Lagrangian Approaches to Forward Reachability in Continuous State Spaces

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Verification: Safety Analysis

• Does there exist a trajectory of system H leading from a state in initial set *I* to a state in terminal set *T*?



Calculating Reach Sets

- Two primary challenges
 - How to represent set of reachable states
 - How to evolve set according to dynamics
- Discrete systems $x_{k+1} = \delta(x_k)$
 - Enumerate trajectories and states
 - Efficient representations: Binary Decision Diagrams
- Continuous systems dx/dt = f(x)?



Typical Systems: ODEs

- Common model for continuous state spaces
- Lipschitz continuity of *f* ensures existence of a unique trajectory
 - Trajectories cannot cross, so boundary of reachable set derives from boundary of initial or target set

ODE $\dot{z}(t) = f(z(t))$ with initial conditions $z(t_0) = z_0$ gives rise to trajectory $\xi_{H_C}(t; z_0, t_0)$ where

- $f: \mathbb{Z} \to \mathbb{T}\mathbb{Z}$ are (Lipschitz) dynamics
- Often $\mathbb{Z} \subseteq \mathbb{R}^{d_z}$

System specified by $H_{C} = (\mathbb{Z}, f)$

Working with Sets

- Optimal control works with a single optimal trajectory
- Verification works with sets of trajectories
 - Takes a nondeterministic (but not probabilistic) viewpoint
- Basic construct is reachability
 - Many versions: forward and backward, sets or tubes
 - When available, what should the input(s) do?
- Many related concepts in control theory
 - Invariant sets, controlled invariant sets, stability
- Safety is not the only verification goal
 - Liveness is a common goal, but often harder to verify

Forward Reachability

• Start at initial conditions and compute forward



Backward Reachability

• Start at terminal set and compute backwards



Exchanging Algorithms

• Algorithms are (mathematically) interchangeable if system dynamics can be reversed in time

Backward dynamic system $\overleftarrow{\mathsf{H}}$ such that $\forall s, t \in \mathbb{T}$ $\xi_{\mathsf{H}}(s; z, t) = \widehat{z} \iff \xi_{\overleftarrow{\mathsf{H}}}(s; \widehat{z}, t) = z.$

- For example: $\overleftarrow{H}_{C} = (\mathbb{Z}, -f)$
- Then

$$F(\mathsf{H}, S, [0, t]) = B(\overleftarrow{\mathsf{H}}, S, [0, t])$$
$$F(\mathsf{H}, S, t) = B(\overleftarrow{\mathsf{H}}, S, t)$$

Lagrangian Approaches

- "Lagrangian" computation is performed along trajectories of the system
 - Compare with "Eulerian" computation, which occurs on a grid which does not move with the trajectories
- Typically defined in terms of forward reach sets & tubes
- Advantages: Compact representation of sets, overapproximation guarantees, demonstrated high dimensions
- Disadvantages: restricted dynamics, reliance on trajectory optimization, restrictive set representation

Examples of Lagrangian Schemes

- Timed automata
 - Derivatives are zero or one; continuous variables are "stopwatches"
 - Uppaal [Larsen, Pettersson...], Kronos [Yovine,...], ...
- Rectangular differential inclusions ("linear" hybrid automata)
 - Derivatives lie in some constant interval
 - Hytech, Hypertech [Henzinger, Ho, Horowitz, Wong-Toi, ...]
- Polyhedra and (mostly) linear dynamics
 - Derivatives are linear (or affine) functions
 - Checkmate [Chutinan & Krogh], d/dt [Bournez, Dang, Maler, Pnueli, ...], PHAVer [Frehse], Coho [Greenstreet, Mitchell, Yan], others [Bemporad, Morari, Torrisi, ...], ...
- Ellipsoids and linear dynamics
 - [Botchkarev, Kurzhanski, Kurzhanskiy, Tripakis, Varaiya, ...]
- Zonotopes and linear dynamics
 - [Girard, le Guernic & Maler]

Four Examples of Lagrangian Schemes

- CheckMate & convex polygons
- Zonotopes
- Ellipsoids
- Coho & projectagons
- Note:
 - Choices are heavily influenced by my expertise
 - I may choose different (and potentially conflicting) variable names in these slides when compared with the assigned papers

CheckMate

- Designed to verify properties of Polyhedral Invariant Hybrid Automata (PIHA)
 - Hybrid automata with invariants/guards defined by conjunctions of linear inequalities (convex polyhedra)
- Works by computing an Approximate Quotient Transition System (AQTS)
 - Discrete transition system which conservatively simulates the hybrid automata's evolution
- Released as an add-on to Mathworks' Simulink / Stateflow
 - Model can be constructed graphically
 - Same model can be simulated and verified

Continuous Algorithm

- Start with an initial set X_0
- Reach set V_{tk}(X₀) at a later time t_k can be determined by simulating trajectories from each vertex of X₀
- Given reach set at t_k and t_{k+1} , initial approximation of reach tube for $[t_k, t_{k+1}]$ is convex hull of $V_{t_k}(X_0)$ and $V_{t_{k+1}}(X_0)$
- Trajectories may curve, so use optimization to push edges of convex hull outward until reach tube contains all reachable states
- For linear dynamics $\dot{x} = Ax$, analytic solution is $\xi(t; x_0, t_0) = e^{A(t-t_0)}x_0$, so optimization is a linear program for any fixed t(easy to solve)



from Chutinan & Krogh, IEEE Trans. AC, fig. 4, p. 68 (2003)

Continuous Algorithm's Issues

- Global nonlinear optimization provides no guarantees
 - Dilated convex hull may not contain all possible trajectories
- Trajectories are approximated numerically
- Accomodating inputs requires additional trust in optimization procedure

CheckMate reach tube examples for 2D Van der Pol model and a 3D linear model



from Chutinan & Krogh, Proc IEEE CDC, fig. 2, p. 2091 & fig. 3, p 2092 (1998)

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Constructing the AQTS

- Reach tube construction is used to determine what set of states on an incoming polyhedral invariant face maps to which set of states on an outgoing polyhedral invariant face
- Sets of states on face are mapped to discrete states in the AQTS (with possible subdivisions)



Primary CheckMate Papers

- Alongkrit Chutinan & Bruce H. Krogh, "Computing Polyhedral Approximations to Flow Pipes for Dynamic Systems," *Proc. IEEE Conference on Decision & Control*, pp. 2089–2094 (1998)
 - Details of the scheme for approximating continuous "flow pipes" (forward reach tubes)
- Alongkrit Chutinan & Bruce H. Krogh, "Verification of Infinite-State Dynamic Systems using Approximate Quotient Transition Systems," *IEEE Trans. on Automatic Control*, vol. 46, num. 9, pp. 1401–1410 (2001)
 - Procedure for constructing the AQTS and hence verifying a model for a continuous system, assuming a scheme for computing continuous reachable sets
- Alongkrit Chutinan & Bruce H. Krogh, "Computational Techniques for Hybrid System Verification," *IEEE Trans. on Automatic Control*, vol. 48, num. 1, pp. 64–75 (2003)
 - Journal version of CDC paper, including proof of flow pipe approximation convergence & detailed batch evaporator example
- Numerous other papers (see CheckMate web site)

CheckMate Outcomes

- Most complete tool for hybrid systems with non-constant dynamics
 - (Partially) integrated with commercial design package
 - Handles hybrid system verification, not just continuous reachability
 - Generates counter-examples on failure
 - Later work integrated Counter-Example Guided Abstraction Refinement (CEGAR) [Clarke, Fehnker, Han, Krogh, Stursberg, Theobald, TACAS 2003]
- Unable to move beyond low dimensions
 - Polyhedral representation grows too complex
 - One proposal: Oriented Rectangular Hull representation [Krogh & Stursberg, HSCC 2003]

A Brief Description of d/dt

- Similar basic idea to CheckMate
 - Encorporates "griddy polyhedron" construction to control complexity of full reach set representation
 - Various continuous reachability extensions: competing inputs, projections, …
- Many publications
 - Eugene Asarin, Olivier Bournez, Thao Dang & Oded Maler, "Approximate Reachability Analysis of Piecewise-Linear Dynamical Systems" in *Hybrid Systems Computation & Control* (Nancy Lynch & Bruce H. Krogh eds.), LNCS 1790, pp. 20-31 (2000)
 - Fig. 2, p. 25 shown at right



Zonotopes

- Representation of general convex polyhedra is too complex in higher dimensional spaces
- Instead, choose a category of sets that can be efficiently represented
- Zonotopes:
 - Image of a hypercube under an affine projection
 - Minkowski sum of a finite set of line segments

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

$$Z = \left\{ x \in \mathbb{R}^n \mid x = c + \sum_{i=1}^{i=p} \lambda_i g_i, \ \lambda_i \in [-1, +1] \right\}$$
where $c, \ g_1, \ g_2, \ \dots, \ g_p$ are vectors in \mathbb{R}^n

 $Z = (c, < g_1, g_2, g_3 >)$

Zonotope Features

- Compact representation: storage cost n(p+1)
- Closed under linear transformation: if $\mathcal{L}x = \mathbf{A}x + b$ then

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

• Closed under Minkowski sum:

$$Z^{(1)} + Z^{(2)} = (c^{(1)} + c^{(2)}, \langle g_1^{(1)}, \dots, g_{p^{(1)}}^{(1)}, g_1^{(2)}, \dots, g_{p^{(2)}}^{(2)} \rangle)$$

- Conversion to other representations can be expensive; for example, a zonotope may have 2p choose n-1 facets
- Computation of intersection and union may be difficult; for example, see [Girard & Le Guernic, HSCC 2006]



Linear Dynamics with Bounded Inputs

Restrict class of ODEs to the form

$$\dot{x} = \mathbf{A}x + u, \qquad u \in U$$

where \boldsymbol{U} in this case is a hypercube

$$U = \{ u \in \mathbb{R}^n \mid ||u||_{\infty} \le \mu \}$$

- f(x, u) = Ax + u is Lipschitz in x, so standard existence and uniqueness results apply
- Trajectories now denoted by $\xi(t; x_0, t_0, u(\cdot))$ where function $u(\cdot) : \mathbb{R} \to U$ is an input signal
- Reach set with fixed (but not necessarily constant) input signal is the same as the input-free case
- Reach set with general input signal is the union over all possible fixed input signals

Continuous Algorithm

• Decompose full reach tube into segments

$$F(I, [0, T]) = \bigcup_{i} F(I, [ir, (i+1)r])$$

for some small timestep \boldsymbol{r}

• Time-independent ODEs have the semigroup property

$$\xi(t_1 + t_2; x_0, 0) = \xi(t_2; \xi(t_1; x_0, 0), t_1)$$

We can use the semigroup property to deduce

$$F(I, [ir, (i+1)r]) = F(F(I, [(i-1)r, ir]), r)$$

• Therefore, if we can conservatively approximate F(I, [0, r])and F(Z, r) for any Z, we can conservatively approximate F(I, [0, T])

Conservative Approximations

- Let $\|\cdot\| = \|\cdot\|_{\infty}$, "+" for sets be interpreted as the Minkowski sum and $\Box(\rho) = \{x \in \mathbb{R}^n \mid \|x\|_{\infty} \le \rho\}$ (which is a zonotope)
- $F(Z,r) \subseteq e^{rA}Z + \Box(\beta_r)$ where $\beta_r = \frac{e^{r||A||} - 1}{||A||} \mu,$ • $F(Z, [0,r]) \subseteq P + \Box(\alpha_r + \beta_r)$ where $\alpha_r = \left(e^{r||A||} - 1 - r||A||\right) \sup_{x \in Z} ||x||$ $P = \frac{1}{2} \left(c + e^{rA}c, \left\langle \begin{array}{c} g_1 + e^{rA}g_1, \dots, g_p + e^{rA}g_p, \\ g_1 - e^{rA}g_1, \dots, g_p - e^{rA}g_p \end{array} \right\rangle \right)$ from Girard, HSCC 2005, fig. 2, p. 295
- These approximations can be shown to converge (in the Hausdorff metric) as $r \rightarrow 0$

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Further Work

- Complexity of zonotopes in basic algorithm grows with time
 - Can conservatively constrain the order of the zonotope
- [Girard, Le Guernic & Maler, HSCC 2006]
 - Refactorizes the Minkowski sum to avoid growth of order
 - Constructs underapproximations and interval hull approximations
 - Discusses extension to hybrid automata (requires set intersection)
- [Girard & Le Guernic, HSCC 2008]
 - "Efficient" Algorithm for zonotope intersection with hyperplane



Reach tube for an oscillatory sink

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Zonotope Outcomes

- Still primarily a research project
 - MATISSE tool implements the continuous reachable set computation (including HSCC 2006?)
- Demonstrated on continuous toy examples in dimension 100 (HSCC 2005) and 200 (HSCC 2006)
- Demonstrated on low dimensional hybrid examples
- Zonotope representation has interesting trade-offs
 - Difficulty of computing set intersection and (presumably) union may make abstraction refinement challenging
 - Complexity (zonotope order) can be controlled over a wide range
 - Infinity norm bounds require well scaled system dynamics and inputs

Ellipsoids

- An alternative class of sets which can be efficiently represented in high dimensions
- Represent as the zero level set of a quadratic function
 - So computational costs in a given dimension are similar to LQR or Kalman filtering

Ellipsoid $\mathcal{E}(z,\mathbf{Z})\subset\mathbb{R}^n$ is specified by

$$\mathcal{E}(z,\mathbf{Z}) = \{x \in \mathbb{R}^d \mid (x-z)^T \mathbf{Z}^{-1} (x-z) \le 1\}$$

where $\mathbf{Z} \in \mathbb{R}^{n \times n}$ is the symmetric positive definite shape matrix and $z \in \mathbb{R}^n$ is the center



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Ellipsoid Features

- Compact representation: $\frac{1}{2}n^2 + O(n)$
- Operations (union, intersection, Minkowski sum, etc.) on ellipsoids rarely give rise to ellipsoids
 - However, inner and/or outer bounding ellipsoids of the results can often be constructed analytically or by convex optimization
 - See various works by Kurzhanski, Kurzhanskiy, Vályi, Varaiya and many others





Two ellipsoids (red & green), their actual Minkowski sum (black), and two ellipsoids bounding their Minkowski sum (cyan & blue)

Ellipsoidal Reachability

• Restrict dynamics to be linear

$$\dot{x} = \mathbf{A}x + \mathbf{B}u$$

where A, B are matrices, and input $u \in U = \mathcal{E}(p, \mathbf{P})$

- Even if $I = \mathcal{E}(x_0, \mathbf{X}_0)$, reach set F(I, t) is not an ellipse
- It is possible to construct tight external and internal bounding ellipses which touch the reach set at known points $\ell^*(t)$
- Choose $\ell^*(t)$ as a solution to the adjoint of the homogenous dynamics

$$\dot{\ell}^* = -\mathbf{A}^T \ell^*$$
 for some $\ell^*(\mathbf{0}) = \ell_0$,

so $\ell^*(t) = e^{-\mathbf{A}^T t} \ell_0$

 We can write a recurrance for the tight ellipsoids' parameters

External Bounding Ellipses

- Construct outer bounding ellipsoid $X_{\ell}^{+}(t) = \mathcal{E}(x_{c}(t), \mathbf{X}_{\ell}^{+}(t))$ such that $F(I, t) \subseteq X_{\ell}^{+}(t)$
- Center is just a trajectory (remember $u \in \mathcal{E}(p, \mathbf{P})$)

$$\dot{x}_c(t) = \mathbf{A}x_c(t) + \mathbf{B}p \qquad x_c(0) = x_0$$

• Shape satisfies a matrix ODE

$$\dot{\mathbf{X}}_{\ell}^{+}(t) = \mathbf{A}\mathbf{X}_{\ell}^{+}(t) + \mathbf{X}_{\ell}^{+}(t)\mathbf{A}^{T} + \pi_{\ell}(t)\mathbf{X}_{\ell}^{+}(t) + \frac{\mathbf{B}\mathbf{P}\mathbf{B}^{T}}{\pi_{\ell}(t)}$$
$$\mathbf{X}_{\ell}^{+}(0) = \mathbf{X}_{0}$$
$$\pi_{\ell}(t) = \left(\frac{\ell^{T}\mathbf{Y}(t)\mathbf{B}\mathbf{P}\mathbf{B}^{T}\mathbf{Y}^{T}(t)\ell}{\ell^{T}\mathbf{Y}(t)\mathbf{X}_{\ell}^{+}(t)\mathbf{Y}^{T}(t)\ell}\right)^{\frac{1}{2}}$$
$$\mathbf{Y}(t) = e^{\mathbf{A}t}$$

• A similar recurrance can be defined for an inner ellipsoid $X_{\ell}^{-}(t)$ such that $X_{\ell}^{-}(t) \subseteq F(I,t)$

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Further Work

- Actual derivation allows dynamics and input set to be time-dependent
- Also derived for systems with two inputs: "control" and "disturbance"
 - State x is reachable if there exists an initial condition in I and a feedback control signal $u(\cdot)$ that drives a trajectory to x for every possible disturbance signal $v(\cdot)$
- In practice, compute bounding ellipsoids for several different ℓ
 - For verification, test if all (outer) or any (inner) ellipsoid intersects with the target
 - For visualization and other operations, can compute bounding ellipsoids for intersections and unions
 - Shown at right: two outer and three inner bounding ellipsoids; actual reach set is contained in the intersection of the outer and the union of the inner





Ellipsoid Outcomes

- Described in a whole series of papers by Kurzhanski & Varaiya
- Implemented in Ellipsoidal Toolbox (ET) by Kurzhanskii
 - Documentation for ET provides concise summary of previous work
- Demonstrated in dozens of dimensions
- Demonstrated on low dimensional hybrid problems [Botchkarev & Tripakis, HSCC 2000] and ET
- Ellipsoid representation has different trade-offs
 - Extensive historical work on geometric operations makes extension to hybrid system reachability seem more feasible
 - Complexity of representation cannot be tuned: always $\frac{1}{2}n^2 + O(n)$
 - General linear input with ellipsoidal bounds adds flexibility



Coho & Projectagons

- Two dimensions is easy: Lots of fast, powerful algorithms
 - Can we design an algorithm that primarily works in two dimensional subsets of the full state space?
- "Projectagons"
 - Subset of high dimensional polyhedrons which can be represented as the intersection of a collection of prisms
 - Each prism is the infinite extension (into the other dimensions) of a bounded (potentially nonconvex) two dimensional polygon
 - We actually track only the two dimensional projections



Evolving a Projection (1)

- Let project agon be P and the prism represented by projection j be $P_j,$ so $P = \cap_j P_j$
- Then $CH(P) \subseteq \cap_j CH(P_j)$, where CH(P) is the convex hull of P
- $CH(P_j)$ is easily computed and can be represented by the conjuction of a set of linear inequalities
- Loosen ("bloat") all inequalities by ϵ
- Now consider an individual edge e_i in the two dimensional projection of P_j , which corresponds to a face of P
- Construct a box bounding all states within ϵ of e_i (also a conjuction of linear inequalities)
- The conjunction of all of the inequalities represents all states within ϵ of the face of P corresponding to e_i

Evolving a Projection (2)

- Construct an affine plus error model $\dot{x} = Ax + b + u$ for $u \in U$ and U a hyperrectangle that is valid within the conjunction of all these linear inequalities
- The forward time mapping of states under this dynamic is linear (if b = 0 and $U = \emptyset$ then it is e^{At})
- Use linear programming to compute the polygonal projection of the forward time mapping of e_i
- Repeat for all edges in the projection
- Compute the union of all forward time polygons (and all states inside that union)
- Simplify if necessary
- Repeat for all projections
- Repeat for next timestep

Practical Aspects

- Geometry and mathematics are well separated
 - Geometry operations in Java, linear programs (LPs) and model computation in Matlab
- LPs are nasty
 - Lots of (nearly) redundant and (nearly) degenerate inequalities
 - Lots of sparsity (only two nonzeros per row)
 - Need to walk the projection (start from nearly optimal point)
 - Need guaranteed optimum for guaranteed overapproximation
 - Led to specialized LP implementation by Laza & Yan: takes advantage of special structure, uses regular floating point calculations to start but guarantees solution accuracy through interval arithmetic and if necessary arbitrary precision arithmetic
- Careful simplification of projections is important
 - Need to keep number of edges under control, but accuracy degrades significantly if nonconvexity is removed
- Choice of projections is not always obvious

Coho Outcomes

- Implemented at UBC in Coho toolset
- Demonstrated on seven dimensional realistic circuit model of a toggle element [Yan & Greenstreet, FMCAD 2007]
 - Included verification of composability to construct a ripple counter
- Projectagons are not as scalable as zonotopes & ellipsoids, but can represent nonconvex reach sets
 - Ample opportunity for parallelization
- Algorithm has considered automatic construction of linear plus error models from nonlinear circuit models





from Greenstreet & Mitchell, HSCC 1999, fig. 6, p. 113 from Yan & G October 2008 Ian Mitchell (UBC Computer Science)

Three Other General Approaches

- Eulerian methods (fixed grid reachability)
- State space decomposition (discrete reachability)
- Lyapunov-like methods

Eulerian Approaches

- Time dependent Hamilton-Jacobi
 - Lygeros, Mitchell, Tomlin, Sastry
 - Finite horizon terminal value
 - Continuous implicit representation
- Static Hamilton-Jacobi
 - Falcone, Ferretti, Soravia, Sethian, Vladimirsky
 - Minimum time to reach
 - (Dis)continuous implicit representation
- Viability kernels
 - Saint-Pierre, Aubin, Quincampoix, Lygeros
 - Based on set valued analysis for very general dynamics
 - Discrete implicit representation
 - Overapproximation guarantee
- Backward reachability approach typical of Eulerian algorithms
 - Representation not moving (although it may adapt)
 - Generally handle nonlinear and multiple inputs
 - No examples beyond four dimensions?

State Space Decomposition

- Partition state space and compute reachability over partition
- Examples
 - Uniform grids: Kurshan & MacMillan, Belta and many others
 - Timed Automata "Region Graph": Alur & Dill
 - Cylindrical Algebraic Decomposition: Tiwari & Khanna
- Advantages: No need to integrate dynamics, direct control over size of representation
- Disadvantages: Restricted classes of dynamics, "wrapping" problem (discrete system has transitions that do not exist in continuous system)

Lyapunov-like Methods

- Invariant sets are isosurfaces of Lyapunov-like functions
- Examples:
 - Convex optimization: Boyd, Hindi, Hassibi
 - Sum of Squares: Prajna, Papachristodoulou, Parrilo
- Advantages: Short certificate proves analytic invariance, no need to integrate dynamics
- Disadvantages: Restricted class of dynamics, no refinement parameter to reduce false negatives, difficult to extract counterexamples

Lagrangian Approaches to Forward Reachability in Continuous State Spaces

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