Robust Satisfaction of Signal Temporal Logics and Applications

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Design and analysis of hybrid systems e.g., embedded systems, mixed-signal circuits, biological systems

Hybrid System $\dot{x} = f_q(x, p) \mid$ Param. p, x_0

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- Signal Temporal Logic (STL): temporal specifications for continuous and hybrid systems
- Quantitative (Robust) satisfaction of STL adapted to deal with uncertainty



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Outline

Temporal Logics for Continuous Time and Space

- Signal Temporal Logic
- Quantitative Satisfaction of STL

An Implementation: The Breach Toolbox

- Simulation of Parametric Hybrid Systems
- Specifying STL Formulas

3 Applications

- Case Study: Voltage Controlled Oscillator
- An Example from Systems Biology

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Temporal logics in a nutshell

Temporal logics allow to specify patterns that timed behaviors of systems may or may not satisfy. They come in many flavors.

The most intuitive is the Linear Temporal Logic (LTL), dealing with discrete sequences of states.

Based on logic operators (\neg, \land, \lor) and temporal operators: "next", "always" (alw), "eventually" (ev) and "until" (U)

Examples:

- $\varphi \ \varphi \ \varphi \ \varphi \ \cdots$ satisfies alw φ
- $\psi \ \psi \ \psi \ \varphi \ \psi \ \cdots$ satisfies ev φ
- $\blacktriangleright \ \varphi \ \varphi \ \varphi \ \varphi \ \psi \ \cdots \ \text{satisfies} \ \varphi \ \mathcal{U} \ \psi$

From Discrete to Continuous

Temporal logics mostly developed for discrete systems

Why not discretizing time and space and reuse existing logics and tools ?

Some reasons:

- Discretization often leads to state-explosion problem
- Specifications should not depend on the discretization used (e.g., "next" depends on time step)

Thus we need:

- Temporal specifications involving dense-time intervals
- Constraints applying on variable in the continuous domain

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Formal Definitions

Definition (STL Syntax)

$$\varphi := \mu \mid \neg \varphi \mid \varphi \land \psi \mid \varphi \ \mathcal{U}_{[a,b]} \ \psi$$

where μ is a predicate of the form $\mu:\mu(x)>0$

Definition (STL Semantics)

The validity of a formula φ with respect to a signal x at time t is

Additionally: $ev_{[a,b]}\varphi = \top \mathcal{U}_{[a,b]} \varphi$ and $alw_{[a,b]}\varphi = \varphi \mathcal{U}_{[a,b]} \perp$

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Consider a simple piecewise affine signal:



Truth value of :

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Truth value of :

$$\blacktriangleright \varphi = x > 2$$

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Truth value of :

$$\blacktriangleright \ \varphi = \mathrm{ev}_{[0,\infty]}(x>2)$$

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Truth value of :

$$\blacktriangleright \ \varphi = \mathrm{ev}_{[0,.5]}(x>2)$$

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Truth value of :

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STL semantics

$$\begin{array}{lll} (x,t)\vDash \mu & \Leftrightarrow & \mu(x[t])>0 \\ (x,t)\vDash \neg \varphi & \Leftrightarrow & (x,t)\nvDash \varphi \\ (x,t)\vDash \varphi_1 \land \varphi_2 & \Leftrightarrow & (x,t)\vDash \varphi_1 \text{ and } (x,t)\vDash \varphi_2 \\ (x,t)\vDash \varphi_1 \mathcal{U}_{[a,b]}\varphi_2 & \Leftrightarrow & \exists t'\in [t+a,t+b] \text{ s.t. } (x,t')\vDash \varphi_2 \\ & \text{ and } \forall t''\in [t,t'], (x,t'')\vDash \varphi_1 \end{array}$$

A Boolean Satisfaction Function χ

Map {false, true} to $\{-\infty, \infty\}$ and define the function $\chi : (x, t) \to \{-\infty, \infty\}$:



STL semantics



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Map {false, true} to $\{-\infty,\infty\}$ and define the function $\chi:(x,t) \to \{-\infty,\infty\}$:

 $\begin{array}{lll} \chi(\mu, x, t) &=& \operatorname{sign}(\mu(x[t])) \times \infty \\ \chi(\neg \varphi, x, t) &=& -\chi(\varphi, x, t) \\ \chi(\varphi_1 \wedge \varphi_2, x, t) &=& \min(\chi(\varphi_1, x, t), \chi(\varphi_2, x, t)) \\ \chi(\varphi_1 \mathcal{U}_{[a,b]}\varphi_2, x, t) &=& \max_{\tau \in t+[a,b]} \min(\chi(\varphi_2, x, \tau), \min_{s \in [t,\tau]} \chi(\varphi_1, x, s)) \end{array}$

We can verify that $(x,t) \models \varphi \Leftrightarrow \chi(\varphi,x,t) = +\infty$

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From Boolean to Quantitative Satisfaction Function

For atomic predicates:

$$\chi(\mu, x, t) = \mathrm{sign}(\mu(x[t])) \times \infty$$

The sign removes the quantitative information in μ to get a boolean signal Simple idea

- \blacktriangleright Get rid of sign to get a quantitative satisfaction function ρ
- Keep the same inductive rules for the quantitative semantics:

 $\begin{array}{lll} \rho(\mu, x, t) & = & \mu(x[t]) \\ \rho(\neg \varphi, x, t) & = & -\rho(\varphi, x, t) \\ \rho(\varphi_1 \wedge \varphi_2, x, t) & = & \min(\rho(\varphi_1, x, t), \rho(\varphi_2, x, t)) \\ \rho(\varphi_1 \mathcal{U}_{[a,b]}\varphi_2, x, t) & = & \max_{\tau \in t + [a,b]} (\min(\rho(\varphi_2, x, \tau), \min_{s \in [t,\tau]} \rho(\varphi_1, x, s)) \end{array}$

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Robust Satisfaction, Examples












Robust Satisfaction, Applications

Assume that x depends on p, we get the following oracle:



Parameter synthesis can be solved by solving

 $p^* = \max \{ \rho(\varphi, p) \mid p \in \mathcal{P} \}$

If $\rho(\varphi, p^*) > 0$ then parameter p^* is such that $(x, p^*) \models \varphi$. Moreover, it maximizes the robustness of satisfaction.

More generally, one can characterize the *validity domain* of φ , given by $d(\varphi, \mathcal{P}) = \{ p \in \mathcal{P} \mid \rho(\varphi, p) > 0 \}$

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$$\begin{array}{ccc} \mathsf{STL} \ \mathsf{Prop.} \ \varphi & & & \\ & \mathsf{Oracle} \\ & \mathsf{Model} \ + \\ & \mathsf{STL} \ \mathsf{Monitor} \end{array} \xrightarrow{} \mathsf{Robust} \ \mathsf{Sat.} \ \rho(\varphi, p) \end{array}$$

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Hybrid Model

Breach deals with piecewise-continuous models of the form

$$\left\{ \begin{array}{rrl} \dot{\mathbf{x}} &=& f(q,\mathbf{x},\mathbf{p}), \ \mathbf{x}(0) = \mathbf{x}_0 \\ \mathbf{y} &=& g(\mathbf{x}) \\ q^+ &=& e(q^-,\mathbf{y}), \ q(0) = q_0 \end{array} \right.$$

where $\mathbf{x} \in \mathbb{R}^n$ is the state variable

- $q \in \mathbb{N}$ is the discrete state,
- $\mathbf{p} \in \mathbb{R}^{n_p}$ is the parameter vector,
- g is the guard function and

e is the event or transition function, where $q^+ \neq q^-$ only if $g(\mathbf{x}) = 0$

Simulation Algorithm

Discontinuity locking + Event detection by zero crossing detection

1. Let $f_k(\mathbf{x}, \mathbf{p}) = f(q(t_k), \mathbf{x}, \mathbf{p})$ (block switching between t_k and t_{k+1})

2. Solve ODE
$$\dot{\mathbf{x}} = f_k(\mathbf{x}, \mathbf{p})$$
 on $[t_k, t_k + h_k]$

- 3. If for all i, sign $(g_i(\mathbf{x})) = \text{Constant}$ on $(t_k, t_k + h_k]$ then let $t_{k+1} = t_k + h_k$
- 4. Else find the minimum time $\tau > t_k$ for which $g_i(\mathbf{x}(\tau)) = 0$ and let $t_{k+1} = \tau$
- 5. Return $\xi_{\mathbf{p}}(t_{k+1})$ and restart with $q(t_{k+1}^+) = e(q(t_k), \lambda(t_{k+1}^-))$

Simulation and Sensitivity Analysis

Simulation based on a state-of-the-art ODE solver CVodes

- Variable-steps variable order implicit methods, efficient for stiff and non-stiff dynamics
- Builtin zero-crossing detection for guards.

Sensitivity functions $s_{ij}(t) = \frac{\partial \mathbf{x}_i}{\partial \mathbf{p}_i}(t)$ are also computed by CVodes solver

Breach implementation adds

- ▶ the computation of sensitivity discontinuities at transitions
- ► an efficient Matlab-C interface:
 - ▶ The solver and the dynamics are in C
 - Matlab manipulates arrays of parameters and externally computed arrays of trajectories
 - \Rightarrow Much more efficient than Matlab native ODE solvers

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Temporal logic formulas: atomic predicates

 $\mathsf{STL} \; \mathsf{Syntax}: \qquad \varphi := \mu \; | \; \neg \varphi \; | \; \varphi \land \varphi \; | \; \varphi \; \mathcal{U}_{[a,b]} \; \varphi$

+ usual syntactic sugars for disjunction, eventually and always.

Predicates: General constraints on the variables: $\mu \equiv \mu(\mathbf{x}, \mathbf{p}, t) \geq 0$

```
% distance to (p0,p1) is more than 2.
(x0[t]-p0)^2 + (x1[t]-p1)^2) >= 4.
% the system reached steady state (very slow evolution)
abs(ddt{x0}[t])+abs(ddt{x1}[t])) <= 1e-3
% x0 is sensitive to parameter p3
abs(d{x0}{p3}[t]) >= 10*x0[t]/p3
```

Temporal logic formulas: formulas

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```
% x0 will become more than -.9 whithin .5 s
ev_[0,.5] (x0[t]>-.9)
% the system will eventually remain close to 0
ev (always (abs(x0)[t] < 1e-6))
% x0 remains low until x1 stabilizes before 10 seconds
(x0[t] < 0.1) until_[0, 10] always ((abs(ddt{x1}[t]) < 1e-6))</pre>
```

Breach computes the function $\rho(\varphi, x, \cdot)$ by induction on the structure of φ .

This reduces to three subproblems: given two functions $y,y':\mathbb{T}\to\mathbb{R},$ and an interval [a,b]

- 1. (operator \neg) compute $\forall t, z[t] = -y[t];$
- 2. (operator \wedge) compute $\forall t, \ z[t] = \min(y[t], y'[t])$
- 3. (operator \mathcal{U}) compute $\forall t, \ z[t] = \max_{\tau \in t+[a,b]} (\min(y'[\tau], \min_{s \in [t,\tau]} y[s])))$
- 1. and 2. are reasonably trivials. 3., less (maybe for a $\min \max$ guru).

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Computational Cost, Some Experiments

(a) Same signal, formula
$$\varphi = (x > 0) \underbrace{\mathcal{U}_{[0,1)} \ (x > 0) \ \mathcal{U}_{[0,1)} \ (x > 0) \dots}_{i \text{ times}}$$

(b) Same formula: $\varphi = alw(x > 1.5 \Rightarrow ev(alw(x < .1)))$, different input sizes

(a)

i	time(s)	
1	0.34747	
2	0.46335	
3	0.60599	
4	0.76067	
5	0.89201	
6	1.03761	

(b)

Computational Cost, Some Experiments

(a)

(a) Same signal, formula
$$\varphi = (x > 0) \underbrace{\mathcal{U}_{[0,1)} \ (x > 0) \ \mathcal{U}_{[0,1)} \ (x > 0) \dots}_{i \text{ times}}$$

(b) Same formula: $\varphi = \mathsf{alw}(x > 1.5 \Rightarrow \mathsf{ev}(\mathsf{alw}(x < .1)))$, different input sizes



i	time(s)	input size	time(s)
1	0.34747	31416	0.18402
2	0.46335	345566	0.40761
3	0.60599	659716	0.75508
4	0.76067	973866	1.09268
5	0.89201	1288016	1.4587
6	1.03761		

Outline

1 Temporal Logics for Continuous Time and Space

- Signal Temporal Logic
- Quantitative Satisfaction of STL

An Implementation: The Breach Toolbox

- Simulation of Parametric Hybrid Systems
- Specifying STL Formulas

3 Applications

- Case Study: Voltage Controlled Oscillator
- An Example from Systems Biology

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Case Study: Voltage Controlled Oscillators

- Characterizing oscillations in a Voltage Controlled Oscillator
- Non linear circuit with 3 state variables (IL1, VD1, VD2) and around 10 parameters (C, Vctrl, L, R, etc)



Specifying Oscillations, Predicates

We look for oscillations of period $\,T\,$ and given minimum and maximum amplitudes around 0

```
% Above and below a minimum amplitude
mu0: IL1[t] > Amin
mu1: IL1[t] < -Amin
% Bounded by a maximum amplitude
mu2: abs(IL1[t]) < Amax
% (almost) Strict periodicity
mu3: (abs(IL1[t] - IL1[t-T]) < epsi)</pre>
```

Specifying Oscillations, Formulas

```
% Alternating above and below a minimum amplitude
phi0: (ev_[0,T] (IL1[t]>Amin)) and (ev_[0,T] (IL1[t]<-Amin))</pre>
```

```
% and holding for 4 periods
phi1: alw_[0,4*T] (phi0)
```

```
% Holding strict periodicity
phi2: alw_[0,4*T] ( (IL1[t] - IL1[t-T])^2 ) < epsi)</pre>
```

```
% Bounding amplitude globally
phi3: alw (IL1[t]<sup>2</sup> < Amax)</pre>
```

% Final formula, the ev operator gets rids of transient phi: ev (phi1 and phi2 and phi3)

Breach Interface



Breach Interface



Robust Satisfaction of STL

Breach Interface


Result on a Single Trace

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Result on a Single Trace





Partitioning the Parameter Region



Partitioning the Parameter Region



Robust Satisfaction of STL

Satisfaction Function

i.e., the resulting cost function



Robust Satisfaction of STL

- We defined 10 uncertain parameters with given ranges
- and picked 5 starting points randomly distributed in this domain

Uncertain Parameters	
V_tp: 0 +/- 1 i.e [-1,1]	٠
K_p: 8.6e-05 +/- 8.6e-05 i.e [0,0.00 Wdl • 960 +/- 960 i.e [0 1920]	
Omega_P: -0.07 +/- 0.007 i.e [-0.07	22
V_DD: 1.8 +/- 1.8 i.e [0,3.6]	
	•
20000	

Using an implementation of the Nelder Mead optimization algorithm, Breach was able to find two parameter valuations satisfying the property in 98 s of computation time.

It turned out those were perfectly valid oscillations

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V_DD: 1.8 +/ - 1.8 i.e [0,3.6] L b: 0.018 +/ - 0.018 i.e [0.0.036]	-
▲ 200000 ►	

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An Enzymatic Network Involved in Angiogenesis

Collagen (C_1) degradation by matrix metalloproteinase (M_2^P) and membrane type 1 metalloproteinase (MT_1).



In [KP04], activation of M_2^P after 12h "Nearly steady state" for $T_2(0)$ between 0 and 200 nM. It turned out that steady state was not reached for $T_2(0) > 20$ nM.

Using $\varphi \equiv \text{ev}$ alw $(|M_2(t)| < \epsilon \times M_2^P(0))$ we could guarantee the correct plot.



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Open Model

We extended the model by introducing production and degradation terms



More complex behaviors becomes possible, such as oscillatory regimes

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We extended the model by introducing production and degradation terms



More complex behaviors becomes possible, such as oscillatory regimes

Oscillations Map



Robust Satisfaction of STL



Robust Satisfaction of STL



Robust Satisfaction of STL



Oscillation, Robustness



Robust Satisfaction of STL

Oscillation, Robustness



Robust Satisfaction of STL

Oscillation, Robustness



Conclusion

Summary

- Specification language for hybrid systems behaviors, with a robust semantics
- An implementation with advanced simulation and parameter exploration features
- Case studies of parameter synthesis problems

Perspectives

- Going further with global robustness and sensitivity analysis for specifications
- Different optimization strategies for parameter synthesis/optimal control
- From robust satisfaction to *formal* specifications