejad, E. Bartocci, and A. Bartoli, Gaia Saveri, Jan Kretisky

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Context and Problem





Need of human-interpretable models

- Starter: Formal specification
 - Signal Temporal Logic (STL)
 - Spatio-Temporal Reach and Escape Logic (STREL)
- Main: Temporal Logic requirement mining
 - STL classifier (supervised and semi-supervised learning)
 - STREL-based clustering (unsupervised learning)
- Dessert: related and ongoing work
 - Fruit Salad
 - Some heavy cake

Formal Specification

Signal Temporal Logic (STL)

STL extends MITL by having signal predicates over real values as atomic formulas:

STL Syntax





 $\varphi \coloneqq true \mid \mu \mid \neg \varphi \mid \varphi_1 \land \varphi_2 \mid \varphi_1 \operatorname{U}_I \varphi_2$

[[]O. Maler, D. Nickovic:, Monitoring Temporal Properties of Continuous Signals. FORMAT 2004]

Monitoring STL



Monitoring STL



Parametric Signal Temporal Logic (PSTL)

Definition (PSTL syntax)

$$\phi \coloneqq (x_i \bowtie \pi) | \neg \varphi | \varphi_1 \land \varphi_2 | \varphi_1 \mathcal{U}_{[\tau_1, \tau_2]} \varphi_2$$

with $\bowtie \in \{>, \leq\}$

- π is **threshold** parameter
- τ_1 , τ_2 are **temporal** parameters
- $\mathbb{K} = (\mathcal{T} \times \mathcal{C})$ be the **parameter space**
- $\theta \in \mathbb{K}$ is a parameter configuration

e.g.,
$$\phi = \mathcal{F}_{[a,b]}(x_i > k), \theta = (0, 2, 3.5)$$
 then $\phi_{\theta} = \mathcal{F}_{[0,2]}(x_i > 3.5).$

Spatio-Temporal Reach and Escape Logic (STREL):

STREL is extension of STL with two spatial operators: Reach and Escape It considers a discrete space described as a weighted (direct) graph



 Somewhere, Everywhere and Surround operators can be derived from Reach and Escape

[Nenzi et al , A Logic for Monitoring Dynamic Networks of Spatially-distributed Cyber-Physical Systems. LMCS, 2022] [Nenzi et al, Monitoring spatio-temporal properties, invited tutorial., 2020]

Reach operator (\mathcal{R})



$$\varphi = yellow R_{[1,4]}green$$

$$l_3 \text{ satisfies } \varphi$$
$$path = l_3, l_{13}l_{14}l_{17}l_{35}$$

$$l_4$$
 does not satisfy φ

Everywhere operator (□)



$$\varphi = \Box_{[2,3]} \frac{\text{yellow}}{\text{yellow}}$$

$$l_1$$
 satisfies $arphi$

$$l_2$$
 does not satisfy φ

Monitoring STREL

INPUTS



Statistical Model Checking



TL Requirement mining

Temporal Logic requirement mining



Source: https://jdeshmukh.github.io/research.html

STL Classifiers ((Semi-)Supervised Learning)



Goal: learning a specification/ classifier as a temporal logic formula to discriminate as much as possible between regular and anomalous behaviours.

We want to learn both the structure and the parameters of the formula

STL Classifier: Problem Statement

We want a way to search in the space of STL formulae considering training data X_{learn}

Supervised two-class classification problem

Training data set: two sets

- regular X_{learn}^+
- anomalous X_{learn}^{-}



Find the best ϕ that better separates the two sets.

Semi-supervised one-class classification prob

Training data set: one set

• regular X_{learn}^+



Find the "tight" ϕ that is satisfied by the set

STL classifier (supervised): ROGE

- Bi-level algorithm:
 - learning formula structure via Genetic Programming (GP)
 - learn parameters of the formula using by Bayesian Optimisation
- A **fitness function** *f* measures the quality of candidate solutions and depends on the kind of problem at hand (two-classes, one-class)

$$f(\varphi; X_{\text{learn}}^+, X_{\text{learn}}^-) = -\frac{\mathbb{E}_{X_{\text{learn}}^+}(\rho_{\varphi}) - \mathbb{E}_{X_{\text{learn}}^-}(\rho_{\varphi})}{\sigma_{\varphi, X_{\text{learn}}^+} + \sigma_{\varphi, X_{\text{learn}}^-}}$$

Require: $\mathcal{D}_p, \mathcal{D}_n, \mathbb{K}, Ne, Ng, \alpha, s$

- 1: $gen \leftarrow GENERATEINITIALFORMULAE(Ne, s)$
- 2: $gen_{\Theta} \leftarrow \text{LEARNINGPARAMETERS}(gen, G, \mathbb{K})$
- 3: **for** i = 1 ... Ng **do**
- 4: $subg_{\Theta} \leftarrow SAMPLE(gen_{\Theta}, F)$
- 5: *newg* \leftarrow **EVOLVE**(*subg* $_{\Theta}, \alpha$)
- 6: $newg_{\Theta} \leftarrow LEARNINGPARAMETERS(newg, G, \mathbb{K})$
- 7: $gen_{\Theta} \leftarrow \text{SAMPLE}(newg_{\Theta} \cup gen_{\Theta}, F)$
- 8: end for
- 9: return gen_{Θ}

[L. Nenzi, S. Silvetti, E. Bartocci, L. Bortolussi: A Robust Genetic Algorithm for Learning Temporal Specifications from Data. QEST 2018]

Crossover Operator



Mutation Operator



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$$f(\varphi; X_{\text{learn}}^+, X_{\text{learn}}^-) = -\frac{\mu_{\varphi, X_{\text{learn}}^+} - \mu_{\varphi, X_{\text{learn}}^-}}{\sigma_{\varphi, X_{\text{learn}}^+} + \sigma_{\varphi, X_{\text{learn}}^-}}$$

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Results: Train Cruise



 $(F_{[22,40]}(vel > 24.48)) \land (F_{[46,49]}(19.00 < vel < 26.44))$

Results: Maritime Surveillance

Synthetic dataset of naval surveillance of 2-dimensional coordinates traces of vessels behaviours.



 $((x_2 > 22.46) \mathcal{U}_{[49,287]} (x_1 \le 31.65))$

- Initial population designed "by hand"
- The learning parameter algorithm can be slow (depending on the size parameter space)

STL Classifier: Context Free Grammar

$$\langle \text{formula} \rangle ::= \langle \text{formula}_1 \rangle \\ \langle \text{formula}_i \rangle ::= \begin{cases} \langle \text{atom} \rangle \mid \langle \text{logic}_i \rangle \mid \langle \text{temp}_i \rangle & \text{if } i < i_{\max} \\ \langle \text{atom} \rangle \mid \langle \text{logic}_i \rangle & \text{otherwise} \end{cases} \\ \langle \logic_i \rangle ::= \neg \langle \text{formula}_i \rangle \mid \langle \text{formula}_i \rangle \wedge \langle \text{formula}_i \rangle \\ \langle \text{temp}_i \rangle ::= \langle \text{formula}_{i+1} \rangle U_{\langle \text{interval} \rangle} \langle \text{formula}_{i+1} \rangle \mid \\ G_{\langle \text{interval} \rangle} \langle \text{formula}_{i+1} \rangle \mid \\ F_{\langle \text{interval} \rangle} \langle \text{formula}_{i+1} \rangle \mid \\ \langle \text{interval} \rangle ::= [\langle \text{num} \rangle, \langle \text{num} \rangle] \\ \langle \text{atom} \rangle ::= \langle \text{attr} \rangle \langle \text{comp} \rangle 0. \langle \text{num} \rangle \\ \langle \text{attr} \rangle ::= a_1 \mid a_2 \mid \dots \mid a_{|A|} \\ \langle \text{comp} \rangle ::= \langle \mid \rangle \\ \langle \text{num} \rangle ::= \langle \text{digit} \rangle \langle \text{digit} \rangle \\ \langle \text{digit} \rangle ::= 0 \mid 1 \mid 2 \mid 3 \mid 4 \mid 5 \mid 6 \mid 7 \mid 8 \mid 9 \end{cases}$$

[F. Pigozzi, E. Medvet, L. Nenzi. Mining Road Traffic Rules with Signal Temporal Logic and Grammar-Based Genetic Programming, Applied Sciences, 2022] [F. Pigozzi, L. Nenzi., E. Medvet, BUSTLE: a Versatile Tool for the Evolutionary Learning of STL Specifications from Data (second revision on Evolutionary Computation]

STL classifier: Building the population

• Candidate formulas are represented as derivation trees of a grammar



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Results

regular

anomalous

0

45 -

40 35 ♀₃₀

> 25 20

> > 0

10 20

0.8

0.6 × 0.4

0.2

0

ż

	Dataset	Algorithm	FNR FPR Acc	Time
egular nomalous	Linear	Random	0.20 0.20 0.80	11
		BUSTLE (single-level)	0.00 0.00 1.00	15
		BUSTLE (bi-level)	0.00 0.00 1.00	112
		Nenzi et al. (2018)	0.00 0.00 1.00	113
4 6 8 10 12 14 sample		Mohammadinejad et al. (2020b)	N/A N/A 0.98	39
regular anomalous 20 40 60 80 100	Train	Random	0.55 0.53 0.46	31
		BUSTLE (single-level)	0.03 0.05 0.96	26
		BUSTLE (bi-level)	0.00 0.03 0.98	523
		Nenzi et al. (2018)	0.10 0.00 0.95	576
		Mohammadinejad et al. (2020b)	N/A N/A 0.98	32
		Random	$0.52 \ \ 0.50 \ \ 0.49$	84
anomaious regular	Maritime	BUSTLE (single-level)	0.00 0.00 1.00	109
		BUSTLE (bi-level)	0.00 0.00 1.00	1477
		Nenzi et al. (2018)	0.00 0.00 1.00	1599
		Mohammadinejad et al. (2020b)	0.05 0.02 0.96	73
20 30 40 50 60 70 80 x1		Bombara and Belta (2021)	N/A N/A 0.98	140

STL Classifier: Fitness Function for the one-class problem



Training data set: one set

• regular X_{learn}^+

Fitness, two high level requirements:

- 1. Tight formulas should be preferred
- 2. Formulas that lead to few false anomalies should be preferred

$$f(\varphi; X_{\text{learn}}^+) = \alpha \frac{1}{|X_{\text{learn}}^+|} \left| \{ \boldsymbol{x} \in X_{\text{learn}}^+ : \boldsymbol{x} \not\models \varphi \} \right| + \frac{1}{\sigma'_{\varphi, X_{\text{learn}}^+} |X_{\text{learn}}^+|} \sum_{\boldsymbol{x} \in X_{\text{learn}}^+} |\rho(\varphi, \boldsymbol{x})|$$

Results

		Two-classes				One-class					
	Variant	FNR	FPR	Acc	Time	c	FNR	FPR	Acc	Time	С
Lin.	Random BUSTLE (single-l.) BUSTLE (bi-l.)	$0.20 \\ 0.00 \\ 0.00$	$0.20 \\ 0.00 \\ 0.00$	$0.80 \\ 1.00 \\ 1.00$	$11 \\ 15 \\ 112$	$8.0 \\ 9.5 \\ 12.5$	$0.98 \\ 0.45 \\ 0.40$	$0.20 \\ 0.00 \\ 0.00$	$0.41 \\ 0.77 \\ 0.80$	$10 \\ 11 \\ 145$	8.0 11.0 11.0
Train	Random BUSTLE (single-l.) BUSTLE (bi-l.)	$0.55 \\ 0.03 \\ 0.00$	$0.53 \\ 0.05 \\ 0.03$	$0.46 \\ 0.96 \\ 0.98$	$31 \\ 26 \\ 523$	$8.0 \\ 12.0 \\ 13.0$	$0.81 \\ 0.30 \\ 0.18$	$0.15 \\ 0.12 \\ 0.08$	$0.52 \\ 0.79 \\ 0.87$	$18 \\ 25 \\ 438$	$8.0 \\ 11.0 \\ 13.5$
Marit.	Random BUSTLE (single-l.) BUSTLE (bi-l.)	$0.52 \\ 0.00 \\ 0.00$	$0.50 \\ 0.00 \\ 0.00$	$0.49 \\ 1.00 \\ 1.00$	$84 \\ 109 \\ 1477$	$8.0 \\ 9.5 \\ 9.0$	$0.77 \\ 0.15 \\ 0.38$	$0.21 \\ 0.49 \\ 0.52$	$0.51 \\ 0.68 \\ 0.55$	73 72 2008	$8.0 \\ 9.5 \\ 12.0$

Results



Limitations:

- There may be several good classifiers
- Finding the best classifier might be unfeasible
- There may not exist a single, good classifier

A one-shot algorithm

An evolutionary algorithm that learns an ensemble of solutions in a single run

- Population update:
 - Divide population in groups, one for each variable
 - The fittest formula of each group goes to next generation (elitism)
 - The remaining offspring is obtained reproducing the individuals
- Solutions update. If some individuals solve the problem (f < ϵ), consider their groups:
 - Remove from the population the individuals in these groups (extinction)
 - Add them to the solutions ensemble
 - Refill the population with new individuals (random immigrants)

Stop once n_{target} variables have been solved



[Patrick Indri, Alberto Bartoli, Eric Medvet, Laura Nenzi: One-Shot Learning of Ensembles of Temporal Logic Formulas for Anomaly Detection in Cyber-Physical Systems. EuroGP 2022: 34-50]

- For "online" anomaly detection
- using Past STL
- a single trajectory *x*, with several variables (> 50)
- x is divided as $x_{train}^+, x_{test}^+, x_{test}^-$
- Sensor readings are numerical variables, whilst actuator readings are ternary non-ordinal variables

Results

	Multi-run G3P (30 runs)				One-shot G3P (n _{target} = 20)			
Dataset	TPR	FPR	AUC	$f_{\rm evals}$	TPR	FPR	AUC	$f_{\rm evals}$
SWaT	0.6648	0.0005	0.8321	43 243	0.6571	0.0007	0.8401	11 767
N-BaloT-1	0.9981	0.0000	0.9990	47 152	0.8952	0.0011	0.9475	3297
N-BaloT-2	0.9996	0.0016	0.9989	355 696	1.0000	0.0422	0.9998	5732
N-BaloT-3	0.9949	0.0000	0.9974	51979	0.9596	0.0076	0.9739	5965
N-BaloT-4	0.0000	0.0002	0.4998	298 158	0.9272	0.0025	0.9632	35 811
N-BaloT-5	0.6152	0.0012	0.8073	156 033	0.7492	0.0010	0.8742	7898
N-BaloT-6	0.7192	0.0011	0.8594	371 358	0.6807	0.0023	0.8387	12 235
N-BaloT-7	0.7070	0.0000	0.8534	269 708	0.6896	0.0009	0.9072	16 736
N-BaloT-8	0.0000	0.0000	0.5000	1015286	0.4166	0.0027	0.7050	88 921
N-BaloT-9	0.7812	0.0005	0.8905	260 259	0.7440	0.0011	0.8702	13 696

Results

- Standard GP more than 60 % of the formulas containing a single variable.
- The one-shot algorithm produces a larger percentage of solutions with more variables, with some STL formulas containing more than 20 variables



Comparison with classical ML: it is

- competitive on SWaT
- it compares unfavourably on N-BaloT, where it reaches a perfect detection rate only on N-BaloT-2. However on N-BaloT at least one anomalous instant for each attack is correctly identified, and all attacks might thus be considered as identified.

Learning STL-based clustering (Unsupervised Learning)



Goal: clusterizing spatio-temporal data using formal logic

[Mohammadinejad et al, Mining Interpretable Spatio-temporal Logic Properties for Spatially Distributed Systems, ATVA, 2021]

Monotonic PSTREL $\varphi(p)$:

- The polarity of a parameter p is:
 - + if it is easier to satisfy φ as we increase the value of p
 - – if it is easier to satisfy φ as we decrease the value of p
- Monotonic PSTREL:
 - All parameters have either + or polarity
- Example: $\Box_{[0,d]}\varphi$
 - Polarity of d is –

Validity Domain of PSTREL $\varphi(p)$

- Given a location *l*
- A set of spatio-temporal traces *X* associated with *l*
- The set of all valuations to *p* such that each trace in *X* satisfies the STREL formula
- Boundary of the validity domain: The robustness value with respect to at least one trace in X is ≈ 0



High-level steps

- Constructing the spatial model
- Projecting each spatio-temporal trace to a tight valuation in the parameter space of a given PSTREL formula
- Clustering the trace projections throught AHC
- Learning bounding boxes for each cluster using a Decision Tree based approach
- Learning a STREL formula for each cluster
- Improving the interpretability of the learned STREL formulas



PSTREL formula: $\circ_{[0,d]} \{F_{[0,\tau]}(x > c)\}$

- We fix τ to 10 days
- Small d and large c are hot spots



0

Longitude

ak 🔷

-118 -117.8

 $\varphi_{red} = \diamond_{[0,4691.29]} \left\{ F_{[0,10]}(x \ge 3181) \right\} \lor \diamond_{[0,15000]} \left\{ F_{[0,10]}(x \ge 5612) \right\}$

BSS data from the city of Edinburgh

PSTREL formula: $\varphi(\tau, d) = G_{[0,3]}(\varphi_{wait}(\tau) \lor \varphi_{walk}(d))$ $\varphi_{wait}(\tau) = F_{[0,\tau]}(B \ge 1) \land F_{[0,\tau]}(S \ge 1),$ $\varphi_{walk}(d) = \diamond_{[0,d]}(B \ge 1) \land \diamond_{[0,d]}(S \ge 1)$



 $\varphi_{red} = \neg G_{[0,3]} (\varphi_{wait}(17.09) \lor \varphi_{walk}(2100)) \land \neg G_{[0,3]} (\varphi_{wait}(50) \lor \varphi_{walk}(1000.98))$

Traditional ML approaches



Dessert

Related Works

- Bartocci et all: Survey on mining signal temporal logic specifications. Inf. Comput., 2022
- Template-Free:
 - Bombara, G et all, A Decision Tree Approach to Data Classification Using Signal Temporal Logic. In: Proc. of HSCC, 2016
 - Bombara, G. and Belta, C. (2021). Offline and Online Learning of Signal Temporal Logic Formulae Using Decision Trees.
 - Mohammadinejad, S., Deshmukh, J. V., Puranic, A. G., Vazquez-Chanlatte, M., and Donze , A. (2020b). Interpretable classification of time-series data using efficient enumerative techniques. Proceedings of the 23rd International Conference on Hybrid Systems: Computation and Control.
 - Andrea Brunello, Dario Della Monica, Angelo Montanari, Nicola Saccomanno, Andrea Urgolo: Monitors That Learn From Failures: Pairing STL and Genetic Programming. IEEE Access 11:
- Only-positive Example:
 - S. Jha, A. Tiwari, S. A. Seshia, T. Sahai, N. Shankar. TeLEx: learning signal temporal logic from positive examples using tightness metric, Formal Methods in System Design
- Clustering
 - Marcell Vazquez-Chanlatte, Jyotirmoy V. Deshmukh, Xiaoqing Jin, Sanjit A. Seshia: Logical Clustering and Learning for Time-Series Data. CAV (1) 2017: 305-325
- Exploiting Monotonicity
 - Marcell Vazquez-Chanlatte, Shromona Ghosh, Jyotirmoy V. Deshmukh, Alberto L. Sangiovanni-Vincentelli, Sanjit A. Seshia: Time-Series Learning Using Monotonic Logical Properties. RV 2018: 389-405

The heavy cake: Can we learn formulae in a continuous space?



Main Idea: define an embedding of STL formulae in continuous space implicitly by defining a kernel for STL (semantic embedding)

Very brief overview

- Using **kernels-based method** we can construct an embeddings
- STL **kernels regression**: given $p(\psi_j | M)$ for randomly chosen formulae ψ_1, \dots, ψ_n , we predict $p(\varphi | M)$ without knowing or executing the system M
- Use Kernel PCA to reduce the dimensionality of the embedded space
- Inverting the embedding: learn invertible encodings using Graph Neural Networks (GNN)
- Combine syntax and semantic based embeddings to get invertible mappings from formulae to real vector spaces and use the framework for STL requirement mining

[Bortolussi, L., Gallo, G. M., Křetínský, J., & Nenzi, L. Learning model checking and the kernel trick for signal temporal logic on stochastic processes. In: TACAS, 2022]



Inverting the embedding

Problem with kernel embeddings: non-invertibility \rightarrow encoding-decoding architecture



Learn invertible encodings using Graph Neural Networks (GNN):

- Encode parse tree of the formula into the latent space
- Decode latent vectors to syntactic trees, ideally with the same semantic meaning of the input formula



$ ho(op, \mathbf{x}, t)$	$= +\infty$
$ ho(\mu, \mathbf{x}, t)$	$= y(\mathbf{x}(t))$ where $\mu \equiv y(\mathbf{x}(t)) \geq 0$
$ ho(eg arphi, \mathbf{x}, t)$	$= - ho(arphi, \mathbf{x}, t)$
$ ho(arphi_1 \wedge arphi_2, \mathbf{x}, t)$	$= \min(ho(arphi_1, \mathbf{x}, t), ho(arphi_2, \mathbf{x}, t))$
$ ho(arphi_1\mathcal{U}_{[a,b]}arphi_2,\mathbf{x},t)$	$= \sup_{t' \in t+[a,b]} (\min(\rho(\varphi_2,\mathbf{x},t'),\inf_{t'' \in [t,t')}(\rho(\varphi_1,\mathbf{x},t''))))$

Learning the Parameters



$$\begin{aligned} \operatorname{Acc}(\hat{\varphi}; X_{\operatorname{test}}^{+}, X_{\operatorname{test}}^{-}; \epsilon) &= \frac{\left| \left\{ \boldsymbol{x} \in X_{\operatorname{test}}^{+} : \rho(\hat{\varphi}, \boldsymbol{x}) > \epsilon \right\} \right|}{\left| X_{\operatorname{test}}^{+} \right| + \left| X_{\operatorname{test}}^{-} \right|} + \frac{\left| \left\{ \boldsymbol{x} \in X_{\operatorname{test}}^{-} : \rho(\hat{\varphi}, \boldsymbol{x}) \le \epsilon \right\} \right|}{\left| X_{\operatorname{test}}^{+} \right| + \left| X_{\operatorname{test}}^{-} \right|} \end{aligned}$$
$$\begin{aligned} \operatorname{FPR}(\hat{\varphi}; X_{\operatorname{test}}^{-}; \epsilon) &= \frac{\left| \left\{ \boldsymbol{x} \in X_{\operatorname{test}}^{-} : \rho(\hat{\varphi}, \boldsymbol{x}) > \epsilon \right\} \right|}{\left| X_{\operatorname{test}}^{-} \right|} \\ \operatorname{FNR}(\hat{\varphi}; X_{\operatorname{test}}^{+}; \epsilon) &= \frac{\left| \left\{ \boldsymbol{x} \in X_{\operatorname{test}}^{+} : \rho(\hat{\varphi}, \boldsymbol{x}) \le \epsilon \right\} \right|}{\left| X_{\operatorname{test}}^{+} \right|} \end{aligned}$$

Results summary:

Case	L	<i>W</i>	runtime(secs)	numC	$ arphi_{cluster} $
COVID-19	235	427	813.65	3	3. $ \phi + 4$
BSS	61	91	681.78	3	2. $ \phi + 4$
Air Quality	107	60	136.02	8	5. $ \phi + 7$
Food Court	20	35	78.24	8	3. $ \phi + 4$

Experimental Results on the stochastic models



(left) Accuracy of satisfiability prediction and (right) MRE of robustness prediction

