**Theory of Reals** 

for Verification and Synthesis of

Hybrid Dynamical Systems

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### **Cyber-Physical Systems**

There is increasing interaction between embedded software/cyber and the physical world

- Aerospace
  - flight control: traditional to adaptive
  - $\circ$  unmanned vehicles
- Automobile
  - powertrain control
  - cooperative adaptive cruise control

How to design, verify, and certify such systems?

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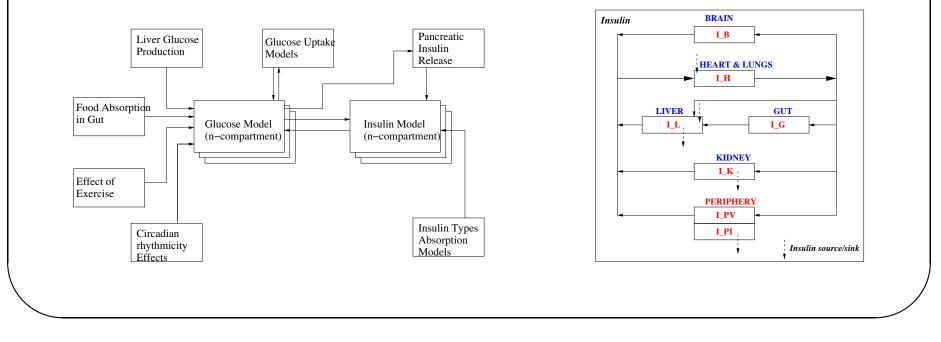
The goal of Systems Biology is to study and understand biological phenomena by building and analyzing dynamic system-level models

Few examples

- *Aplysia*: Neural circuitry of the feeding behavior
- *B.Subtilis*: Sporulation initiation network

### **Symbolic Systems Biology**

The goal of Symbolic Systems Biology is to study and understand biological phenomena by building and analyzing dynamic system-level models symbolically



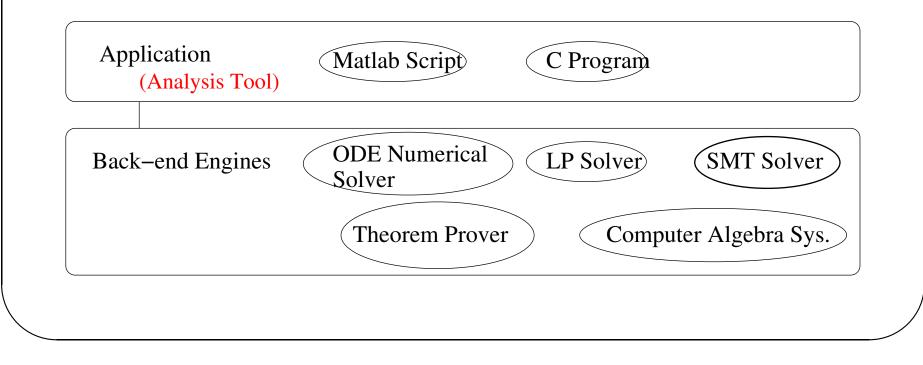
Human Insulin-Glucose Metabolism

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# **Backend Engines**

We need general-purpose symbolic+numeric reasoning engines to enable analysis of these rich models

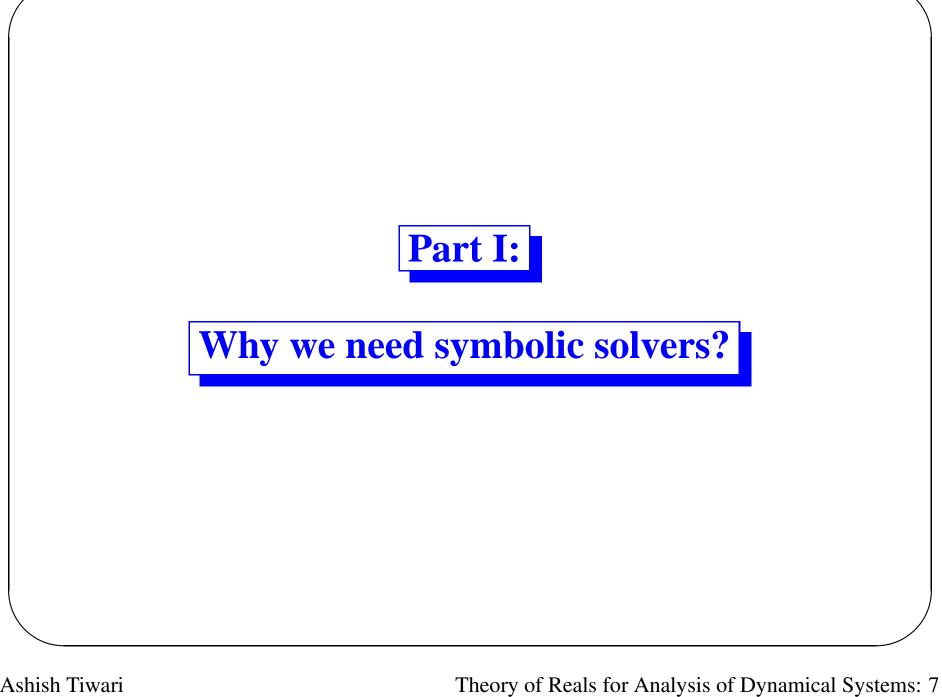
A popular architecture for building analysis tools



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- 1. Part I: Why we need symbolic solvers?
- 2. Part II: What are **SMT** solvers? How to overcome complexity barriers?
- 3. Part III: Theory of Reals = Gröbner basis + ?



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#### **Safety of Cruise Control**

Example. Consider a cruise control:

$$\dot{v} = a$$
  
$$\dot{a} = -4v + 3v_f - 3a + gap$$
  
$$g\dot{a}p = -v + v_f$$

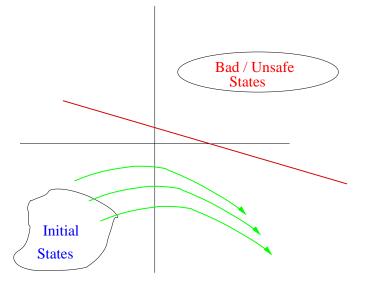
where v, a is the velocity and acceleration of this car,  $v_f$  is the velocity of car in front, and *gap* is the distance between the two cars.

Suppose we enter the cruise control mode whenever *Init* holds. Prove that the cars will not crash.

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#### **Invariants / Barriers**

We can prove cars will not crash if we can find an invariant set whose boundary separates unsafe states from initial states



Suppose I guess that the invariant is of the form:

$$c_1v + c_2v_f + c_3a + c_4gap \le c_5$$

How can I find 
$$c_1, \ldots, c_5$$
?

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**Invariants / Barriers** 

I need to solve:

$$\exists c_1, \dots, c_5 : \forall v, v_f, a, gap : Init(v, v_f, a, gap) \Rightarrow c_1v + c_2v_f + c_3a + c_4gap \le c_5 \land c_1v + c_2v_f + c_3a + c_4gap = c_5 \Rightarrow \frac{d}{dt}(c_1v + c_2v_f + c_3a + c_4gap) \le 0 \land c_1v + c_2v_f + c_3a + c_4gap \le c_5 \Rightarrow gap > 0$$

Need backend solvers to decide satisfiability of above.

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#### **Dynamical Systems**

A lot of engineering and science concerns dynamical systems

- State Space: The set of states, X
  - Discrete: **X** is  $\mathbb{N}^n$
  - Continuous: **X** is  $\mathbb{R}^n$
  - $\circ$  Hybrid: **X** is  $\mathbb{N}^{n_1} \times \mathbb{R}^{n_2}$
- Dynamics: The evolutions,  $\mathbf{T}\mapsto \mathbf{X}$ 
  - $\circ\,$  Discrete: T is  $\mathbb N$
  - $\circ\;$  Continuous: T is  $\mathbb R$
  - $\circ\,$  Hybrid: T is  $\mathbb{R}\times\mathbb{N}$

These systems can be modeled using differential equations, (Finite) state machines, or hybrid automata.

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#### **Typical Properties of Systems**

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
  - $\circ~$  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 and evaluated over the semantic structure defined by the formal models.

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#### **Verification Problem for Dynamical Systems**

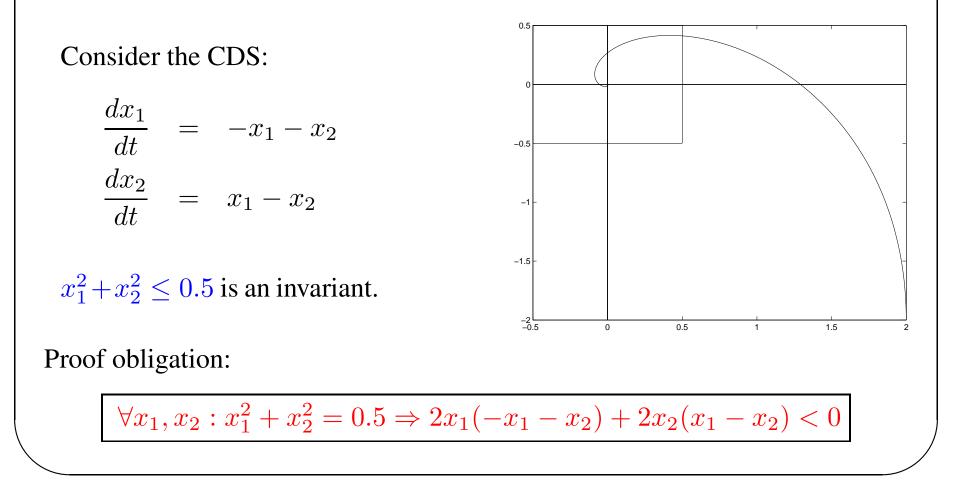
- Given a dynamical system
- And a property: safety, reachability, liveness
- Show that the property is true of the model

#### **Approaches**:

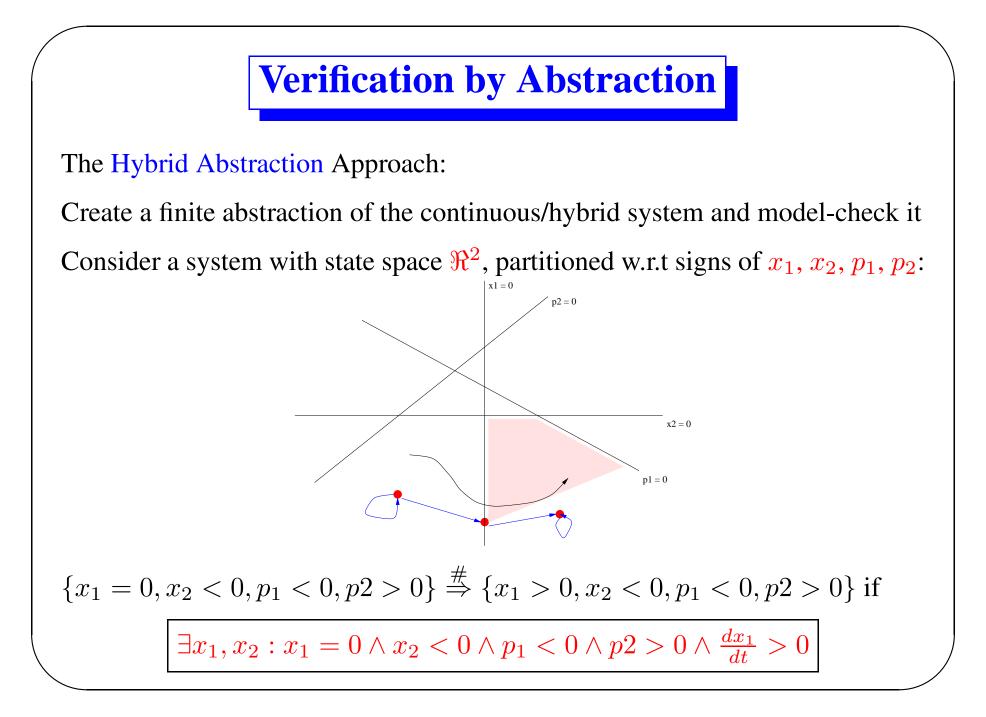
- model checking (MC), bounded MC (BMC), infinite BMC (iBMC)
- deductive verification, k-induction
- Abstract interpretation

### **Verification by Invariance Checking**

Also called **Barrier Certificates** 



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#### **Verification by Invariant Generation**

Consider the system:

$$\frac{dx_1}{dt} = -x_1 - x_2$$
$$\frac{dx_2}{dt} = x_1 - x_2 + x_d$$

Initially:  $x_1 = 0, x_2 = 1$ 

Property:  $|x_1| \leq 1$  always

Guess

- Template for witness  $W := ax_1^2 + bx_2^2 + c$
- Template for assumption  $A := |x_d| < d$

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#### **Example Continued**

Verification Condition:  $\exists a, b, c, d : \forall x_1, x_2, x_d :$ 

$$x_1 = 0 \land x_2 = 1 \quad \Rightarrow \quad W \le 0$$
$$A \land W = 0 \quad \Rightarrow \quad \frac{dW}{dt} < 0$$
$$W \le 0 \quad \Rightarrow \quad |x_1| \le 1$$

Ask contraint solver for satisfiability of above formula

Solver says: 
$$a = 1, b = 1, c = -1, d = 1$$
  
 $x_1 = 0 \land x_2 = 1 \implies x_1^2 + x_2^2 - 1 \le 0$   
 $|x_d| < 1 \land x_1^2 + x_2^2 - 1 = 0 \implies 2x_1(-x_1 - x_2) + 2x_2(x_1 - x_2 + x_d) < 0$   
 $x_1^2 + x_2^2 - 1 \le 0 \implies |x_1| \le 1$ 

This proves that  $|x_1| \leq 1$  always.

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**Stability Verification** 

Consider the aircraft model:

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

where  $\vec{x}$  is a state vector consisting of airspeed, angle of attack, pitch rate, pitch angle, . . .

Property: System is asymptotically stable

Guess template for Lyapunov function  $V := \vec{x}^T A \vec{x}$ 

Verification Condition:

$$\exists A: \forall \vec{x}: V \ge 0 \land (V > 0 \Rightarrow \frac{dV}{dt} \le 0)$$

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# **Summary So Far**

• Formulas in the theory of real-closed fields arise when verifying continuous and hybrid dynamical systems

 $\forall \text{ and } \exists \forall \text{ formulas}$ 

- We need embeddable solvers that are
  - incremental and fast,
  - support rich API,
  - generate small unsatisfiable core
- We need practical methods: detect inconsistency of "easy" instances efficiently
- Ideally integrate with Satisfiability Modulo Theory (SMT) solvers



- 1. Part I: Why we need symbolic solvers?
- 2. Part II: What are **SMT** solvers? How to overcome complexity barriers?
- 3. Part III: Theory of Reals = Gröbner basis + ?

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# **SMT Solvers**

Decide satisfiability modulo theories using symbolic + algebraic techniques!

- Employ a propositional satisfiability solvers for Boolean reasoning
- Employ decision procedures for reasoning over theories
  - $\circ$  rational linear arithmetic: simplex
  - uninterpreted function symbols: congruence closure
  - linear arithmetic over integers
  - theory of arrays
  - theory of bitvectors
  - theory of datatypes

Example: Yices http://yices.csl.sri.com/



Consider the following constraints:

$$\begin{array}{rrrr} x>3 & \lor & x<1,\\ x<2 & \Rightarrow & f(y)=2,\\ x>2 & \Rightarrow & y=x,\\ f(x)=f(y) & \Rightarrow & x=0,\\ f(y)>0 & \Rightarrow & x>1 \end{array}$$

Is there a value for x, y and f such that the above constraints are satisfiable?

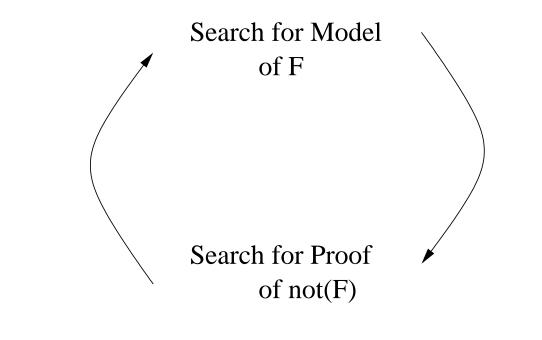
SMT solvers can solve such problems – with 1000s of variables and constraints

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#### Why are SMT Solvers So Effective?

SMT is a revolution

Successful combination of model searching and proof searching



The system now learns from failures, making the search feasible SMT has realized the dream of having embedded deduction

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### **Nonlinear Constraint Solving**

SMT solvers currently have limited support for things a computer algebra system can do

Very limited reasoning about nonlinear constraints

Nonlinear constraint solving is essential for analyzing

- complex cyber-physical systems and
- models from systems biology

SMT + CAS : Challenge is to not compromise speed and scalability of SMT solvers

Can we do it? Can we overcome the complexity barrier?

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# **Canonical Application Area: Analysis**

Model analysis is the canonical application area for symbolic engines such as SMT solvers

Most important problems in verification are undecidable

• Safety verification of infinite-state systems

and they can not be directly reduced to (decidable) SMT problems

Applications make a choice...

#### **View from the Application Layer**

Any application that solves an undecidable problem L, when given an instance  $\phi$ , focuses on either

- showing  $\phi \in L$ , or
- proving  $\phi \not\in L$

#### but not both

A verification tool will target either

- exhibiting an error or
- proving correctness

#### but not both

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#### **View from the Application Layer**

Depending on what the application targets, the needs are different

Verification Approach	Commitment	Useful definitive answer
Abstraction	Proving correctness	Proof of not(F)
Invariant Checking	Proving correctness	Proof of not(F)
Bounded Model-Checking	Showing a bug	Model for F

Both SAT and UNSAT answers are useful

But only ONE answer needs to be definitive for soundness claims

#### **Skewing the Symmetry**

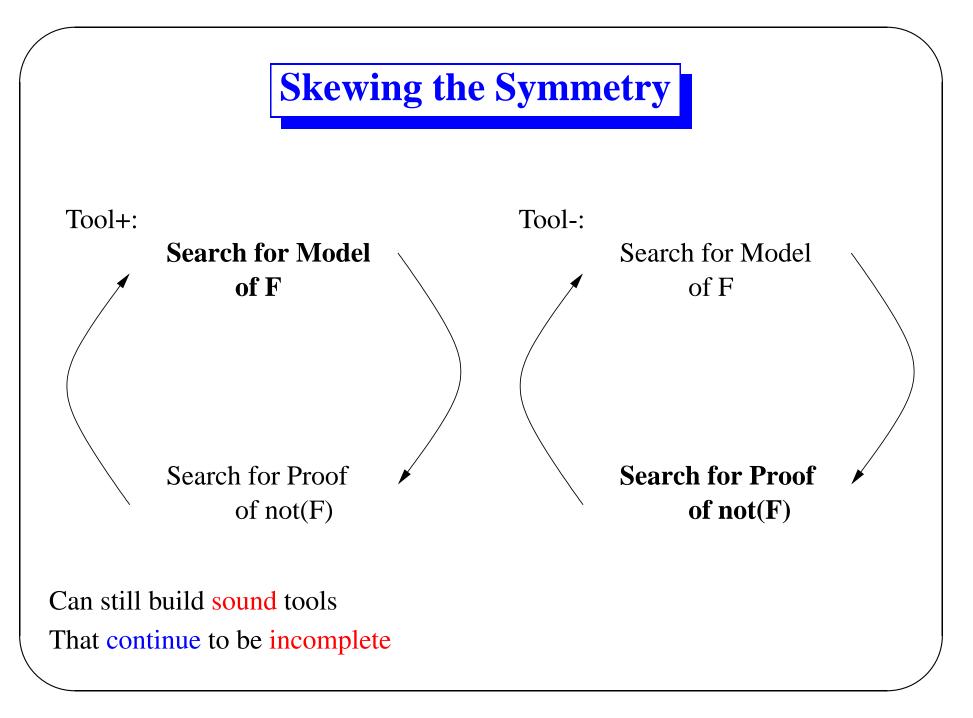
There is a market for asymmetric tools

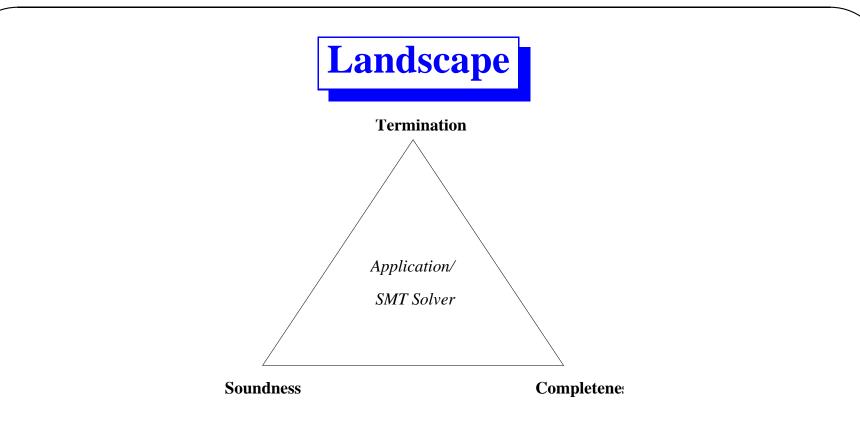
Tool+( $\phi$ ): Input:  $\phi$ Output: DEFINITELY SAT or MAYBE UNSAT

Tool-( $\phi$ ): Input:  $\phi$ Output: DEFINITELY UNSAT or MAYBE SAT

If output = DEFINITELY SAT, then  $\phi$  should indeed be satisfiable If output = DEFINITELY UNSAT, then  $\phi$  should indeed be unsatisfiable If output = MAYBE SAT/UNSAT, then nothing can be inferred about  $\phi$ .

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If a certain problem is **undecidable**, then we cannot have a sound, complete and terminating technique.

Application will compromise completeness, so backend solver can compromise completeness too!

Applications overcome undecidability, backend solvers overcome inefficiency/undecidability

# Outline

- 1. Part I: Why we need symbolic solvers?
- 2. Part II: What are **SMT** solvers? How to overcome complexity barriers?
- 3. Part III: Theory of Reals = Gröbner basis + ?



Focus on  $\forall$  formulas first

Given a set of nonlinear equations and inequalities:

p = 0,	$p \in P$
q > 0,	$q \in Q$
$r \ge 0,$	$r \in R$

where  $P, Q, R \subset \mathbb{Q}[\vec{x}]$  are sets of polynomials over  $\vec{x}$ 

Is the above set unsatisfiable over the reals?

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Examples of satisfiable constraints:

$$\{x^2 = 2\}$$
  
$$\{x^2 = 2, x < 0, y \ge x\}$$

Examples of unsatisfiable constraints:

$$\{x^2 = -2, \ y \ge x\}$$
$$\{x^2 = 2, \ 2x > 3\}$$

Applications in: control, robotics, solving games, static analysis, hybrid systems, ...

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### **Known Results**

- The full FO theory of reals is decidable [Tarski48] Nonelementary decision procedure, impractical
- Double-exponential time decision procedure [Collins74, MonkSolovay74]
- Exponential space lower bound
- Collin's algorithm based on "cylindrical algebraic decomposition" has been improved over the years and implemented in QEPCAD.
   In practice, could fail on p > 0 ∧ p < 0.</li>

Obtaining efficient, sound and complete method unlikely

SMT+/SMT-: Can we obtain efficiency by relaxing completeness?

#### **SMT- Procedure for NRA**

The approach is reminiscent of **Simplex** 

• Introduce slack variables s.t. all inequality constraints are of the form v > 0, or  $w \ge 0$ 

$$\begin{split} P &= 0, \quad Q > 0, \qquad R \ge 0 \qquad &\mapsto \\ \underline{P = 0}, \quad \underline{Q - \vec{v} = 0}, \quad \underline{R - \vec{w} = 0}, \quad \vec{v} > 0, \ \vec{w} \ge 0 \end{split}$$

• Search for a polynomial *p* s.t.

$$P = 0 \land Q = \vec{v} \land R = \vec{w} \quad \Rightarrow \quad p = 0$$
$$\vec{v} > 0, \ \vec{w} \ge 0 \quad \Rightarrow \quad p > 0$$

• If we find such a *p*, return "unsatisfiable" else return "maybe satisfiable"

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#### How to search for p?

Witness for unsatisfiability p satisfies:

$$P = 0 \land Q = \vec{v} \land R = \vec{w} \quad \Rightarrow \quad p = 0 \tag{1}$$

$$\vec{v} > 0, \ \vec{w} \ge 0 \quad \Rightarrow \quad p > 0$$
 (2)

We need efficient sufficient checks

Sufficient check for Condition 1: $p \in Ideal(P, Q - \vec{v}, R - \vec{w})$ Sufficient check for Condition 2:p is a positive polynomial over  $\vec{v}, \vec{w}$ 

To search for p, compute the Gröbner basis for P making  $\vec{v}, \vec{w}$  smaller in the ordering

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#### **Example: Easy Instance**

Consider  $E = \{x^3 = x, x > 2\}.$ 

$x^3 - x = 0,$	x - v - 2 = 0
$(v+2)^3 - (v+2) = 0,$	x - v - 2 = 0
$v^3 + 6v^2 + 11v + 6 = 0,$	x - v - 2 = 0
	$\perp$

Computing GB and projecting it onto the slack variables discovers the witness p for unsatisfiability

```
May not work always ...
```

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#### **Example: Harder Instance**

Let  $I = \{v_1 > 0, v_2 > 0, v_3 > 0\}.$ 

 $v_1 + v_2 - 1 = 0, \qquad v_1 v_3 + v_2 - v_3 - 2 = 0$   $v_1 + v_2 - 1 = 0, \qquad (1 - v_2)v_3 + v_2 - v_3 - 2 = 0$   $v_1 + v_2 - 1 = 0, \qquad v_2 v_3 - v_2 + 2 = 0$ 

This is a Gröbner basis.

There is an unsatisfiability witness p for this example, but we failed to find it.

Recall that in the linear case, Simplex performs pivoting What is the nonlinear analogue of pivoting

First, let us revisit GB computation

# **Gröbner Basis**

Algorithm for computing Gröbner basis is a completion algorithm

Idea behind completion:

- Starting with a set of facts
- Add new facts (saturation)

 $\circ$  that do not have a smaller proof using existing facts

- Delete any fact (simplification)
  - that do have a smaller proof using other facts

#### **Gröbner Basis: Example**

View as completion enables optimizations

$$\begin{array}{c} xy^2 - x = 0, \ x^2y - y^2 = 0 \\ \hline xy^2 \to x, \ x^2y \to y^2 \\ \hline xy^2 \to x, \ x^2y \to y^2[y], \ x^2 = y^3 \\ \hline xy^2 \to x, \ x^2y \to y^2[y], \ y^3 \to x^2 \\ \hline xy^2 \to x[y], \ x^2y \to y^2[y], \ y^3 \to x^2, \ xy = x^3 \\ \hline xy^2 \to x[y], \ x^2y \to y^2[y], \ y^3 \to x^2, \ x^3 \to xy \\ \hline xy^2 \to x[y, x^2], \ x^2y \to y^2[y, x], \ y^3 \to x^2, \ x^3 \to xy \end{array}$$

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If

 $p' \in Ideal(P)$ 

G : Gröbner basis for P

#### Then

$$p' \leftrightarrow_P^* 0$$
 definition of ideal  
 $p' \to_G^* 0$  definition of GB

Claim. If there is no  $p'' \prec p'$  s.t.  $p'' \in Ideal(P)$ , then  $p' \in G$ . *Proof.* If  $p' \rightarrow_G p'' \rightarrow_G^* 0$ , then  $p' \succ p''$  and both  $p', p'' \in Ideal(P)$ .

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#### **Example: Easy Instance**

Recall: We prove unsatisfiability of  $P = 0 \land Q > 0 \land R \ge 0$  by searching for a polynomial p s.t.

$$P = 0 \land Q = \vec{v} \land R = \vec{w} \quad \Rightarrow \quad p = 0$$
$$\vec{v} > 0, \ \vec{w} \ge 0 \quad \Rightarrow \quad p > 0$$

Consider  $E = \{x^3 = x, x > 2\}.$  $\frac{x^3 - x = 0, \qquad x - v - 2 = 0}{(v+2)^3 - (v+2) = 0, \qquad x - v - 2 = 0}$  $\frac{v^3 + 6v^2 + 11v + 6 = 0, \qquad x - v - 2 = 0}{\bot}$ 

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We know  $p \in Ideal(P)$ .

If p is "small-enough" in the ordering  $\succ$ , then p will appear explicitly in the Gröbner basis for P constructed using  $\succ$ .

Example:  $P = \{w_1 - 2w_3 + 2, w_2 + 2w_3 - 1\}$  and  $I = \{w_1 \ge 0, w_2 \ge 0\}$ . If  $w_1 \succ w_2 \succ w_3$ , then  $GB_{\succ}(P) = P$ .

If we make  $w_3 \succ w_1$  and  $w_3 \succ w_2$  in the ordering, then

$$GB_{\succ}(P) = \{2w_3 - w_1 - 2, \ \underline{w_2 + w_1 + 1}\}.$$

For linear polynomials, this is pivoting, but what is its analogue for nonlinear systems ?

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# **Finding** *p***: Nonlinear Issues**

It is not always possible to change  $\succ$  to get witness  $p \in GB_{\succ}(P)$ .

• Problem 1:

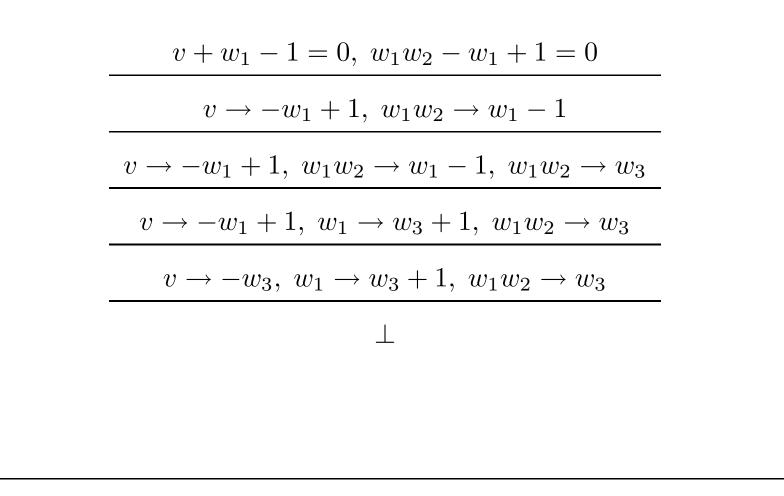
$$P_1 = \{v + w_1 - 1, w_1 w_2 - w_1 + 1\}$$

Need  $w_1 \succ w_1 w_2$  to "get"  $v + w_1 w_2$  in  $GB(P_1)$ .

Solution: Introduce new definitions and get flexibility in choosing  $\succ$ Add  $w_1w_2 - w_3$  to  $P_1$  and have  $w_1 \succ w_3$ .

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## **Problem 1: Example**



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# **Finding** *p***: Nonlinear Issues**

It is not always possible to change  $\succ$  to get witness  $p \in GB_{\succ}(P)$ .

• Problem 2:

$$P_2 = \{w_1^2 - 2w_1w_2 + w_2^2 + 1\}$$

Need  $w_1, w_2 \succ (w_1 - w_2)^2$  to "get" the witness  $(w_1 - w_2)^2 + 1$  in  $GB(P_2)$ .

Solution: Introduce new definitions and get flexibility in choosing  $\succ$ Add  $(w_1 - w_2)^2 - w_3$  to  $P_2$  and have  $w_1, w_2 \succ w_3$ .

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**Problem 2: Example** 

$$\begin{split} & w_1^2 - 2w_1w_2 + w_2^2 + 1 = 0 \\ & w_1^2 \to 2w_1w_2 - w_2^2 - 1 \\ & w_1^2 \to 2w_1w_2 - w_2^2 - 1, \ (w_1 - w_2)^2 = w_3 \\ & w_1^2 \to 2w_1w_2 - w_2^2 - 1, \ w_1^2 \to 2w_1w_2 - w_2^2 + w_3 \\ & w_3 \to -1, \ w_1^2 \to 2w_1w_2 - w_2^2 + w_3 \\ & \bot \end{split}$$

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Positivstellensatz

What guarantees the existence of such a witness?

The constraint

 $\{p=0: p \in P\} \cup \{q \ge 0: q \in Q\} \cup \{r \ne 0: r \in R\}$ 

is unsatisfiable (over the reals) iff

there exist polynomials p, q, and r such that

 $p \in Ideal(P) \qquad \{\Sigma_i p_i q_i : p_i \in P\}$   $q \in Cone[Q] \qquad \{\Sigma_i s_i^2 q_1 q_2 \dots q_k : q_j \in Q\}$   $r \in [R] \qquad \{r_1 r_2 \dots r_k : r_i \in R\}$   $p + q + r^2 \equiv 0$ 

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#### **Positivstellensatz Corollary**

The constraint

$$\{p = 0 : p \in P\} \cup \{v > 0 : v \in \vec{v}\} \cup \{w \ge 0 : w \in \vec{w}\}$$

is unsatisfiable iff  $\neg u'$  and that

 $\exists p' \text{ such that }$ 

$$p' \in Ideal(P) \cap (Cone[\vec{v}, \vec{w}] + [\vec{v}])$$

Hence, the method is "refutationally complete"

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#### **Example: Harder Instance**

Let 
$$I = \{v_1 > 0, v_2 > 0, v_3 > 0\}$$
.  

$$\begin{array}{c}
v_1 + v_2 - 1 = 0, \quad v_1 v_3 + v_2 - v_3 - 2 = 0 \\
\hline
v_1 + v_2 - 1 = 0, \quad (1 - v_2)v_3 + v_2 - v_3 - 2 = 0 \\
\hline
v_1 + v_2 - 1 = 0, \quad v_2 v_3 - v_2 + 2 = 0 \\
\hline
v_1 + v_2 - 1 = 0, \quad v_2 v_3 - v_2 + 2 = 0, \quad v_2 v_3 - v_4 = 0 \\
\hline
v_1 + v_2 - 1 = 0, \quad -v_2 + v_4 + 2 = 0, \quad v_2 v_3 - v_4 = 0 \\
\hline
v_1 + v_4 + 1 = 0, \quad -v_2 + v_4 + 2 = 0, \quad v_2 v_3 - v_4 = 0 \\
\hline
\bot
\end{array}$$

The polynomial  $v_1 + v_4 + 1$  is the required witness to the unsatisfiability of the constraints.

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# **Summary of the Procedure**

- Turn all inequalities into equations by introducing slack variables
- Compute Gröbner basis of the equations
- If a positive polynomial is ever generated, return unsatisfiable
- If not, introduce new definitions to try different orderings and repeat

# **Solving** $\exists \forall$ **Formulas**

Farkas' Lemma converts  $\forall$  to  $\exists$  in linear arithmetic

Its generalization can be used for nonlinear arithmetic

 $\forall \vec{x} : p_1 \ge 0 \land p_2 \ge 0 \Rightarrow p_3 \ge 0$ , if

$$\exists s_1, s_2, s_3 : s_3 p_3 = s_1 p_1 + s_2 p_2 \land s_1 \ge 0 \land s_2 \ge 0 \land s_3 \ge 0$$

A sufficient condition for guaranteeing  $s_1, s_2 \ge 0$  is that they are sums of squares

Once  $\forall$  is eliminated, we can use the procedure for  $\exists$ 

# **Solving** ∃∀ **Formulas**

Another approach we are pursuing is based on Combining symbolic and numeric techniques

Suppose we wish to solve  $\exists x_1, x_2 : \forall y : p(x_1, x_2, y) \ge 0 \land q(x_1, x_2, y) \ge 0$ 

- Use QEPCAD to eliminate  $\forall$  from  $\forall y : p(x_1, x_2, y) \ge 0$
- Use numerical techniques to get a value for  $x_1$
- Use QEPCAD to eliminate  $\forall$  from  $\forall y : q(x_1, x_2, y) \ge 0$  with  $x_1$  instantiated

#### **Sum-of-Squares Programming**

The need for nonlinear reasoning and optimization has been recognized by several communities

This has lead to the formulation of SOS programming

```
\min_{\vec{u}\in\mathbb{R}^n}c_1u_1+\cdots+c_nu_n
```

subject to

 $p_{i1}u_1 + \dots + p_{in}u_n$  is a SOS,  $i = 1, 2, \dots, k$ 

SOS programs can be converted into semidefinite programs using the observation that p is SOS iff  $p = z^T Q z$  for some symmetric positive-semidefinite matrix Q (z is a vector of all monomials of degree deg(p)/2)

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#### **Semidefinite Programming**

Semidefinite Programming:

 $\min_{\vec{u}\in\mathbb{R}^n}c_1u_1+\cdots+c_nu_n$ 

subject to

 $F_0 + u_1F_1 + \cdots + u_nF_n$  is positive semidefinite

where  $c_i$ 's are given constants and  $F_i$ 's are given symmetric matrices.

SDPs can be solved using numerical convex optimization toolboxes

Is there a good way to combine SOS techniques with symbolic techniques?

# Conclusion

Symbolic and algebraic techniques will play increasingly important role as we design, build and understand complex systems

We need fast and scalable tools that can be embedded in applications: SMT+CAS?

There is a market for incomplete but fast tools

Reasoning about nonlinear constraints is presently a critical bottleneck

We will need to augment sound symbolic techniques with fast numerical approaches