15-819M: Data, Code, Decisions

13: Real Arithmetic

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Outline

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Real Computation and Floating-Point Arithmetic

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```
r=a-1; q=1; p=1/2;
while (2*p*r >= err) {
  if (2*r - 2*q - p >= 0) {
    r = 2*r - 2*q - p;
    q = q+p;
    p = p/2;
  } else {
    r = 2*r;
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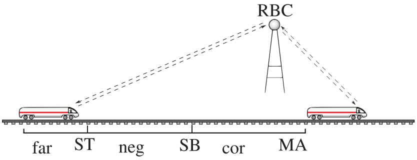
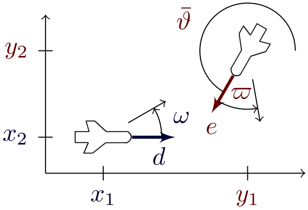
@loop_invariant(a = q^2+2*p*r)

Motivation + Applications of Real Arithmetic

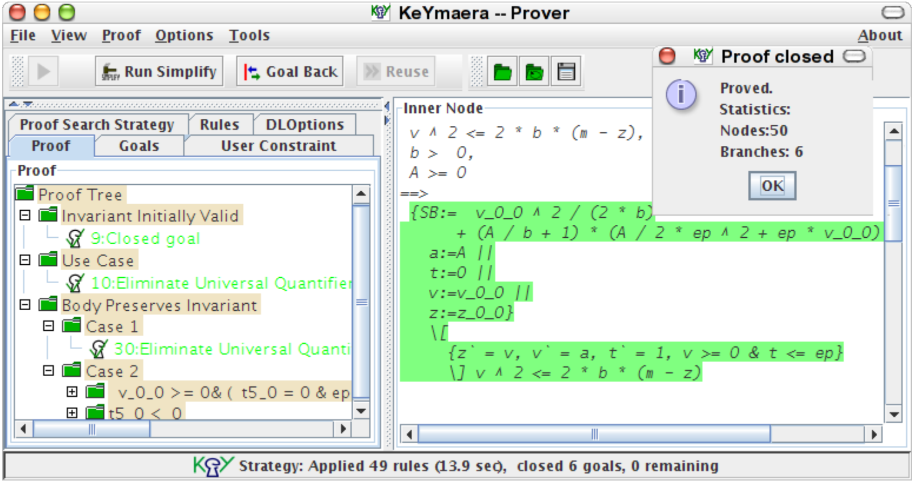
Real arithmetic is used in:

- Mathematical algorithms in real or floating-point arithmetic
- Hybrid systems, i.e., joint discrete and continuous dynamics
- Geometric problems

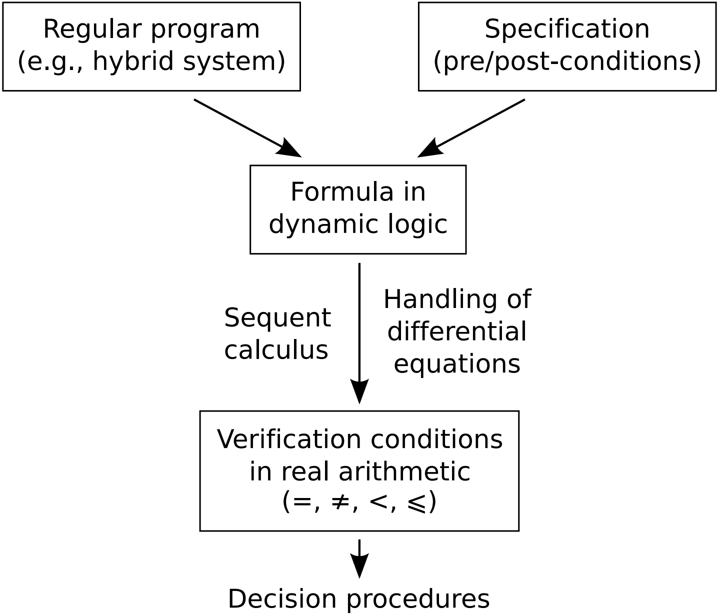




KeYmaera = KeY + Math for Hybrid Systems



Overall Verification Approach



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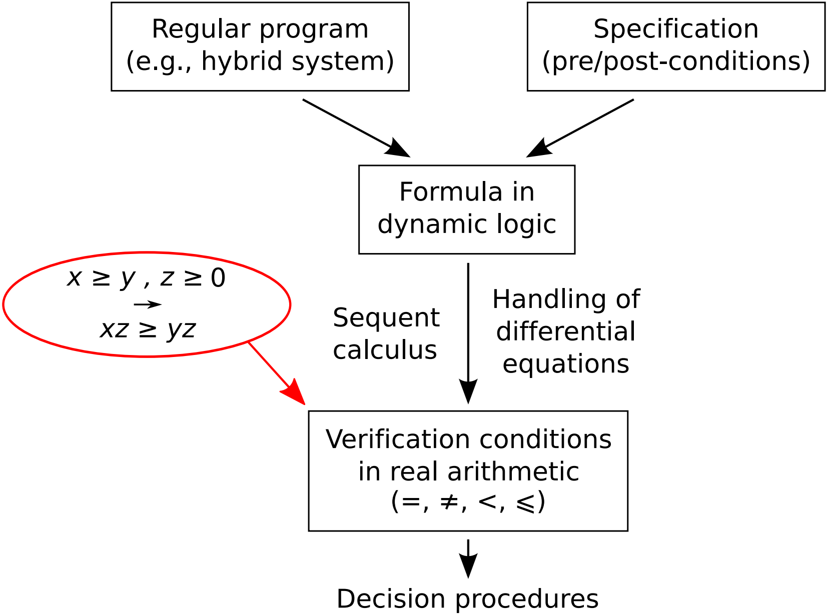

Outline

Interpreted First-order Logic of Real Arithmetic

- In a formula like

$$(x_1 - y_1)^2 + (x_2 - y_2)^2 > p^2$$

  how do we get "$+$" and "$-$" and "ˆ2" and "$>$" to mean what we want?

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- Interpreted first-order logic is like first-order logic, except that some symbols have a fixed semantics (all interpretations agree on the semantics of those symbols).
- Our primary focus: first-order real arithmetic $\text{FOL}_{\mathbb{R}}$

First-order Logic of Real Arithmetic: Syntax

Definition (Interpreted $\text{FOL}_{\mathbb{R}}$ Term t)

$t ::=$

x	for variable $x \in V$
r	for rational number r
$t_1 + t_2$	(infix notation)
$t_1 - t_2$	(infix notation)
$t_1 \cdot t_2$	(infix notation)
$f(t_1, \dots, t_n)$	for function $f/n \in \Sigma$ of arity $n \geq 0$

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$F ::=$

$t_1 \geq t_2$	(infix notation)
$t_1 > t_2$	(infix notation)
$t_1 = t_2$	(infix notation)
$p(t_1, \ldots, t_n)$	for predicate $p/n \in \Sigma$ of arity $n \geq 0$
$\neg F$	“not”
$(F \land G)$	“and”
$(F \lor G)$	“or”
$(F \to G)$	“implies”
$(F \leftrightarrow G)$	“equivalent/bi-implies”
$\forall x\, F$	“universal quantifier/forall” for $x \in V$
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$\forall x\, F$	"universal quantifier/forall" for $x \in V$
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Quiz

Is this a formula of first-order real arithmetic?

1. $F \lor (G \land (H \leftrightarrow \neg F) \to J)$
2. $\forall x\, (p(x) \to \exists y\, (p(y) \land \exists x\, \neg r(x, y)))$
3. $\forall x\, \forall y\, (x > y \leftrightarrow x - y > 0)$
4. $x < y \land \exists z\, x > z^2$
5. $x > 0 \land \forall y\, \exists z\, (x > z^2 + y \cdot z - 5)$
6. $\forall x\, \exists y\, x > x^y$
7. $\exists x\, \forall y\, x > y + \pi$
8. $(\exists x\, \neg \exists y\, x > y + 3.1415926) \to \forall x\, (x^2 > x^3)$

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First-order Logic of Real Arithmetic: Semantics

Definition ($\text{FOL}_{\mathbb{R}}$ Interpretation I)

1. $D = \mathbb{R}$
2. I assigns relations and functions on $\mathbb{R}$ to all symbols in Σ
   - function $I(f) : \mathbb{R}^n \to \mathbb{R}$ for each function symbol f of arity n
   - relation $I(p) \subseteq \mathbb{R}^n$ for each predicate symbol p of arity n
   - element $I(c) \in \mathbb{R}$ for each constant symbol (function of arity 0)
   - truth-value $I(p) \in \{true, false\}$ for each predicate symbol of arity 0

   such that

   - $I(+)$ is addition on $\mathbb{R}$
   - $I(-)$ is subtraction on $\mathbb{R}$
   - $I(\cdot)$ is multiplication on $\mathbb{R}$
   - $I(=)$ is equality on $\mathbb{R}$
   - $I(>)$ is the greater relation on $\mathbb{R}$
   - $I(\geq)$ is the greater-equals relation on $\mathbb{R}$
   - $I(r) = r$ for all numbers $r \in \mathbb{Q}$

Quiz

(Validity of) which of the following logics is decidable/semidecidable/undecidable/not semidecidable?

1. PL_0
2. FOL
3. $\text{FOL}_{\mathbb{N}}[+,\cdot,=]$
4. $\text{FOL}_{\mathbb{R}}[+,\cdot,=,<]$
5. $\text{FOL}_{\mathbb{Q}}[+,\cdot,=]$
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✓ PL_0 decidable

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- ✓ $FOL_{\mathbb{R}}[+, \cdot, =, <]$ decidable [Tarski'51]
5. $FOL_{\mathbb{Q}}[+, \cdot, =]$
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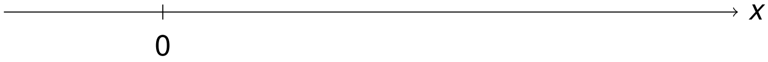
Quantifier Elimination by Example



Can we get rid of the quantifier without changing the semantics of the formula?

$$\exists x (x > 2 \land x < \frac{17}{3})$$

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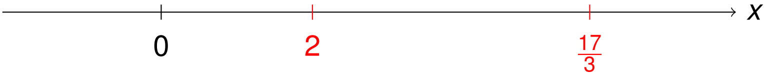

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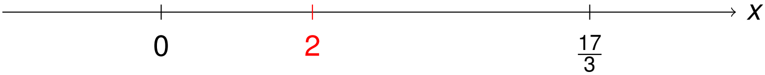

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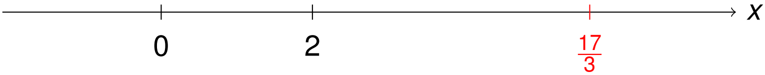

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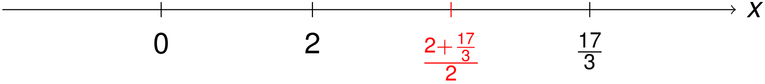

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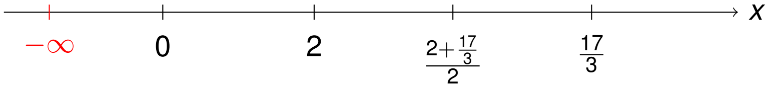

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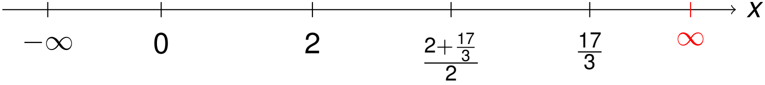

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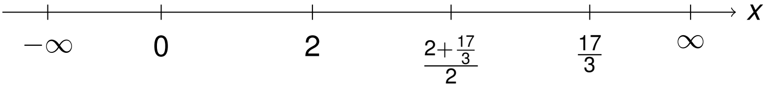

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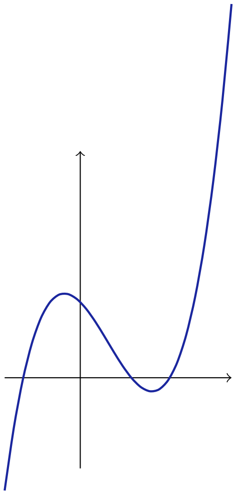
\lor & (\infty > 2 \land \infty < \frac{17}{3}) & \text{extremal case “}x = \infty\text{”} \\
\equiv & \mathit{true} & \text{evaluate}
\end{array}
$$

Quantifier Elimination and Projection



$$\exists y\,(y \geq 0 \land 1 - x - 1.83x^2 + 1.66x^3 > y)$$

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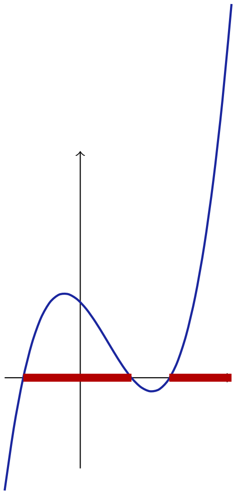

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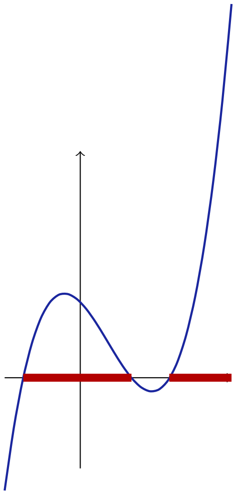
Quantifier Elimination and Projection

$\exists y\, (y \geq 0 \land 1 - x - 1.83x^2 + 1.66x^3 > y)$



$0.75 < x \land x < 0.68 \lor x > 1.17$

Quantifier Elimination in Real-Closed Fields

Definition (Quantifier elimination)

A first-order theory admits *quantifier elimination* if to each formula ϕ, a quantifier-free formula QE(ϕ) can be effectively associated that is equivalent (i.e., $\phi \leftrightarrow$ QE(ϕ) is valid) and has no other free variables. The operation QE is further assumed to evaluate ground formulas (i.e., without variables), yielding a decision procedure for this theory.

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Theorem (Complexity, Davenport&Heintz'88,Weispfenning'88)

(Time and space) complexity of QE *for* $\mathbb{R}$ *is doubly exponential in the number of quantifier (alternations).*

Quiz

(Validity of) which of the following logics is
decidable/semidecidable/undecidable/not semidecidable?

- ✓ PL_0 decidable
- ? FOL undecidable but semidecidable
- × $\mathrm{FOL}_{\mathbb{N}}[+,\cdot,=]$ not semidecidable “Peano arithmetic” [Gödel’31]
- ✓ $\mathrm{FOL}_{\mathbb{R}}[+,\cdot,=,<]$ decidable [Tarski’51]
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15. Sup “Non-empty subsets with upper bounds have supremum”

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Theorem (downward Skolem-Löwenheim'1915-20)

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But the first-order "view" of the reals is still fairly amazing

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3. R admits an ordering that makes R an ordered field.

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5. R is a real field such that no proper algebraic extension is a formally real field.

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- Computable numbers, i.e., those that can be approximated by a computable function up to any desired precision. π lives here!
- ZFC-Definable numbers, i.e., those real numbers $a \in \mathbb{R}$ for which there is a first-order formula φ in set theory with one free variable such that a is the unique real number for which φ holds true.

$$I \models \varphi \text{ iff } I(x) = a$$

The advantages of implicit definition over construction are roughly those of theft over honest toil [Russell]

First-Order Axiom Schemes of Real-Closed Fields

1. Commutative group $(\mathbb{R}, +)$: $\forall x\, \forall y\, \forall z\, x + (y + z) = (x + y) + z$
2. Neutral $\forall x\, x + 0 = x$
3. Inverse $\forall x\, \exists y\, x + y = 0$
4. Abelian $\forall x\, \forall y\, (x + y = y + x)$
5. Commutative group $(\mathbb{R} \setminus \{0\}, \cdot)$: $\forall x\, \forall y\, \forall z\, x \cdot (y \cdot z) = (x \cdot y) \cdot z$
6. Neutral $\forall x\, x \cdot 1 = x$
7. Inverse $\forall x\, (x \neq 0 \rightarrow \exists y\, x \cdot y = 1)$
8. Abelian $\forall x\, \forall y\, (x \cdot y = y \cdot x)$
9. Distributive $\forall x\, \forall y\, \forall z\, (x \cdot (y + z) = (x \cdot y) + (x \cdot z))$
10. $\neg \exists x_1 \, \dots \exists x_n\, (-1 = x_1^2 + \cdots + x_n^2)$ for any n
11. $\forall x\, \forall y\, (x < y \land p(x)p(y) < 0 \rightarrow \exists z\, (x < z < y \land p(z) = 0))$ for polynomial p (intermediate value property)

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History of Symbolic Methods in Real Arithmetic

1930	First quantifier elimination procedure by Tarski (Non-elementary)
1965	Buchberger introduces Gröbner bases
1973	Real Nullstellensatz and Positivstellensatz by Stengle
1975	Cylindrical algebraic decomposition (CAD) by Collins (Doubly exponential)
1983	Cohen-Hörmander elimination procedure
1993	Virtual substitution by Weispfenning
2003	Parrilo introduces semidefinite programming for the Positivstellensatz (Later refined by Harrison)
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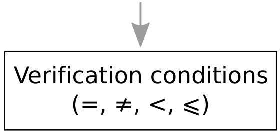
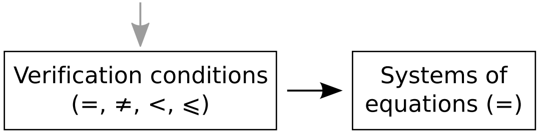
Outline

Gröbner Bases for Quantifier-Free Real Arithmetic



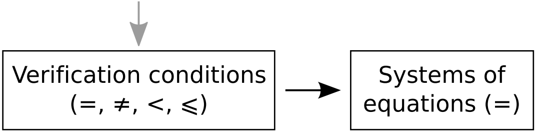
Inequalities and disequations?



Gröbner Bases for Quantifier-Free Real Arithmetic

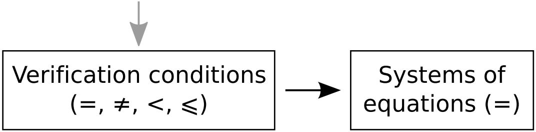
Inequalities and disequations can be eliminated:

$$
\begin{aligned}
f \neq g &\equiv \exists z.\, (f-g)z = 1 \\
f \geq g &\equiv \exists z.\, f-g = z^2 \\
f > g &\equiv \exists z.\, (f-g)z^2 = 1
\end{aligned}
$$



Goal: prove unsatisfiability of:

$$\bigwedge_i t_i = 0$$

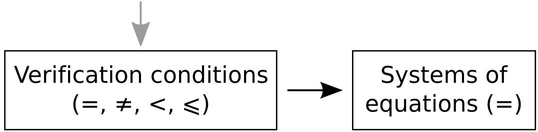


Gröbner Bases for Quantifier-Free Real Arithmetic

Witnesses for unsatisfiability:

$$\left(\sum_i s_i t_i\right) = 1 \quad \Longrightarrow \quad \bigwedge_i t_i = 0 \text{ unsatisfiable}$$

How to determine coefficients s_i?



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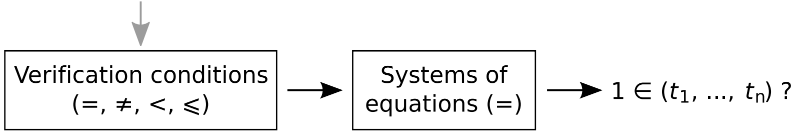
Need some more notation:

- Ideal generated by $\{t_1, \ldots, t_n\} \subseteq \mathbb{Q}[X_1, \ldots, X_n]$:

$$(t_1, \ldots, t_n) \ = \ \left\{ \sum_i s_i t_i \mid s_1, \ldots, s_n \in \mathbb{Q}[X_1, \ldots, X_n] \right\}$$



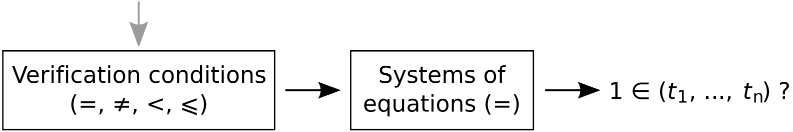
Gröbner Bases for Quantifier-Free Real Arithmetic

Gröbner bases to solve the ideal membership problem:

- Monomial ordering $\prec$: admissible total well-founded ordering on monomials (Gives the order in which to try eliminating monomials)
- Reduction of a polynomial s w.r.t. $B = \{t_1, \ldots, t_n\}$:

$$\begin{aligned} s &\succ s + u_1 t_{i_1} \\ &\succ s + u_1 t_{i_1} + u_2 t_{i_2} \\ &\succ \cdots \\ &\succ \mathrm{red}_B\, s \end{aligned}$$

- B is called Gröbner basis if $\mathrm{red}_B\, s = 0$ for all $s \in (B)$



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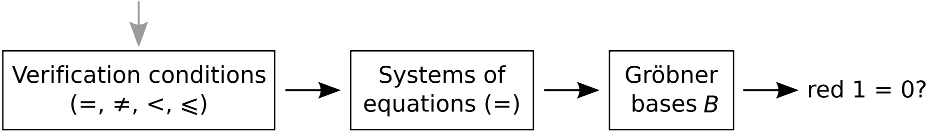

Gröbner Bases for Quantifier-Free Real Arithmetic

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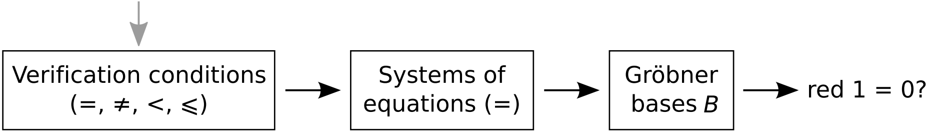
- Monomial ordering $\prec$: admissible total well-founded ordering on monomials
- $\prec$ admissible iff its reflexive closure $\preceq$ satisfies
  1. $X^\nu \preceq X^\mu$ then $X^\nu X^\lambda \preceq X^\mu X^\lambda$ for all $\nu, \mu, \lambda \in \mathbb{N}^n$
  2. $X^\nu | X^\mu$ then $X^\nu \preceq X^\mu$ for all $\nu, \mu \in \mathbb{N}^n$



The Nullstellensatz

Method is sound and complete over complex numbers:

Theorem (Hilbert's Nullstellensatz)

$$\neg\exists x \in \mathbb{C}^n : \bigwedge_i t_i(x) = 0 \quad \textit{iff} \quad 1 \in (t_1, \ldots, t_n)$$

What about the real numbers?

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e.g.	$x^2 + 1 = 0$	is unsatisfiable
but	$(x^2 + 1)$	does not contain 1

Next: an extension that is complete over the reals

Gröbner Bases

Definition (Gröbner basis)

Finite set $G \subseteq k[X_1, \dots, X_n]$ with $(G) = I$ is *Gröbner basis* of ideal I iff, equivalently:

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Can be computed effectively by Buchberger's algorithm

Buchberger's Algorithm for Computing Gröbner Bases

GB(finite $F \subset k[X_1, \ldots, X_n]$):

1. choose $f, g \in F$
2. $s := \frac{lcm(\ell(f),\ell(g))}{\ell(f)} f - \frac{lcm(\ell(f),\ell(g))}{\ell(g)} g$
   let the leading terms $\ell(...)$ cancel by construction
3. $F := F \cup \{\mathrm{red}_F\, s\}$

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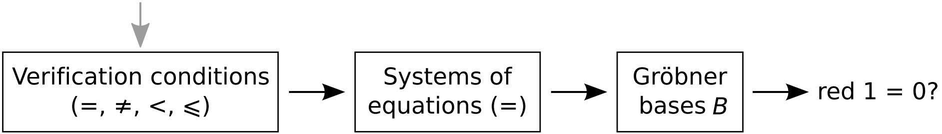
Next: an extension that is complete over the reals

The Real Nullstellensatz

Theorem (Stengle's Real Nullstellensatz, 1973)

$$\neg\exists x \in \mathbb{R}^n : \bigwedge_i t_i(x) = 0 \quad \textit{iff}$$

$$\exists s_1, \ldots, s_k \in \mathbb{R}[X_1, \ldots, X_m] :\ 1 + s_1^2 + \cdots + s_k^2 \in (t_1, \ldots, t_n)$$

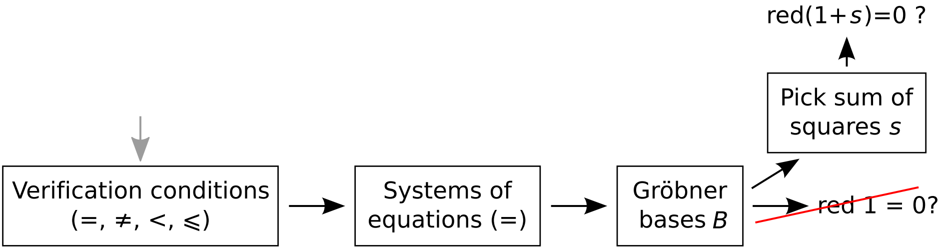


The Real Nullstellensatz

Theorem (Stengle's Real Nullstellensatz, 1973)

$$\neg\exists x \in \mathbb{R}^n : \bigwedge_i t_i(x) = 0 \quad \textit{iff}$$

$$\exists s_1, \ldots, s_k \in \mathbb{R}[X_1, \ldots, X_m] : \ 1 + s_1^2 + \cdots + s_k^2 \in (t_1, \ldots, t_n)$$



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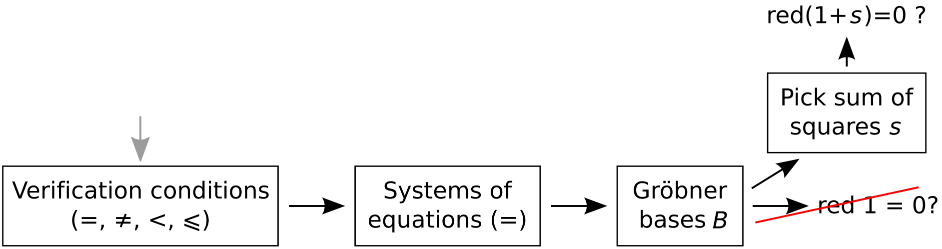
How to pick sum of squares $s_1^2 + \cdots + s_n^2$?

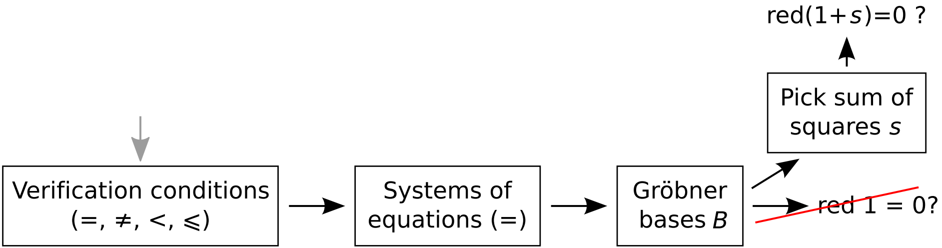


The Real Nullstellensatz

Observation: [Parrilo, 2003]
Sums of squares can be represented as scalar products

E.g.

$$2x^2 - 2xy + y^2 \;=\; x^2 + (x-y)^2 \;=\; \begin{pmatrix} x \\ y \end{pmatrix}^t \begin{pmatrix} 2 & -1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$



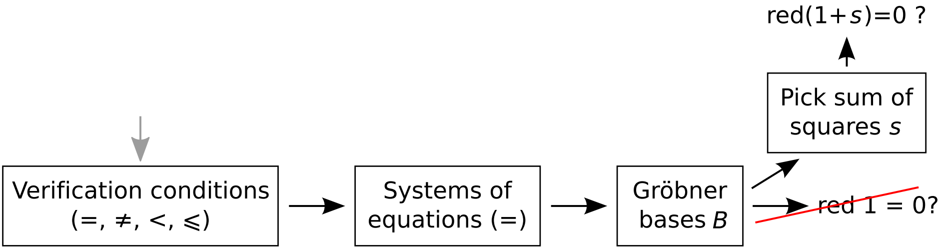
The Real Nullstellensatz

Lemma

Every sum of squares can be represented as $p^t X p$, where $p \in \mathbb{R}[X_1, \ldots, X_m]^k$ and X is positive semi-definite (and vice versa).

Matrix X is called positive semi-definite if

1. X is symmetric (i.e., $X^t = X$)
2. $x^t X x \geq 0$ for all $x \in \mathbb{R}^n$.



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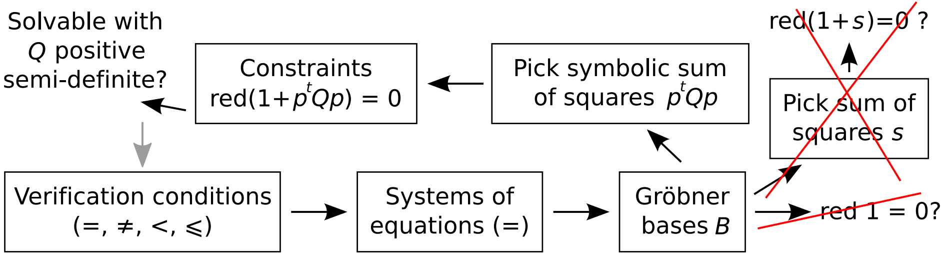
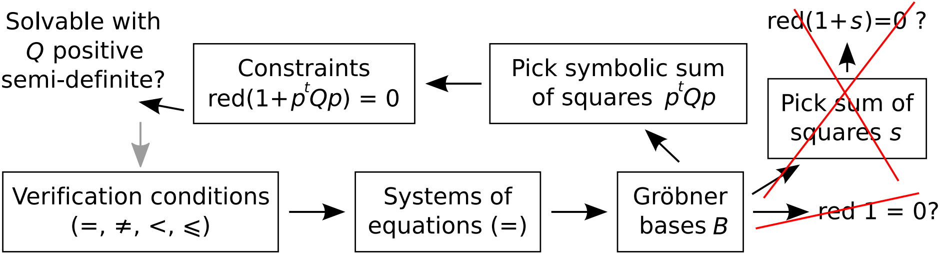


The Real Nullstellensatz

Constraint solving by semidefinite programming (convex optimisation):

- Has been used successfully in combination with Positivstellensatz [Parrilo, 2003; Harrison, 2007]



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$$x \geq y,\ z \geq 0,\ yz > xz$$

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Pick basis monomials p and symmetric matrix Q:

$$p \;=\; \begin{pmatrix} 1 \\ a^2 \\ abc \end{pmatrix} \qquad Q \;=\; \begin{pmatrix} q_{1,1} & q_{1,2} & q_{1,3} \\ q_{1,2} & q_{2,2} & q_{2,3} \\ q_{1,3} & q_{2,3} & q_{3,3} \end{pmatrix}$$

$$p^t Q p \;=\; q_{1,1}1^2 + 2q_{1,2}a^2 + 2q_{1,3}abc + 2q_{2,3}a^3bc + q_{3,3}a^2b^2c^2$$

Example (2)

$$p^t Q p \;=\; q_{1,1} 1^2 + 2 q_{1,2} a^2 + 2 q_{1,3} abc + 2 q_{2,3} a^3 bc + q_{3,3} a^2 b^2 c^2$$

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Reduce $1 + p^t Qp$ w.r.t. B:

$$\begin{aligned} \mathrm{red}_B(1 + p^t Qp) = & \ 1 + q_{1,1} - q_{3,3} + 2q_{1,2}x - 2q_{1,2}y + \\ & 2q_{1,3}abc + 2q_{2,3}abcx - 2q_{2,3}abcy \end{aligned}$$

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Solve the program: $q_{3,3} = 1$ and $q_{i,j} = 0$ for all $(i, j) \neq (3, 3)$

$$1 + p^t Qp \;=\; \underbrace{1 + (abc)^2}_{\text{Witness for unsatisfiability}} \;\in (B)$$

Gröbner Bases for the Real Nullstellensatz (GRN)

Properties of the procedure

- Sound + “complete” method for quantifier-free real arithmetic
- Sums of squares as certificates (“proof producing”)
- Termination criteria can be given → decision procedure
- In practice:
  Enumerate basis monomials with ascending degree

Numerical issues

- Existing solvers for semidefinite programming are numeric
  (we use CSDP)
- Solution:
  Solve program numerically, then round to exact solution
  [Harrison, 2007]

Optimizations

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  $\rightsquigarrow$ replace by $m_1, \ldots, m_n$

Outline

Other Approaches

Positivstellensatz methods [Parrilo, 2003; Harrison, 2007]:

- Positivstellensatz [Stengle, 1973]:
  Extension of Real Nullstellensatz for inequalities
- Differences: Gröbner bases, simpler certificates

Tiwari's method [Tiwari, 2005]:

- Differences: less heuristic $\Rightarrow$ completeness, semidefinite programming

Proof-producing quantifier elimination [McLaughlin, Harrison, 2005]:

- Differences: universal fragment vs. full real arithmetic, performance

Numeric methods:

- Differences: soundness + completeness

Empirical Comparison of Decision Procedures

- Gröbner basis approaches
  - **GM**, **GO**: pure Gröbner bases (inequalities → equations)
  - **GK**: Gröbner bases combined with Fourier-Motzkin
  - **GRN**: Gröbner bases for the Real Nullstellensatz
- Quantifier elimination procedures
  - **QQ**, **QM**, **QR**$_c$: cylindrical algebraic decomposition (CAD)
  - **QR**$_s$: CAD + virtual substitution
  - **QC**, **QH**: Cohen-Hörmander
- Semidefinite programming for the Positivstellensatz
  - **PH**: Harrison's implementation
  - **PK**: our implementation in KeYmaera

Benchmarks: 100 problems taken from . . .

- Case studies in hybrid systems verification
- Verification of mathematical algorithms, geometry
- (A few) synthetic problems

Experiments