Progress on the reachability analysis and verification methods for hybrid systems

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Reachability analysis

Reachable set computations are useful for

• Verification

problems such as proving that the system does not reach a 'bad' state

• Controller synthesis

problems such as determining the set of states from which it is possible to reach a target set while avoiding a forbidden set

Many existing methods and tools (see the next slide)

Reachability analysis

Direct methods

- Track the evolution of the reachable set under the flow of the system. Various set representations: *e.g.* polyhedra, ellipsoids, level sets
- Exact results, or accurate approximations with error bounds. Using symbolic or numerical computations
- Tools: Coho, CheckMate, d/dt, HysDel, VeriShift, Vertdict, Requiem, Level-set toolbox, ..

Indirect methods

- Abstraction methods: reducing to a simpler system that preserves the property (*e.g.* Tiwari & Khanna 02; Alur et al. 02; Clarke et al. 03)
- Prove the property without computing reachable sets: *e.g.* Barrier certificates Prajna & Jadbabaie04, polynomial invariants Tiwari & Khanna04.

*** Scalability** is still challenging (complexity and size of real-life systems)

Our progress in reachability analysis

Accurate approximations

- Complexity of the dynamics
 - Hybridization methods for non-linear systems
 - Extension to differential algebraic systems
- Size of the system
 - Reachability technique using zonotopes \Rightarrow large scale systems

Abstraction methods: predicate abstraction, projection

Plan

- Hybridization methods for non-linear systems
- Extension to differential algebraic systems
- Reachability computations using zonotopes
- Abstraction by projection

Plan

- Hybridization methods for non-linear systems [Asarin, Dang, Girard 03, 05]
- Extension to differential algebraic systems
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Hybridization: Principle

System Δ : $\dot{x} = f(x), x \in \mathcal{X}, f$ is Lipschitz

Step 1: Construction of the approximate system:

- Partition the state space \mathcal{X} into disjoint regions of size **h** and assign to each region an approximate vector field
- h: space discretization size
- $f_{\rm h}$: resulting vector field over the whole state space \mathcal{X}
- Approximation error $\boldsymbol{\varepsilon}(\mathbf{h}) = \sup_{x \in \mathcal{X}} ||\mathbf{f}(\mathbf{x}) \mathbf{f}_{\mathbf{h}}(\mathbf{x})||$
- Conservative approximate system

System
$$\Delta_{\mathbf{h}}$$
: $\dot{x} = f_{\mathbf{h}}(x) + u$

 $u(\cdot):$ disturbance taking values in $Ball(\boldsymbol{\varepsilon}(\mathbf{h}))$

Hybridization: Principle (cont'd)

Step 2. Using $\Delta_{\mathbf{h}}$ to yield approximate analysis results for Δ

Convergence results: If $\Delta_{\mathbf{h}}$ is continuous

- The distance between the reachable sets $d_H(Reach(\Delta), Reach(\Delta_h))$ is $\mathcal{O}(\boldsymbol{\varepsilon}(\mathbf{h}))$
- The reachable set of $\Delta_{\mathbf{h}}$ converges to the reachable sets of Δ with the same rate as $f_{\mathbf{h}}$ converges to f

We developed two methods for constructing approximate systems with good error bound $\pmb{\varepsilon}(\mathbf{h})$

- Piecewise affine systems
- Piecewise multi-affine systems

Piecewise affine approximation

- Using a simplicial mesh, each cell C_i is a simplex of size **h** (edge length)
- Define for each C_i a linear function f_h interpolating f at its vertices
- Piecewise linear function $f_{\rm h}$ is continuous over the state space

Approximation error

If f is C^2 on \mathcal{X} with bounded second order derivatives \Rightarrow quadratic error: $\boldsymbol{\varepsilon}(\mathbf{h}) = \mathcal{O}(\mathbf{h}^2)$.

Mesh construction: decompose a hypercube into n! simplices



- Reachability computations for $\Delta_{\mathbf{h}}$: various existing techniques
- Our implementation using reachability procedures of the tool d/dt

Piecewise multi-affine approximation

- Using a rectangular mesh, each cell C_i is a hypercube of size **h**
- Define for each cell C_i a multi-linear function f_h interpolating f at its vertices \Rightarrow iteratively applying linear interpolation on each dimension
- Piecewise multi-linear function $f_{\mathbf{h}}$ is continuous over the state space

Approximation error: If f is C^2 on \mathcal{X} with bounded second order derivatives \Rightarrow quadratic error: $\boldsymbol{\varepsilon}(\mathbf{h}) = \mathcal{O}(\mathbf{h}^2)$.



Piecewise multi-affine approximation (cont'd)

 \star Advantage comparison

Simplicial meshes	Rectangular meshes			
	smaller number of cells			
	less complex geometric structure			
available techniques	???			
for approximate systems				

 \star Reachability computations for piecewise multi-affine systems with input

- Use projection to obtain a uncertain bilinear control system
- Then, use our reachability technique for bilinear control systems

Plan

- Hybridization methods for nonlinear systems
- Extension to differential algebraic systems [Dang, Donze, Maler FMCAD04]
- Reachability computations using zonotopes
- Abstraction by projection

Differential Algebraic Equations

Motivations

- DAEs arise in numerous applications: *e.g.* electrical circuits, constrained mechanical systems, chemical reaction kinetics, singular perturbation problems
- Our interest in applications of hybrid systems techniques to verification of analog and mixed-signal circuits

Reachability analysis of DAEs

 $F(x, \dot{x}) = 0$

- DAEs differ from ODEs (in theoretical and numerical properties)
- Differential index: minimal number of differentiations required to solve for the derivatives $\dot{\mathbf{x}}$
- We focus on **DAEs of index 1**

Extension to DAEs

Reachability analysis of DAEs (cont'd)

We study the equivalent semi-explicit form:

$$\dot{x} = f(x, y)$$
$$0 = g(x, y)$$

• Transforming into ODEs :

Differentiating the algebraic eq. once gives $\dot{y} = -g_y^{-1}g_x f$ where $g_y(x,y) = \partial g/\partial y$. (Note that the DAEs are of index 1) \Rightarrow Obtain augmented ODEs with variables $z = (x,y)^T$:

$$\dot{z} = (f, -g_y^{-1}g_x f)^T = \tilde{f}$$

• Retain the algebraic constraint and integret the original DAEs as the augmented ODEs on a manifold :

$$\dot{z} = \tilde{f}(z)$$
$$0 = g(z)$$

ODEs on manifolds

Remark: ODEs on manifolds are useful to study systems with invariants

Combining reachability computations techniques for ODEs and ideas from *geometric integration using projection* [Lubich, Hairer, Wanner 2003]



Algorithm for ODEs on manifolds

$$\begin{array}{l} R_0: \text{ initial set} \\ \textbf{repeat} \quad k = 0, 1, \dots \\ \hat{R}_{k+1} = \textbf{Reach}_{[0,r]}(R_k) \ /^* \ computed \ for \ the \ augmented \ ODEs \ */ \\ R_{k+1} = \Pi_{\mathcal{M}}(\hat{R}_{k+1}) \qquad /^* \ project \ on \ the \ manifold \ \mathcal{M} \ */ \\ \textbf{until} \quad R_{k+1} = \bigcup_{i=1}^k R_i \end{array}$$

• Projection:

$$\Pi_{\mathcal{M}}(\hat{z}) = \arg\min_{z} |\hat{z} - z| \text{ subject to } g(z) = 0$$

- Convergence : same order as the convergence order of the technique for ODEs (projection does not deteriorate the convergence)
- Second order method

Approximation of the projection

Manifold \mathcal{M} : g(x) = 0

P is a convex polyhedron, computing $\Pi_{\mathcal{M}}(P)$??

- If the algeb. constraint is linear, $\Pi_{\mathcal{M}}$ is computed using linear algebra.
- { v^1, \ldots, v^m }: vertices of $P, \overline{\Pi}_{\mathcal{M}}(P) = conv \{ \Pi_{\mathcal{M}}(v^1), \ldots, \Pi_{\mathcal{M}}(v^m) \}.$
- Using $\overline{\Pi}_{\mathcal{M}}(P)$ to over-approximate the projection
 - Estimate ρ , the maximum radius of curvature of \mathcal{M} for $x \in \overline{\Pi}_{\mathcal{M}}(P)$
 - Estimate the diameter δ of $\overline{\Pi}_{\mathcal{M}}$
 - If $\rho \leq \kappa \delta$, subdivide $\overline{\Pi}_{\mathcal{M}}(P)$ and then repeat the procedure for each subpolyhedron. Otherwise, find a polyhedron enclosing $\Pi_{\mathcal{M}}(P)$.





Example: Biquad lowpass filter

[Hartong, Hedrich, Barke 2002]



$$\dot{u}_{C1} = \frac{u_{C2} + u_o - u_{C1}}{C_1 R_2} \qquad \dot{u}_{C2} = \frac{U_i - u_{C2} - u_o}{C_2 R_1} - \frac{u_{C2} + u_o - u_{C1}}{C_2 R_2},\tag{1}$$

$$u_o - V_{max} \tanh(\frac{(u_{C2} - u_o)V_e}{V_{max}}) + U_{om} = 0,$$
(2)

$$U_{om} = \mathcal{V}(i_0), \quad i_o = -C_2 \,\dot{u}_{C2},$$
(3)

$$\mathcal{V}(i_o) = K_1 i_o + 0.5 \sqrt{K_1 i_o^2 - 2K_2 i_o I_s + K_1 I_s^2 + K_2 - 0.5} \sqrt{K_1 i_o^2 + 2K_2 i_o I_s + K_1 I_s^2 + K_2}.$$
 (4)

Biquad lowpass filter: verification results

The property to verify is the *absence of overshoots*.



- $C_1 = 0.5e 8$, $C_2 = 2e 8$, and $R_1 = R_2 = 1e6$ (highly damped case)
- The initial set: $u_{C1} \in [-0.3, 0.3], u_{C2} \in [-0.3, 0.3]$ and $u_o \in [-0.2, 0.2]$
- Reachability for the ODE part is done using a simplicial mesh

Plan

- Hybridization methods for nonlinear systems
- Extension to differential algebraic systems
- Reachability computations using zonotopes [A. Girard 2005]
- Abstraction by projection

Linear Systems with uncertain inputs $\dot{x} = Ax + u, ||u(\cdot)|| \le \mu$

• $Reach_r(X_0) \subseteq \mathbf{e}^{\mathbf{r}\mathbf{A}}X_0 + Ball(\alpha_r)$

•
$$\alpha_r = \frac{e^{r||A||} - 1}{||A||} \mu$$

- Two required operations:
 - -Linear operator e^{rA}
 - Minkowski sum ('expanding' the reachable set of the autonomous system by α_r)
- On **zonotopes**, these two operations can be efficiently performed (see next)

Reachability computations using zonotopes

Zonotopes

• Zonotope: Minkowski sum of a finite number of segments:

$$Z = \{ x \in \mathbb{R}^n \mid x = \mathbf{c} + \sum_{i=1}^p x_i \mathbf{g_i}, \ -1 \le x_i \le 1 \}.$$

• **c** is the center of the zonotope, $\{\mathbf{g}_1, \ldots, \mathbf{g}_p\}$ are the generators. The ratio p/n is the order of the zonotope.



Two-dimensional zonotope with 3 generators

Computational advantages of zonotopes

- Encoding of a zonotope has a **polynomial complexity** wrt dimension (vs. **exponential complexity** for general convex polyhedra)
- Zonotopes are closed under **linear transformation**

 $Z = (\mathbf{c}, \langle \mathbf{g_1}, \dots, \mathbf{g_p} \rangle)$

$$LZ = (L\mathbf{c}, \langle L\mathbf{g}_1, \dots, L\mathbf{g}_p \rangle)$$

• Zonotopes are closed under the **Minkowski sum**

$$\mathbf{Z}_1 = (\mathbf{c}_1, \langle \mathbf{g}_1, \dots, \mathbf{g}_p \rangle), \quad Z_2 = (c_2, \langle h_1, \dots, h_q \rangle)$$
$$\mathbf{Z}_1 + Z_2 = (\mathbf{c}_1 + c_2, \langle \mathbf{g}_1, \dots, \mathbf{g}_p, h_1, \dots, h_q \rangle)$$

 \Rightarrow **Important properties** needed for reachability computations

Complexity reduction

At each iteration, the order of the zonotope increases (due to the Minkowski sum) \Rightarrow Complexity is $\mathcal{O}(\mathbb{N}^2)$ where \mathbb{N} is the number of iterations

Controlling the order growth

- When the order is greater than m, over-approximate by a zonotope of lower order \Rightarrow Efficient zonotope order reduction techniques exist
- \bullet Thus, the complexity of the algorithm is $\mathcal{O}(N)$



Performance

Dimension	5	10	20	50	100
CPU time (s)	0.05	0.33	1.5	9.91	43.7

(Computation of $Reach_{[0,1]}$, 100 iterations, zonotope order=5)

A 5-dimensional system



Projections of $Reach_{[0,1]}$, 200 iterations, order of the zonotopes 40.

Reachability computations using zonotopes: Summary

• Efficient and scalable

- Handle systems up to **100 dimensions**
- Can be extended to **non-linear** systems and **hybrid** systems
- **Future work:** Computational methods for zonotopes (intersection, union)

Plan

- Hybridization methods for nonlinear systems
- Extension to differential algebraic systems
- Reachability computations using zonotopes
- Abstraction by projection [Asarin & Dang 04]

Introduction

- Basic idea: **project away** some variables the evolution of which is modeled as input
- **Dimension reduction** method for continuous systems
- A 'hybridization' method using ideas of qualitative simulation
- Goals:
 - more precise than qualitative simulation
 - less expensive than analyzing the original system (due to lower dimension)

Principle

 $\left\{ \begin{array}{ll} \dot{x} &= f(x,y,z) \\ \dot{y} &= g(x,y,z) \\ \dot{z} &= h(x,y,z) \end{array} \right. \label{eq:constraint}$

- \bullet We want to abstract away variable ${\bf z}$
- Partition the domain of \mathbf{z} into k disjoint intervals

$$\{[l^1, u^1), [l^2, u^2), \dots [l^k, u^k]\}$$

where $l^{i+1} = u^i$ for all i

• If $z \in I_z^i = [l^i, u^i]$, the dynamics of x and y can be approximated by **differential inclusion** :

$$\begin{cases} \dot{x} \in F_i(x, y) = \{ f(x, y, z) \mid z \in I_z^i \} \\ \dot{y} \in G_i(x, y) = \{ g(x, y, z) \mid z \in I_z^i \} \end{cases}$$

Hybridization

- The original system is thus approximated by 2-dimensional **hybrid** system with **k** different continuous dynamics
- Switching between adjacent intervals I_z^i :
 - Transition from $I_z^i = [l^i, u^i)$ to $I_z^{i+1} = [l^{i+1}, u^{i+1})$ is possible if at the boundary the derivative of **z** is positive, i.e. $h(x, y, u_i) > 0$
 - Similarly, transition from I_z^{i+1} to I_z^i if $h(x, y, u_i) < 0$
 - These switching conditions are not sufficient \Rightarrow conservative approximation



Remedy Discontinuities

- Our hybridization method introduces **discontinuities**
- "Convexify" the dynamics at switching surfaces (to guarantee existence of solution, error bound)
- Between adjacent intervals I_z^i and I_z^j (j = i + 1), add a location:

$$\begin{cases} \dot{x} \in F_{ij}(x,y) = co\{F_i(x,y), F_j(x,y)\} \\ \dot{y} \in G_{ij}(x,y) = co\{G_i(x,y), G_j(x,y)\} \end{cases}$$



Convergence result

- Resulting abstract system is upper semi-continuous and one-sided Lipschitz
 - \Rightarrow We can prove **error bound**:
 - Distance between trajectories of the original system and the abstract system is $\mathcal{O}(\delta)$
 - $-\delta$: bound on the distance between the derivatives (which depends on the size of the **z**-mesh)
- First order method

Abstraction with timing information

- So far, only the sign of \dot{z} is used to determine switching conditions
- The time the system can stay with a dynamics is omitted
- Inlude timing information to obtain more precise abstraction
 - Additionally **discretize derivatives** \dot{z} into disjoint intervals
 - Each location corresponds to an interval I_z^i of z and an interval $I_{\dot{z}}^j$ of \dot{z}
 - Then, we can estimate **bounds on the staying times** \Rightarrow embed in the switching conditions.

Computation Issues

- Linear Systems: abstract system is a linear system with uncertain input.
- Non-linear systems: abstract system is a **general differential in**clusions
- We focus on the case of **multi-affine systems** (which have numerous applications in biology, economy)

Abstraction of multi-affine systems

Given a system

$$\begin{cases} \dot{x}_1 = a_1 x_1 + b_1 x_2 + c_1 x_1 x_2 \\ \dot{x}_2 = a_2 x_1 + b_2 x_2 + c_2 x_1 x_2 \end{cases}$$

Abstract away $x_2 \Rightarrow$ Dynamics of each cell:

$$\begin{cases} \dot{x}_1 = a_1 x_1 + b_1 \mathbf{u} + c_1 \mathbf{u} x_2 \\ ||\mathbf{u}(\cdot)|| \le \mu \end{cases}$$

 \Rightarrow bilinear control system

Reachability analysis of Bilinear Control Systems

A bilinear control system with additive and multiplicative inputs

$$\dot{x}(t) = f(x(t), u(t)) = Ax(t) + \sum_{j=1}^{l} u_j(t)B_jx(t) + Cu(t)$$

Basic idea: Applying the Maximum principle to find 'optimal' input $\tilde{u} \Rightarrow$ require solving an optimal control problem for a bilinear system.

For tractability purposes,

- 1. Restrict to piecesiwe constant inputs
- 2. To solve bilinear diff equations, treat the bilinear term as independent input (see next)

Applying the Maximum Principe

* Represent the initial set X_0 as intersection of half-spaces. * For each half-space H = (q, x) with normal vector q and supporting point x.

$$\begin{split} \dot{\tilde{x}} &= A\tilde{x} + \tilde{u}B\tilde{x} + C\tilde{u} \\ \dot{\tilde{q}} &= -\frac{\partial H}{\partial x}(\tilde{x}, \tilde{q}, \tilde{u}) \text{ where } H(q, x, u) = \langle q, Ax + ubx + cu \rangle \\ \tilde{u}(t) &\in argmax\{\langle \tilde{q}(t), \ uB\tilde{x}(t) + Cu \rangle \mid u \in U\} \end{split}$$

with initial conditions: $\tilde{q}(0) = q$, $\tilde{x}(0) = x$.

Then,

- For all t > 0, the half-space $H(\tilde{q}(t), \tilde{x}(t))$ contains $Reach_t(X_0)$
- Its hyperplane is a supporting hyperplane of $Reach_t(X_0)$.

Bilinear Control Systems

★ Solving the optimal control problem for arbitrary inputs is hard ⇒ restrict to **piecewise constant inputs** $u(t) = u^k$ for $t \in [t_k, t_{k+1})$.

 \star Solving bilinear systems with piecewise constant input: r is time step

$$x^{k+1} = e^{Ah}x^k + \int_0^r e^{A(r-\tau)}u^k b \,\mathbf{x}(\tau) \,d\tau + \int_0^r e^{A(r-\tau)}c u^k \,d\tau$$

• Approximate $x(\tau)$ for $\tau \in [0, r)$ by: $\pi(\tau) = \alpha \tau^3 + \beta \tau^2 + \gamma \tau + \sigma$ satisfying Hermite interpolation conditions: $\pi(0) = x(t_k), \ \dot{\pi}(0) = \dot{x}(t_k), \ \pi(r) = x(t_{k+1}), \ \dot{\pi}(r) = \dot{x}(t_{k+1})$

• Replacing $\mathbf{x}(\tau)$ by $\pi(\tau)$ in the integral, we obtain: $Mx^{k+1} = Dx^k + d$

• We can prove that the **error is quadratic** in time step $O(r^2)$

Example: A biological system

A multi-affine system, used to model the gene transcription control in the *Vibrio fischeri* bacteria [Belta et al 03].

$$\begin{cases}
\dot{x_1} = k_2 x_2 - k_1 x_1 x_3 + u_1 \\
\dot{x_2} = k_1 x_1 x_3 - k_2 x_2 \\
\dot{x_3} = k_2 x_2 - k_1 x_1 x_3 - n x_3 + n u_2
\end{cases}$$
(5)

State variables x_1 , x_2 , x_3 represent cellular concentration of different species

Parameters k_1 , k_2 , n are binding, dissociation and diffusion constants. Control variables u_1 and u_2 are plasmid and external source of autoinducer.

Goal: drive the system through to the face $x_2 = 2$

Example: A biological system (cont'd)

Results obtained by abstracting away x_1 . Location $x_1 \in [1.0, 1.5]$

uncontrolled system (u = 0)



controlled system



Ongoing and Future work

- Zonotopic calculus
- Efficient method for multi-affine systems
- \bullet Hybridization: Hierarchical mesh construction
- Randomized simulation with coverage criteria
- Guided abstraction refinement

