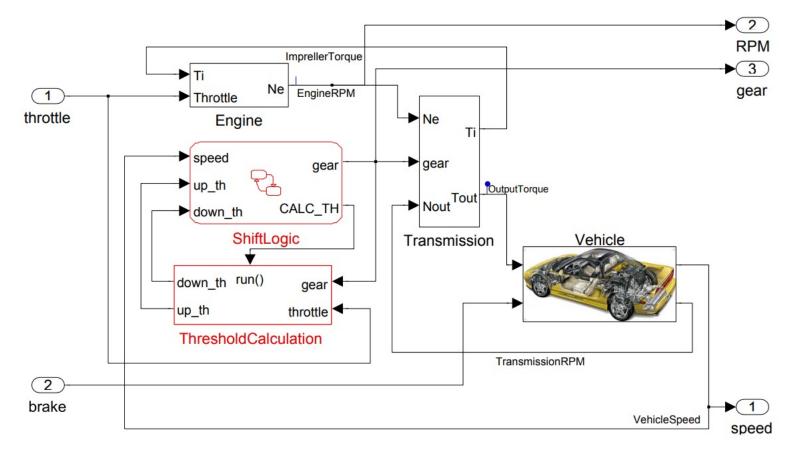
Cyber-Physical Systems

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Lecture: STL learning 2

Specification Mining



- What is the maximum speed that the vehicle can reach?
- What is the minimum d well time in a given gear ?

Parametric Signal Temporal Logic

Definition (PSTL syntax)

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

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

- π is **threshold** parameter
- $ightharpoonup au_1$, au_2 are **temporal** parameters

- $\mathbb{K} = (\mathcal{T} \times \mathcal{C})$ be the **parameter space**
- ▶ $\theta \in \mathbb{K}$ is a parameter configuration

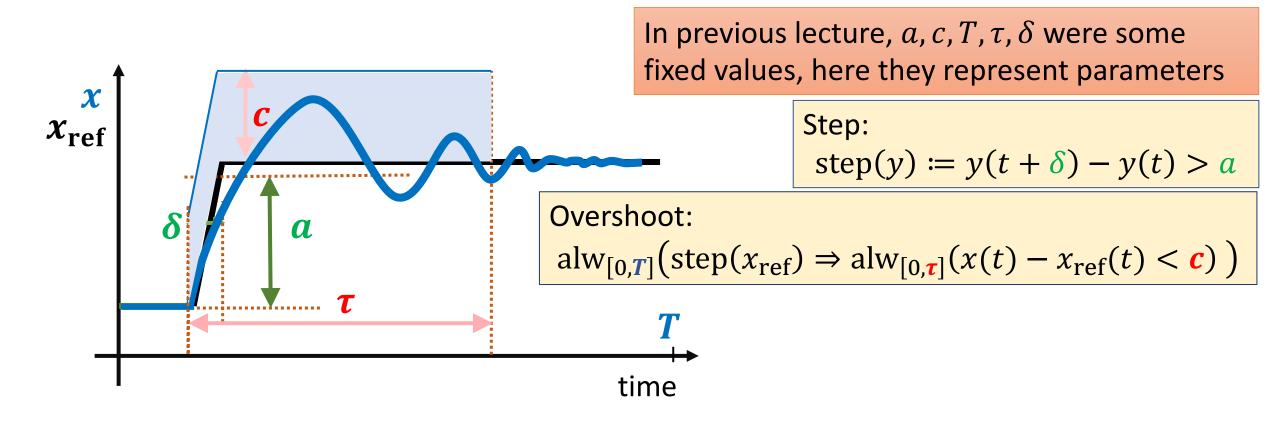
e.g.,
$$\phi = \mathcal{F}_{[a,b]}(x_i > k), \theta = (0,2,3.5)$$
 then $\phi_{\theta} = \mathcal{F}_{[0,2]}(x_i > 3.5)$.

Specification Mining

Specification Mining: Try to find values of parameters of a PSTL formula from a given model

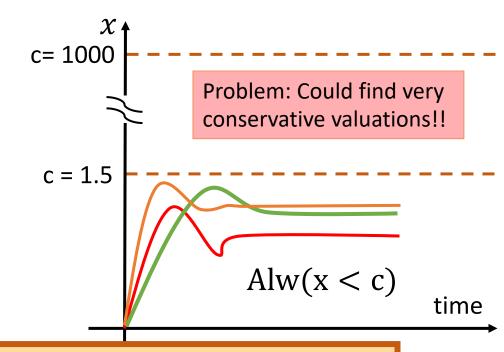
- ► Why?
 - Good to know "as-is" properties of the model
 - Finds worst-case behaviors of the model
 - Discriminates between regular and anomalous behaviours

Specification Templates using PSTL



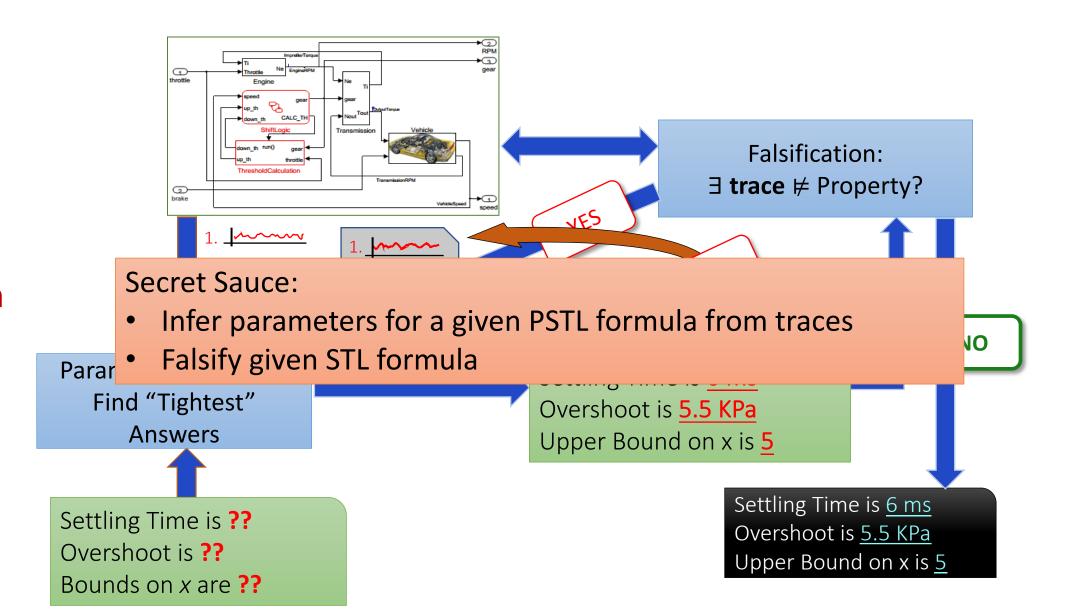
Parameter inference for PSTL

- Given:
 - ▶ PSTL formula $\varphi(\mathbf{p})$, $[\mathbf{p} = (p_1, p_2, ..., p_m)]$
 - ightharpoonup Traces x_1, \dots, x_n
- Find:
 - ▶ Valuation $\nu(\mathbf{p})$ such that: $\forall i : x_i \models \varphi(\nu(\mathbf{p}))$ δ -tight valuation
 - and $\exists i: x_i \not\models \varphi(\nu(\mathbf{p}) \pm \delta):$ i.e. small perturbation in $\nu(\mathbf{p})$ makes some trace not satisfy formula



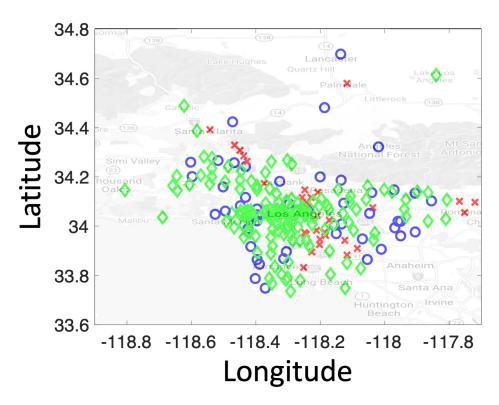
formula sat for given valuation ⇒ ∀ greater (or lesser) valuations sat

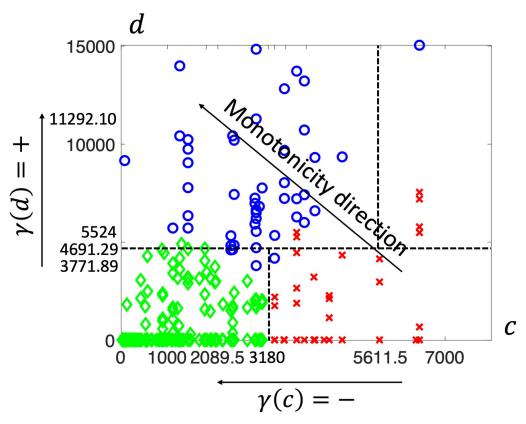
Binary search on parameter space



Specification Mining

Learning STL-based clustering (Unsupervised Learning)





Goal: clusterizing spatio-temporal data using formal logic

Motivation

► Spatially distributed systems generate a large volume of spatiotemporal data

Designers are interested in analyzing and extracting high-level structure from such data

Traditional ML for time-series clustering:

- ► Popular techniques:
 - ► Kmeans
 - Hierarchical Clustering
 - Agglomerative clustering
 - ▶ Shapelets
- ▶ Pros:
 - ► Fast
- ► Cons:
 - Based on shape-similarity
 - May lack interpretability

STL-based clustering of time-series data:

► Considerable interest in learning logical properties of temporal data using logics such as Signal Temporal Logic (STL)

Algorithms for unsupervised learning of spatio-temporal data using formal logics

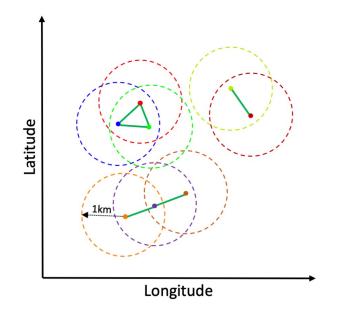
Spatial Model:



We model the spatial configuration as a weighted graph $S = \langle L, W \rangle$

L: set of locations

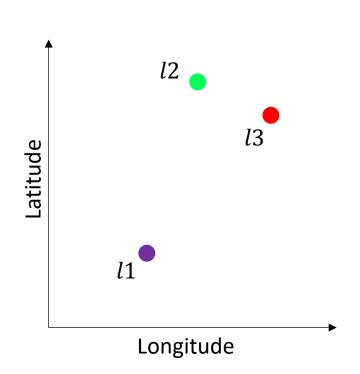
W: proximity relation between locations

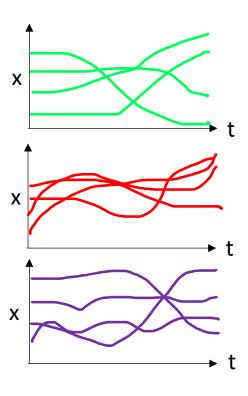


Connectivity graph
W: spatial proximity

Spatio-temporal trace:

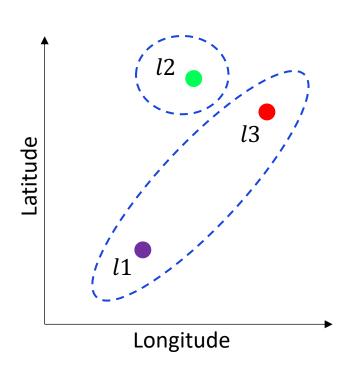
- ► Time-series data (trace/signal): a sequence of data values indexed by time stamps
- ► A spatio-temporal trace associates each location in a spatial model with a time-series trace

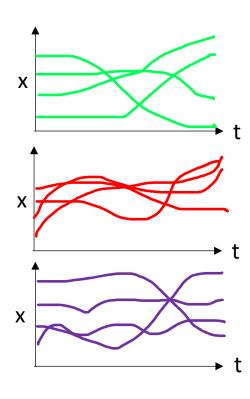




Spatio-temporal data clustering:

► It is a process of grouping data with similar spatial attributes, temporal attributes, or both





Parametric STREL (PSTREL):

► Replacing values in STREL by parameters

 $\varphi_1 R_{[0,1000]} \varphi_2$



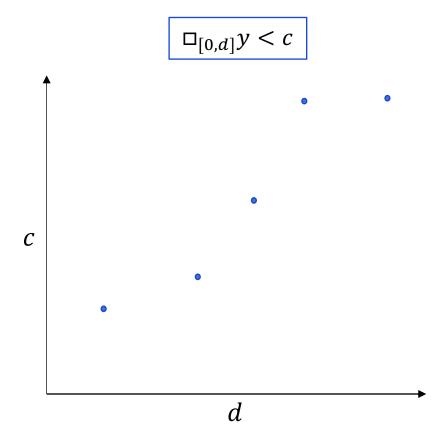
 $\varphi_1 R_{[d_1,d_2]} \varphi_2$

Monotonic PSTREL $\varphi(p)$:

- ► The polarity of a parameter p is:
 - \blacktriangleright + if it is easier to satisfy φ as we increase the value of p
 - \triangleright 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*
- lacktriangle 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
- ► Robustness means distance to satisfaction or violation

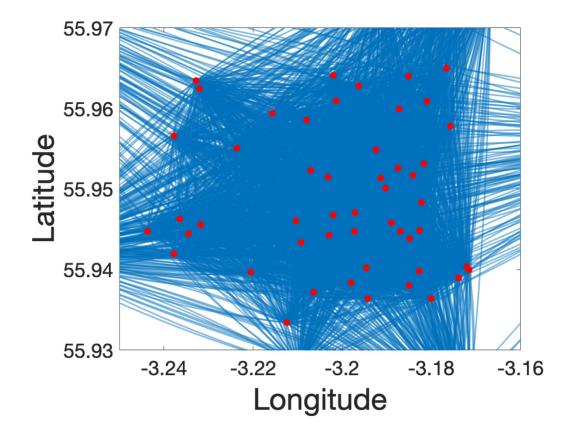


High-level steps:

- ► 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
- ► 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

Approach 1: fully connected graph

- ▶ Pros: gives the most accurate result
- ► Cons: computationally expensive

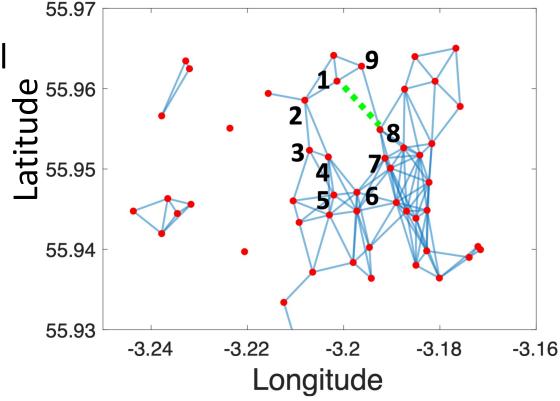


Approach 2: Connectivity graph that connects locations with distance less than a threshold

▶ Pros: lower cost

► Cons: disconnected spatial model

which affects the accuracy

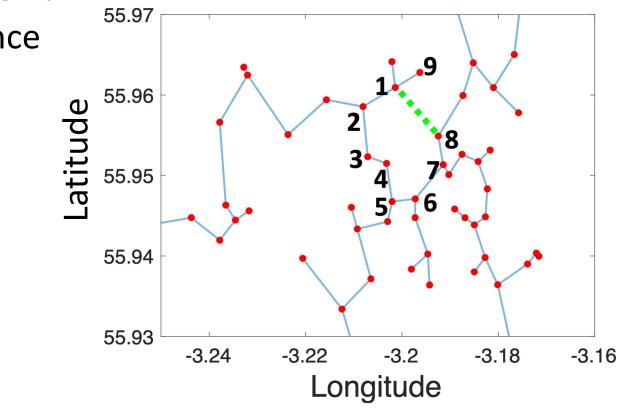


Approach 3: Minimum Spanning Tree (MST)

Pros: low cost and connected graph

► Cons: overestimation of distance

between some nodes

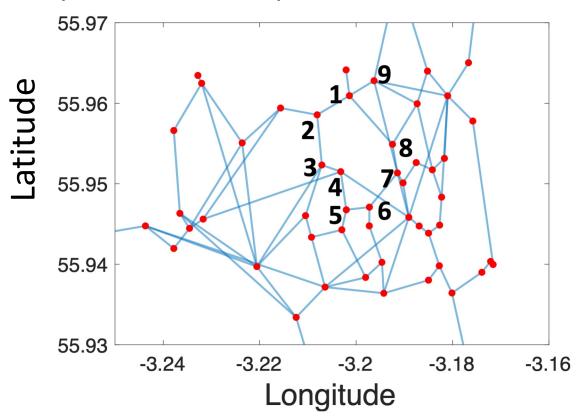


Approach 4: Enhanced Minimum Spanning Graph

Step1: create an MST

Step2: connect nodes that their shortest distance through MST is more than α times their actual distance (default $\alpha = 2$)

- ► Pros: low cost, connected graph and more accurate distance between nodes
- Cons: not as accurate as fully connected graph

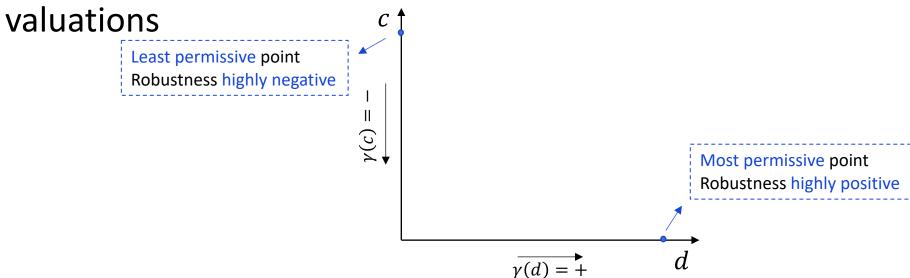


Spatio-temporal trace projection:

► The user provides a PSTREL formula

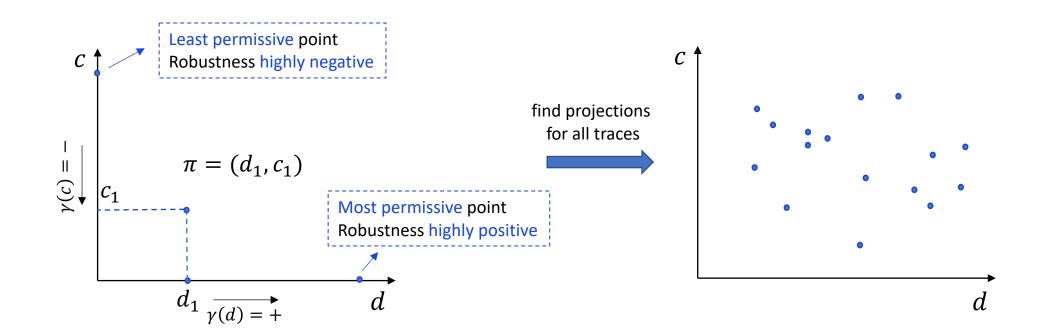
$$G_{[0,3hours]} \diamond_{[0,d]} (Bikes > c)$$

- ► The goal is to learn the tight parameter valuations for each spatiotemporal trace
- ► Tight parameter valuation is not unique, and each point on the boundary of validity domain corresponds to a tight parameter



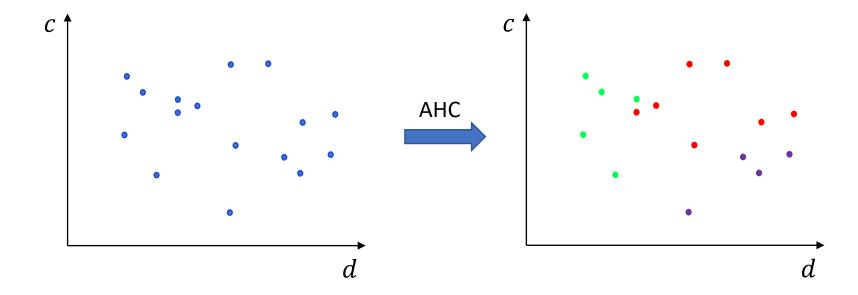
Spatio-temporal trace projection:

- We assume some ordering or priority on parameter space, e.g., $d>_p c$, provided by user
 - 1. Bisection search on d
 - 2. Bisection search on c



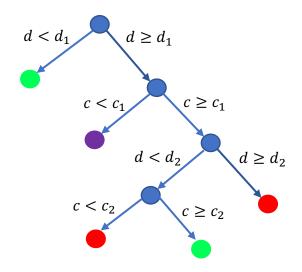
Clustering:

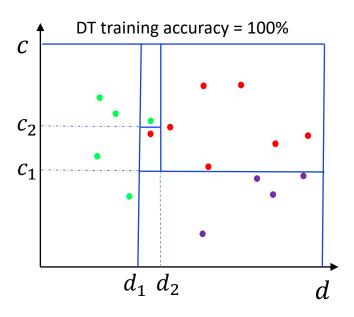
- ► The parameter valuation points serve as features for off-the-shelf clustering algorithms
- ► We use the Agglomerative Hierarchical Clustering (AHC) technique
- Number of clusters to choose:
 - ► Domain knowledge/Silhouette metric



Learning bounding boxes for each cluster:

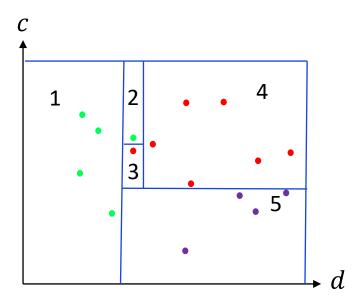
- ► We label each parameter valuation with its cluster
 - ► Labels = (green, red, purple)
- We use off-the-shelf Decision Tree (DT) algorithms to learn bounding boxes



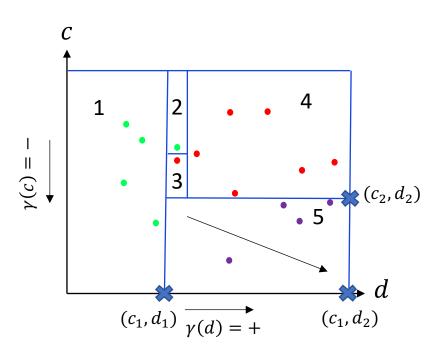


Learning a STREL Formula for each Cluster:

- $\blacktriangleright \varphi_{green} = \varphi_1 \lor \varphi_2$
- $\blacktriangleright \varphi_{red} = \varphi_3 \lor \varphi_4$
- $\blacktriangleright \varphi_{purple} = \varphi_5$



Learning a STREL Formula for each Cluster:



$$\varphi_{5} = \varphi(c_{1}, d_{2}) \land \neg \varphi(c_{1}, d_{1}) \land \neg \varphi(c_{2}, d_{2})$$

$$\varphi = G_{[0,3hours]} \diamond_{[0,d]} (Bikes > c)$$

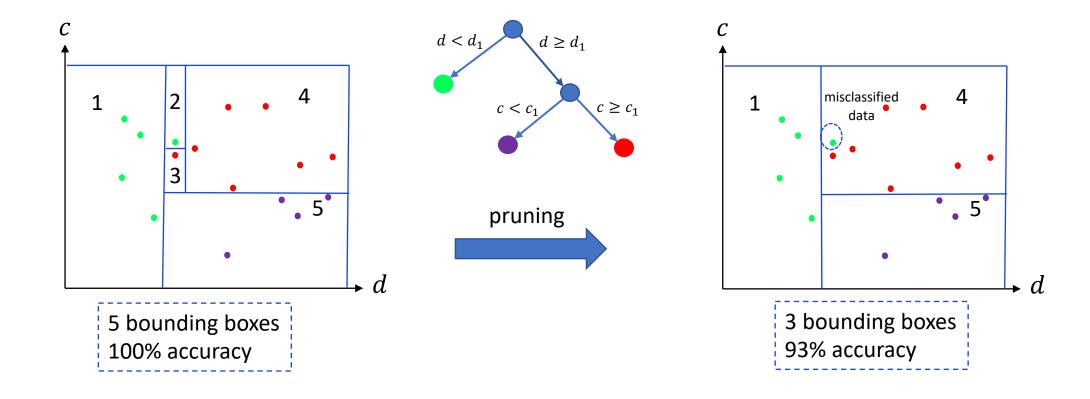
$$\varphi_{5} = G_{[0,3hours]} \diamond_{[0,d_{2}]} (Bikes > c_{1})$$

$$\land \neg G_{[0,3hours]} \diamond_{[0,d_{1}]} (Bikes > c_{1})$$

$$\land \neg G_{[0,3hours]} \diamond_{[0,d_{2}]} (Bikes > c_{2})$$

Pruning the Decision Tree:

- In some cases, achieving 100% accuracy can result in long and hence less interpretable formulas
- ► We prune the DT using a K-fold cross validation approach



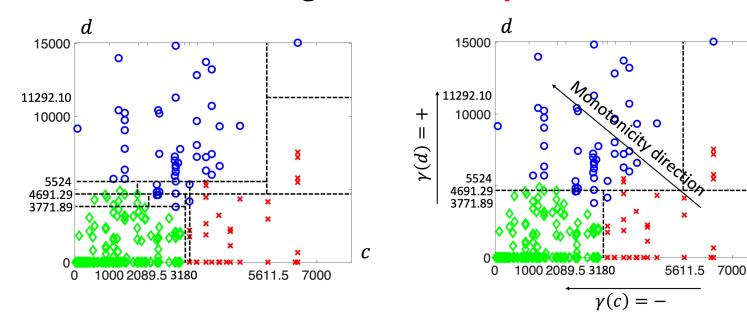
Benchmarks:

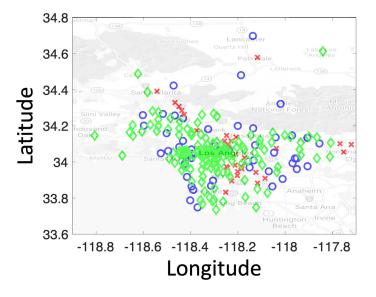
- ► COVID-19 data from LA County
 - ► COVID-19 pandemic has extremely affected our lives
 - ► Understanding the spread pattern of COVID-19 in different areas is vital to stop the spread of the disease.
 - We focus on number of new positive cases in each region of the LA county
- ▶ BSS data from the city of Edinburgh
 - ► The BSS consists of a number of bike stations, distributed over a geographic area
 - ► We focus on the number of bikes (B) and empty slots (S) in each bike station
 - We are interested in analyzing the behavior of each station
- Outdoor Air Quality data from California
- ► Synthetic data for a food court building

COVID-19 data from LA County

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

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





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

BSS data from the city of Edinburgh

PSTREL formula:

$$\varphi(\tau, d) = G_{[0,\tau]} (\varphi_{wait}(\tau) \vee \varphi_{walk}(d))$$

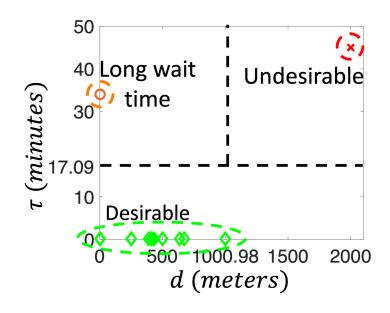
▶ Within the next 3 hours either $\varphi_{wait}(\tau)$ or $\varphi_{walk}(d)$ is True

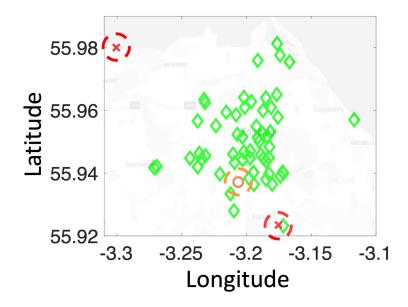
$$\varphi_{wait}(\tau) = F_{[0,\tau]}(B \ge 1) \land F_{[0,\tau]}(S \ge 1),$$

$$\varphi_{walk}(d) = \diamond_{[0,d]}(B \ge 1) \land \diamond_{[0,d]}(S \ge 1)$$

- Locations with large τ : long wait times
- ► Locations with large d: far from stations with Bikes/Slots availability

BSS data from the city of Edinburgh





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

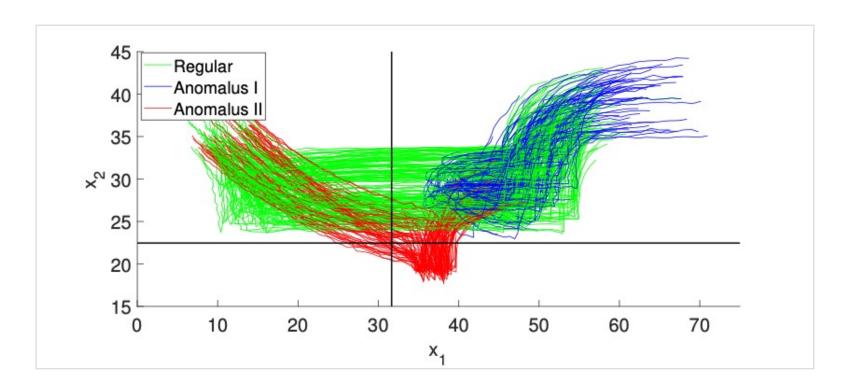
Results summary:

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

In a nutshell:

- ► We proposed a technique to learn interpretable STREL formulas from spatio-temporal data
- We proposed a new method for creating a spatial model with a restrict number of edges that preserves connectivity of the spatial model.
- ► We leveraged robustness of STREL combined with bisection search to extract features for spatiotemporal time-series clustering.
- ► We applied AHC on the extracted features followed by a DT based approach to learn an interpretable STREL formula for each cluster
- ► The results show that our method performs slower than ML approaches, but it is more interpretable

Learning STL classifiers



Goal: learning a specification/ classifier as a temporal logic formula to discriminate as much as possible between bad and good behaviours

Advantages: explicability, easy to build monitors

Application: anomaly detection, specification synthesis

Methodology

• *Single-level* variant: learning formula structure and parameter using Context Free Grammar Genetic Programming (CFGGP)

- *Bi-level* variant:
 - learning formula structure CFGGP
 - 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)

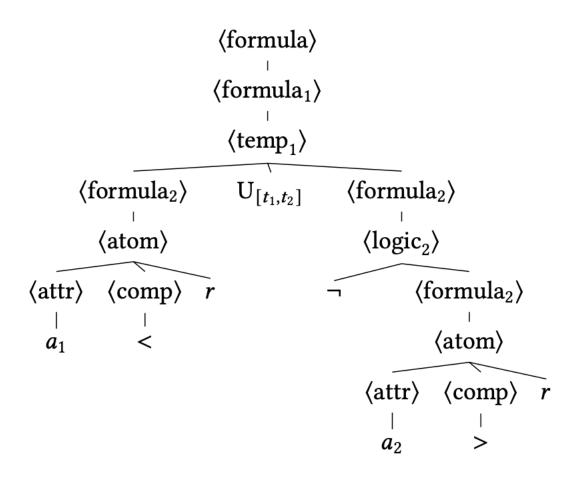
Evolutionary algorithm

- It builds the offspring population P'
- It merges the parent and offspring populations
- It shrinks the resulting new population P

```
1 function evolve():
           P \leftarrow \text{initialize}(\mathcal{G}, n_{\text{pop}})
           foreach i \in \{1, \ldots, n_{\text{gen}}\} do
                  P' \leftarrow \emptyset
                  while |P'| \leq n_{pop} do
 5
                         i \leftarrow 0
 6
                         repeat
                               if \sim U(0,1) \leq p_{xover} then
                                      (\varphi_{p,1}, f_{p,1}) \leftarrow \operatorname{select}(P)
                                      (\varphi_{p,2}, f_{p,2}) \leftarrow \operatorname{select}(P)
 10
                                      \varphi_c \leftarrow \mathsf{crossover}(\varphi_{p,1}, \varphi_{p,2}; \mathcal{G})
11
                               else
12
                                      (\varphi_p, f_p) \leftarrow \text{select}(P)
 13
                                      \varphi_c \leftarrow \mathsf{mutate}(\varphi_p; \mathcal{G})
 14
                                end
15
                               i \leftarrow i + 1
16
                         until (\varphi_c \notin P \cup P') \land (i \leq n_{atts})
17
                        P' \leftarrow P' \cup \{(\varphi_c, f_{\text{opt}}(\varphi_c; \mathcal{L}))\}
18
                  end
19
                  P \leftarrow P \cup P'
20
                  while |P| \ge n_{pop} do
21
                       P \leftarrow P \setminus \{ worst(P) \}
22
                  end
23
           end
24
           return best(P)
26 end
```

Building the populations

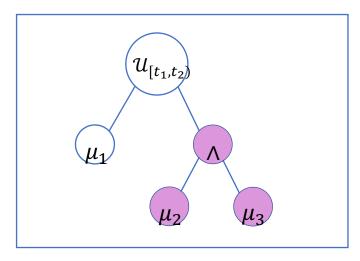
► Candidate formulas are represented as derivation trees of a grammar

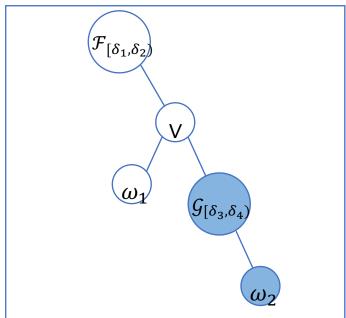


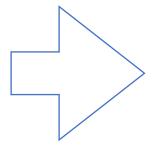
Context Free Grammar

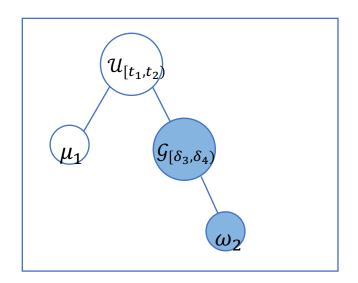
```
\langle \text{formula} \rangle ::= \langle \text{formula}_1 \rangle
\langle \text{formula}_i \rangle ::= \begin{cases} \langle \text{atom} \rangle \mid \langle \text{logic}_i \rangle \mid \langle \text{temp}_1 \rangle & \text{if } i < i_{\text{max}} \\ \langle \text{atom} \rangle \mid \langle \text{logic}_i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

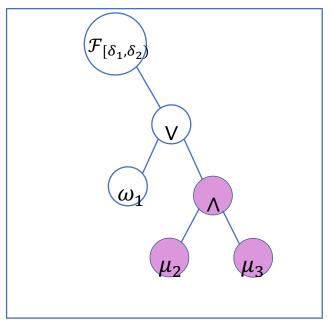
Crossover operator



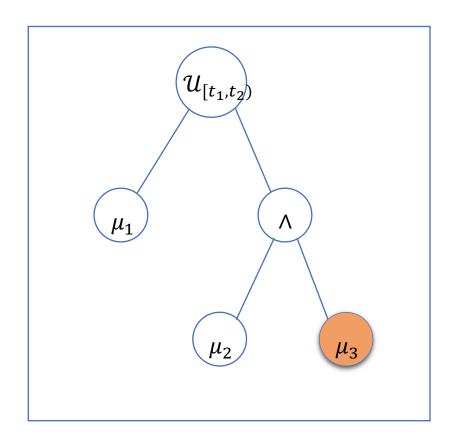


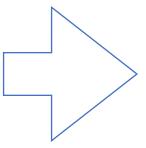


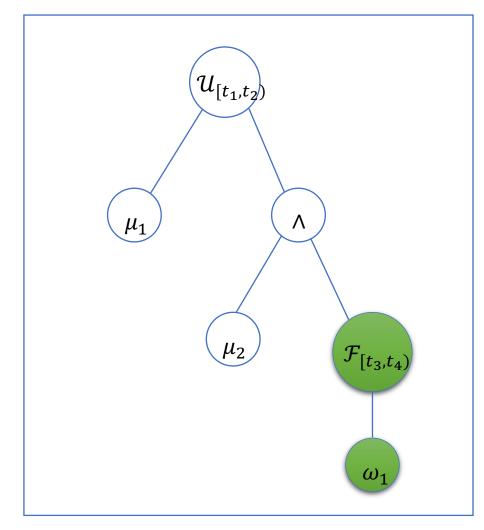




Mutation operator







Learning the Parameters

Problem

Given a PSTL formula φ , a parameter space K, find Θ^* that maximises the discrimination function $f_{opt}(\varphi_\Theta)$

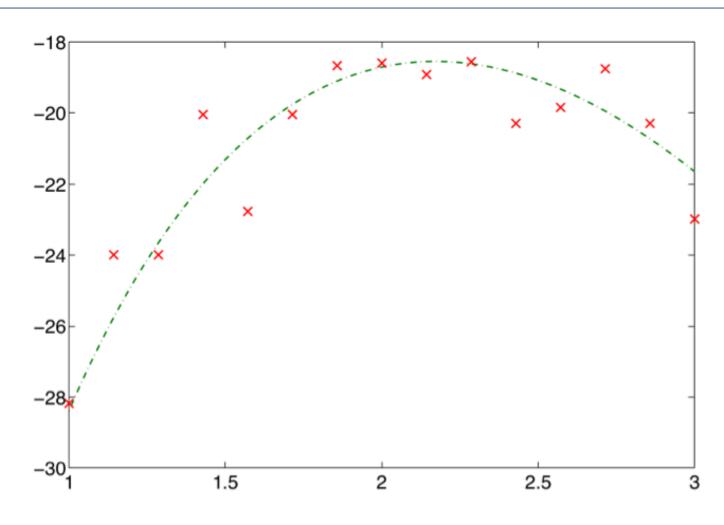


Methodology

- 1. Sample $\{(\theta_{(i)}, y_{(i)}), i = 1,...,n\}$
- 2. Emulate (**GP Regression**): $G[R_{\phi}] \sim GP(\mu,k)$
- 3. Optimize the emulation via **GP-UCB algorithm**, new $\theta_{(n+1)}$

(1) The G(φ_s) Computation

Collection of the training set $\{(\theta_0, y_0), i = 1,...,m\}$ for parameters values θ .

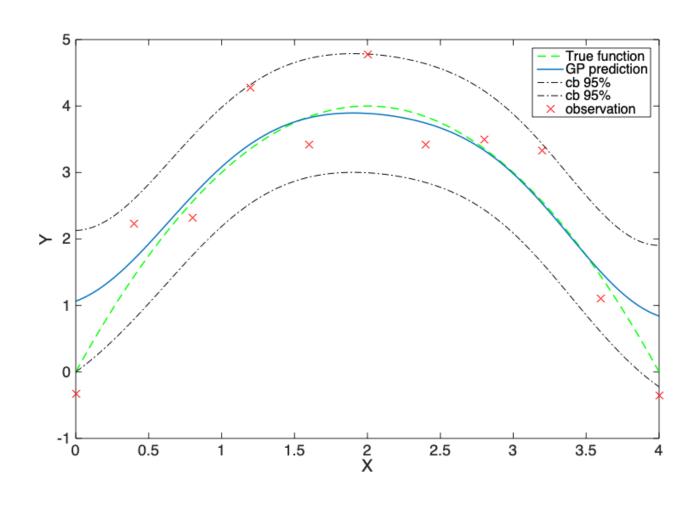


(2) The GP Regression

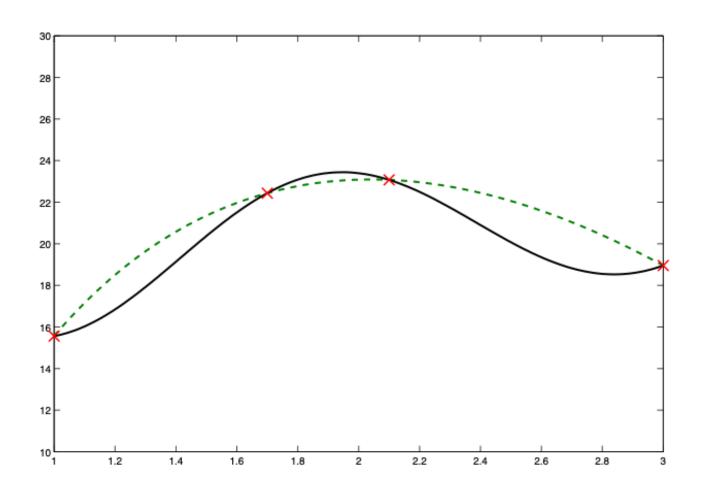
We have noisy observations y of the function value distributed around an unknown true value $f(\theta)$ with spherical Gaussian noise

(2) The GP Regression

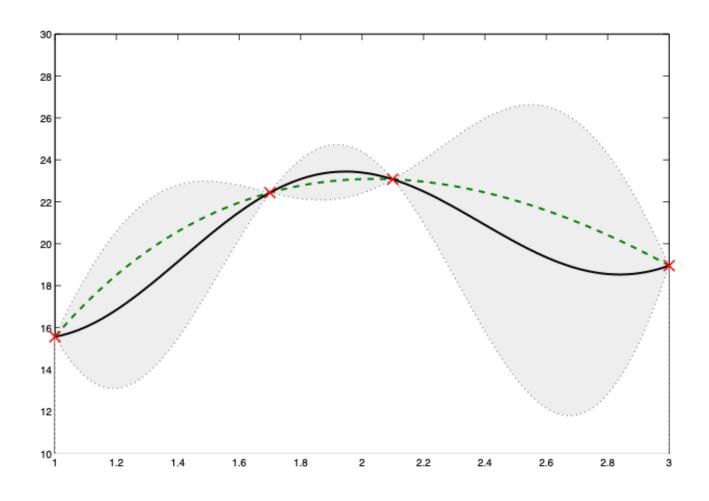
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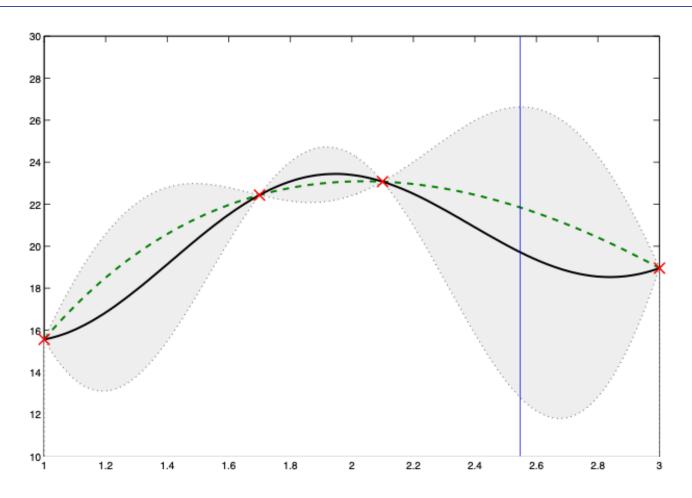
Balance Exploration and Exploitation: we maximise the



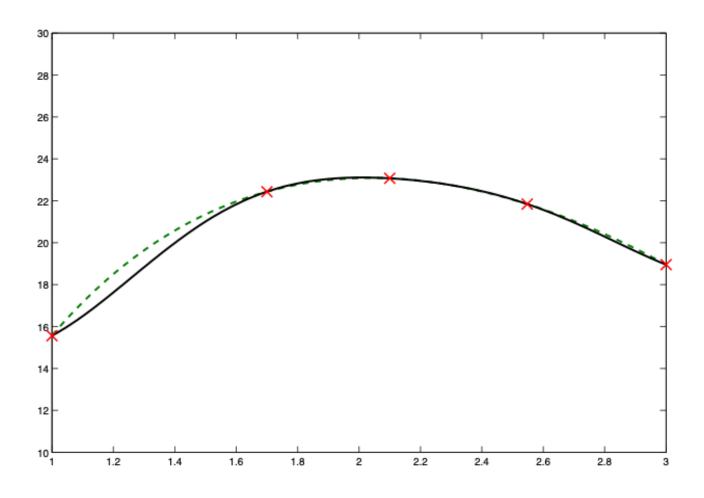
Balance Exploration and Exploitation: we maximise the



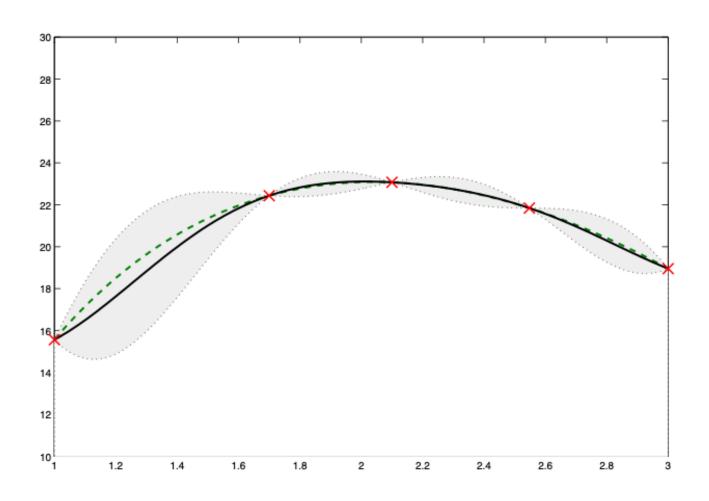
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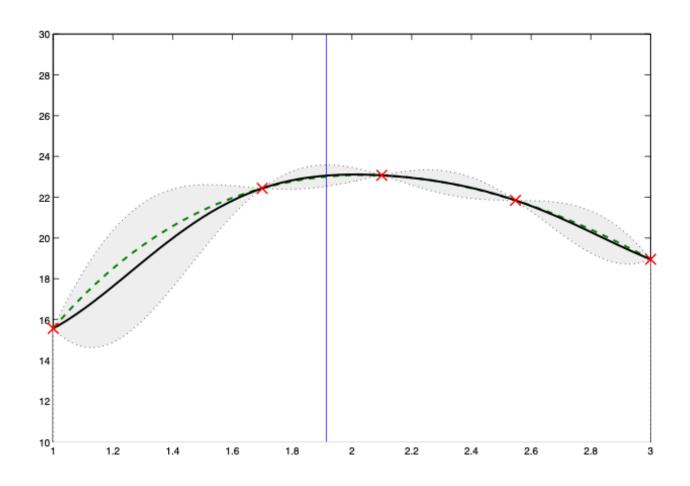
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Fitness Function for the two-classes problem

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

$$\mu_{\varphi,X} = \frac{1}{|X|} \sum_{\boldsymbol{x} \in X} \rho(\varphi, \boldsymbol{x})$$

$$\sigma_{\varphi,X} = \sqrt{\frac{1}{|X|}} \sum_{\boldsymbol{x} \in X} (\rho(\varphi, \boldsymbol{x}) - \mu_{\varphi,X})^{2}$$

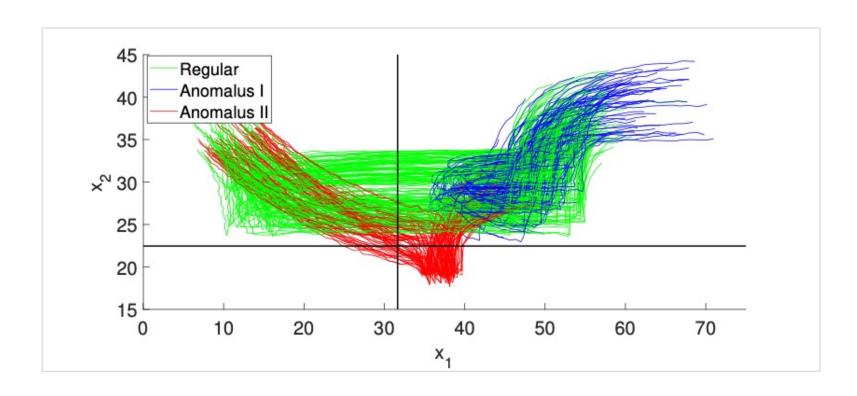
Fitness Function for the one-class problem

$$f(\varphi; X_{\mathcal{L}}^{+}) = \alpha \frac{1}{\left|X_{\mathcal{L}}^{+}\right|} \left| \left\{ \boldsymbol{x} \in X_{\mathcal{L}}^{+} : \boldsymbol{x} \not\models \varphi \right\} \right| + \frac{1}{\sigma_{\varphi, X_{\mathcal{L}}^{+}}^{+} \left|X_{\mathcal{L}}^{+}\right|} \sum_{\boldsymbol{x} \in X_{\mathcal{L}}^{+}} \left|\rho(\varphi, \boldsymbol{x})\right|$$

$$\sigma'_{\varphi,X} = \sqrt{\frac{1}{|X|} \sum_{\boldsymbol{x} \in X} \left(|\rho(\varphi, \boldsymbol{x})| - \frac{1}{|X|} \sum_{\boldsymbol{x} \in X} |\rho(\varphi, \boldsymbol{x})| \right)^2}$$

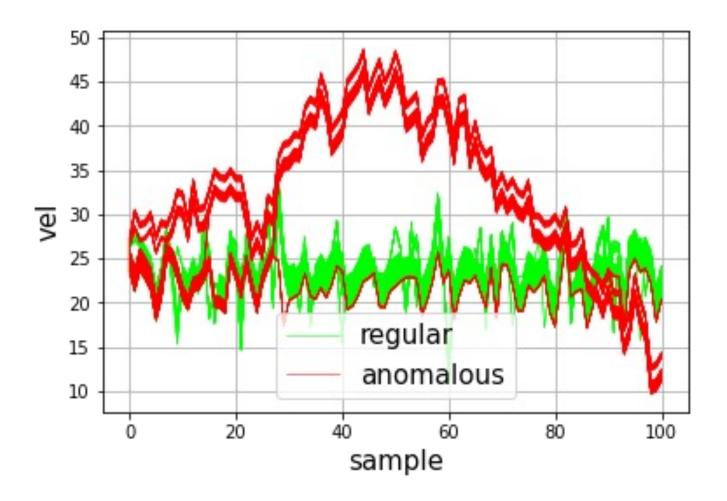
Maritime Surveillance

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



$$\phi_1 = ((x_2 > 22.46) \mathcal{U}_{[49,287]} (x_1 \le 31.65))$$

Train Cruise

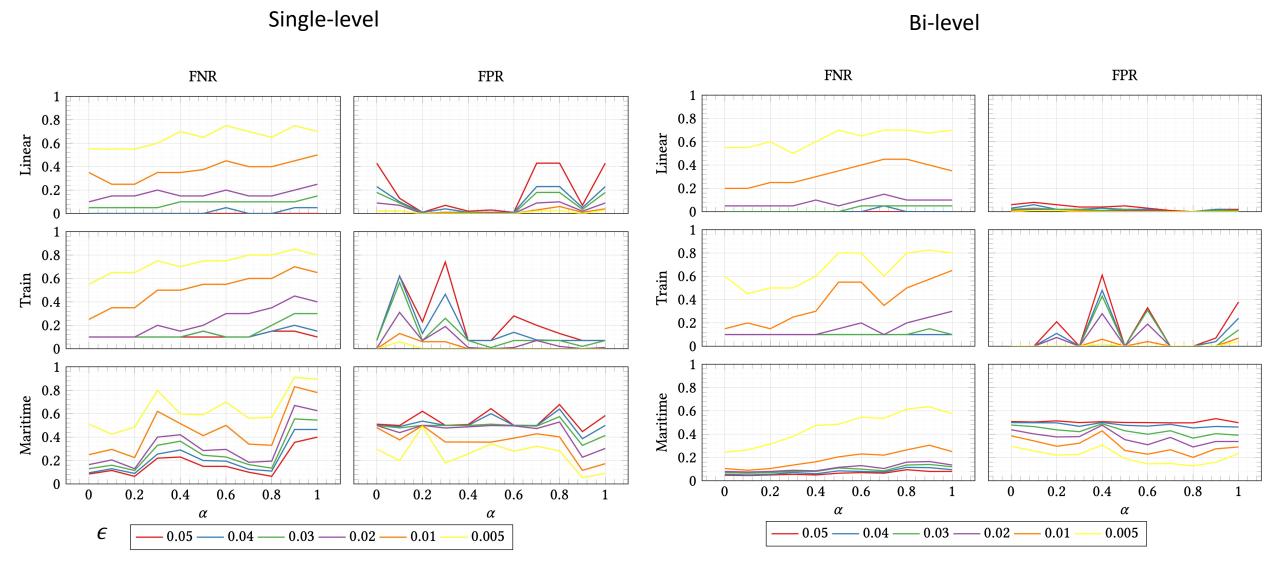


$$(F_{[22,40]}(\text{vel} > 24.48)) \land (F_{[46,49]}(19.00 < \text{vel} < 26.44))$$

Results (supervised learning)

Dataset	Algorithm	FNR	FPR	MCR	Time
Maritime	BUSTLE (single-level)	0.00	0.00	0.00	109
	BUSTLE (bi-level)	0.00	0.00	0.00	1477
	[23]	0.00	0.00	0.00	N/A
	[22]	0.05	0.02	0.04	73
	[6]	N/A	N/A	0.02	140
Linear	BUSTLE (single-level)	0.00	0.00	0.00	15
	BUSTLE (bi-level)	0.00	0.00	0.00	112
	[23]	0.01	0.01	0.01	N/A
	[22]	N/A	N/A	0.02	39
Train	BUSTLE (single-level)	0.03	0.05	0.04	26
	BUSTLE (bi-level)	0.00	0.03	0.02	523
	[23]	0.07	0.32	0.19	N/A
	[22]	N/A	N/A	0.02	32

Results (semi-supervised learning)



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