Using the Theory of Reals in Analyzing Continuous and Hybrid Systems

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Dynamical Systems

A lot of engineering and science concerns dynamical systems

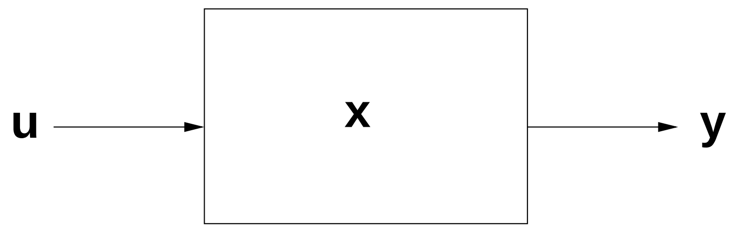
- State Space: The set of states, $\mathbf{X}$
- Dynamics: The evolutions, $\mathbf{T} \mapsto \mathbf{X}$
  - Discrete Systems: $\mathbf{T}$ is $\mathbb{N}$
  - Continuous Systems: $\mathbf{T}$ is $\mathbb{R}$
  - Hybrid Systems: $\mathbf{T}$ is $\mathbb{R} \times \mathbb{N}$

Formal Models I

Modeling languages:

- Continuous systems: Differential equations
  - The state space formulation

$$\begin{aligned} \dot{x}(t) &= f(x(t), u(t), t) \\ y(t) &= h(x(t), t) \end{aligned}$$

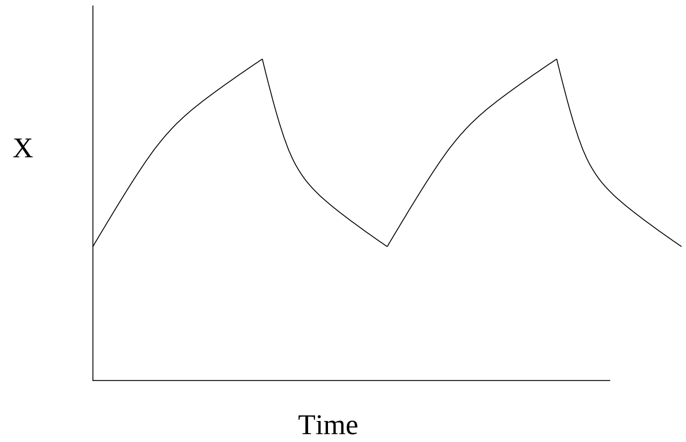


- Discrete systems: (Finite) state machines
  - $t(\vec{x}, \vec{x}')$ is a formula in some theory

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

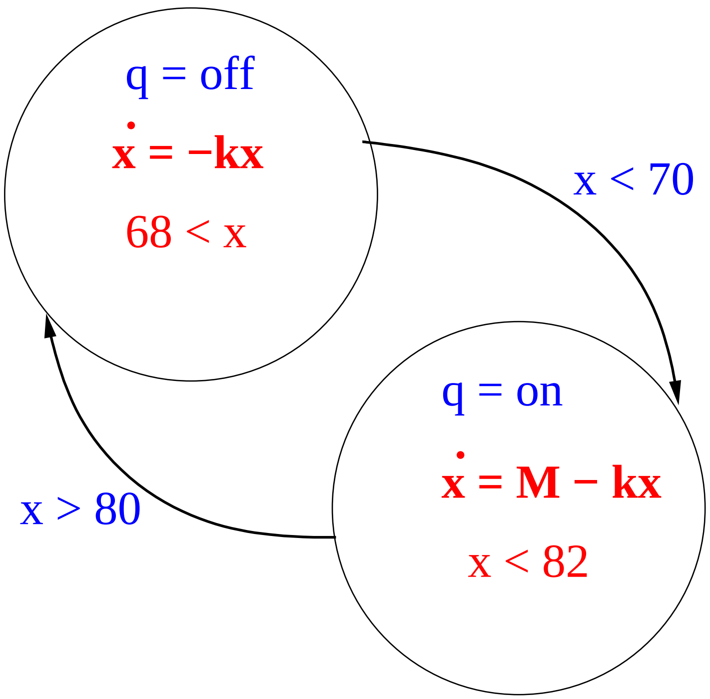


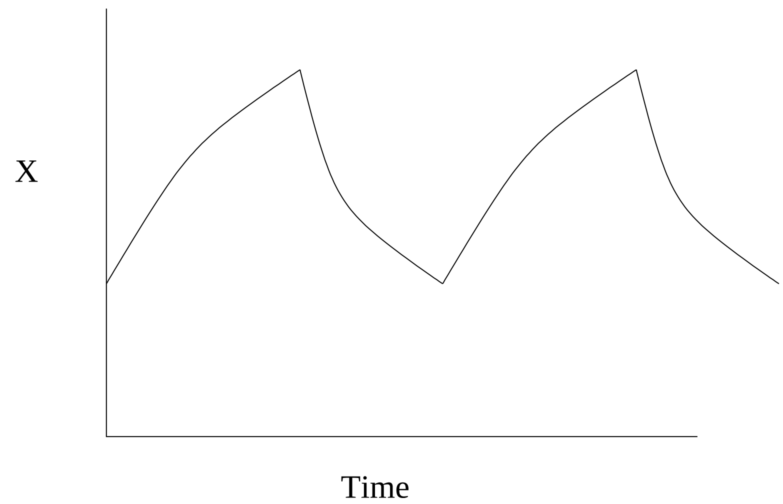
Hybrid Automata

A tuple $(Q, X, \mathbf{S}_0, F, Inv, R)$:

- Q: finite set of discrete variables
- X: finite set of continuous variables
- $\mathbf{X} = \Re^{|X|}$, $\mathbf{Q}$ = set of all valuations for Q
- $\mathbf{S} = \mathbf{Q} \times \mathbf{X}$
- $\mathbf{S}_0 \subseteq \mathbf{S}$ is the set of initial states
- $F : \mathbf{Q} \mapsto (\mathbf{X} \mapsto \Re^{|X|})$ specifies the rate of flow, $\dot{x} = F(q)(x)$
- $Inv : \mathbf{Q} \mapsto 2^{\Re^{|X|}}$ gives the invariant set
- $R \subseteq \mathbf{Q} \times 2^{\mathbf{X}} \mapsto \mathbf{Q} \times 2^{\mathbf{X}}$ captures discontinuous state changes

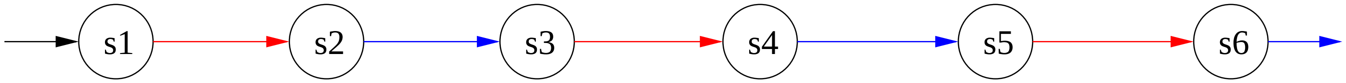
Hybrid Automata: In picture





Dense Time: Time does not elapse during discrete transition

Semantics of Hybrid Systems



- $s1 \in \mathbf{S}_0$ 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 $f : \Re^{|X|} \mapsto \Re^{|X|}$ and $\delta > 0$ such that

$$\begin{array}{rclcrcl} x_{i+1} & = & f(\delta) & & x_i & = & f(0) \\ \dot{f} & = & F(l) & & f(t) & \in & Inv(l) \; for \; 0 \leq t \leq \delta \end{array}$$

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 $Reach := \exists t : (x = x_0 + t \wedge y = y_0 + t)$

$\dot{\vec{x}} = A\vec{x}$, then $Reach := \exists t : \vec{x} = e^{At}\vec{x_0}$

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

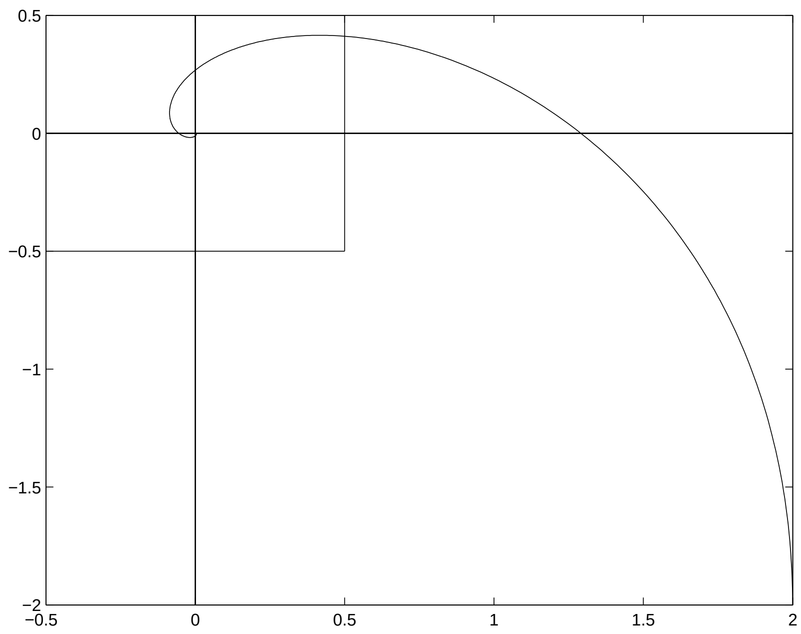
Consider the CDS:

$$\begin{aligned}\dot{x}_1 &= -x_1 - x_2\\ \dot{x}_2 &= x_1 - x_2\end{aligned}$$

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

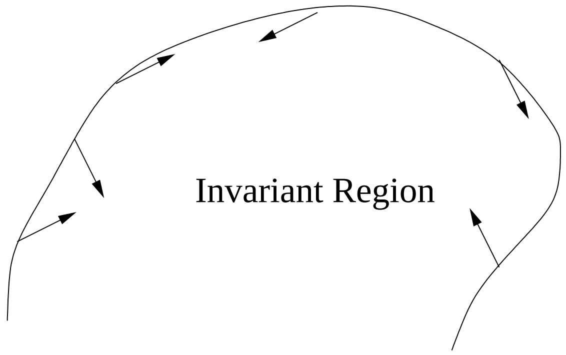
But there are more invariants:

$$|x_1| \leq 0.5 \wedge |x_2| \leq 0.5$$

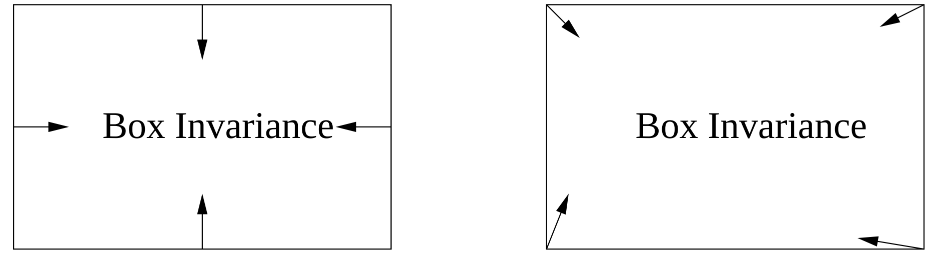


Invariants for Dynamical Systems

Illustration of invariant sets in 2-D:



Arbitrarily shaped



Box shaped

Box Invariants

A positively invariant rectangular box

$$\vec{l} \leq \vec{x} \leq \vec{u}$$

i.e., invariants of the form,

$$l_1 \leq x_1 \ \wedge \ x_1 \leq u_1 \ \wedge \ l_2 \leq x_2 \ \wedge \ x_2 \leq u_2 \ \wedge \ \ldots$$

Related Concepts—

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

Unstable systems can have useful box invariants

Why 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

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

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 = matrix obtained from A s.t. $a^m_{ii} = a_{ii},\ a^m_{ij} = |a_{ij}|$ for $i \neq j$.

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

- Is $\dot{\vec{x}} = A\vec{x}$ strictly box invariant?
- Is $\dot{\vec{x}} = A^m\vec{x}$ strictly box invariant?
- Is there a $\vec{z} > 0$ such that $A^m\vec{z} < 0$?
- 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

Linear Systems, Box Invariance, Metzler Matrices

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 τ s.t.:

1. τ is real; furthermore, $\tau > Re(\lambda)$, where λ is any other eigenvalue of A^m different from τ;
2. τ 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 $-(A^m)^{-1} > 0$.

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

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

$$\exists \vec{l}, \vec{u} : \forall \vec{x} : \bigwedge_{1 \le j \le n} ((\vec{x} \in FaceL^j(\vec{l}, \vec{u}) \Rightarrow \frac{dx_j}{dt} \ge 0) \wedge (\vec{x} \in FaceU^j(\vec{l}, \vec{u}) \Rightarrow \frac{dx_j}{dt} \le 0)), \tag{2}$$

If $\vec{p}$ are all polynomials, then
inductive properties of the form $|\vec{x}| \le c$ can be computed

Efficiency is an issue

Nonlinear Systems: Multiaffine

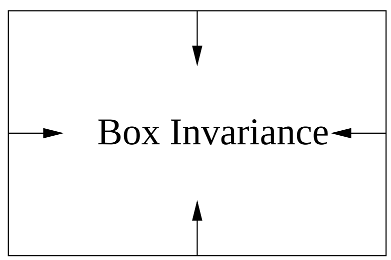
$$\frac{d\vec{x}}{dt} = \vec{p}(\vec{x})$$

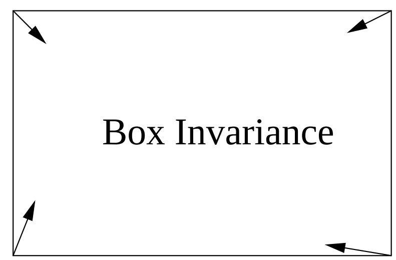
Multiaffine: Degree at most one in each variable

Example: $x_1x_2 - x_2x_3$ is multiaffine

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

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





Generalize: Degree of x_j can be arbitrary in p_j

Nonlinear Systems: Monotone

Generalize multiaffine systems

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

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

Examples:

$\dot{\vec{x}} = 1 - x^2$ is monotone, but not multiaffine

$\dot{\vec{x}} = x^3 + x$ is monotone, but not multiaffine

$\exists\forall(2n)$ 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

$$\begin{array}{lll} 1 - u_1 - \frac{u_1 l_2}{4} \leq 0, & u_2(2u_3 - 1) \leq 0, & \frac{u_1}{4} - 2u_3^2 \leq 0, \\ 1 - l_1 - \frac{l_1 u_2}{4} \geq 0, & l_2(2l_3 - 1) \geq 0, & \frac{l_1}{4} - 2l_3^2 \geq 0. \end{array}$$

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

Summary

- 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)