Relational Program Synthesis with Numerical Reasoning

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Motivation: learning programs with numerical values



zendo(Structure) ← piece(Structure,Piece1), contact(Piece1,Piece2), size(Piece2,Size), geq(Size,**7**).

Motivation: learning programs with numerical values



pharma3(Molecule) ← zincsite(Molecule,Zinc),
hacc(Molecule,Hydrogen),
dist(Molecule,Zinc,Hydrogen,Distance),
geq(Distance, 1.7),
leq(Distance, 3.5).
pharma3(Molecule) ← hacc(Molecule,Hydrogen1),
hacc(Molecule,Hydrogen2),
bond(Molecule,Hydrogen1,Hydrogen2,du),
dist(Molecule,Hydrogen1,Hydrogen2,Distance),
leq(Distance, 2.7).

Related Work

- Existing approaches:
 - cannot scale to infinite domains (ASPAL, ILASP, HEXMIL, ProSynth, Popper, δILP)
 - cannot reason from multiple examples jointly (Progol, MagicPopper)
 - cannot learn chained numerical literals sharing variables (Aleph)
 - cannot learn recursive programs, optimal programs (textually minimal) (Progol, Aleph)

Program synthesis approach to learn programs with numerical values

- infinite and continuous domains
- complex numerical reasoning
- reason from multiple examples

Decompose the learning task in two stages:

- Program search: generate partial hypotheses with variables in place of numerical values
- **Numerical search**: searches for numerical values to fill in the numerical variables.



Program search: generate partial hypotheses with variables in place of numerical values

 $H: f(List) \leftarrow length(List,Length), leq(Length,N), @numerical(N)$



Numerical search: searches for numerical values to fill in the numerical variables.

- finds values for the intermediate variables given the positive and negative examples
- $H: f(List) \leftarrow length(List,Length), geq(Length,N), @numerical(N)$
- $S_{P}(Length) = \{5, 4\} \text{ and } S_{N}(Length) = \{3, 2\}$

Positive	Negative
f([3,7,8,2,4])	f([8,0,4])
f([2,7,0,1])	f([1,2])

- translates the numerical search as a SMT formula

 $H: f(List) \leftarrow length(List,Length), geq(Length,N), @numerical(N)$

 $S_{p}(Length) = \{5, 4\} and S_{N}(Length) = \{3, 2\}$

 $5 \ge N \land 4 \ge N \land \neg (3 \ge N) \land \neg (2 \ge N)$

Positive	Negative
f([3,7,8,2,4])	f([8,0,4])
f([2,7,0,1])	f([1,2])

- substitutes numerical variables with a solution to the SMT formula

 $H: f(List) \leftarrow length(List,Length), geq(Length,N), @numerical(N)$

 $S_{p}(Length) = \{5, 4\} and S_{N}(Length) = \{3, 2\}$

 $5 \ge N \land 4 \ge N \land \neg (3 \ge N) \land \neg (2 \ge N)$

 $f(List) \leftarrow length(List,Length), geq(Length, 4)$

Positive	Negative
f([3,7,8,2,4]) f([2,7,0,1])	f([8,0,4]) f([1,2])

Implementation

We implement our approach in NumSynth:

- It is based on the program synthesis system Popper.
- It uses the SMT solver Z3 in the numerical search stage.

Implementation: built-in numerical literals

Literal	Definition	Example
geq(A,N)	$A \ge N$	geq(A,3)
leq(A,N)	$A \leq N$	leq(A,5.2)
add(A,B,C)	A + B = C	add(A,B,C)
mult(A,N,C)	A * N = C	<pre>mult(A,2,C)</pre>

Implementation: supported fragments

Fragment	NUMSYNTH	Example
Linear real arithmetic	\checkmark	$X + 6.3 * Y \le 3$
Linear integer arithmetic	\checkmark	$U + 6 * V \le 3$
Mixed real / integer	\checkmark	$X + 6.3 * V \le 3$
Integer difference logic	\checkmark	$U-V \leq 4$
Real difference logic	\checkmark	$X - Y \le 4$
Unit two-variable / inequality	\checkmark	$X+Y \le 4$
Polynomial real arithmetic	Х	$X^2 + Y^2 = 2$
Non-linear integer arithmetic	Х	$U^{2} = 2$



Q1: Can NumSynth learn programs with numerical values?

Q2: How well does NumSynth perform compared to other approaches?

Q1: comparison with other approaches

Task	ALEPH	MAGICPOPPER	NUMSYNTH
interval	69 ± 1	70 ± 0	99 ± 1
halfplane	99 ± 0	84 ± 7	96 ± 1
zendo1	98 ± 0	68 ± 3	99 ± 0
zendo2	51 ± 1	56 ± 1	96 ± 1
zendo3	71 ± 1	51 ± 1	96 ± 1
zendo4	63 ± 1	52 ± 1	94 ± 1
pharma1	82 ± 1	64 ± 3	99 ± 0
pharma2	83 ± 1	77 ± 2	95 ± 1
pharma3	81 ± 1	82 ± 1	98 ± 1
pharma4	76 ± 1	62 ± 2	$\textbf{92}\pm\textbf{1}$
member_between	49 ± 0	75 ± 4	97 ± 1
last_leg	50 ± 0	51 ± 1	98 ± 1
next_geq	50 ± 0	50 ± 0	92 ± 5

Predictive accuracies

Q1: comparison with other approaches

Task	ALEPH	MAGICPOPPER	NUMSYNTH
interval			0 ± 0
halfplane	1 ± 0	60 ± 26	2 ± 1
zendo1	25 ± 8	KARS AN	10 ± 1
zendo2			17 ± 1
zendo3			69 ± 2
zendo4			76 ± 2
pharma1	2 ± 0		1 ± 0
pharma2	10 ± 2	7 ± 0	2 ± 0
pharma3	24 ± 3	66 ± 5	20 ± 1
pharma4	3 ± 0		20 ± 0
member_between		161 ± 38	2 ± 0
last_leq			13 ± 1
next_geq			39 ± 6

Learning times

Q1: comparison with other approaches

- > NumSynth can learn programs with numerical values
- NumSynth can outperform existing approaches in terms of learning times and predictive accuracies



Q3: How well does NumSynth scale with the number of examples?

Q3: scalability with respect to the number of examples



Q3: scalability with respect to the number of examples

- NumSynth can scale well better than Aleph and MagicPopper with respect to the number of examples
- Numerical search stage can be expensive and limit scalability

Conclusion

NumSynth, approach to learn programs with numerical values. It can:

- outperform state-of-the art approaches,
- learn in infinite and continuous domains,
- learn optimal programs and recursive programs.

Future Work and Limitations

• Scalability with respect to the complexity of the numerical reasoning stage

• Noise: identify numerical values from noisy examples

References

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zendo4(A):- piece(A,B), size(B,C), geq(C,**1.23**), leq(C,**4.66**). zendo4(A):- piece(A,B), position(B,X,Y), leq(X,**3.45**), leq(Y,**6.87**). zendo4(A):- piece(A,B), contact(B,C), rotation(C,D), leq(D,**1.18**).

pharma4(A):- zincsite(A, B), hacc(A, C), dist(A, B, C, D), leq(D,**4.18**),geq(D,**2.22**). pharma4(A):- hacc(A, C), hacc(A, E), dist(A, B, C, D), geq(D,**1.23**), leq(D,**3.41**). pharma4(A):- zincsite(A, C), zincsite(A, B), bond(B,C,du), dist(A, B, C, D), leq(D,**1.23**).

f(A):- head(A,19),tail(A,E),head(E,C),geq(C,**27**). f(A):- tail(A,B),f(B).