Nonlinear Polynomials, Interpolants and Invariant Generation for System Analysis

Deepak Kapur

Department of Computer Science
University of New Mexico
Albuquerque, NM, USA

with Rodriguez-Carbonell, Zhihai Zhang, Hengjun Zhao, Stephan Falke, Naijun Zhan, Ting Gan, Bican Xia and others
(work in progress)

Outline

- Ideal-theoretic approach for generating nonlinear polynomial equalities as invariants.

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- Challenges for symbolic computation community.

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- Automation and scalability are critical for success.

Invariants: Integer Square Root

Example

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x := 1, y := 1, z := 0;
while (x <= N) {
  x := x + y + 2;
  y := y + 2;
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Explore methods that can generate (strong) loop invariants (useful program properties) automatically for a large class of programs

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Papers with Enric Rodríguez-Carbonell in ISSAC (2004), SAS (2004), ICTAC (2004), Science of Programming (2007), Journal of Symbolic Computation (2007)

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Interplay of Computational Logic and Algebra

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- Using quantifier elimination, find constraints on parameters $A, B, C, D, E, F, G, H, J, K$ which ensure that the verification conditions are valid for all possible program variables.

Quantifier Elimination from Verification Conditions

Considering **VC2:**

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- Simplifying using the hypothesis gives:
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- Since this should be 0 for all values of x, y, z: we have: $A + D = 0$; $A = 0$; $E = 0$ which implies $D = 0$; using these gives: $2C + 2F = 0$ which implies $C = -F$; using all these: $G = -4B - F$, $H = -G - K - B$ and $J = -2B - F + 2K$.

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- $B = 1, J = -2, G = -4, H = 3$ gives $y^2 - 4x + 3y - 2z = 0$.
- The most general invariant describing all invariants of the above form is a conjunction of:

  $$y = 2z + 1; \quad z^2 - yz + z + x - y = 0 \quad y^2 - 2z - 4x + 3y = 0,$$

  from which $x = (z + 1)^2$ follows.

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- Find a formula expressed in terms of parameters eliminating all program variables (using quantifier elimination).

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- If all assignments making the formula true can be finitely described, invariants generated may be the strongest of the hypothesized form. Invariants generated are guaranteed to be the strongest if no approximations are made, while generating verification conditions.

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  - Output is huge and difficult to decipher.
  - In practice, they often do not work (i.e., run out of memory or hang).
- Linear constraint solving on rationals and reals (polyhedral domain), while of polynomial complexity, has been found in practice to be inefficient and slow, especially when used repeatedly as in abstract interpretation approach [Miné]

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Making QE based Method Practical

- Identify (atomic) formulas and program abstractions resulting in verification conditions with good shape and structure.
- Develop QE heuristics which exploit *local* structure of formulas (e.g. two variables at a time) and geometry of state space defined by formulas.
- Among many possibilities in a result after QE, identify those most likely to be useful.
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- Combination of Octagonal and Max formulas.

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for every pair of variables x_i, x_j, where $a_{i,j}$, $b_{i,j}$, $c_{i,j}$, $d_{i,j}$, e_i, f_i, g_j, h_j are parameters.

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- **Goal:** Performance of QE heuristic should be at least as good.

A Simple Example

Example

```
 x := 4; y := 6;
while (x + y >= 0) do
 if (y >= 6) then { x := -x;  y := y - 1 }
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- A program path is a sequence of assignment statements interspersed with tests. Its behavior may have to be approximated to generate the post condition in which both the hypothesis and the conclusion are each conjunctions of atomic octagonal formulas.

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- Analysis of a big conjunctive constraint on every possible pair of variables can be considered individually by considering the subformula on each distinct pair.

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- Analyze how a general octagon gets transformed due to assignments. For each assignment case, a table is built showing the effect on the parameter values.

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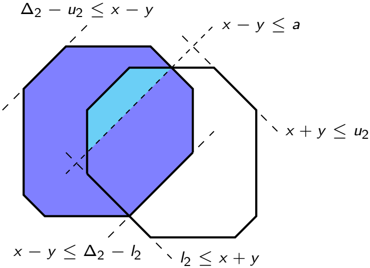
- In the case of many possibilities, the one likely to generate the most useful invariant is identified.
- Quantifier elimination heuristics to generate constraints on lower and upper bounds by table look ups in $O(n^2)$ steps, where n is the number of program variables.

Table 3: Sign of exactly one variable is changed

$$x := -x + A$$
$$y := y + B$$

$$\Delta_1 = A - B, \quad \Delta_2 = A + B.$$



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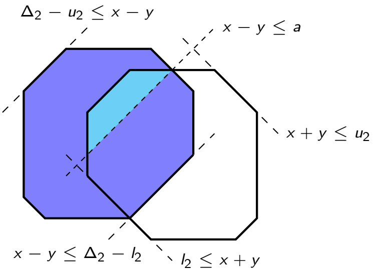

constraint	present	absent	side condition
$x - y \leq a$	$a \leq \Delta_2 - l_2$	$u_1 \leq \Delta_2 - l_2$	–
$x - y \geq b$	$\Delta_2 - u_2 \leq b$	$\Delta_2 - u_2 \leq l_1$	–
$x + y \leq c$	$c \leq \Delta_1 - l_1$	$u_2 \leq \Delta_1 - l_1$	–
$x + y \geq d$	$\Delta_1 - u_1 \leq d$	$\Delta_1 - u_1 \leq l_2$	–
$x \leq e$	$e \leq A - l_3$	$u_3 \leq A - l_3$	–
$x \geq f$	$A - u_3 \leq f$	$A - u_3 \leq l_3$	–
$y \leq g$	$u_4 \geq g + B$	$u_4 = +\infty$	$B > 0$
$y \geq h$	$l_4 \leq h + B$	$l_4 = -\infty$	$B < 0$

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Generating Constraints on Parameters

- **VC0:**
  $l_1 \leq -2 \leq u_1 \wedge l_2 \leq 10 \leq u_2 \wedge l_3 \leq 4 \leq u_3 \wedge l_4 \leq 6 \leq u_4.$

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  x: $l_3 \le -6.$
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- Make l_i's as large as possible and u_i's as small as possible:
  $l_1 = -10, u_1 = 9, l_2 = -11, u_2 = 10,$
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  $l_3 = -6, u_3 = 6, l_4 = -5, u_4 = 6.$
- The corresponding invariant is:
  $-10 \leq x - y \leq 9 \wedge -11 \leq x + y \leq 10$
  $\wedge -6 \leq x \leq 6 \wedge -5 \leq y \leq 6.$

Generating Invariants using Table Look-ups

- Parameter constraints corresponding to a specific program path are read from the corresponding entries in tables.

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- Parameter constraints corresponding to a specific program path are read from the corresponding entries in tables.
- Accumulate all such constraints on parameter values. They are also **octagonal**.
- Every parameter value that satisfies the parameter constraints leads to an invariant.
- Maximum values of lower bounds and minimal values of upper bounds satisfying the parameter constraints gives the strongest invariants. Maximum and minimum values can be computed using Floyd-Warshall's algorithm.

Complexity and Parallelization

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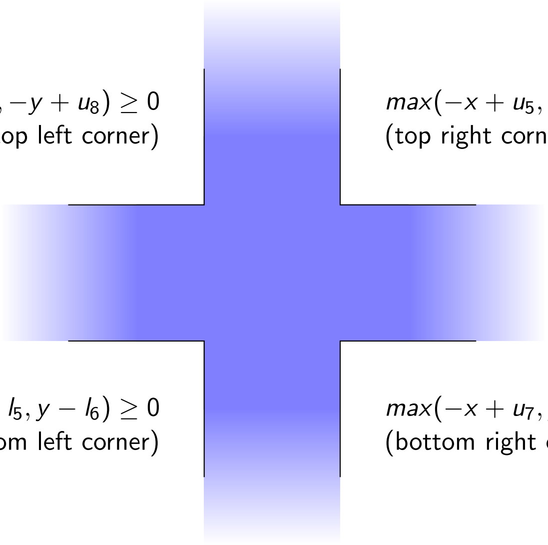
- Program paths can be analyzed in parallel. Parametric constraints can be processed in parallel.

Max Formulas

Pictorial representation of all possible cases of $max(\pm x + l, \pm y + h)$. Observe that every defined region is nonconvex.

$max(x - l_8, -y + u_8) \geq 0$ (top left corner)

$max(-x + u_5, -y + u_6) \geq 0$ (top right corner)



$max(x - l_5, y - l_6) \geq 0$ (bottom left corner)

$max(-x + u_7, y - l_7) \geq 0$ (bottom right corner)

Max Formulas

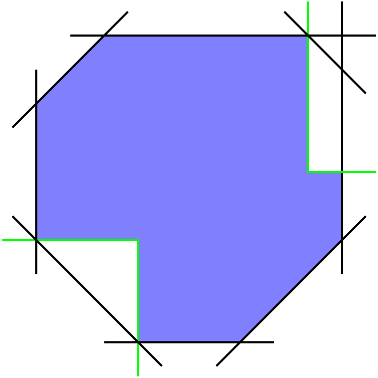
A typical template: octagonal formulas and max formulas.

$$
\begin{aligned}
l_1 \leq \quad & x - y \quad \leq u_1 \\
l_2 \leq \quad & x + y \quad \leq u_2 \\
l_3 \leq \quad & x \quad \leq u_3 \\
l_4 \leq \quad & y \quad \leq u_4 \\
max(\ \ x - \ l_5, \ \ y - \ l_6) & \geq 0 \\
max(\ \ x - \ l_8, -y + u_8) & \geq 0 \\
max(-x + u_7, \ \ y - \ l_7) & \geq 0 \\
max(-x + u_5, -y + u_6) & \geq 0
\end{aligned}
$$

Max Formulas – some nonconvex regions

An octagon with two corners cut out.

A square that turns into 2 disconnected components.



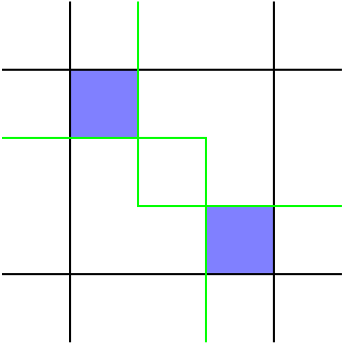


Table 6: Parametric Constraints for assignments with sign of one variable reversed

Assignments: $x := -x + A, y := y + B$

Bottom left and bottom right corners:
$max(x - l_5, y - l_6) \geq 0$ and $max(-x + u_7, y - l_7) \geq 0$

	$y \geq h$ absent	$y \geq h$ present
$x \geq f$ absent	$(l_5 + u_7 \geq A \wedge l_7 - l_6 \leq B)$ $\vee\, l_5 + u_7 \leq A \vee l_7 - l_4 \leq B$ $\vee\, l_2 - l_7 + u_7 \geq A - B$	$l_7 \leq h + B$
$x \geq f$ present	$u_7 \geq -f + A$	$u_7 \geq -f + A \vee l_6 \leq h + B$

The constraints for two absent tests can also be used as disjuncts in the other cases.

	$y \geq h$ absent	$y \geq h$ present
$x \leq e$ absent	$(l_5 + u_7 \leq A \wedge l_6 - l_7 \leq B)$ $\vee\, l_5 + u_3 \leq A \vee l_6 - l_4 \leq B$ $\vee\, l_5 + l_6 - u_1 \geq A + B$	$l_6 \leq h + B$
$x \leq e$ present	$l_5 \leq -e + A$	$l_5 \leq -e + A \vee l_6 \leq h + B$

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Table 6 Contd: Parametric Constraints for assignments with sign of one variable reversed

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Top left and top right corners:
$max(x - l_8, -y + u_8) \geq 0$ and $max(-x + u_5, -y + u_6) \geq 0$

	$y \leq g$ absent	$y \leq g$ present
$x \geq f$ absent	$(l_8 + u_5 \geq A \wedge u_6 - u_8 \geq B)$ $\vee\ l_3 + u_5 \geq A \vee u_6 - u_4 \geq B$ $\vee\ l_1 + u_5 + u_6 \geq A + B$	$u_6 \geq g + B$
$x \geq f$ present	$u_5 \geq -f + A$	$u_5 \leq -f + A \vee u_6 \geq g + B$

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Example: Stairs Program

```
x := 1; y := 4;
while (y>1) {
  if (x<2)
    x++;
  else if (y>3)
    y--;
  else if (x<3)
    x++;
  else if (y>2)
    y--;
  else if (x<4)
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  else
    y--;
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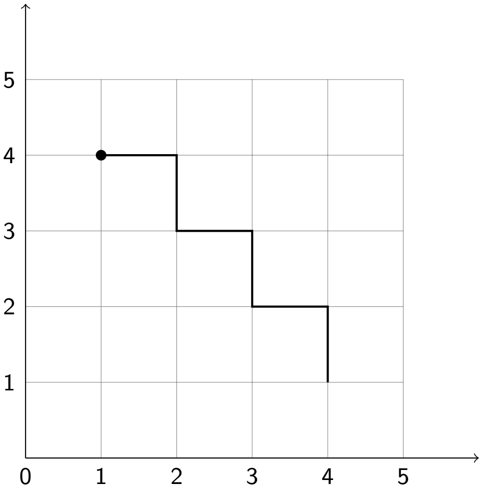

Example: Stairs Program

Parametric Constraints due to the initialization `x := 1; y := 4`:

$$
\begin{aligned}
l_1 &\leq -3 \leq u_1 & \qquad l_5 \leq 1 &\vee l_6 \leq 4 \\
l_2 &\leq 5 \leq u_2 & \qquad u_5 \geq 1 &\vee u_6 \geq 4 \\
l_3 &\leq 1 \leq u_3 & \qquad l_7 \leq 1 &\vee u_7 \geq 4 \\
l_4 &\leq 4 \leq u_4 & \qquad l_8 \geq 1 &\vee u_8 \geq 4
\end{aligned}
$$

Example: Stairs Program

Parametric Constraints from Table look up for

- Program paths in which x is increasing:

$$u_1 = +\infty$$
$$u_2 = +\infty$$
$$u_3 \geq 2$$
$$u_3 \geq 3$$
$$u_3 \geq 4$$
$$u_5 \geq 2$$
$$u_5 \geq 3 \vee u_6 \geq 3$$
$$u_5 \geq 4 \vee u_6 \geq 2$$

- Program Paths in which y is decreasing:

$$u_1 = +\infty$$
$$l_2 = -\infty$$
$$l_4 \leq 3$$
$$l_4 \leq 2$$
$$l_4 \leq 1$$
$$l_5 \geq 2 \vee l_6 \geq 5$$
$$l_5 \geq 3 \vee l_6 \geq 4$$
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Example: Stairs Program

Putting all parametric constraints together and deriving the strongest max invariant

(contrasted with the strongest octagonal invariant)

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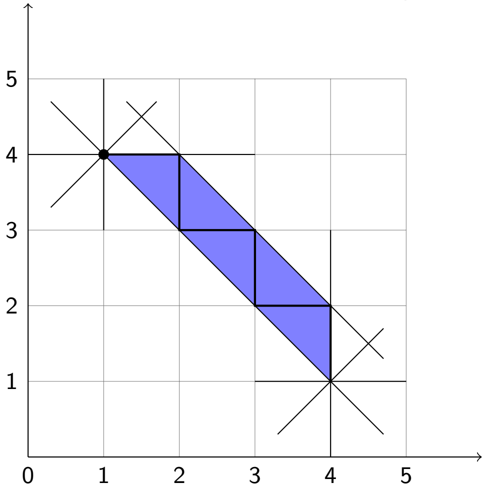

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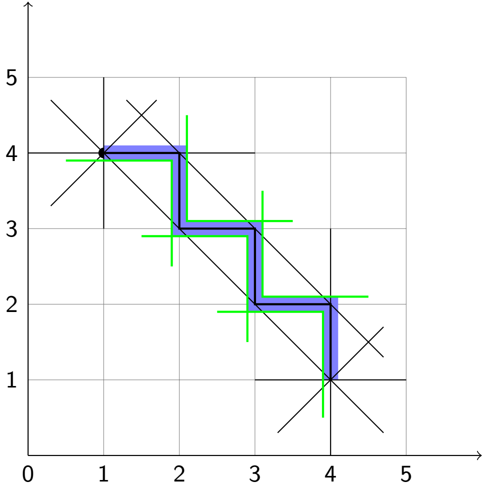
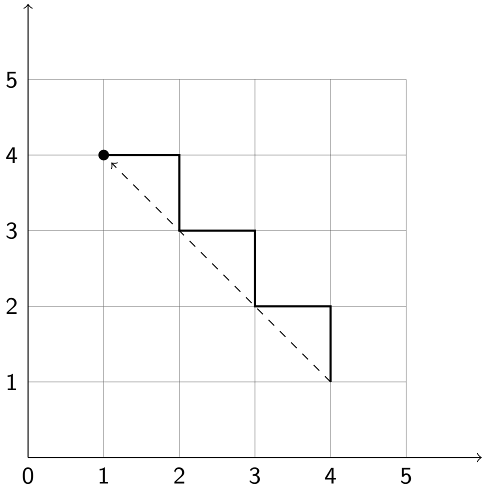


Invariants of a Program with a nested loop

```
x := 1; y := 4;
while (true) {
  if (x<2)
    x++;
  else if (y>3)
    y--;
  else if (x<3)
    x++;
  else if (y>2)
    y--;
  else if (x<4)
    x++;
  else if (y>1)
    y--;
  else
    while (x>1) {
      x--; y++;
    }
}
```



Invariants of a Program with a nested loop

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x := 1; y := 4;
while (true) {
  if (x<2)
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  else if (y>3)
    y--;
  else if (x<3)
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  else if (y>2)
    y--;
  else if (x<4)
    x++;
  else if (y>1)
    y--;
  else
    while (x>1) {
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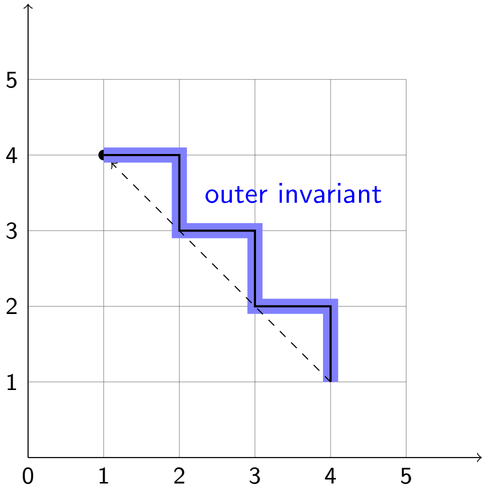
    }
}
```



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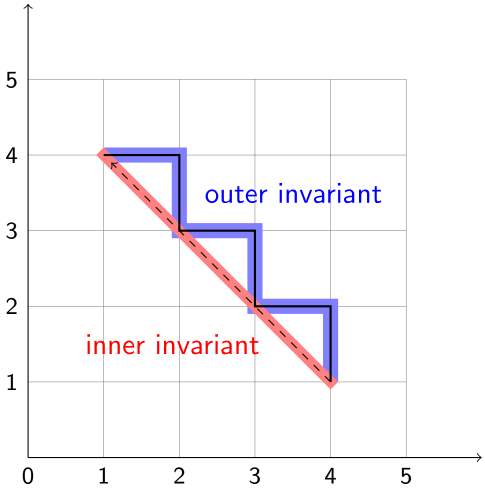

Max Invariants vs Octagonal Invariants

- 16 instead of 8 parameters per variable pair:
  $l_1, u_1, \ldots, l_4, u_4, \quad l_5, u_5, \ldots, l_8, u_8$

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  Max: Multiple noncomparable values for parameter tuples.
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  - Sacrificing efficiency to generate stronger invariants.
- Same asymptotic complexity if a single parametric constraint in every table entry is selected.

Termination Analysis based on Quantifier Elimination

Ranking functions can be synthesized by hypothesizing poiynomials in program variables and unary predicates on program variable in a loop body.

Example

```
while (n>1) {
  if  n mod 2 = 0 then n := n/2
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Theorem There does not exist any polynomial in n that can serve as a ranking function.

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Must use the function $n \ mod \ 2$. Consider $n + 2(n \ mod \ 2)$ as a possible ranking function (which can be generated from $An + B(n \ mod \ 2) + C$).

1. $n \ mod \ 2 = 0$: tricky but with the loop condition $n > 1$, easy.
2. otherwise: $n' = n + 1$: easy.

Interpolant Generation using Quantifier Elimination

Craig: Given $\alpha \implies \beta$, an intermediate formula γ in common symbols of α and β exists and can be constructed such that

$$\alpha \implies \gamma \wedge \gamma \implies \beta$$

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In Kapur et al (FSE06) we showed an obvious connection between interpolation and quantifier elimination.

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- The above assertions assume complete quantifier elimination.
- This interpolant generated from α can serve as an interpolant all β's whose uncommon symbols with α are precisely remain invariant. Other properties of such interpolants can also be established.

Interpolants over Equality with Uninterpreted Symbols

α, a finite conjunction of equality and disequalities over constants and function symbols, with their subset UC being uncommon symbols with β's (UC may or may not include nonconstant function symbols).

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  - Define a total ordering in which all uncommon nonconstant symbols are bigger than all uncommon constant symbols, followed by all common nonconstant symbols which are made bigger than all common constant symbols, run congruence closure which is ground completion.
  - This is in contrast to Kapur's algorithm in which all nonconstant symbols are bigger than constant symbols.

Interpolants over Equality with Uninterpreted Symbols

- The result is a finite set of rewrite rules of the form
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- **Horn clause introduction** From

$$f(a, b) \to e, \quad f(c, d) \to g,$$

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  where f is uncommon or least one of a, b, c, d is uncommon.
- **Normalize Horn clauses** Run congruence closure on the antecedent and normalize the consequent. If a Horn clause becomes trivially true, it is discarded. This is done every time a new Horn clause is generated.

Interpolants over Equality with Uninterpreted Symbols

- **Conditional Rewriting** The consequent of a Horn clause may have a uncommon symbol on its left side, which may also appear in an antecedent. That can be replaced in all such antecedents by carrying the conditions of this antecedent,

$$(c_1 = d_1 \wedge \cdots \wedge c_k = d_k) \Longrightarrow c = d$$

$$(a_1 = b_1 \wedge \cdots \wedge a_l = b_l) \Longrightarrow a = b$$

If a is some c_i or d_i, then

$$(a_1 = b_1 \wedge \cdots \wedge a_l = b_l) \wedge (c_1 = d_1 \wedge b = d_i \wedge \cdots c_k = d_k) \Longrightarrow c = d$$

DIsequalities do not play since at best they can do is to delete a Horn clause or identify unsatisfiability. But if α is assumed to be satisfiable in the input, then the result of this includes an interpolant which is all the equations and Horn clauses which only have common symbols.

An Example of Interpolant Generation on EUF

Mutually contradictory $\alpha = \{x_1 = z_1, z_2 = x_2, z_3 = f(x_1), f(x_2) = z_4, x_3 = z_5, z_6 = x_4, z_7 = f(x_3), f(x_4) = z_8\}$ and

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Our algorithm gives:
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Interpolant Generation over Octagonal formulas

Let α to be a conjunction of $\pm x_i \leq c_i$ and $\pm x_i \pm x_j \leq c_{i,j}$, where x_i and x_j are distinct.

1. For each uncommon symbol x_i in α, consider two octagon formulas in which the sign of x_i is positive in one and negative in the other.
   x_i is eliminated by adding the two formulas. This must be done for every pair of such formulas.

The result of all uncommon symbols is an interpolant generated from α. This is illustrated below.

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3. If some uncommon symbol only appears positively or negatively, all octagonal formulas containing it can be eliminated as they do not occur in the interpolant.

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Griggio's example of Octagonal Formulas

Mutually contradictory
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Griggio's algorithm gives the conditional interpolant
$(-x_6 - x_5 \geq 0) \Longrightarrow (x_1 - x + 3 \geq 3)$

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   $\{-x_3 + x_5 \geq 2, x_1 + x_6 \geq 0, x_1 + x_5 \geq -7, \quad -x_3 + x_6 \geq 9\}$.
2. No literal from α is included.
3. Interpolant:
   $I_\alpha = \{-x_3 + x_5 \geq 2, x_1 + x_6 \geq 0, x_1 + x_5 \geq -7, -x_3 + x_6 \geq 9\}$.

Griggio's algorithm gives the conditional interpolant
$(-x_6 - x_5 \geq 0) \implies (x_1 - x + 3 \geq 3)$
The strongest interpolant is an octagonal formula and is generated by our algorithm.

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- ψ is an abductor for $(I \wedge cond, I')$.

Saturation based Invariant Strengthening and Abductor Generation

Example

var x, y, z: integer **end var**
$x := 0, \quad y := 0, \quad z := 9;$
while $x \leq N$ **do**
$x := x + 1; \quad y := y + 1; \quad z := z + x - y;$
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Quantifier elimination comes to the rescue

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- Let us call a spade a spade.

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- Can we have **better, effective** interfaces between a computer algebra system and a theorem prover?
- Can certificates be generated for outputs computed by a symbolic computation algorithm so that a theorem prover/SMT solver can trust it?

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  5. a small step: interpolant generation for concave quadratic polynomial inequalities (over EUF).