Machine Learning for Quantifiers

Mikoláš Janota

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Czech Technical University

CTU CZECH TECHNICAL UNIVERSITY IN PRAGUE

MINISTRY OF EDUCATION, YOUTH AND SPORTS

ROBOPROX

Outline

Intro: QBF, Expansion, Games, Careful expansion

Solving QBF

Learning in QBF

Targeting SMT

Towards Synthesizing Terms

Towards Infinite Models

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SAT and QBF

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  ($\forall = \wedge$, $\exists = \vee$)

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  2. $\forall x.\ (x \leftrightarrow 0) \vee (x \leftrightarrow 1)$

SAT and QBF

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  4. 1 (True)

Satisfiability Modulo Theories (SMT)

- Example (single instantiations)

$$f : \mathbb{Z} \to \mathbb{Z}$$
$$(\forall x : \mathbb{Z})(f(x) > 0)$$
$$f(0) < 0$$

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\begin{aligned}
&f : \mathbb{Z} \to \mathbb{Z} \\
&(\forall x : \mathbb{Z})(f(x) > 0) \\
&f(0) < 0
\end{aligned}
$$

- Example (many instantiations)

$$
\begin{aligned}
&f : \mathbb{Z} \to \mathbb{Z} \\
&(\forall x : \mathbb{Z})(f(x) < f(x+1)) \\
&f(0) > f(100)
\end{aligned}
$$

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$$(\forall u \exists e)(u \leftrightarrow e)$$

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Example

$$(\forall u \exists e)(u \leftrightarrow e)$$

$\exists$-player wins by playing $e \triangleq u$.

Solving QBF

Solving by CEGAR Expansion

$$(\exists \vec{E} \forall \vec{U})(\phi) \equiv (\exists \vec{E}) \bigwedge_{\mu \in 2^{\vec{U}}} \phi[\mu]$$

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- $(\exists x)(1 \Rightarrow x \wedge 1 \Rightarrow \neg x)$

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- Expansion by definition: 2^3
- Sufficient: $u = z = w = 1$ and $u = z = w = 0$
- $(\exists x)(1 \Rightarrow x \wedge 1 \Rightarrow \neg x)$
- What is a good expansion?

Solving by CEGAR Expansion Contd.

$$(\exists \vec{E} \forall \vec{U})\ \phi \equiv (\exists \vec{E})\ \bigwedge_{\mu \in 2^{\vec{U}}} \phi[\mu]$$

Expand gradually instead: [J. and Marques-Silva, 2011]

- Pick τ_0 arbitrary assignment to $\vec{E}$

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- $\texttt{SAT}(\neg\phi[\tau_1]) = \mu_2$ assignment to $\vec{U}$
- $\texttt{SAT}(\phi[\mu_0] \wedge \phi[\mu_1]) = \tau_2$ assignment to $\vec{E}$

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- $\mathtt{SAT}(\neg\phi[\tau_1]) = \mu_2$ assignment to $\vec{U}$
- $\mathtt{SAT}(\phi[\mu_0] \wedge \phi[\mu_1]) = \tau_2$ assignment to $\vec{E}$
- After n iterations

$$(\exists\vec{E}\,)\ \bigwedge_{i\in 1..n} \phi[\tau_i]$$

Strengths and Weaknesses

Careful Expansion: Good Example

$$(\exists x \ldots \forall y \ldots)(\phi \wedge y)$$

Setting counter-move $y \triangleq 0$ yields false. Stop.

Careful Expansion: Good Example

$$(\exists x \ldots \forall y \ldots)(\phi \land y)$$

Setting counter-move $y \triangleq 0$ yields false. Stop.

$$(\exists x \ldots \forall y \ldots)(x \lor \phi)$$

Setting candidate $x \triangleq 1$ yields true. Stop.

Careful Expansion: Bad Example

$$(\exists x \forall y)(x \Leftrightarrow y)$$

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Necessarily you need to use both:

$\mathtt{SAT}(x \Leftrightarrow 0 \wedge x \Leftrightarrow 1) \ldots$ UNSAT Stop

Careful Expansion: Ugly Example

$$(\exists x_1 x_2 \forall y_1 y_2)(x_1 \Leftrightarrow y_1 \vee x_2 \Leftrightarrow y_2)$$

Careful Expansion: Ugly Example

$$(\exists x_1 x_2 \forall y_1 y_2)(x_1 \Leftrightarrow y_1 \vee x_2 \Leftrightarrow y_2)$$

Necessarily need 2^2 values of y_1, y_2

Learning in QBF

Issue

- CEGAR requires 2^n SAT calls for the formula

$$(\exists x_1 \ldots x_n \forall y_1 \ldots y_n) \left(\bigvee_{i \in 1..n} x_i \Leftrightarrow y_i \right)$$

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- BUT: The formula immediately false if we set $y_i \triangleq \neg x_i$.

$$\left(\exists x_1 \ldots x_n \forall y_1 \ldots y_n. \bigvee_{i \in 1..n} x_i \Leftrightarrow \neg x_i\right) \equiv \left(\exists x_1 \ldots x_n.\ 0\right)$$

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- Idea: plug in functions rather than constants.

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- Idea: plug in functions rather than constants.
- **Where do we get the functions?**

Use Machine Learning

[J., 2018]

1. Enumerate some candidate-countermove pairs.

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4. Repeat.

Machine Learning Example

x_1	x_2	$\dots$	x_n	y_1	y_2	$\dots$	y_n
0	0	$\dots$	0	1	1	$\dots$	1
1	0	$\dots$	0	0	1	$\dots$	1
0	0	$\dots$	1	1	1	$\dots$	0
0	1	$\dots$	1	1	0	$\dots$	0

Machine Learning Example

x_1	x_2	...	x_n	y_1	y_2	...	y_n
0	0	...	0	1	1	...	1
1	0	...	0	0	1	...	1
0	0	...	1	1	1	...	0
0	1	...	1	1	0	...	0

- After 2 steps: $y_1 \leftarrow \neg x_1$, $y_i \leftarrow 1$ for $i \in 2..n$.

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- $SAT(x_1 \Leftrightarrow \neg x_1 \vee \bigvee_{i \in 2..n} x_2 \Leftrightarrow 1)$

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- After 4 steps: $y_1 \leftarrow \neg x_1 \; y_2 \leftarrow \neg x_2 \ldots$

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- $SAT(x_1 \Leftrightarrow \neg x_1 \vee \bigvee_{i \in 2..n} x_2 \Leftrightarrow 1)$
- After 4 steps: $y_1 \leftarrow \neg x_1$ $y_2 \leftarrow \neg x_2$ $\ldots$
- Eventually we learn the right functions.

Implementation Notes (2018)

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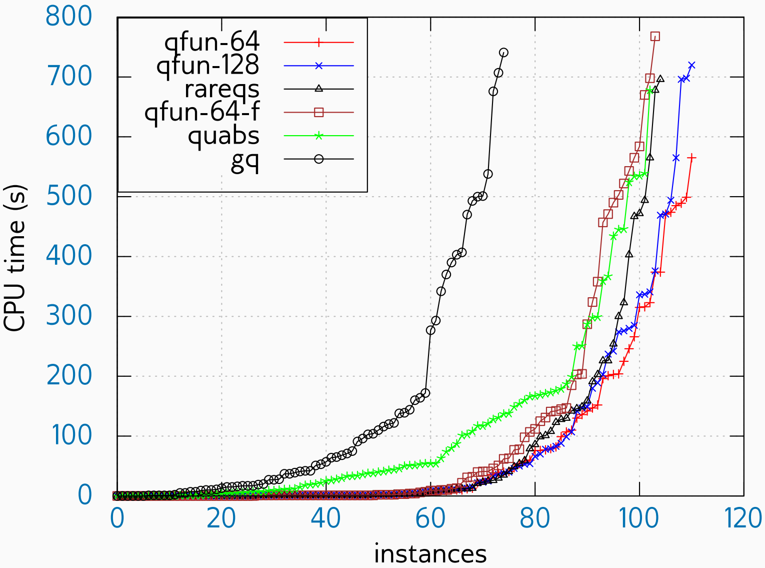
- Recursion to generalize to multiple levels as before.
- Refinement as before.
- Every K refinements, learn new functions from last K samples. Refine with them.
- Learning using decision trees by ID3 algorithm.
- Additional heuristic: If a learned function still works, keep it. "Don't fix what ain't broke."

Experiments



Targeting SMT

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\begin{array}{ll}
 & f(f(c)) \neq c \\
\wedge & (\forall x)(f(x) = x)
\end{array}
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Instantiation:

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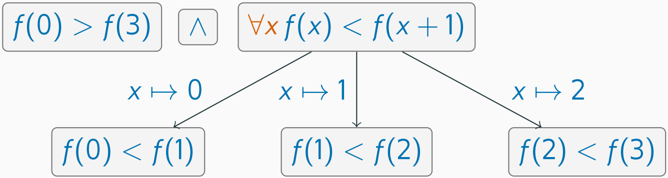
 & f(f(c)) \neq c \\
\wedge & f(c) = c \\
\wedge & f(f(c)) = f(c)
\end{array}
$$

Instantiations for UnSAT

$f(0) > f(3)$ $\wedge$ $\forall x\, f(x) < f(x+1)$

Instantiations for UnSAT



Instantiations for UnSAT

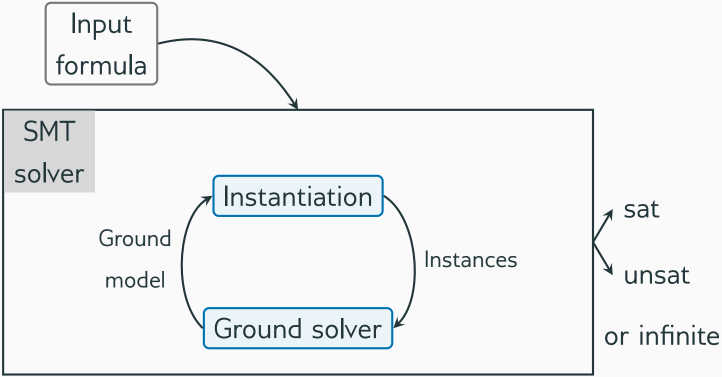
$f(0) > f(3)$ $\wedge$ $\forall x\, f(x) < f(x+1)$

$x \mapsto 0$ $x \mapsto 1$ $x \mapsto 2$

$f(0) < f(1)$ $f(1) < f(2)$ $f(2) < f(3)$

$\Rightarrow \bot$

Setup for Machine Learning



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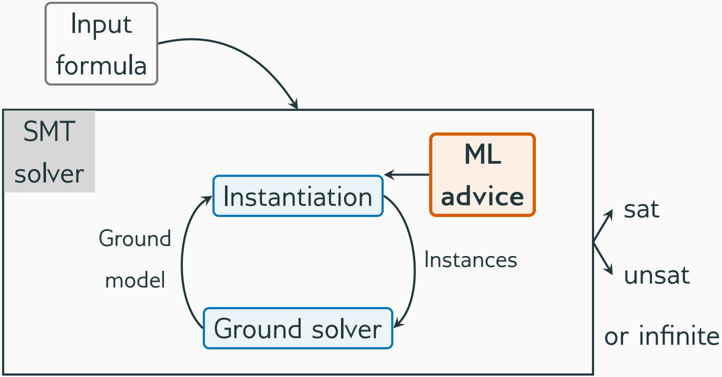
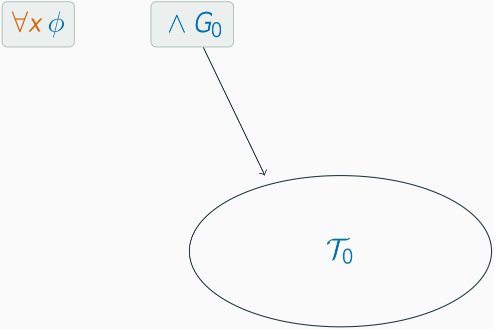


Strengthened Herbrand Theorem

$\forall x \, \phi$

$\wedge \, G_0$

Strengthened Herbrand Theorem



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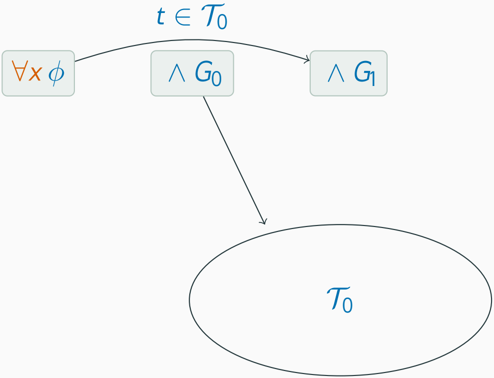
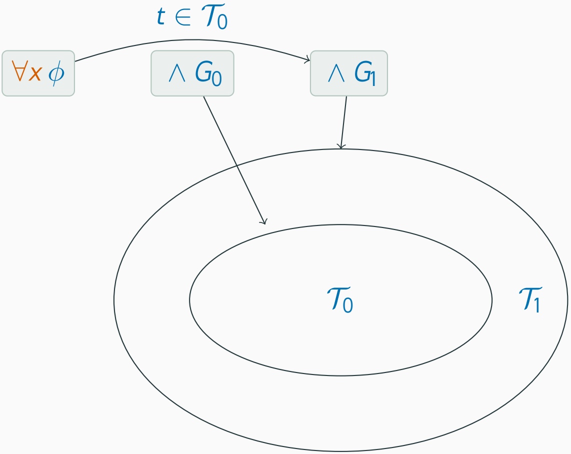


Strengthened Herbrand Theorem



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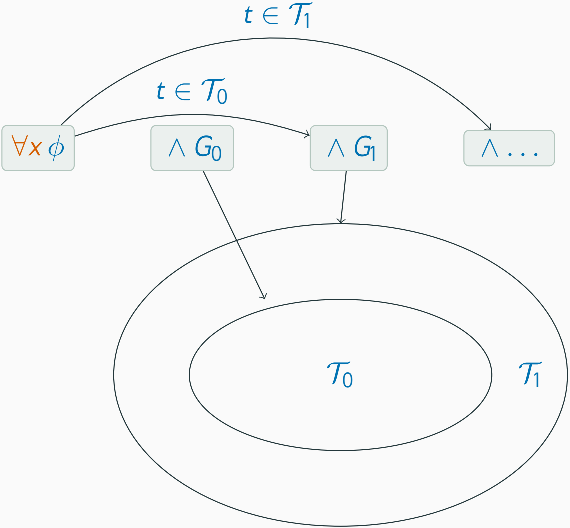

Ordering Possible Candidates

$$\forall \quad x \quad y \quad z \quad (x < y) \vee (x < z)$$

Ordering Possible Candidates

$\forall$	x	y	z
	0	1	11
	3	5	7
	10	9	2

$(x < y) \vee (x < z)$

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$$(x < y) \vee (x < z)$$

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...	...	...

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Ordering Possible Candidates

∀	x	y	z
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$(x < y) \vee (x < z)$

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...	...	...

Task for ML

Input:

Set of terms for quantified variable

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Objective:

Order the terms to increase likelihood of UnSAT

High-level ML Design

[J. et al., 2022]

- Gradient boosted trees (LightGBM)

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    - **anonymous** for **uninterpreted** symbols, e.g. f, g.

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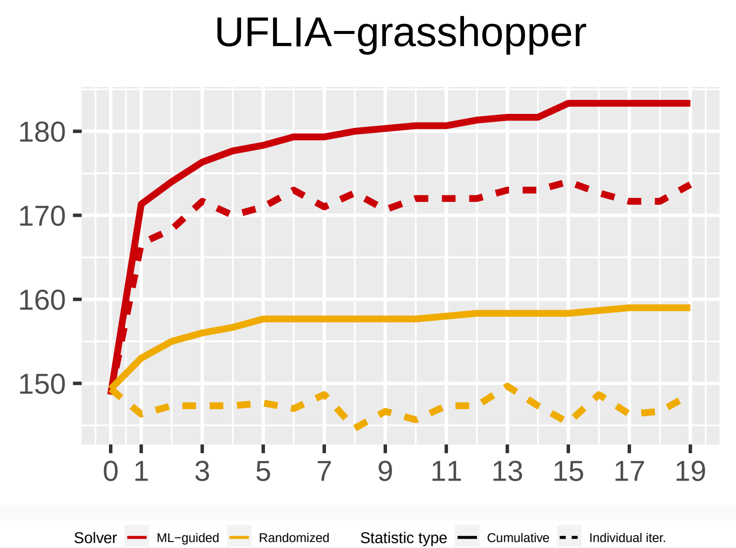
Solved instances – Target set



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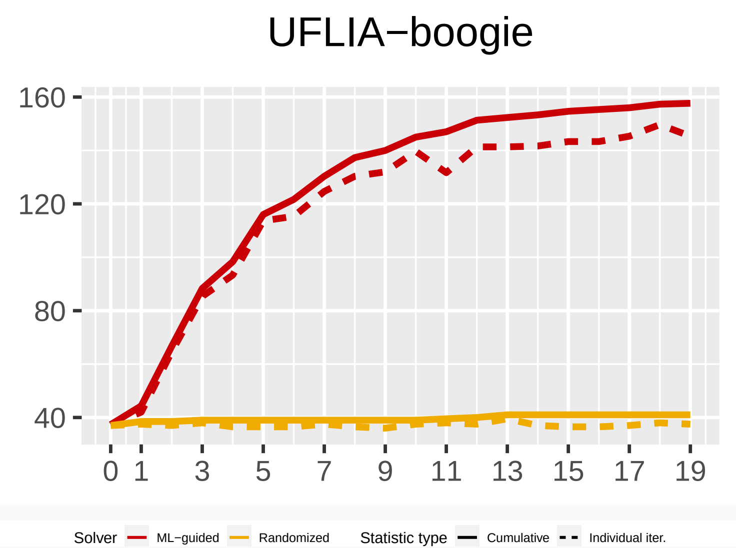
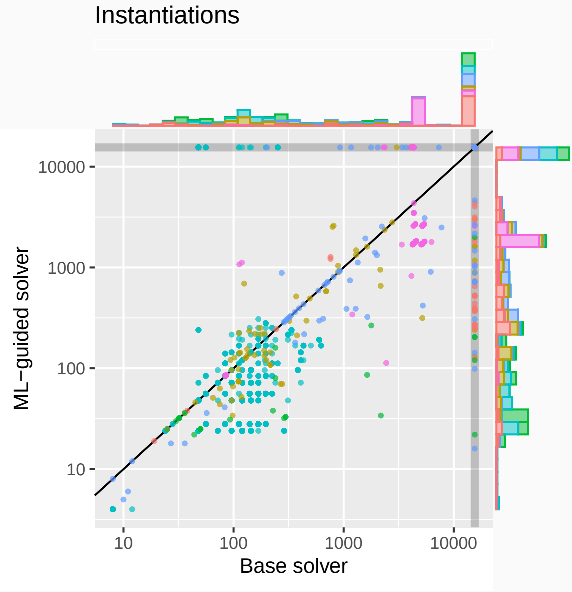
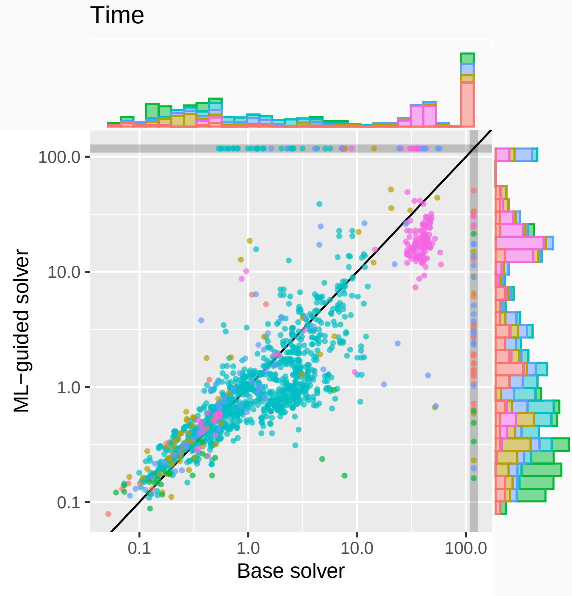


Holdout Set: Instantiation Count



Holdout Set: Time Comparison

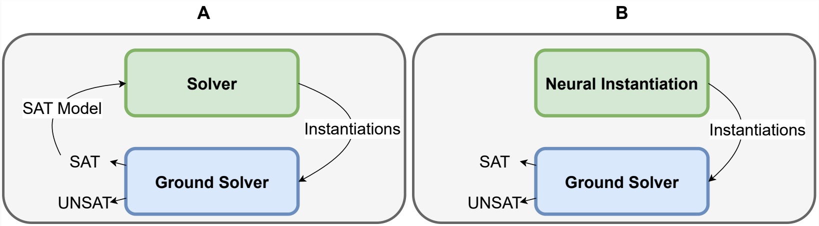


Towards Synthesizing Terms

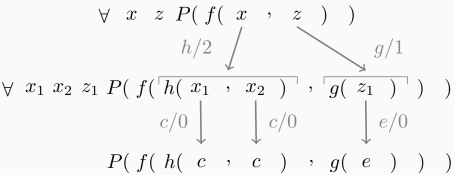
ML Maximalist — Proving By Instantiation

[Piepenbrock et al., 2025]

- A GNN analyzes the formula, and predicts how to instantiate clauses by growing terms
- SAT solver (+ congruence closure) does the rest



Synthesizing Terms



(1) instantiate x by head symbol h with arity 2 and z by g of arity 1 (going from level_0 to level_1)

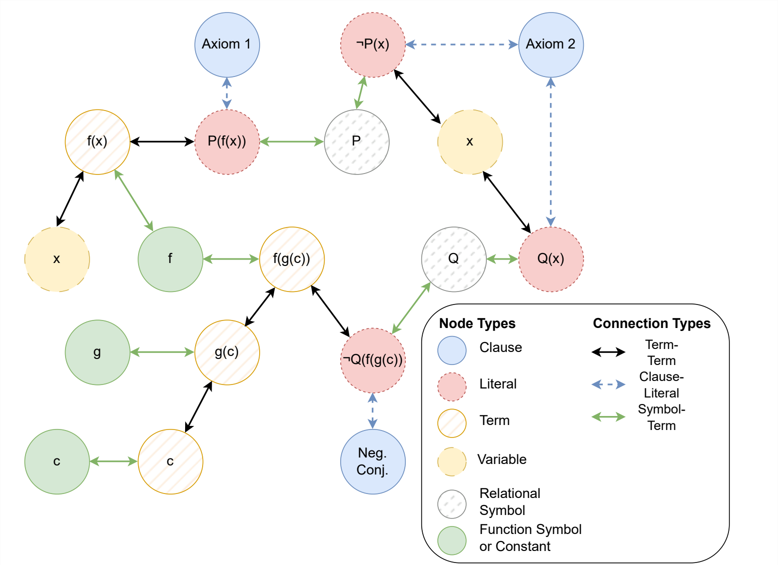
(2) instantiate x_1, x_2, z_1 by constants c, c, and e, respectively (going from level_1 to level_2)

Synthesizing Terms by GNN2RNN

$\forall xz.\, P(f(x,z))$	$x : h \quad z : g$
$\forall x_1 x_2 z_1.\, P(f(h(x_1,x_2),g(z_1)))$	$x_1 : c \xrightarrow{\text{RNN}} x_2 : c \xrightarrow{\text{RNN}} z : e$
$P(f(h(c,c),g(e)))$	

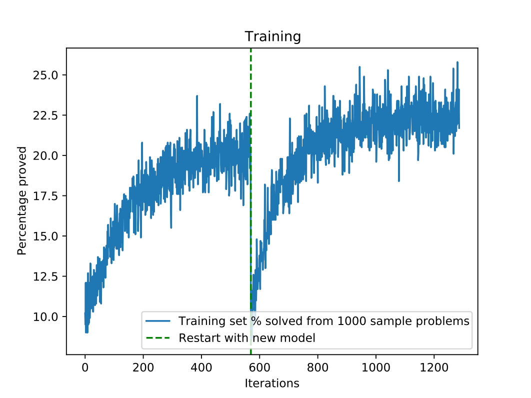
GNN

GNN Example



Axiom 1
¬P(x)
Axiom 2
f(x)
P(f(x))
P
x
x
f
f(g(c))
Q
Q(x)
g
g(c)
¬Q(f(g(c)))
c
c
Neg. Conj.
Node Types
Clause
Literal
Term
Variable
Relational Symbol
Function Symbol or Constant
Connection Types
Term-Term
Clause-Literal
Symbol-Term

System Can Learn



Dedicated Provers are Still Better

Table 1: Performance of various methods. iProver is used in pure instantiation mode. Random is 1 run of the 2-level random grounding. In parentheses, we indicate which dataset was used.

Time limit	1s	10s	60s	Inst. + 30s
Random (all)	—	—	—	3.44%
Neural (train)	—	—	—	26.25%
Neural (test)	—	—	—	19.74%
iProver (train)	43.28%	59.99%	67.6%	—
iProver (test)	43.16%	59.75%	68.69%	—
CVC5 (test)	83.44%	85.6%	86.28%	—

Towards Infinite Models

SMT Models: Constants

```
(declare-fun c () Int)
(declare-fun d () Int)
(assert (< c d))
(check-sat)
(get-model)
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$c < d$

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```
:!z3 ex1.smt2
sat
(
  (define-fun d () Int
    1)
  (define-fun c () Int
    0)
)
```

$c = 0, d = 1$

SMT Models: Functions

```
(declare-fun f (Int) Int)
(assert (< (f 0) (f 1)))
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$$f(0) < f(1)$$

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```
:!z3 ex2.smt2
sat
(
  (define-fun f ((x!0 Int)) Int
    (ite (= x!0 1) 1
      0))
)
```

$fx \triangleq (1 \text{ if } x = 1 \text{ else } 0)$

SMT Models: Quantifiers

```
(declare-fun f (Int) Int)
(assert (forall ((x Int))
           (<= (f x) x)))
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```

$$(\forall x)(fx \leq x)$$

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```
:!z3 -T:60 ex4.smt2
timeout
```

Not Solved!

Learn infinite models from finite ones?

Model-Based Guided Quantifier Instantiation

For $\forall x \phi$ construct a sequence of:

- candidate models M_i

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- s.t. $M_i \not\models \phi[x/\sigma_i]$

Example

$$(\forall x)(fx > x)$$

$\bigwedge_{j\in 1..i-1}\phi[x/\sigma_j]$	M_i	σ_i
true	$fx \triangleq 0$	$x \mapsto 0$

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$\bigwedge_{j\in 1..i-1} \phi[x/\sigma_j]$	M_i	σ_i
$f(0) > 0$	$fx \triangleq (x = 0\,?\,1 : 2)$	$x \mapsto 2$
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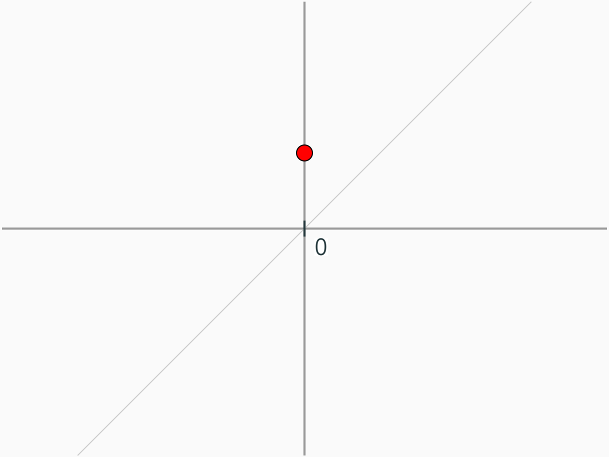

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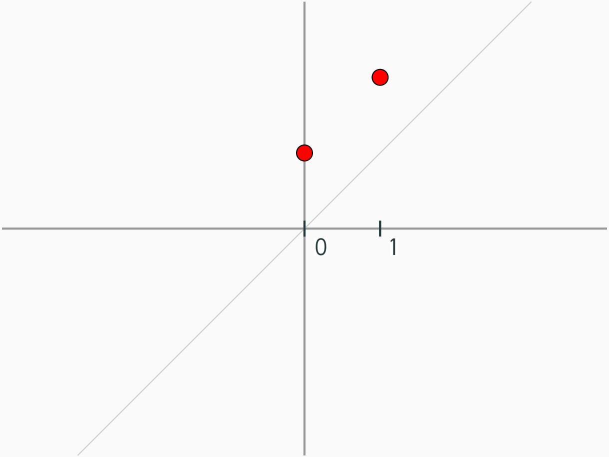

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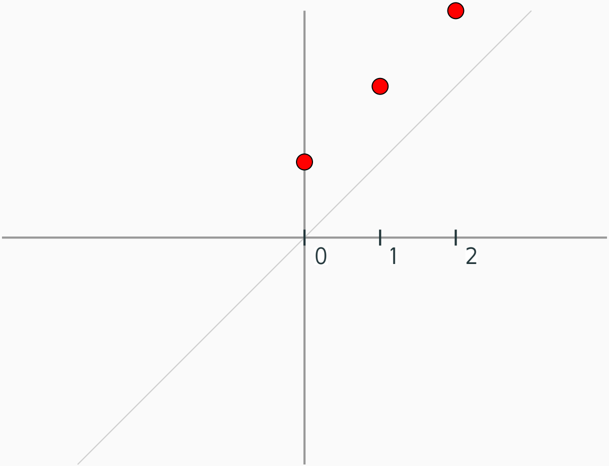

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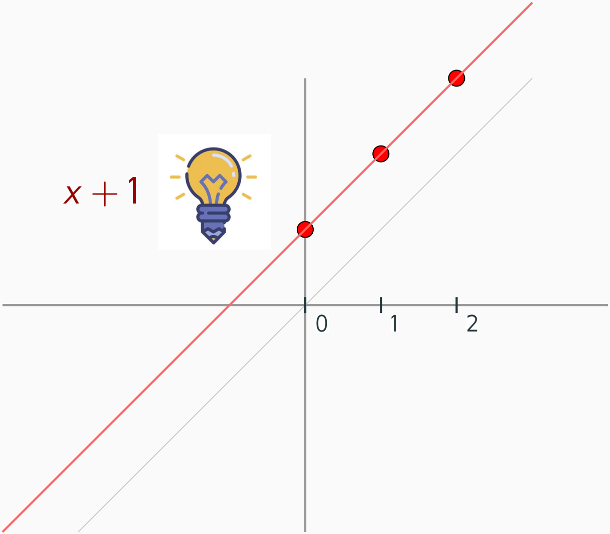

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- Keep the same hyper-plane as long as possible
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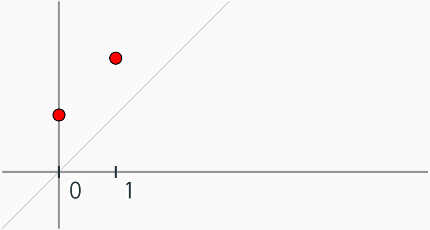

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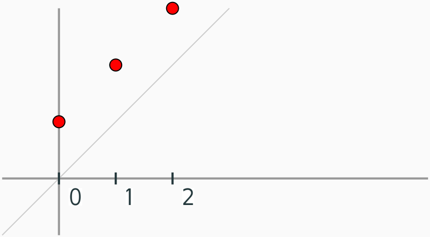

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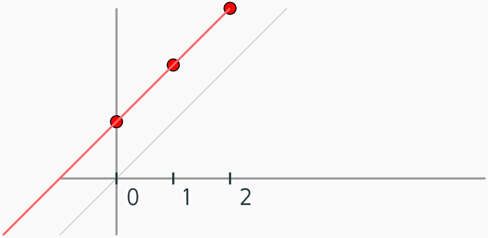

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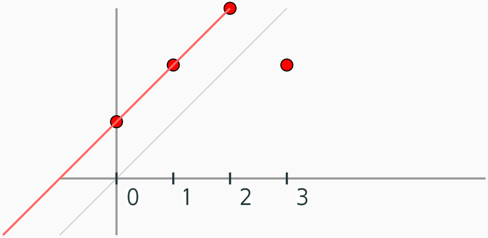

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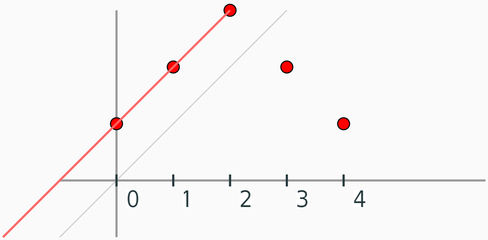

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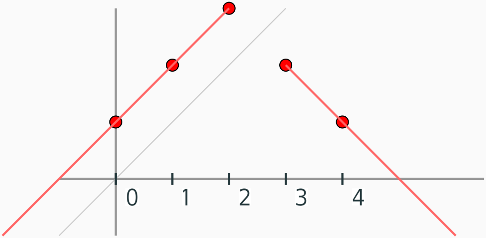

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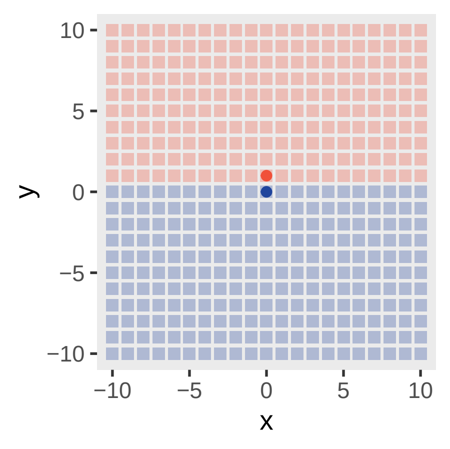

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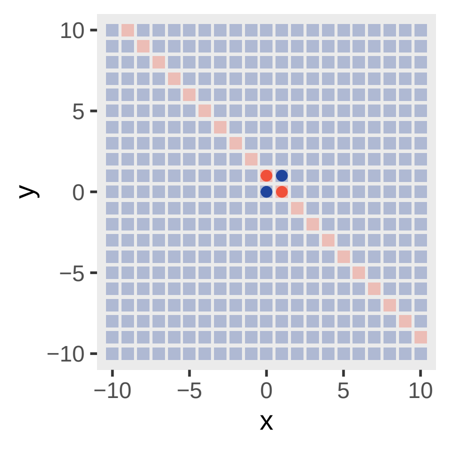

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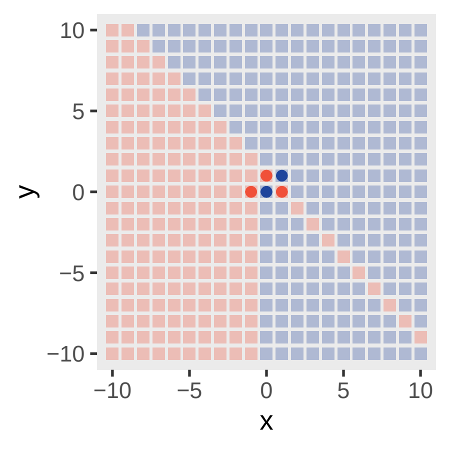

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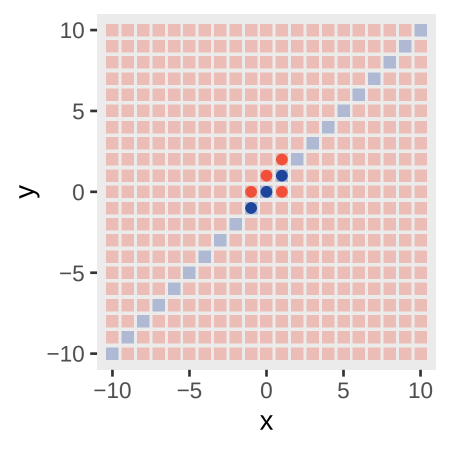

Results UFLIA

- Implemented in cvc5
- Run on [J. et al., 2023]

solver	SAT	UNSAT	total
standard MBQI	18,843	7,863	26,706
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ours smart MBQI	31,977	7,863	39,840
Z3	28,380	7,482	35,862

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- In SMT instantiations can be ordered by ML.
- Synthesizing new terms is possible, but harder.
- Synthesizing new models is also possible but
  What are the appropriate ML techniques?

J., M. (2018).
Towards generalization in QBF solving via machine learning.

J., M., Brown, C. E., and Kaliszyk, C. (2023).
A benchmark for infinite models in SMT.

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Piepenbrock, J., Urban, J., Korovin, K., Olšák, M., Heskes, T., and J., M. (2025).
Invariant neural architecture for learning term synthesis in instantiation proving.