Synthesis of Optimal Numerical Algorithms using Real Quantifier Elimination

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Quantifier Elimination (QE) over Real-Closed Fields (RCF)

Problem QE over RCF

Input : ϕ - a formula in the first-order theory of RCF

Output : ψ - a quantifier-free-formula equivalent to ϕ.

Toy Example

Input: $\underset{y}{\exists}\,(x^2 + y^2 - 4 < 0 \;\wedge\; y^2 - 2x + 2 < 0)$

Output: $1 < x < 2.$

History

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1975 Collins	First algorithm with elementary complexity	
	Based on Cylindrical Algebraic Decomposition	2^{2^n}
1975 —	Doubly exponential in the number of quantifier blocks	
1975 —	Faster algorithms for special but important subclasses of formulas.	

Software:

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- Redlog
- SyNRAC
- Mathematica (Reduce command)

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QE over Real-Closed Fields (cont'd)

Applications (see *Stefan Ratschan – Applications of Quantified Constraint Solving over the Reals. Bibliography*):

- Electrical Engineering/Electronics
- Numerical analysis
- Control theory
- Computational Geometry/Motion Planning/Collision Detection
- Constraint Databases
- Theorem Proving in Real Geometry
- Program Analysis
- *Others*: camera motion, constraint logic programming, mechanical engineering, biology, automated theorem proving, optimization, termination of rewrite systems, flight control, hybrid systems, computer assisted proofs, parameter estimation, etc.

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Numerical Algorithms

Problem:

in: x - real number

ε - error bound

out: an interval I s.t. $width(I) < \varepsilon \wedge\ y \in I\ \wedge\ f(y) = x$.

Algorithm schema: Interval refining

Initialize I

while width(I) $> \varepsilon$

$I \leftarrow R(I, x)$

return I

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Numerical Algorithms (Square Root)

Problem:

in: x - real number greater than 0

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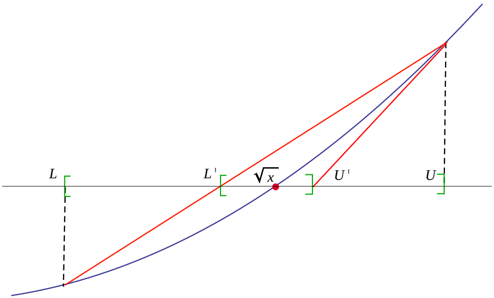

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Analysis:

- Partial Correctness
- Termination
- Complexity

Analysis – Partial Correctness

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Partial Correctness:

$$\mathit{LoopInv}(L, U) \iff 0 < L \leq \sqrt{x} \leq U$$

To show:

1. the invariant holds at the beginning of the loop
2. the invariant holds after one loop iteration
3. the invariant implies the postcondition

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Termination:

$$LoopInv(L, U) \iff 0 < L \leq \sqrt{x} \leq U$$

$$width(L, U) = U - L$$

To show:

- $\exists_{c \in (0,1)}$ s.t. $c = \sup_{\substack{L,U,x \\ LoopInv(L,U,x)}} \frac{width(f(L,U))}{width(L,U)}$

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Complexity:

The number of loop iterations n is given by

$$n = \left\lceil \frac{\log_2 \frac{\max(1,x) - \min(1,x)}{\varepsilon}}{\log_2 \frac{1}{c}} \right\rceil$$

where

$$c = \sup_{\substack{L, U, x \\ LoopInv(L, U, x)}} \frac{width(f(L, U))}{width(L, U)}$$

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Complexity:

# iter	$U' - L'$
0	$\leq l_0$
1	$\leq c \cdot l_0$
2	$\leq c^2 \cdot l_0$
...	...
n	$\leq c^n \cdot l_0 \quad \leq \varepsilon$

$$\Rightarrow n \leq \log_c \frac{\varepsilon}{l_0} \quad \Rightarrow \quad n \leq \left\lceil \log_c \frac{\varepsilon}{l_0} \right\rceil = \left\lceil \frac{\log_2 \frac{\varepsilon}{l_0}}{\log_2 c} \right\rceil = \left\lceil \frac{\log_2 \frac{l_0}{\varepsilon}}{\log_2 \frac{1}{c}} \right\rceil$$

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Complexity:

Rate of convergence

$$\underset{x>0}{\forall} \ \underset{c>0}{\exists} \ \underset{\substack{L,U \\ LoopInv(L,U)}}{\forall} \quad width(f(L, U)) \leq c(U - L)^2$$

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in: x - real number greater than 0

ε - error bound

out: an interval I s.t. $width(I) < \varepsilon \ \wedge \ y \in I \wedge y^2 = x$.

Algorithm schema: Interval refining

$I \leftarrow [\min(1,x), \max(1,x)]$

while width(I) $> \varepsilon$

$\quad I \leftarrow \left[L + \frac{x-L^2}{L+U}, U + \frac{x-U^2}{2U}\right]$

return I

Complexity:

Rate of convergence

$$\underset{x>0}{\forall} \ \underset{c>0}{\exists} \ \underset{\substack{L,U \\ LoopInv(L,U)}}{\forall} \ width(f(L,U)) \leq c(U-L)^2$$

Numerical Algorithms (Square Root) Synthesis

Problem: solve $y^2 = x$

in: x - real number

ε - error bound

out: an interval I with width less than ε such that $y \in I \ \wedge \ y^2 = x$.

Algorithm schema: Interval refining

$I \leftarrow [\min(1, x), \max(1, x)]$

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$I \leftarrow \left[L + \frac{x - L^2}{L+U}, U + \frac{x - U^2}{2U}\right]$

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Numerical Algorithms (Square Root) Synthesis

Problem: solve $y^2 = x$

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$$I \leftarrow \left[L + \frac{x + p_0 L^2 + p_1 LU + p_2 U^2}{p_3 L + p_4 U}, U + \frac{x + q_0 U^2 + q_1 UL + q_2 L^2}{q_3 U + q_4 L}\right]$$

Quadratic Refining Map

return I

Numerical Algorithms (Square Root) Synthesis

Problem: solve $y^2 = x$

in: x - real number

ε - error bound

out: an interval I with width less than ε such that $y \in I \ \wedge \ y^2 = x$.

Algorithm schema: Interval refining

$I \leftarrow [\min(1, x), \max(1, x)]$

while width$(I) > \varepsilon$

$$I \leftarrow \left[L + \frac{x+(-1)L^2+0LU+0U^2}{1L+1U}, U + \frac{x+(-1)U^2+0UL+0L^2}{2U+0L}\right]$$ Secant-Newton

return I

Numerical Algorithms (Square Root) Synthesis Optimal

$$L' = L + \frac{x + p_0 L^2 + p_1 LU + p_2 U^2}{p_3 L + p_4 U} \qquad U' = U + \frac{x + q_0 U^2 + q_1 UL + q_2 L^2}{q_3 U + q_4 L}$$

Minimize

$$E(p,q) = \sup_{\substack{L,U,x \\ 0<L\leq\sqrt{x}\leq U \\ L\neq U}} \frac{U'-L'}{U-L}$$

Subject to

$$Correctness(p,q) :\Longleftrightarrow \forall_{\substack{L,U,x \\ 0<L\leq\sqrt{x}\leq U}} \quad 0 < L' \leq \sqrt{x} \leq U'$$

$$QuadraticConv(p,q) :\Longleftrightarrow \forall_{\substack{x \\ x>0}} \ \exists_{\substack{c \\ c>0}} \ \forall_{\substack{L,U \\ 0<L\leq\sqrt{x}\leq U}} \quad U' - L' \leq c\,(U-L)^2$$

Standard numerical optimization methods cannot be applied because:

1. The objective function is itself the result of parametric optimization (sup).
2. The constraints are quantified formulas.
3. It turns out that there are infinitely many values of p and q with the same minimum.

Numerical Algorithms (Square Root) Synthesis Optimal

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Numerical Algorithms (Square Root) Synthesis Optimal by QE

$$L' = L + \frac{x + p_0 L^2 + p_1 LU + p_2 U^2}{p_3 L + p_4 U} \qquad U' = U + \frac{x + q_0 U^2 + q_1 UL + q_2 L^2}{q_3 U + q_4 L}$$

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$$Optimality(p,q) :\iff \ldots$$

Trouble: state-of-the-art QE software take very long time ($\gg$ several days)

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$$Optimality(p, q) :\Longleftrightarrow \; \ldots$$

Strategies:

1. divide the QE problems into several simpler ones
2. apply state of the art QE software
3. manual simplification on the remaining ones

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Numerical Algorithms (Square Root) Synthesis Optimal by QE (cont'd)

1. Find $Correctness(p, q)$

   Strategies:

   - Split conjunction in the goal
   - Eliminate universal quantifier using the properties of convex functions

2. Compute $E(p, q) = \sup\limits_{\substack{L,U,x \\ 0<L\leq\sqrt{x}\leq U \\ L\neq U}} \frac{U'-L'}{U-L}$, where

   $$E(p, q) = E_j(p, q) \text{ if } G_j(p, q)$$

   $$G_j(p, q) \text{– a conjunction of equations/inequalities in } p, q$$

   Strategies:

   - Variable elimination using monotonicity of functions

3. Find the minimum of $E_j(p, q)$ over
   $\bigwedge\limits_j Correctness(p, q) \wedge QuadraticConv(p, q) \wedge G_j(p, q)$.

Numerical Algorithms (Square Root) Synthesis Optimal by QE (cont'd)

1. Find *Correctness*(p, q)

   Strategies:

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Numerical Algorithms (Square Root) Synthesis Optimal by QE (cont'd)

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Numerical Algorithms (Square Root) Synthesis Optimal by QE (cont'd)

Key steps in the proof:

$$a_3>0 \wedge a_4 \geq 0 \wedge \underset{\substack{L,W \\ 0<L\leq L+W}}{\forall} \; \underset{\substack{y \\ L\leq y\leq L+W}}{\forall} \; y^2 - y(a_3L+a_4W) - L^2 + a_1LW + a_2W^2 + L(a_3L+a_4W) \leq 0 \iff \ldots$$

$$b_3>0 \wedge b_4 \geq 0 \wedge \underset{\substack{L,W \\ 0<L\leq L+W}}{\forall} \; \underset{\substack{y \\ L\leq y\leq L+W}}{\forall} \; y^2 - y(b_3L+b_4W) - L^2 + b_1LW + b_2W^2 + (L+W)(b_3L+b_4W) \geq 0 \iff \ldots$$

Numerical Algorithms (Square Root) Synthesis Optimal **by QE** (cont'd)

Key steps in the proof:

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Numerical Algorithms (Square Root) Synthesis Optimal by QE (cont'd)

Key steps in the proof:

$$
\begin{aligned}
E(p,q) &= \sup_{\substack{0<L\le\sqrt{x}\le U\\ L\ne U}} \left[\frac{U'-L'}{U-L}\right]\\
&\quad \cdots\\
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Numerical Algorithms (Square Root) Synthesis Optimal **by QE** (cont'd)

Key steps in the proof:

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Numerical Algorithms (Square Root) Synthesis Optimal by QE (cont'd)

Main Result:

(a) $E(p,q) \geq \frac{1}{4}$ $\left(E(p^*,q^*) = \frac{1}{2},\ \text{where } p^*, q^* \text{ are for Secant-Newton}\right)$

(b) $E(p,q) = \frac{1}{4}$ iff $p = (-1,0,0,1,1) \wedge q = \left(-\frac{3}{4}, -\frac{1}{2}, \frac{1}{4}, 1, 1\right)$

In other words

$$L' = L + \frac{x - L^2}{L + U}$$

$$U' = U + \frac{x - \frac{3}{4}U^2 - \frac{1}{2}LU + \frac{1}{4}L^2}{U + L}$$

How much improvement?

	Secant-Newton Map $R^*(I, x)$	Synthesized Map $\tilde{R}(I, x)$	
Original	$\left[L + \frac{x - L^2}{L+U}, U + \frac{x - U^2}{2U}\right]$	$\left[L + \frac{x - L^2}{L+U}, U + \frac{x - \frac{3}{4}U^2 - \frac{1}{2}LU + \frac{1}{4}L^2}{U+L}\right]$	
Rewritten	$\left[\frac{x+LU}{L+U}, \frac{x}{U+U} + \frac{1}{4}(U+U)\right]$	$\left[\frac{x+LU}{L+U}, \frac{x}{U+L} + \frac{1}{4}(U+L)\right]$	
# of ops.	9	9	The same
Convergence	Quadratic	Quadratic	The same
Lipschitz	$\frac{1}{2}$	$\frac{1}{4}$	Better
# of loop iters.	$\log_2 \frac{I_0}{\varepsilon}$	$\frac{\log_2 \frac{I_0}{\varepsilon}}{2}$	Better

Input: $x = 150$ $\quad \varepsilon = 10^{-5}$

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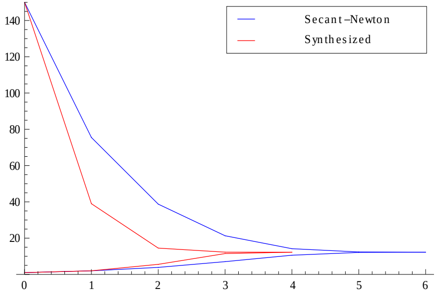

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(1) Carried out a case study on the synthesis of optimal numerical algorithms for square root computation.

(2) Semi-automatically an algorithm faster than Secant-Newton.

Current and future work:

(b) derive the result *completely* automatically

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