Combining Symbolic Expressions and Black-box Function Evaluations in Neural Programs

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Neural Programming

- Learning black-box functions
- Observations:
  - black-box function evaluations (*fEval*)
  - program execution traces (*eTrace*)
- Challenges: Lack of generalization due to:
  - *fEval*: Insufficient structural information
  - *eTrace*: Computational issues affecting the domain coverage
- Solution:
  - Most problems have access to symbolic representations (*sym*)
  - Combine *sym* and *fEval* data:
    - *sym*: preserve problem's structure
    - *fEval*: enable function evaluation

- Case study: Modeling mathematical equations
- Summary of contributions:
  - Combine symbolic representation and function evaluation
  - Equation verification and equation completion using TreeLSTMs
  - Balanced dataset generation method

Mathematical Equation Modeling

- Grammar rules:

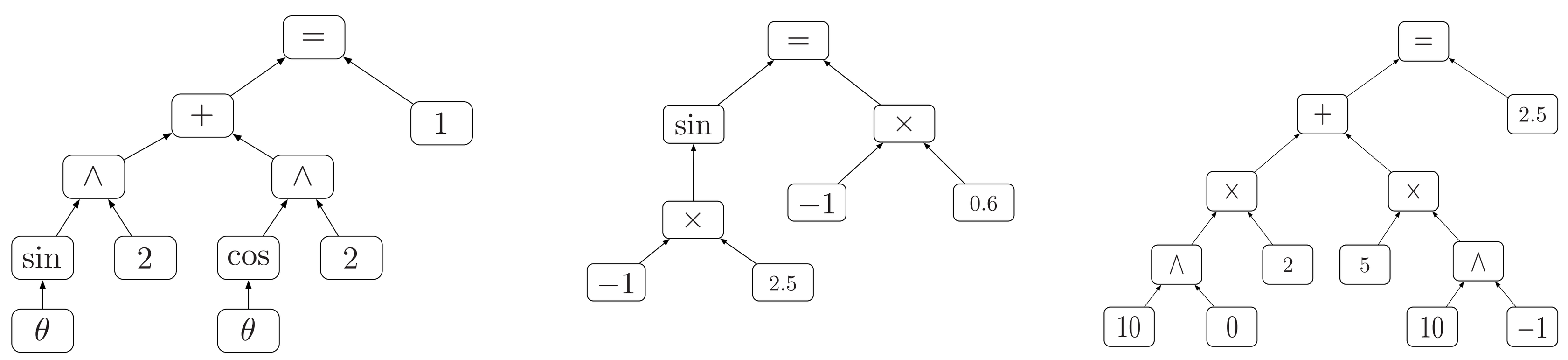
$$
\begin{aligned}
&I \to =(E,E),\ \neq(E,E)\\
&E \to T, F_1(E), F_2(E,E)\\
&F_1 \to \sin, \cos, \tan, \ldots\\
&F_2 \to +, \wedge, \times, \ldots\\
&T \to -1, 0, 1, 2, \pi, x, y, \ldots, \text{any number in [-3.14,+3.14]}
\end{aligned}
$$

- Covered domain:

Table: Symbols in our grammar, i.e. the functions, variables, and constants

Unary functions, F_1					Terminal, T		Binary, F_2
sin	cos	csc	sec	tan	0	1	$+$
cot	arcsin	arccos	arccsc	arcsec	2	3	$\times$
arctan	arccot	sinh	cosh	csch	4	10	$\wedge$
sech	tanh	coth	arsinh	arcosh	0.5	-1	
arcsch	arsech	artanh	arcoth	exp	0.4	0.7	
					π	x	

- Examples of equation trees:



$\sin^2(\theta) + \cos^2(\theta) = 1$ $\sin(-2.5) = -0.6$ decimal tree for 2.5

Dataset Generation Scheme:

Generating Symbolic Equations

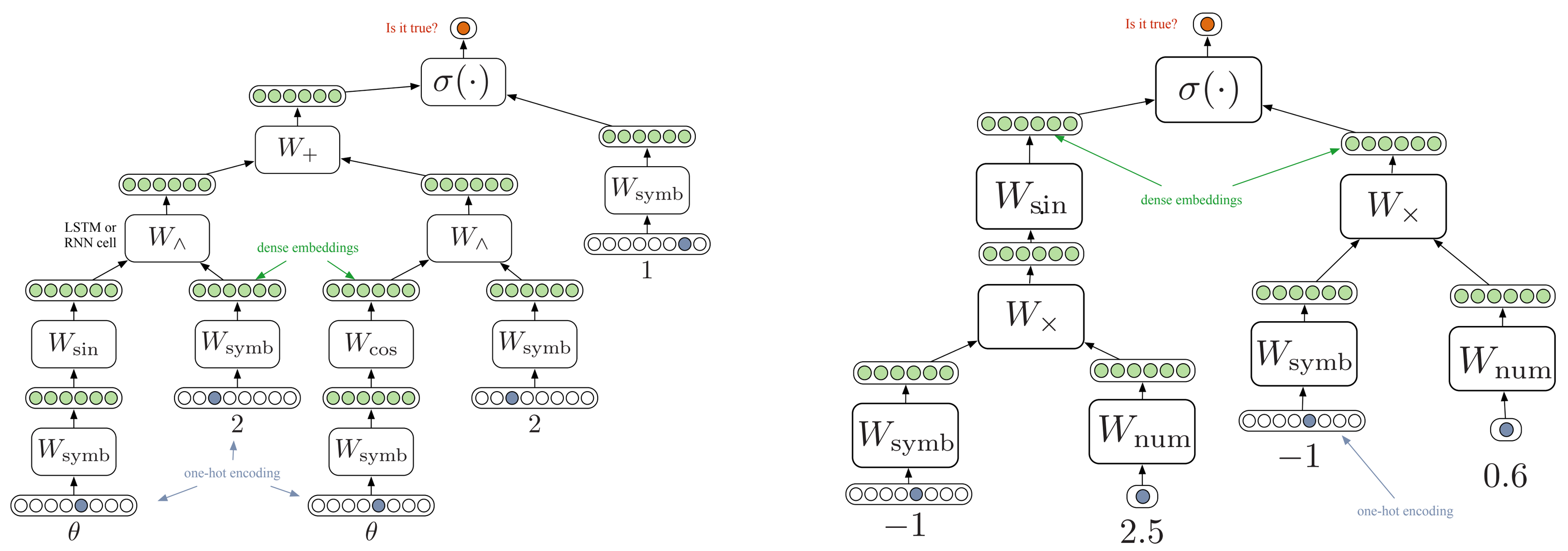
- Generate possible equations valid in the grammar
  - Start from a small initial set of axioms
  - For each axiom, choose a random tree node
  - Make local random changes to the node:
  - Problem: More incorrect equations than correct
  - Solution: Sub-tree matching
- Generate additional correct equations
  - *mathDictionary*: A dictionary of valid mathematical statements.
    - E.g. $(x+y : y+x)$ forms a key-value pair
  - For each correct equation in the dataset, chose a random tree node
  - Find a dictionary key whose pattern matches the chosen sub-tree
  - Replace the sub-tree with the value's pattern, e.g:
    - Equation: $\sin^2\theta + \cos^2\theta = 1$
    - Chosen node: $+$
    - Key-value pair: $(x+y : y+x)$
    - output: $\cos^2\theta + \sin^2\theta = 1$

Generating function evaluation equations

- Function Evaluation
  - Range of floating point numbers of precision 2: [-3.14, 3.14]
  - For each unary function: draw a random number and evaluate
  - For each binary function: draw two random numbers and evaluate
- Representation of numbers
  - For all numbers in the dataset, form the decimal tree expansion
  - E.g. $2.5 = 2 \times 10^0 + 5 \times 10^{-1}$

Tree LSTMs for Modeling Equations

- Tree LSTM whose structure mirrors the input equation
  - Function blocks are LSTM cells
    - Weight sharing between occurrences of the same function
  - Symbol block is a 1-layer feed-forward net for embedding terminals
  - Number block is a 2-layer feed-forward net for embedding numbers



- Baselines:
  - Sequential Recurrent Neural Networks
  - Sequential LSTMs
  - Tree-structured RNNs without function evaluation data
  - Tree-LSTMs without function evaluation data
  - Tree-structured RNNs with function evaluation data

Experiments and Results

Complexity of an equation: its expression tree depth

- Equation Verification: Generalization to unseen identities

Table: **Generalization Evaluation:** the train and the test contain equations of the same depth [1,2,3,4]. Results are on unseen equations. *Sym* and *F Eval* refer to accuracy on Symbolic and function evaluation expressions, respectively. Test set sizes shown as the counts in (Sym + F Eval) data.

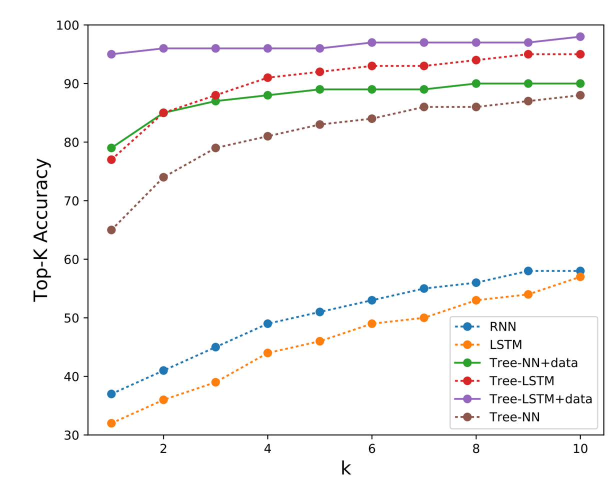
Approach	Sym	F Eval	depth 1	depth 2	depth 3	depth 4
Test set size	3527	401	5+2	542+158	2416+228	563+13
Majority Class	50.24	50.00	20.00	45.75	52.85	43.69
Sympy	81.74	-	80.00	89.11	82.98	69.44
RNN	66.37	-	50	62.93	65.13	72.32
LSTM	81.71	-	80.00	79.49	80.81	83.86
TreeNN	92.06	-	**100**	95.37	94.16	87.45
TreeLSTM	95.18	-	80.00	96.50	95.07	94.50
TreeNN + data	93.38	92.81	87.5	94.43	92.32	93.58
TreeLSTM + data	**97.11**	**97.17**	75.00	**98.14**	**97.01**	**97.05**

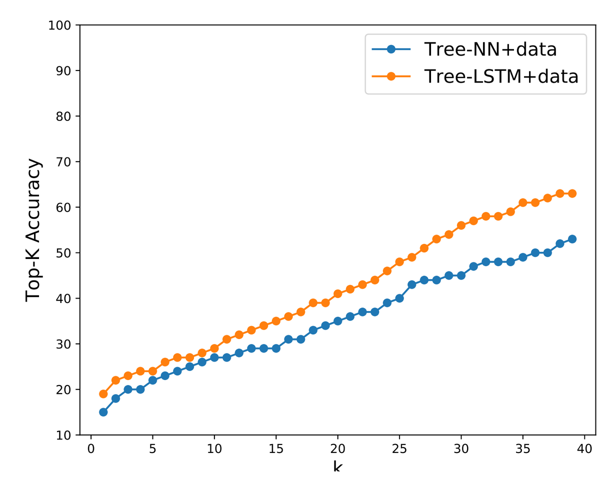
- Equation Verification: Extrapolation to unseen depths

Table: **Extrapolation Evaluation** to measure capability of the model to generalize to unseen depth. Acc: Accuracy, Prec: Precision, Rec: Recall

Approach	Train:1,2,3; Test on 4			Train:1,3,4; Test on 2		
	Acc	Prec	Rec	Acc	Prec	Rec
Majority Class	55.22	0	0	56.21	0	0
RNN	65.15	68.61	75.51	71.27	82.98	43.27
LSTM	76.40	71.62	78.35	79.31	75.27	79.31
TreeNN	88.36	87.87	85.86	92.58	89.04	94.71
TreeLSTM	93.27	90.20	95.33	94.78	94.15	93.90
TreeNN + data	92.71	88.07	93.66	94.09	91.06	93.19
TreeLSTM + data	**96.17**	**92.97**	**97.15**	**97.37**	**96.08**	**96.86**

- Equation Completion





$4^{\tanh(0)} = \blacksquare^x$	
-2^0	0.9999
1^0	0.9999
7^0	0.9999
-3^0	0.999
8^0	0.999

$\tan(\blacksquare) = 0.29$	
0.28	0.9977
0.27	0.9977
0.29	0.9977
0.26	0.9977
0.25	0.9977