Towards Practical Provably Correct Algorithms for Real Quantifier Elimination

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Problem

- Real arithmetic questions involving the **∃ (exists) and ∀ (for all) quantifiers** (ranging over the reals) are difficult for computers
- **Quantifier elimination (QE)**: The process of transforming a quantified statement into a ***logically equivalent*** quantifier-free statement

Examples

Example

$$\forall x.\ x^2 + 1 > 0$$

QE

True

Example*

$$\forall x \forall y.\ ((x^2 + ay^2 \leq 1) \Rightarrow (ax^2 - a^2xy + 2 \geq 0))$$

QE

$$(a \geq 0) \text{ and } (a^3 - 8a - 16 \leq 0)$$

QE is identifying exactly what conditions on a will make the original formula true!

*This example is taken from some of Pablo Parrilo's lecture notes (Lecture 18 of his 2006 course, "Algebraic Techniques and Semidefinite Optimization"). Accessible through his webpage: https://www.mit.edu/~parrilo/index.html

A Miraculous Result

- Algorithms for QE exist (Tarski, 1930)
- Algorithms for QE are complicated

Alfred Tarski

Terminology

- **Formulas:** Conjunctions and disjunctions of polynomial inequalities and equations (with rational coefficients)
- If a formula in a QE problem involves only one variable, we call it a **univariate** QE problem. Else it is a **multivariate** QE problem
- **Decision problems** are problems where all variables are quantified

Examples, Revisited

Example

$\forall x.\ x^2 + 1 > 0$

⬇ QE

True

A univariate decision problem

Example*

$$\forall x \forall y.\ ((x^2 + ay^2 \leq 1) \Rightarrow (ax^2 - a^2xy + 2 \geq 0))$$

⬇ QE

$$(a \geq 0) \text{ and } (a^3 - 8a - 16 \leq 0)$$

A multivariate QE question
***Not* a decision problem**

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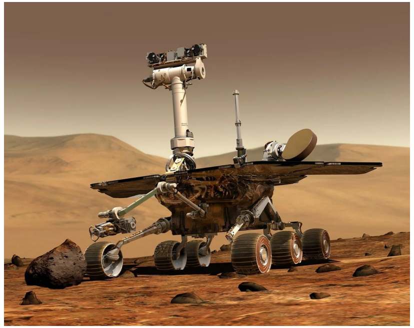
Motivation

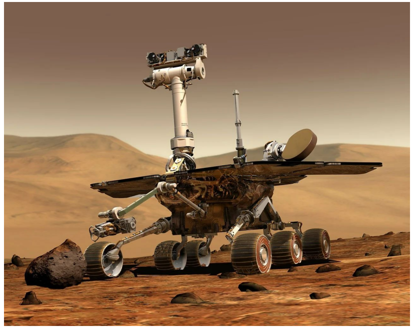
- Quantified statements arise in a number of applications
  - Geometry proofs
  - Stability analysis
  - Verification of cyber-physical systems (like robots!)



For more information, see:
Sturm, T. A Survey of Some Methods for Real Quantifier Elimination, Decision, and Satisfiability and Their Applications. *Math.Comput.Sci.* 11, 483–502 (2017).

Motivation

- Quantified statements arise in a number of applications
  - Geometry proofs
  - Stability analysis
  - Verification of cyber-physical systems (like robots!)
- Two conclusions
  - We want to know how to do QE
  - We want to be sure that we know how to do QE **correctly**



Doing QE correctly

- Formally verified QE algorithms
    - Implemented in theorem provers
    - Have proofs of correctness
    - Significantly more trustworthy than unverified algorithms

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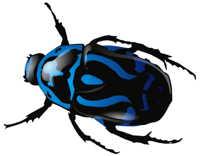
There are QE algorithms (Tarski), we'll just verify them and be done…?

Doing QE correctly

- **Challenge:** Verified QE is much more difficult than unverified QE
- **Problem:** Dearth of efficient verified QE support
  - CPS theorem prover KeYmaera X outsources QE to unverified software
  - This can introduce bugs





Related Work

✓ = YES

✗ = NO

■ = IN BETWEEN

	Efficient?	Verified?	Multivariate case builds directly on univariate?
Cohen-Hörmander	✗	✓	✓
Tarski	✗	✓	✓
CAD	✓	■	✗

Our Approach

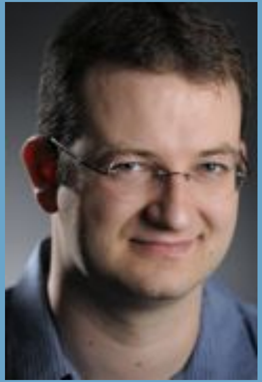
Twofold Approach

- Verify the **Ben-Or, Kozen, and Reif (BKR)** decision procedure (and its extension to a full QE algorithm by Renegar), **which fits in a sweet spot in between practicality and ease of formalization**
- Verify **virtual substitution (VS)**, an extremely efficient QE algorithm that works on a fragment of QE problems

Our Approach: Verifying Virtual Substitution (VS)

Matias Scharager

Stefan Mitsch



André Platzer

Fabian Immler

M. Scharager, **K. Cordwell**, S. Mitsch, and A. Platzer. Verified Quadratic Virtual Substitution for Real Arithmetic. Accepted to Formal Methods (FM) 2021, to appear.

What is Virtual Substitution?

- A **highly efficient** QE method that works on a fragment of QE problems
- Targets problems with **low-degree polynomials** (linear or quadratic)
- Two flavors: Equality VS and General VS

Equality Virtual Substitution

- Works when a formula has a linear or quadratic **equation**:

$$\exists\, x.\ (ax^2 + bx + c = 0 \wedge F)$$

- Can we directly substitute $x = \dfrac{-b \pm \sqrt{b^2 - 4ac}}{2a}$ into F?

Equality Virtual Substitution

- Works when a formula has a linear or quadratic **equation**:

$$\exists x. (ax^2 + bx + c = 0 \land F)$$

- Can we directly substitute $x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$ into F?

  Not without leaving the first-order logic of real arithmetic (FOL_R)

  Instead: "virtually" substitute

Equality Virtual Substitution

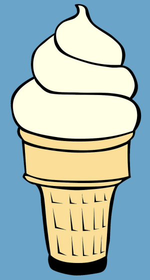
- Example: $\exists x. (x > 0 \land x^2 = 2 \land xy = 1)$
- We'd like to virtually substitute $x = \sqrt{2}$ into $xy = 1$

Equality Virtual Substitution

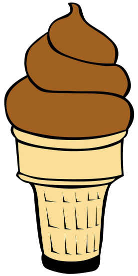
- Example: $\exists$ **x. (x > 0 ∧ x^2 = 2 ∧ xy = 1)**
- We'd like to virtually substitute x = $\sqrt{2}$ into xy = 1
- An appropriate FOL_R formula: **y > 0 ∧ y^2 = 1/2**

Key Takeaways

- VS "simulates" direct substitution in that it captures all of the logical meaning in direct substitution, but maintains formulas in FOL_R
- The presence of low-degree equalities automatically gives us a finite number of points to virtually substitute

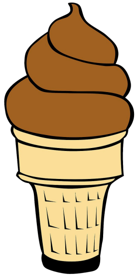


General Virtual Substitution



- General VS allows for the presence of inequalities
- ...but then what points do we substitute?

General Virtual Substitution



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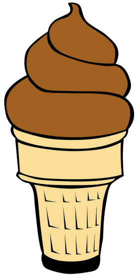
In every interval between the roots, the polynomials have constant sign

General Virtual Substitution



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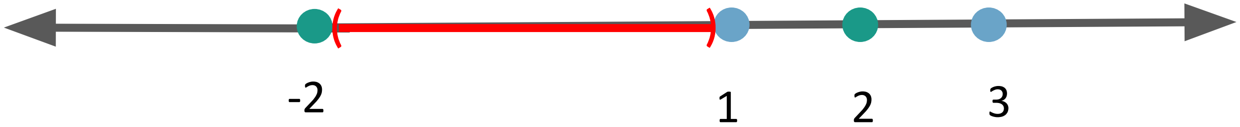

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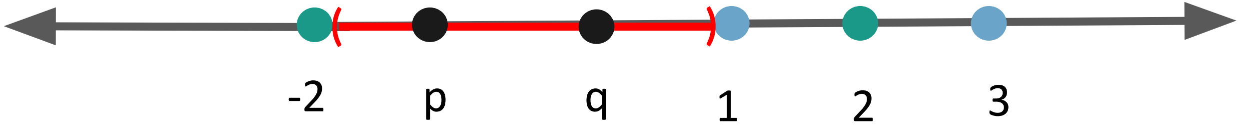

$p^2 - 4$ and $q^2 - 4$ have the same sign

$p^2 - 4p + 3$ and $q^2 - 4q + 3$ have the same sign

General Virtual Substitution

- General VS allows for the presence of inequalities
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$$\exists x. (x^2 - 4 > 0 \wedge x^2 - 4x + 3 < 0)$$

ANY point from this interval captures information for the entire interval!

This allows us to discretize with sample points

General Virtual Substitution

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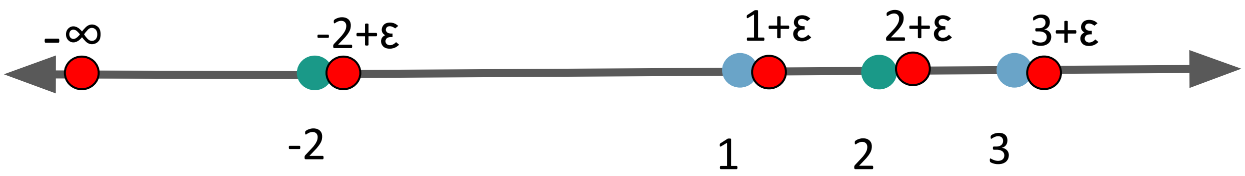

Here are the sample points VS will pick (in red)

General Virtual Substitution

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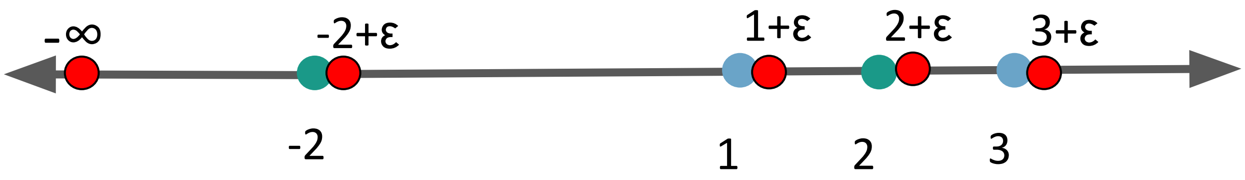

Why $-\infty$ and the ε's? Why not -3, 0, 1.5, 2.5, and 4?

General Virtual Substitution

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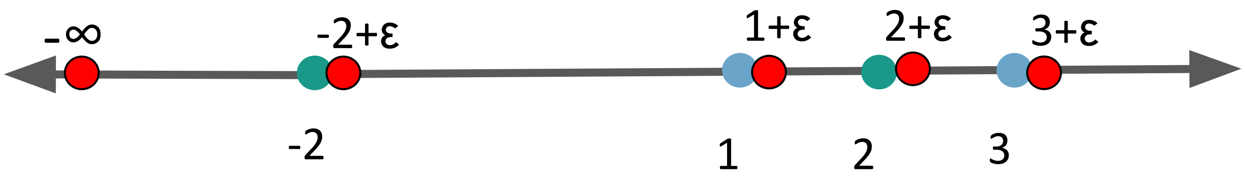
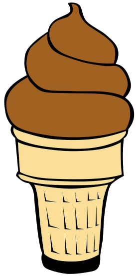


Why $-\infty$ and the ε's? Why not -3, 0, 1, 1.5, 2.5, 3, and 4?
VS needs to be able to generalize to arbitrary examples; can't overfit for the current example

General Virtual Substitution



- General VS allows for the presence of inequalities
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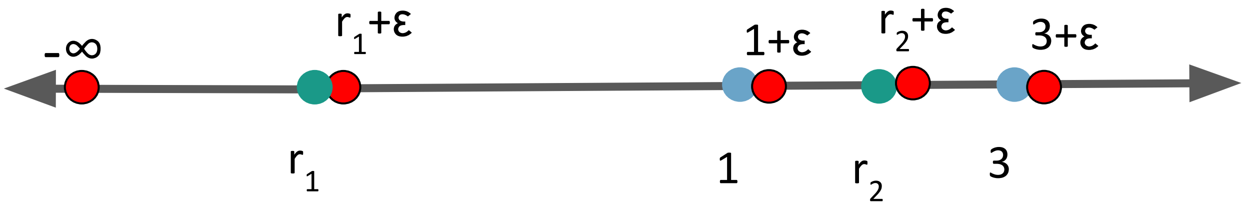
$$\exists\, x.\ (ax^2 + bx + c > 0 \wedge x^2 - 4x + 3 < 0)$$



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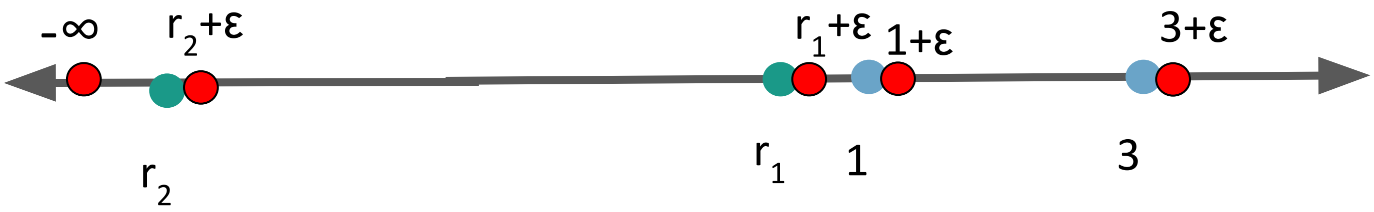

General Virtual Substitution

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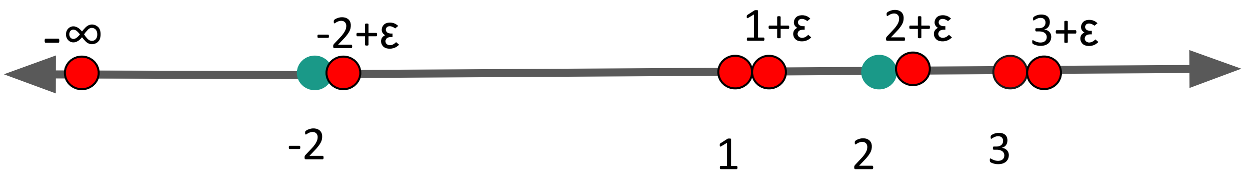

Note: We can only use general VS when we know all of the roots of the polynomials in our formula: i.e. when all of the polynomials are linear or quadratic in the variable of interest.

Formalizing this in Isabelle/HOL!

Substituting -∞

```
lemma infinity_evalUni: shows "(∃y. ∀x<y. aEvalUni At x) =
  (evalUni (substNegInfinityUni At) x)"
```

The intuition: VS for -∞ should be equivalent to sampling from in the leftmost interval on the number line

Substituting -∞

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Checks whether ax^2 + bx + c satisfies the sign condition specified by At

At is a triple of real numbers (a, b, c) and a sign condition: <, =, ≤, or ≠

Substituting -∞

```
lemma infinity_evalUni: shows "(∃y. ∀x<y. aEvalUni At x) =
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Decide: Is there some sufficiently negative y so that, for all $x < y$, $ax^2 + bx + c$ satisfies the sign condition specified by *At*?

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Evaluate a formula at a point

Given *At*, virtually substitute -∞

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Why is this substitution lemma only stated for univariate polynomials?

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Why is this substitution lemma only stated for univariate polynomials?

A clever trick: The multivariate VS proof proceeds by valuation. So we can state most of our correctness lemmas for univariate polynomials. Then later, naturally extend them to multivariate.

Substituting ε

```
lemma infinitesimal_quad:
  fixes A B C D:: "real"
  assumes "D≠0"
  assumes "C≥0"
  shows "(∃y::real>((A+B * sqrt(C))/(D)).
      ∀x::real ∈{((A+B * sqrt(C))/(D))<..y}. aEvalUni At x)
      = (evalUni (substInfinitesimalQuadraticUni A B C D At) x
```

This is stated for a quadratic polynomial, with a root (A + B*sqrt(C))/D

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```

This is stated for a quadratic polynomial, with a root (A + B*sqrt(C))/D

VS of (A + B*sqrt(C)/D) + ε is equivalent to **sampling from the interval directly "above" (A + B*sqrt(C)/D)**

Formalizing VS: Related Work

- We formalize both Equality VS and General VS
- Related work: Tobias Nipkow (linear VS), Amine Chaeib (quadratic equality VS)
  - Nipkow's work is more theoretically oriented
  - Chaeib's formalization is not publicly available; we chose not to build on it

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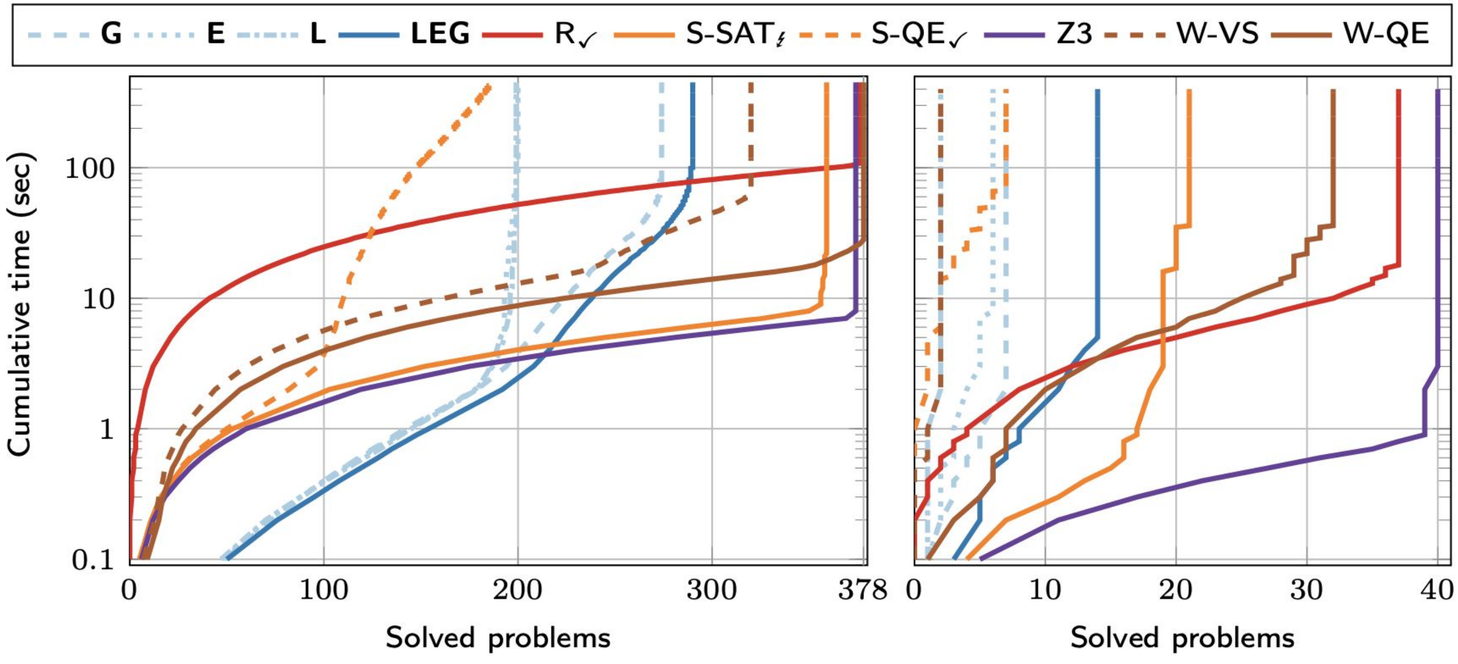
Different goals: We want practical verified real QE

Code Export and Experiments

Formalizing VS

- We export our code to SML for experimentation
  - 378 benchmarks from the literature
  - Compare to Mathematica, Z3, Redlog, SMT-RAT

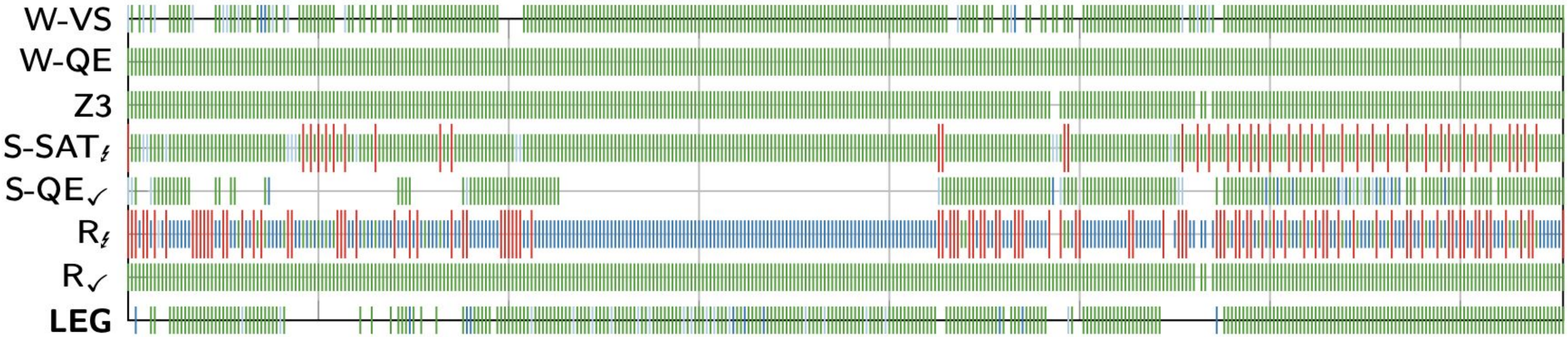
Some Experimental Results

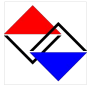


(a) CADE09 (378 examples) (b) Economics (45 examples)

Some Experimental Results

We find longstanding errors in existing tools with a consistency comparison:



W:  Z3:  S:  R:  **LEG**: us!

Green: consistent

Blue: only one solved

Red: inconsistent

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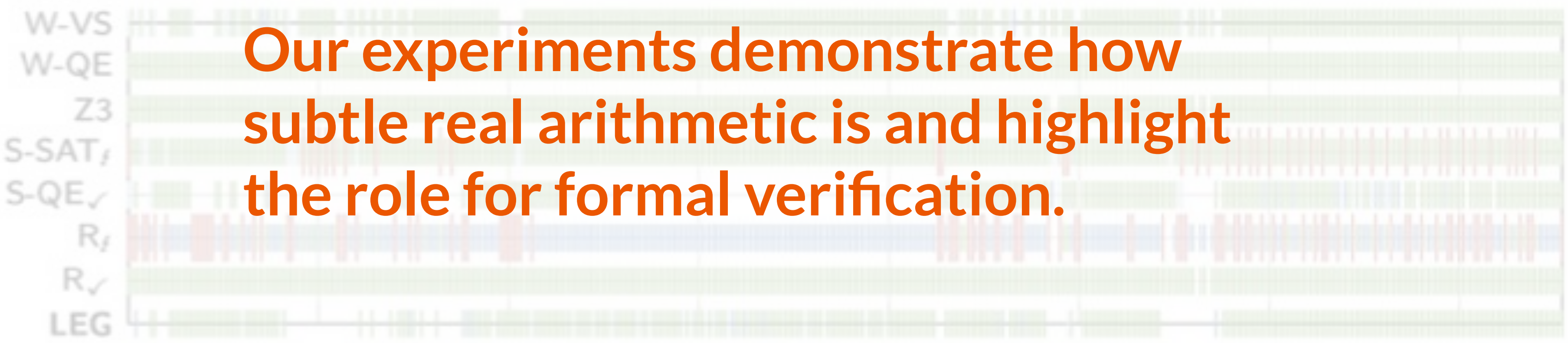

Our experiments demonstrate how subtle real arithmetic is and highlight the role for formal verification.

W: Z3: S: R: **LEG**: us!

Green: consistent Blue: only one solved Red: inconsistent

Our Approach: Verifying BKR/Renegar

Yong Kiam Tan

André Platzer

Related Work

✓ = YES
✗ = NO
▭ = IN BETWEEN

	Efficient?	Verified?	Multivariate case builds directly on univariate?
Cohen-Hörmander	✗	✓	✓
Tarski	✗	✓	✓
CAD	✓	▭	✗
BKR & Renegar Potential sweet spot!	▭	✗	✓

We formally verify* the univariate cases of BKR and Renegar in Isabelle/HOL.

K. Cordwell, Y. K. Tan, and A. Platzer. A Verified Decision Procedure for Univariate Real Arithmetic with the BKR Algorithm. Interactive Theorem Proving (ITP) 2021.

*Available on the Archive of Formal Proofs at: https://www.isa-afp.org/entries/BenOr_Kozen_Reif.html

High-level Context

- ~7000 LOC
    - Algorithm: ~110 LOC
    - Matrix library extensions: ~1800 LOC

High-level Context

- ~7000 LOC
  - Algorithm: ~110 LOC
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- Why Isabelle/HOL?
  - Well-suited to formalizing mathematics
  - Strong math libraries
  - Sledgehammer

Univariate BKR: Bird's Eye View

- Transform the problem:
  1. Decision problems to sign determination
  2. Sign determination to restricted sign determination
  3. To solve restricted sign determination, set up a matrix equation.

The main formalization challenge

Step 1: Decision to Sign Determination

- Solve decision problems by finding the ***consistent sign assignments (CSAs)*** for a set of polynomials (sign determination)

Definition (sign assignment for $\{g_1, \ldots, g_n\}$). A mapping $\sigma: \{g_1, \ldots, g_n\} \to \{+, -, 0\}$
σ is **consistent** if there is a real x where, for all i, the sign of $g_i(x)$ matches $\sigma(g_i)$.

Step 1: Decision to Sign Determination

- Solve decision problems by finding the ***consistent sign assignments (CSAs)*** for a set of polynomials (sign determination)

Decision Problem:
$\exists x. (x^2+1 \geq 0 \land 3x < 0)$

Find all consistent sign assignments for $x^2 + 1$ and $3x$

CSAs: (+, -), (+, 0), (+, +)

CSA (+, -) indicates the existence of a point k with $(k^2+1 \geq 0 \land 3k < 0)$

Correctness Results for Step 1

```
theorem decision_procedure:
  "(∀x::real. fml_sem fml x) ⟷ decide_universal fml"
  "(∃x::real. fml_sem fml x) ⟷ decide_existential fml"
```

Canonical semantics for formulas (defines what it means for a formula to hold at x in the standard way)

Our algorithms

Step 2: Restricted Sign Determination

- Restrict sign determination to finding all **CSAs** for a set of univariate polynomials $\{q_1, \ldots, q_n\}$ ***at the roots of*** an auxiliary nonzero polynomial p

Technical detail: BKR imposes some conditions on $\{q_1, \ldots, q_n\}$, p

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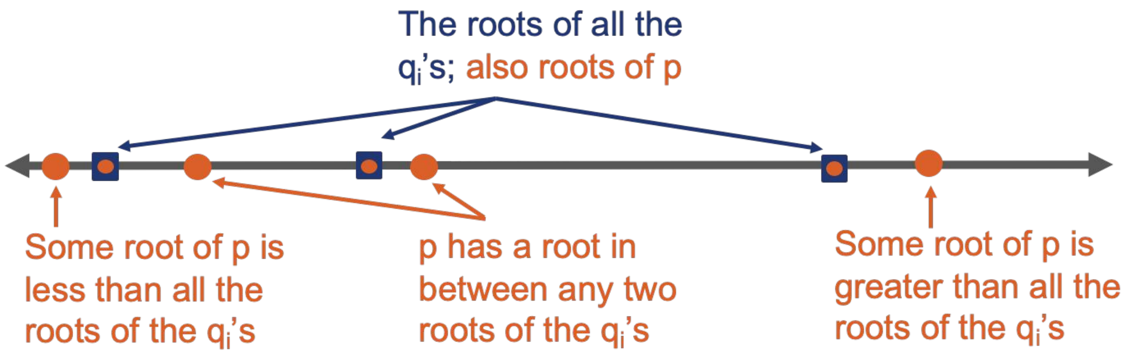

Correctness Results for Step 2

```
definition roots :: "real poly ⇒ real set" where "roots p = {x. poly p x = 0}"

definition consistent_signs_at_roots :: "real poly ⇒ real poly list ⇒ rat list set"
where "consistent_signs_at_roots p qs = (sgn_vec qs) ` (roots p)"
```

Plug in the roots to the q_i's, take the resulting signs

Solve for the roots of a polynomial

Correctness Results for Step 2

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definition roots :: "real poly ⇒ real set" where "roots p = {x. poly p x = 0}"

definition consistent_signs_at_roots :: "real poly ⇒ real poly list ⇒ rat list set"
where "consistent_signs_at_roots p qs = (sgn_vec qs) ` (roots p)"

theorem find_consistent_signs_at_roots:
assumes "p ≠ 0"
assumes "⋀q. q ∈ set qs ⟹ coprime p q"
shows "set (find_consistent_signs_at_roots p qs) = consistent_signs_at_roots p qs"
```

our (constructive) algorithm

the nonconstructive definition

Step 3: The Matrix Equation

- Stores all relevant information for sign determination
- Idea dates back to Tarski; similarities to Cohen and Mahboubi's formalization*
- **But BKR does it efficiently**

Alfred Tarski

*Cyril Cohen and Assia Mahboubi. Formal proofs in real algebraic geometry: from ordered fields to quantifier elimination. Log. Methods Comput. Sci., 8(1), 2012. doi:10.2168/ LMCS-8(1:2)2012.

Step 3: The Matrix Equation

Find sign assignments to $q_1, \dots, q_n$ at the roots of p

Tarski

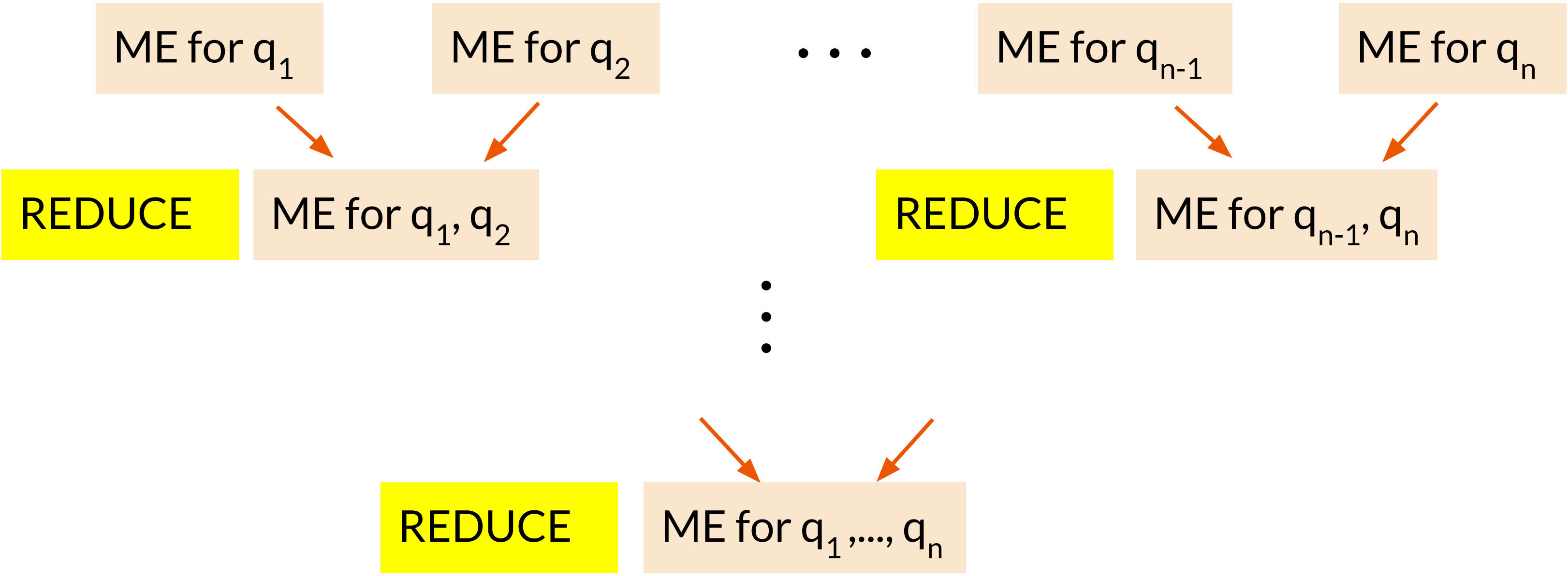
TQ stands for "Tarski query", refers to invoking the (computational) Sturm-Tarski theorem

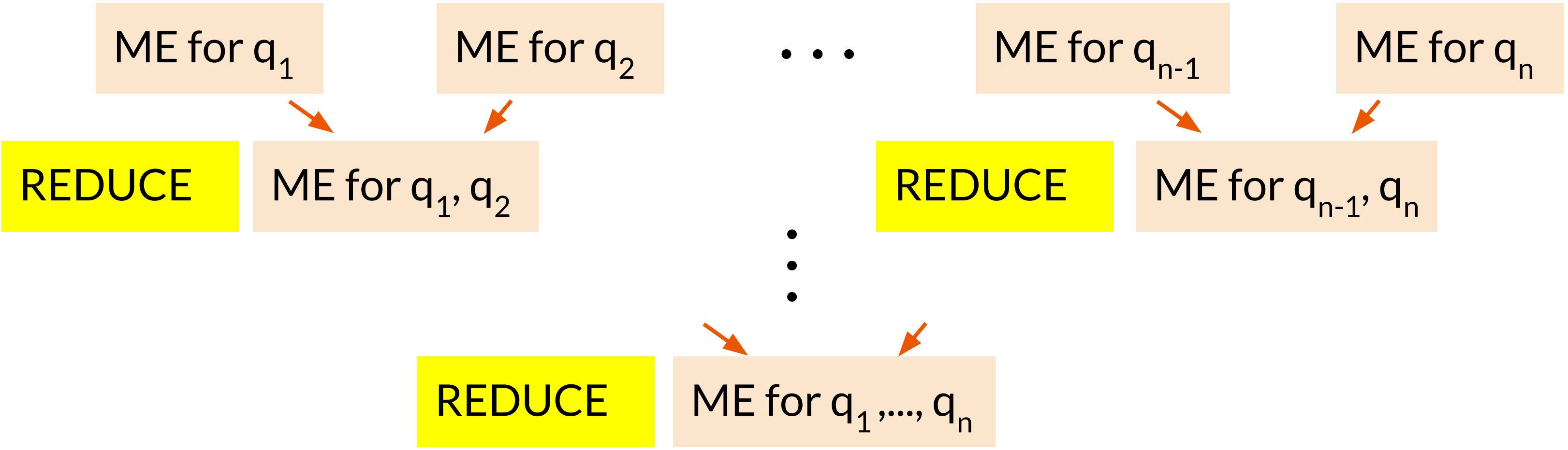
$$\begin{pmatrix} \text{\# of } (+,\dots,+,+) \\ \text{\# of } (+,\dots,+,-) \\ \vdots \\ \text{\# of } (-,\dots,-,-) \end{pmatrix} = M^{-1} * \begin{pmatrix} \text{TQ subset } 1 \\ \text{TQ subset } 2 \\ \vdots \\ \text{TQ subset } 2^n \end{pmatrix}$$

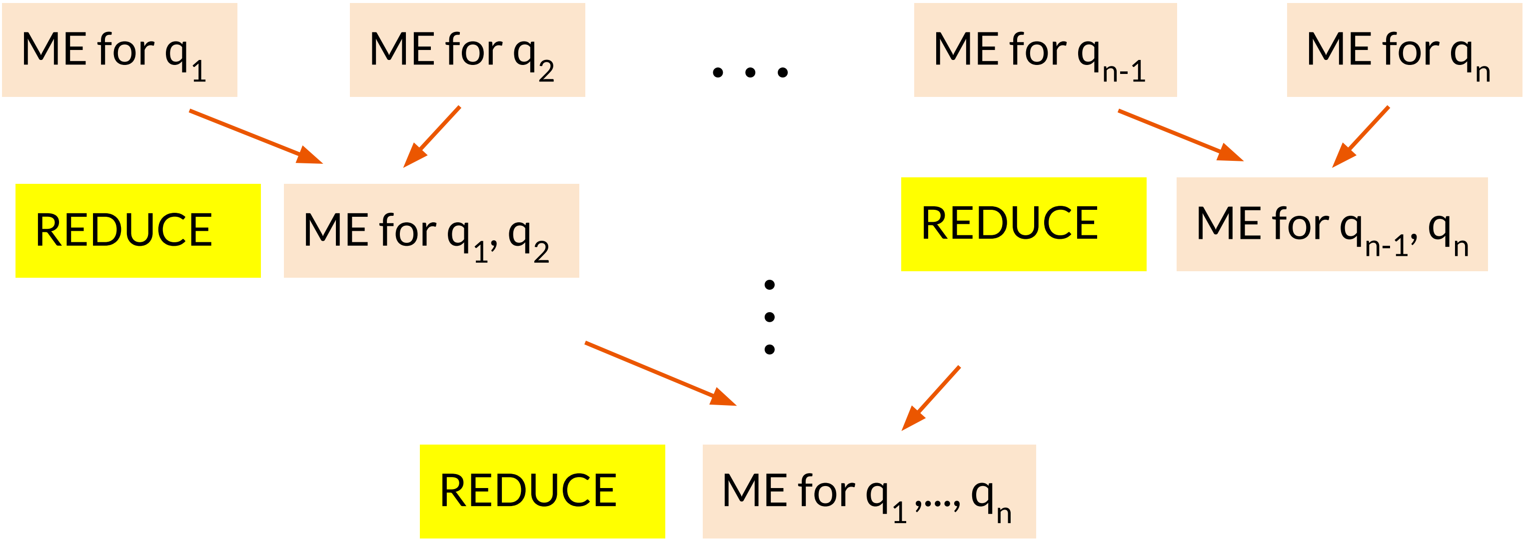
Invertible matrix
Size $2^n \times 2^n$
Can be computed

Step 3: The Matrix Equation

Find sign assignments to $q_1, \ldots, q_n$ at the roots of p
BKR builds its matrix equation (ME) inductively




ME for q_1
ME for q_2
. . .
ME for q_{n-1}
ME for q_n
REDUCE
ME for q_1, q_2
REDUCE
ME for q_{n-1}, q_n
REDUCE
ME for $q_1 ,..., q_n$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Step 3: The Matrix Equation

After each combination, remove all inconsistent sign assignments
(reduction step)

$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{bmatrix} \cdot \begin{bmatrix} 1 \\ 1 \\ 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 3 \\ 1 \\ 1 \\ -1 \end{bmatrix} \Rightarrow \begin{bmatrix} 1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{bmatrix} \cdot \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 3 \\ 1 \\ 1 \end{bmatrix}$$

Signs: ++, + - , - +, --

Signs: ++, + - , - +

Reflections on Formalizing the Matrix Equation

- Inductive construction, inductive proof!
    - It took some work to identify the right inductive invariant
    - The reduction step poses the biggest challenge
- The reduction step requires extra proofs

*Wenda Li. The Sturm-Tarski theorem. Archive of Formal Proofs, September 2014. https://isa-afp.org/entries/Sturm_Tarski.html, Formal proof development.

Reflections on Formalizing the Matrix Equation

- Isabelle/HOL has well-developed libraries
  - The Sturm-Tarski theorem is already formalized* (the key computational tool for the matrix equation)
  - A number of linear algebra libraries are available

*Wenda Li. The Sturm-Tarski theorem. Archive of Formal Proofs, September 2014. https://isa-afp.org/entries/Sturm_Tarski.html, Formal proof development.

Extending the Matrix Libraries

- We build on a matrix library by Thiemann and Yamada*
- Our additions (~1800 LOC):
  - A computational notion of the Kronecker product
  - An algorithm to extract a basis from the rows of a matrix
    - Involved proving that row rank equals column rank

*Rene Theimann and Akihisa Yamada. Matrices, Jordan normal forms, and spectral radius theory. *Archive of Formal Proofs,* August 2015.

Code Export and Experiments

Experiments with SML code

- We export our formally verified algorithm to SML for experimentation
- Compare to:
    - A naive (unverified) version of Tarski's algorithm
    - Li, Passmore, and Paulson*

*Wenda Li, Grant Olney Passmore, and Lawrence C. Paulson. Deciding univariate polynomial problems using untrusted certificates in Isabelle/HOL. J. Autom. Reason., 62(1):69–91, 2019.

Experiments with SML code

- We export our formally verified algorithm to SML for experimentation
- Compare to:
  - A naive (unverified) version of Tarski's algorithm
  - Li, Passmore, and Paulson*
- Li et. al is faster:
  - CAD is generally faster than BKR
  - Their procedure is highly optimized
  - They use Mathematica as an untrusted oracle

*Wenda Li, Grant Olney Passmore, and Lawrence C. Paulson. Deciding univariate polynomial problems using untrusted certificates in Isabelle/HOL. J. Autom. Reason., 62(1):69–91, 2019.

Experiments with SML code

*Compiled with mlton
*Run on a laptop
*Dashes indicate timeout
*Times in seconds

Benchmarks from [18]

Formula	#Poly	$\#N(p,q)$ (Naive)	$\#N(p,q)$ (BKR)	Time (Naive)	Time (BKR)	Time ([18])
ex1	4 (12)	20	31	0.003	0.006	3.020
ex2	5 (6)	576	180	5.780	0.442	3.407
ex3	4 (22)	112	120	1794.843	1865.313	3.580
ex4	5 (3)	112	95	0.461	0.261	3.828
ex5	8 (3)	576	219	28.608	8.333	3.806
ex6	22 (9)	50331648	-	-	-	6.187
ex7	10 (12)	6144	-	-	-	-
ex1 $\wedge$ 2	9 (12)	2816	298	317.432	3.027	3.033
ex1 $\wedge$ 2 $\wedge$ 4	13 (12)	28672	555	-	51.347	3.848
ex1 $\wedge$ 2 $\wedge$ 5	16 (12)	131072	826	-	436.575	3.711

3s startup time for Mathematica

[18] Wenda Li, Grant Olney Passmore, and Lawrence C. Paulson. Deciding univariate polynomial problems using untrusted certificates in Isabelle/HOL. J. Autom. Reason., 62(1):69–91, 2019.

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Putting it all together: Future directions

Future Directions

BKR

- Optimize univariate BKR
- Formally verified complexity analysis (ambitious!)
- Formalizing multivariate BKR

VS

- Continue to optimize
- Add support for division
- Extend to higher-degree?

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Towards a practical verified QE method: link together BKR, VS

Conclusion

- We have formally verified the univariate case of BKR's QE algorithm
  - BKR hits a potential **sweet spot** in between practicality and ease of verification
- We have formally verified linear and quadratic VS, a **highly effective** (but limited) QE method
  - Our experiments demonstrate the role of verification for QE

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$\exists$ Questions?