Using the Theory of Reals in

Analyzing Continuous and Hybrid Systems

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A lot of engineering and science concerns dynamical systems

- **State Space**: The set of states, $X$
- **Dynamics**: The evolutions, $T \mapsto X$
  - Discrete Systems: $T$ is $\mathbb{N}$
  - Continuous Systems: $T$ is $\mathbb{R}$
  - Hybrid Systems: $T$ is $\mathbb{R} \times \mathbb{N}$
Modeling languages:

- **Continuous systems**: Differential equations
  - The state space formulation
    
    \[
    \begin{align*}
    \dot{x}(t) & = f(x(t), u(t), t) \\
    y(t) & = h(x(t), t)
    \end{align*}
    \]

- **Discrete systems**: (Finite) state machines
  - \( t(\vec{x}, \vec{x}') \) is a formula in some theory
Formal Models II

Putting the two formal models together, Hybrid Automata:

- Embed a continuous dynamical system inside each state

- World now evolves in two different ways
  - Move from one state to another via a discrete transition
  - Remain in the state and let the continuous world evolve

- System has different modes of operation, while some discrete logic performs mode switches

![Graph showing continuous evolution over time](image-url)
A tuple \((Q, X, S_0, F, Inv, R)\):

- \(Q\): finite set of discrete variables
- \(X\): finite set of continuous variables
- \(X = \mathcal{R}^{|X|}\), \(Q\) = set of all valuations for \(Q\)
- \(S = Q \times X\)
- \(S_0 \subseteq S\) is the set of initial states
- \(F : Q \mapsto (X \mapsto \mathcal{R}^{|X|})\) specifies the rate of flow, \(\dot{x} = F(q)(x)\)
- \(Inv : Q \mapsto 2^{\mathcal{R}^{|X|}}\) gives the invariant set
- \(R \subseteq Q \times 2^X \mapsto Q \times 2^X\) captures discontinuous state changes
Hybrid Automata: In picture

Dense Time: Time does not elapse during discrete transition
Semantics of Hybrid Systems

- $s_1 \in S_0$ is an initial state

- **Discrete Evolution**: $s_i \rightarrow s_{i+1}$ iff $R(s_i, s_{i+1})$

- **Continuous Evolution**: $s_i = (l, x_i) \rightarrow s_{i+1} = (l, x_{i+1})$ iff there exists a $f : \mathbb{R}^{|X|} \rightarrow \mathbb{R}^{|X|}$ and $\delta > 0$ such that

  \[
  x_{i+1} = f(\delta) \quad x_i = f(0) \\
  \dot{f} = F(l) \quad f(t) \in \text{Inv}(l) \text{ for } 0 \leq t \leq \delta
  \]
Questions

What can we say (deduce, compute) about the model?

- **Reachability.** Is there a way to get from state $\vec{x}$ to $\vec{x}'$?

- **Safety.** Does the system stay out of a bad region
  - Can the car ever collide with the car in front?

- **Liveness.** Does something good always happen

- **Stability.** Eventually remain in good region

- **Timing Properties.** Something good happens in 10 seconds

Does the model satisfy some property.

Property is described in a logic interpreted over the formal models.
Problem

- Given a hybrid automata
- And a property: safety, reachability, liveness
- Show that the property is true of the model

- Discrete systems: mc, bmc, abs. inter., inf-bmc, k-induction, deductive rules
- Continuous systems: ?
- Hybrid systems: ...
Continuous Systems

Approach 1: Solve the ODE and eliminate $t$

Eg. If $\dot{x} = 1$, $\dot{y} = 1$, then $\text{Reach} := \exists t : (x = x_0 + t \land y = y_0 + t)$

$\dot{x} = A\vec{x}$, then $\text{Reach} := \exists t : \vec{x} = e^{At}\vec{x}_0$

If $A$ is nilpotent: $e^{At}x_0$ is a polynomial

If $A$ has all rational eigenvalues: $e^{At}x_0$ is a polynomial with $e$

If $A$ has all imaginary rational eigenvalues: $e^{At}x_0$ is a polynomial with $\sin, \cos$

In all cases, reduces to $\exists$ elimination over RCF
Continuous Systems

**Approach 2:** Use inductive invariants

cf. Barrier Certificates, Lyapunov Functions

Consider the CDS:

\[
\begin{align*}
\dot{x}_1 &= -x_1 - x_2 \\
\dot{x}_2 &= x_1 - x_2
\end{align*}
\]

\[x_1^2 + x_2^2 \leq 0.5\] is an invariant set.

But there are more invariants:

\[|x_1| \leq 0.5 \land |x_2| \leq 0.5\]
Invariants for Dynamical Systems

Illustration of invariant sets in 2-D:

Arbitrarily shaped

Box shaped

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Box Invariants

A positively invariant rectangular box

\[ \vec{l} \leq \vec{x} \leq \vec{u} \]

i.e., invariants of the form,

\[ l_1 \leq x_1 \land x_1 \leq u_1 \land l_2 \leq x_2 \land x_2 \leq u_2 \land \ldots \]

Related Concepts—

- Component-wise Asymptotic Stability (CWAS)
- Lyapunov stability under the infinity vector norm

Unstable systems can have useful box invariants
An Empirical Law for Biological Models: If a model of a biological system is stable, then it also has a rectangular box of attraction—if the system enters this box, then it remains inside it.

This “law” allows verification and parameter estimation for models of biological systems.

Natural intuitive meaning
Computing Box Invariants

Find $Box(\vec{l}, \vec{u})$ such that vector field points inwards on the boundary

$$\exists \vec{l}, \vec{u} : \forall \vec{x} : \bigwedge_{1 \leq j \leq n} ((\vec{x} \in FaceL^j(\vec{l}, \vec{u}) \Rightarrow \frac{dx_j}{dt} \geq 0)$$

$$\wedge (\vec{x} \in FaceU^j(\vec{l}, \vec{u}) \Rightarrow \frac{dx_j}{dt} \leq 0)), \quad (1)$$

If $\frac{dx_j}{dt}$ is a polynomial expression, then existence of box invariants is decidable.
Linear Systems: Deciding Box Invariance

\[ A \in \mathbb{Q}^{n \times n} \]

\[ A^m = \text{matrix obtained from } A \text{ s.t. } a^m_{ii} = a_{ii}, \quad a^m_{ij} = |a_{ij}| \text{ for } i \neq j. \]

The following problems are all equivalent and can be solved in \( O(n^3) \) time:

- Is \( \dot{x} = Ax \) strictly box invariant?
- Is \( \dot{x} = A^m x \) strictly box invariant?
- Is there a \( \bar{z} > 0 \) such that \( A^m \bar{z} < 0 \)?
- Does there exist a positive diagonal matrix \( D \) s.t. \( \mu(D^{-1}A^mD) < 0 \) (in the infinity norm)?
- Is \( -A^m \) a \( P \)-matrix?

Box invariance is stronger than stability for linear systems.
Matrices with non-negative off-diagonal terms, such as $A^m$, are known as Metzler matrices.

$A^m \in \mathbb{R}^{n \times n}$ is Metzler and irreducible. Then it has an eigenvalue $\tau$ s.t.:

1. $\tau$ is real; furthermore, $\tau > \text{Re}(\lambda)$, where $\lambda$ is any other eigenvalue of $A^m$ different from $\tau$;

2. $\tau$ is associated with a unique (up to multiplicative constant) positive (right) eigenvector;

3. $\tau \leq 0$ iff $\exists \vec{c} > \vec{0}$, such that $A^m \vec{c} \leq \vec{0}$; $\tau < 0$ iff there is at least one strict inequality in $A^m \vec{c} \leq \vec{0}$;

4. $\tau < 0$ iff all the principal minors of $-A^m$ are positive;

5. $\tau < 0$ iff $-(A^m)^{-1} > 0$. 

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Examples

Glucose/Insulin metabolism in Human Body:

- Compartmental model of whole body is typically box invariant.
- Boxes give bounds on blood sugar concentration in different organs.

EGFR / HER2 trafficking model:
Proposed affine model is box invariant.

Delta-Notch lateral signaling model:
The stable modes are box invariants

Tetracycline Antibiotics Resistance:
The resistant mode is box invariant
Nonlinear Systems

\[ \frac{d\vec{x}}{dt} = \vec{p}(\vec{x}) \]

\[ \exists \vec{l}, \vec{u} : \forall \vec{x} : \bigwedge_{1 \leq j \leq n} ((\vec{x} \in \text{Face} L^j (\vec{l}, \vec{u})) \Rightarrow \frac{dx_j}{dt} \geq 0) \]

\[ \wedge (\vec{x} \in \text{Face} U^j (\vec{l}, \vec{u}) \Rightarrow \frac{dx_j}{dt} \leq 0)) \], \quad (2) \]

If \( \vec{p} \) are all polynomials, then inductive properties of the form \( |\vec{x}| \leq c \) can be computed.

Efficiency is an issue.

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Nonlinear Systems: Multiaffine

\[
\frac{d\bar{x}}{dt} = \bar{p}(\bar{x})
\]

Multiaffine: Degree at most one in each variable

Example: \(x_1 x_2 - x_2 x_3\) is multiaffine

If \(p\) is multiaffine and \(\bar{x} \in Box(\bar{l}, \bar{u})\), then \(p(\bar{x})\) is bounded by values of \(p\) at vertices of the box

\[∃∀(2n) \text{ to } ∃(n2^n): \]

Generalize: Degree of \(x_j\) can be arbitrary in \(p_j\)
Generalize multiaffine systems

If $f$ is a monotone function, then $f(\bar{x})$ is bounded by values $f(\bar{v})$ at the vertices $v$

\[ \dot{x} = \bar{p} \] is monotone if $p_i$ is monotone wrt $x_j$ for all $j \neq i$.

Examples:
\begin{itemize}
  \item $\dot{x} = 1 - x^2$ is monotone, but not multiaffine
  \item $\dot{x} = x^3 + x$ is monotone, but not multiaffine
\end{itemize}

\[ \exists (2n) \text{ to } \exists (n2^n) \]
Nonlinear Systems: Uniformly Monotone

$f$ is uniformly monotone wrt $y$ if it is monotone in the same way for all choices of $\vec{x} - y$

Examples:

$xy - yz$ is not uniformly monotone wrt $y$, whereas it is monotonic wrt $y$

$xy - yz$ is uniformly monotone wrt $x$ in domain \( \{y \geq 0\} \)

\( \exists \forall (2n) \) to \( \exists (n2^n) \) to \( \exists (2n) \)

Linear systems are uniformly monotone

Linear \( \subseteq \) Uniformly monotone \( \subseteq \) Monotone
Uniformly Monotone Nonlinear Example

Phytoplankton Growth Model:

$$\dot{x}_1 = 1 - x_1 - \frac{x_1 x_2}{4}, \quad \dot{x}_2 = (2x_3 - 1)x_2, \quad \dot{x}_3 = \frac{x_1}{4} - 2x_3^2,$$

Monotone, but not multiaffine

Uniformly monotone in the positive quadrant

Box invariant sets can be computed by solving

$$1 - u_1 - \frac{u_1 l_2}{4} \leq 0, \quad u_2 (2u_3 - 1) \leq 0, \quad \frac{u_1}{4} - 2u_3^2 \leq 0,$$

$$1 - l_1 - \frac{l_1 u_2}{4} \geq 0, \quad l_2 (2l_3 - 1) \geq 0, \quad \frac{l_1}{4} - 2l_3^2 \geq 0.$$

One possible solution: $\vec{l} = (0, 0, 0)$ and $\vec{u} = (2, 1, 1/2)$
Continuous to Hybrid Systems

Hybrid systems = control flow graph over continuous systems

- Analysis of each node
- Control flow: loops

If dynamics are simple (timed, multirate), discrete control flow can be complex

If dynamics are complex, control flow needs to be restricted
Continuous and Hybrid Systems can model biological and control systems.

We can use ideas, such as, inductive invariants, for analysis.

All symbolic analysis requires reasoning over the reals.

Biological systems tend to be box invariant.

Monotonicity — interesting property that can be utilized for analysis.

Biological systems are monotone or nearly-monotone (Sontag).