Proofs from Simulations and Modular Annotations

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Background

- Invariant verification for dynamical systems.
 - Through computing the set of state the system can reach (reach set)
 - Exact Reach set computation is in general undecidable ⇒ Over-approximation
- Static analysis and symbolic approaches
 - E.g. SpaceEx, PHAVer, CheckMate, d/dt
- Dynamic+Static analysis using numerical simulations
 - E.g. S-TaLiRo, Breach, C2E2

Simulation-based Reachability

- $\dot{x} = f(x), \Theta \subseteq \mathbb{R}^n$
- Denote $\xi(\theta, t)$ as a trajectory from $\theta \in \Theta$
- Simulation-based Verification
 - Finite cover of Θ (
 - Simulate from the center of each cover.
 - Bloat the simulation with some factor, such that the bloated tube contains all trajectories starting from the cover.
 - Union of all such tubes gives an over-approximation of reach set
- In [1], we expect the bloating factor to be given by the user as an annotation to the model



Annotation: Discrepancy Function

Definition. Functions $V: X \times X \to \mathbb{R}^{\geq 0}$ and $\beta: \mathbb{R}^{\geq 0} \times T \to \mathbb{R}^{\geq 0}$ define a discrepancy of the system if for any two states θ_1 and $\theta_2 \in \Theta$, For any t, $V(\xi(\theta, t), \xi(\theta', t)) \leq \beta(|\theta - \theta'|, t)$ where, $\beta \to 0$ as $\theta \to \theta'$

- Stability not required
- Discrepancy can be found automatically for linear systems
- For nonlinear systems, several template-based heuristics were proposed



Key challenge: Finding Discrepancy Functions for Large Models

Models of Cardiac Cell Networks

- FitzHugh–Nagumo (FHN) model [1]
- Invariant property
 - Threshold of voltage
 - Periodicity of behavior



[1] FitzHugh. Biophysical J. 1961[2] Aylward, Parrilo, Slotine. Automatica. 2008

• Find quadratic contraction metric [2]:

•
$$J(v, w) = \begin{bmatrix} 0.5 - 3v^2 & -1 \\ 1 & -1 \end{bmatrix}$$

• Search for $\beta \in \Re$ and the coefficients of $R(v,w) = \begin{bmatrix} \sum a_{ij} v^i w^j & \sum b_{ij} v^i w^j \\ \sum b_{ij} v^i w^j & \sum c_{ij} v^i w^j \end{bmatrix},$

s.t. $0 \le i + j \le 2, R > 0$, and $J^T R + RJ + \dot{R} < -\beta M$



Scalability of Finding Annotation



Input-to-State (IS) Discrepancy

Definition. Functions $V: X_1 \times X_1 \to \mathbb{R}^{\geq 0}$, $\beta: \mathbb{R}^{\geq 0} \times \mathbb{R}^{\geq 0} \to \mathbb{R}^{\geq 0}$ and $\gamma: \mathbb{R}^{\geq 0} \to \mathbb{R}^{\geq 0}$ define a IS discrepancy of the system:

 $V_1(\xi_1(\theta_1, u_1, t), \xi(\theta_1', u_1', t)) \le \beta_1(|\theta_1 - \theta_1'|, t) + \int_0^T \gamma_1(|u_1(s) - u_1'(s)|) ds$

and
$$\gamma_1(\cdot) \rightarrow 0$$
 as $u_1 \rightarrow u_1'$

 $\begin{aligned} &(\xi_1, \xi_2) \text{ and } (\xi_1', \xi_2') \text{ are a pair of trajectories} \\ & \text{ of the overall ring:} \\ & \left\{ V_1(\xi_1(t), \xi_1'(t)) \le \beta_1(|\theta_1 - \theta_1'|, t) + \int_0^t \gamma_1(|\xi_2(s) - \xi_2'(s)|) ds \\ & V_2(\xi_2(t), \xi_2'(t)) \le \beta_2(|\theta_2 - \theta_2'|, t) + \int_0^t \gamma_2(|\xi_1(s) - \xi_1'(s)|) ds \\ \end{aligned} \right. \end{aligned}$



More on IS Discrepancy

• IS Discrepancy:

$$V\big(\xi(\theta, u, t), \xi(\theta', u', t)\big) \le \beta(|\theta - \theta'|, t) + \int_0^t \gamma(|u(s) - u'(s)|)ds$$

- Incremental integral input-to-state stability [1], except no stability property is required.
- Most methods of finding discrepancy of $\dot{x} = f(x)$ can be modified to find IS discrepancy systems with linear input $\dot{x} = f(x) + Bu$.

IS Discrepancy \Rightarrow Reachability

• We will build a reduced model $M(\delta)$ with a unique trajectory $\mu(t)$ using the IS Discrepancy.



• **Theorem**: for small enough δ and precise enough simulation, the over-approximation can be computed arbitrarily precise.

Construction of the Reduced Model

• Reduced model $M(\delta)$

•
$$\dot{x} = f_M(x)$$
 with $x = \langle m_1, m_2, clk \rangle$
• $\begin{bmatrix} \dot{m_1} \\ m_2 \\ clk \end{bmatrix} = \begin{bmatrix} \dot{\beta}_1(\delta, clk) + \gamma_1(m_2) \\ \dot{\beta}_2(\delta, clk) + \gamma_2(m_1) \\ 1 \end{bmatrix}$
• $m_i(0) = \beta_i(\delta, 0), clk(0) = 0$

 ξ_1, u_2

 ξ_2, u_1

• $M(\delta)$ has a unique trajectory $\mu(t)$.

Reduced Model \Rightarrow Bloating Factor

The ODE of the reduced model $M(\delta)$:

$$\begin{pmatrix} \dot{m_1} \\ m_2 \\ c l k \end{pmatrix} = \begin{pmatrix} \dot{\beta_1}(\delta, c l k) + \gamma_1 (m_2) \\ \dot{\beta_2}(\delta, c l k) + \gamma_2 (m_1) \\ 1 \end{pmatrix}$$

The IS Discrepancy functions: $\begin{cases}
V_1(\xi_1(t), \xi_1'(t)) \leq \beta_1(|\theta_1 - \theta_1'|, t) + \int_0^t \gamma_1(|\xi_2(s) - \xi_2'(s)|) ds \\
V_2(\xi_2(t), \xi_2'(t)) \leq \beta_2(|\theta_2 - \theta_2'|, t) + \int_0^t \gamma_2(|\xi_1(s) - \xi_1'(s)|) ds
\end{cases}$

• Lemma: $|\theta_1 - \theta'_1| \leq \delta$, and $|\theta_2 - \theta'_2| \leq \delta \implies$ $V_1(\xi_1(t), \xi'_1(t)) \leq m_1(t)$, and $V_2(\xi_2(t), \xi'_2(t)) \leq m_2(t)$.

• Thus, bloating $\xi(\theta, t)$ by $\mu(t)$ gives an overapproximation of reach set from a ball.



Simulation & Modular Annotation \Rightarrow Proof



Soundness and Relative Complete

- Robustness Assumption:
 - Invariant is closed.
 - If an initial set Θ satisfies the invariant, $\exists \epsilon > 0$, such that all trajectories are at least ϵ distance from the boundary of the invariant.
- **Theorem**: the Algorithm is sound and relatively complete
- We verify systems with upto 30 dimensions in minutes.

System	# Variables	# Module	# Init. cover	Run Time
Lin. Sync	24	6	128	135.1
Nonli. WT	30	6	128	140.0
Nonli. Robot	6	2	216	166.8

Conclusion

- A scalable technique to verify nonlinear dynamical systems using modular annotations
- Modular annotations are used to construct a reduced model of the overall system whose trajectory gives the discrepancy of trajectories
- Sound and relatively complete
- Ongoing: extension to hybrid, cardiac cell network with 5 cells each has 4 continuous var. and 29 locations

• Thank you for your attention!