





Chronosymbolic Learning

Efficient CHC Solving with Symbolic Reasoning and Inductive Learning

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What are CHCs?

SAT Problem
$$(x \land y) \lor (x \land \neg z)$$
 SMT Problem
$$\forall a, b, c, \ a > 0 \ \land \ b \leq a \ \land \ c = 0 \ \rightarrow a + b + c \geq 0$$
 Constrained Horn Clause
$$(CHC)$$

$$\forall a, b, c, \ a > 0 \ \land \ b \leq a \ \land \ c = 0 \ \rightarrow p(a, b, c)$$
 CHC System
$$(C_1 : \forall a, b, c, c_1, \ c_1 = 1 + c \land p(a, b, c) \rightarrow q(a, b, c_1)$$

$$(C_2 : \forall a, b, c, b < a \cdot c \ \land \ q(a, b, c) \rightarrow \bot$$

Problem: find (synthesize) such interpretations of p, q, or prove it UNSAT!

(Solution interpretations, Def. 1)

CHC System, Terminologies

Unknown predicate symbols (relation)

$$\forall \mathcal{V} \cdot (\varphi \land p_1(X_1) \land \cdots \land p_k(X_k) \to h(X)), \text{ for } k \geq 1$$
 For all variables ("Constrained") Conjunction Implication p->q means ~p or q

Can be omitted
$$\begin{cases} (\varphi \wedge p_1(X_1) \wedge \cdots \wedge p_k(X_k)) & \to h(X)), \text{ for } k \geq 1 \\ \text{Body} & \to h(X), \text{ for } k \geq 1 \end{cases}$$
 Head
$$\mathcal{C}_0: \forall a,b,c,\ a > 0 \ \wedge \ b \leq a \ \wedge \ c = 0 \to p(a,b,c) \quad \text{Fact (also a Rule)}$$

$$\mathcal{C}_1: \forall a,b,c,c_1, \ c_1 = 1 + c \land p(a,b,c) \to q(a,b,c_1) \quad \text{Rule}$$

$$\mathcal{C}_2: \forall a,b,c,\ b < a \cdot c \ \wedge \ q(a,b,c) \to \bot \qquad \text{Query}$$

For simplicity, trivial rules that have pre-determined truth value are omitted

CHC solver can be a *backbone* for program verification

- CHC system is SAT ⇔ Program is safe
- Cast the program verification problem as constraint solving problem
- Naturally handles *loop invariant* generation problem (but not limited to)

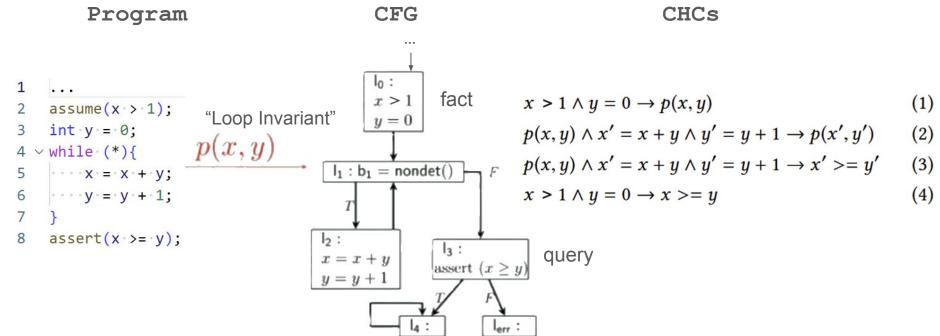
Known as the biggest challenge in program verification!

```
An abstract interpretation of a loop
  x > 1 \land y = 0 \rightarrow p(x, y)
                                                           (1)
  p(x, y) \wedge x' = x + y \wedge y' = y + 1 \rightarrow p(x', y')
                                                           (2)
  p(x, y) \wedge x' = x + y \wedge y' = y + 1 \rightarrow x' >= y'
                                                           (3)
  x > 1 \land y = 0 \rightarrow x >= y
                                                           (4)
   assume(x > 1);
                                      Pre-condition
   int y = 0;

∨ while (*){
                                  nondeterministic
   \times \times \times = \times \times + \times \times;
                                                       Command
                                  expression of x, y
   \cdot \cdot \cdot \cdot y = y + 1;
   assert(x >= y);
                                     Post-condition
```

CHC solver can be a backbone for program verification





We will use programs to explain CHCs

Table 5. Mapping of program verification concepts to CHC solving concepts.

Program Verification Concept	CHC Solving Concept			
Verification Conditions (VCs)	CHC system \mathcal{H}			
Initial program state	Fact \mathcal{C}_f			
Transition	Rule C_r			
Assertion/Unsafe condition	Query C_q			
Inductive invariant/Loop invariant	Solution Interpretation $\mathcal{I}^*[p]$ to predicate p			
Counterexample trace	Refutation proof \mathcal{R}			
Reachable program states	Positive samples s^+			
Unsafe program states	Negative samples s^-			

White-box vs. black-box approaches





 Bounded model checking (BMC): encode the initial states, k loop transitions, and bad states into logical formula (Can prove UNSAFE if the formula is SAT) main() {

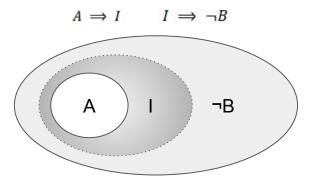
$$Init(V) \wedge \underbrace{Tr(V, V') \wedge Tr(V', V'') \wedge \ldots \wedge Tr(V^{(k-1)}, V^{(k)})}_{k} \wedge Bad(V^{(k)})$$

SMT encoding for k=2:

$$x = 1, y = 0 \land x_1 = x + y, y_1 = y + 1 \land x_2 = x_1 + y_1, y_2 = y_1 + 1 \land x_2 < y_2$$

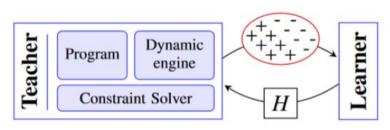
```
main() {
  int x,y;
  x=1; y=0; Some
  while(*){-> nondeterministic
    x=x+y; expression of x, y
  y++;}
  assert(x>=y);}
```

- Unbounded model checking: find a fixed-point through inductive generalization heuristics
 - (e.g., Craig interpolants (CI), IC3, PDR, Spacer, GSpacer)
 - ✓ Efficiently maximize the power of the solvers
 - X Often rely on heuristics to do inductive generalization
 - X Not flexible with data samples (which is cheap sometimes)

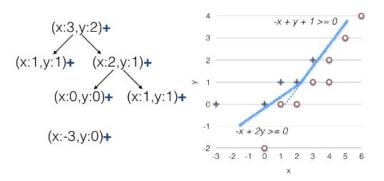


White-box vs. <u>black-box</u> approaches

- Teacher and Learner paradigm, "Guess-and-check"
- Hypothesize interpretations by induction learning
- Iteratively refine the hypothesis
- ✓ Can take global information into account, better *generalization* (using ML rather than CI)
- ✓ For arbitrary guesses, it's relatively easy to get data samples as counterexamples
- x Cheap prior knowledge in CHC systems is ignored
- x State explosion issue exists



ICE: A Robust Framework for Learning Invariants, Garg et al., 2014



A Data-Driven CHC Solver, Zhu et al., 2018 (LinearArbitrary)



Motivation

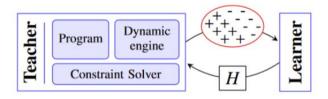
- Black-box approaches is sample inefficient
- White-box methods is 1) difficult to deal with data samples
 2) hard to do inductive generalization

$$x > 1 \land y = 0 \to p(x, y) \tag{1}$$

$$p(x,y) \wedge x' = x + y \wedge y' = y + 1 \rightarrow p(x',y') \tag{2}$$

$$p(x,y) \wedge x' = x + y \wedge y' = y + 1 \rightarrow x' >= y' \qquad (3)$$

$$x > 1 \land y = 0 \to x >= y \tag{4}$$



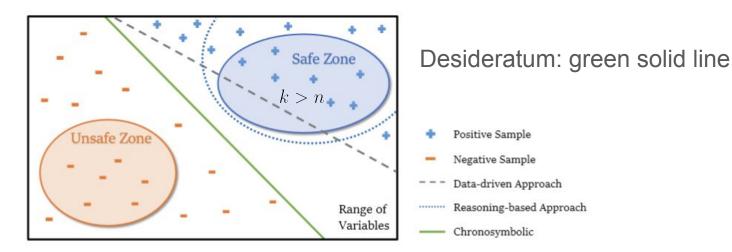
- Need many samples to "relearn" $x > 1 \land y = 0$
- Each learning iteration gives only 1 additional sample
- Might have infinite interpretations for a set of positive and negative samples

Motivation

Can we find a way to finding global patterns of CHCs without the resort to any hand-crafted heuristics?

Can we make the data-driven methods more sample efficient?

Can we present symbolic and data-driven methods in a *unified framework*?



Contributions

- Identify and formulate the key concepts in CHC solving: samples, zones,
 counterexample, and etc. Their connection is also discussed.
 - Enable synergistic working for symbolic methods and learning-based methods
 - Here we don't assume any specific algorithm for learner and reasoner
- Design a modular framework, <u>Chronosymbolic Learning</u> to realize the desiderata
 - Naming: Synchronous, CHC, symbolic, no. (number)
- Propose a minimal instance, showing how components interact in our framework
- Provide artifacts for the minimal instance
- Give an evaluation of the instance and show the potential

(Inspired by and generalized from program verification)

Samples

query $x > 1 \land y = 0 \rightarrow x >= y$

Definition 4 (Positive Sample). A data point s^+ is a positive sample of predicate p in \mathcal{H} iff $p(s^+) = \top$ must hold to make all rules in \mathcal{H} SAT.

```
2 assume(x > 1);
             3 int y = 0;
            4 \sim \text{while} (*)
             5 x = x + y;
             6 y = y + 1;
                assert(x >= y);
      \int x > 1 \wedge y = 0 \rightarrow p(x, y)
rules p(x,y) \wedge x' = x + y \wedge y' = y + 1 \rightarrow p(x',y')
       p(x, y) \wedge x' = x + y \wedge y' = y + 1 \rightarrow x' >= y'
```

For predicate p(x, y)

• Positive samples:

$$(2, 0), (2, 1), (3, 2), (5, 3), \dots$$

Negative samples:

• Implication samples:

$$((2,0),(2,1)),((-1,0),(-1,1)),\ldots$$

(Forward) Reachable program configurations

Program configurations that is unsafe (backward reachable starting from the unsafe condition)

Not necessarily samples that appears in program But should *depict the "semantics" of the loop*

Zones

Definition 7 (Safe and Unsafe Zones). A safe (unsafe) zone of a predicate p, S_p (U_p), is a set of positive (negative) samples of p.

```
x > 1 \land y = 0 \rightarrow p(x, y)
p(x, y) \land x' = x + y \land y' = y + 1 \rightarrow p(x', y')
p(x, y) \land x' = x + y \land y' = y + 1 \rightarrow x' >= y'
x > 1 \land y = 0 \rightarrow x >= y
```

- Zone is a set of samples; samples are zones (with cardinality of 1)
- Sometimes it's easy to know some zones (Lemma 7,8)

Zones can be symbolically represented: For predicate p(x, y)

- Example of a safe zone: $\{x > 1 \land y = 0\}$
- Example of an unsafe zone: {x < y}
 (Or any zones that can be implied by current zones, conceptually)

Some immediate useful lemmas

Connection of solutions and samples

Lemma 1. If \mathcal{H} is SAT, for each solution interpretation \mathcal{I}^* of \mathcal{H} ,

- (1) if s^+ is a positive sample of p in \mathcal{H} , we have $\mathcal{I}^*[p](s^+) = \top$.
- (2) if s^- is a negative sample of p in \mathcal{H} , we have $\mathcal{I}^*[p](s^-) = \bot$.
- (3) if $s^{\rightarrow} = (s_1^{\rightarrow}, \dots, s_n^{\rightarrow}, s_h^{\rightarrow})$ is a implication sample of body predicates (p_1, \dots, p_n) and head predicate h in \mathcal{H} , $\mathcal{I}^*[p_1](s_1^{\rightarrow}) \wedge \dots \wedge \mathcal{I}^*[p_n](s_n^{\rightarrow}) \rightarrow \mathcal{I}^*[h](s_h^{\rightarrow})$.

A valid solution interpretation should separate any positive and negative samples.

Valid zones can directly extracted from the fact and query

Lemma 7 (Initial Safe Zones). A fact $C_f : \phi_f \to h_f(T)$ produces a safe zone for $h_f : S_{h_f}^0(T) = \exists \mathcal{X}_{\varphi}, \phi_f$.

Lemma 8 (Initial Unsafe Zones). A linear query $C_q : \phi_q \wedge p_q(T) \to \bot$ produces an unsafe zone for $p_q : \mathcal{U}_{p_q}^0(T) = \exists \mathcal{X}_{\varphi}, \phi_q$.

Why we need Zones?



1. Integrated into the learner's hypothesis to enhance it (Lemma 2)

Add S: $x > 1 \land y = 0$ to the hypothesis, and the new data samples will never be in $x > 1 \land y = 0$

2. Provide the learner with additional samples (Sampling)

Zones Sampling Samples s* and s

Sample from S: $x > 1 \land y = 0$ to get positive samples like (2, 0), (100, 0), ...

3. Simplify the UNSAT checking of the CHC system

We assume there is a solution interpretation and make hypotheses, until there is a **conflict**

Lemma 5 (sample-sample conflict): samples cannot be both positive and negative

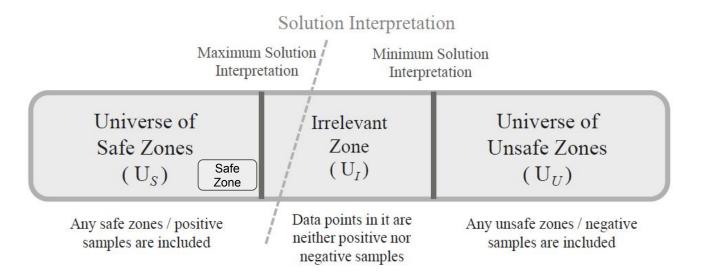
Lemma 6 (sample-zone conflict): a positive sample cannot be in unsafe zones

Lemma 11: safe and unsafe zones cannot overlap

Solution space of a CHC system

The universes of safe and unsafe zones are disjoint

Zones ensure more efficient "data coverage" of Us and Uu than samples



Counterexamples

Definition 8 (Counterexample). A counterexample $c = ((s_{p_1}, \dots, s_{p_k}), s_h)$ for a CHC \mathcal{C} and an interpretation \mathcal{I} is a set of data points¹⁵ such that under $c, \mathcal{I}[\mathcal{C}'] = \bot$, where \mathcal{C}' is the same constraint as \mathcal{C} but without the quantifier.

- A situation that current interpretation fails
- Formulate the information the teacher provides to the learner
- Can be converted into positive / negative samples (Lemma 3,4)
- The information can potentially extended to zonal representation

$$x > 1 \land y = 0 \to p(x, y) \tag{1}$$

$$p(x,y) \wedge x' = x + y \wedge y' = y + 1 \rightarrow p(x',y') \tag{2}$$

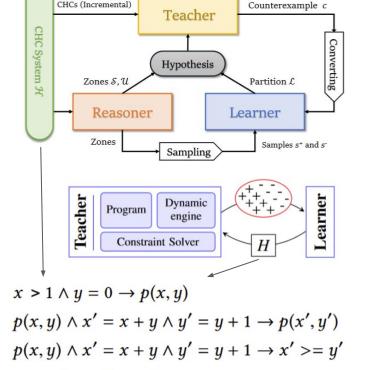
$$p(x,y) \wedge x' = x + y \wedge y' = y + 1 \rightarrow x' >= y' \qquad (3)$$

$$x > 1 \land y = 0 \to x >= y \tag{4}$$

For CHC (2) and $p(x, y) \equiv x = y + 2$:

- Example of a counterexample: (((2,0)), (2,1))
- It makes CHC (2) $\top \rightarrow \bot$
- SMTModel(\neg (CHC (2) \land p(x, y) \equiv x = y + 2))

Chronosymbolic Learning



 $x > 1 \land y = 0 \rightarrow x >= y$

Solution Interpretation Maximum Solution Interpretation Interpretation Universe of Universe of Irrelevant Unsafe Zones Safe Zones Zone (U_r) (Ue) (\mathbf{U}_{II}) Data points in it are Any safe zones / positive Any unsafe zones / negative neither positive nor samples are included samples are included negative samples

In each iteration:

- The reasoner and learner propose new <u>zones</u> and <u>partition</u> based on current <u>zones</u> and samples
- Make a hypothesis based on them
- The teacher checks the satisfiability for one certain interpreted CHC
- If SAT, switch to another CHC
- If not SAT, return a counterexample, convert it into data samples
- Do UNSAT checking for CHC system (Lemma 5, 6,
 11) using samples and zones
- Sample data from <u>zones</u>
- If all CHC is SAT, we find the solution interpretation

Instantiations of Chronosymbolic Learning

- Previous methods can be seen as special instances of our framework
- (6): Better state-space coverage and more efficient UNSAT checking (Lemma 2)
- For some instances, w/o S/U (4, 5) is better
 - Can be seen as different exploration strategies

Table 1. Several candidates of making hypotheses.

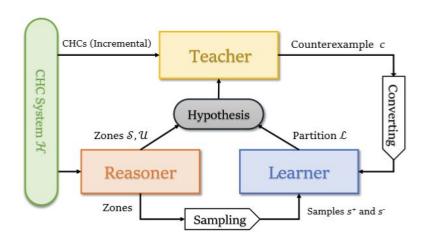
Methods	Candidate Hypothesis	
BMC-styled	$\left \tilde{\mathcal{I}}_s \left[p_i \right] = \mathcal{S}_{p_i} \right $	(2)
LinearArbitrary-styled	$\tilde{\mathcal{I}}_l\left[p_i\right] = \mathcal{L}_{p_i}$	(3)
Chronosymbolic w/o safe zones	$\tilde{\mathcal{I}}_{lu}\left[p_i\right] = \mathcal{L}_{p_i} \land \neg \ \mathcal{U}_{p_i}$	(4)
Chronosymbolic w/o unsafe zones	$\tilde{\mathcal{I}}_{sl}\left[p_i\right] = \mathcal{S}_{p_i} \vee \mathcal{L}_{p_i}$	(5)
Chronosymbolic	$\tilde{\mathcal{I}}_{slu}\left[p_{i}\right] = \mathcal{S}_{p_{i}} \vee \left(\mathcal{L}_{p_{i}} \wedge \neg \mathcal{U}_{p_{i}}\right)$	(6)

Our instance of Chronosymbolic Learning

- A data-driven learner (L) + a BMC-styled reasoner (S, U)
- makeHypothesis() is done by:
 - Chronosymbolic-single: Always using (6)
 - Chronosymbolic-cover: alternates from (2, 3, 4, 5, 6) using some scheduling heuristics
 - Ablation study: Always using (2, 3, 4, 5)

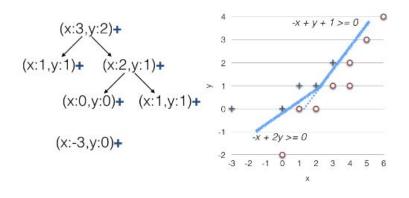
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Learner

- Collect the counterexample and convert them to positive and negative samples
- The learner contains a *dataset* and a *machine learning toolchain (SVM+DT)*
 - SVM (learn arbitrary hyperplanes) + Decision Tree (tune and recombine those hyperplanes)
 - Refer to our paper for further details



A Data-Driven CHC Solver, Zhu et al., 2018 (LinearArbitrary)

Reasoner

- BMC-styled image/pre-image computation

$$Init(V) \wedge \underbrace{Tr(V, V') \wedge Tr(V', V'') \wedge \ldots \wedge Tr(V^{(k-1)}, V^{(k)})}_{k} \wedge Bad(V^{(k)})$$

Append a transition to the current zone to expand the zone

Lemma 9 (Forward Expansion). From given safe zones $S_{p_i}^m$, we can expand them in one forward transition by a non-fact rule $C_r: \phi \wedge p_1(T_1) \wedge \cdots \wedge p_k(T_k) \rightarrow h(T)$ to get an expanded safe zone S_h^{m+1} , where $S_h^{m+1}(T) = \exists \mathcal{X}_{\varphi}, \phi \wedge S_{p_1}^m(T_1) \wedge \cdots \wedge S_{p_k}^m(T_k)$.

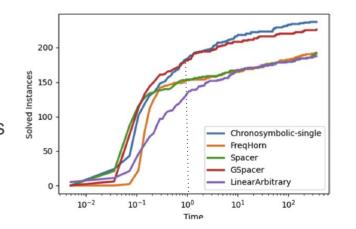
Lemma 10 (Backward Expansion). From a given unsafe zone \mathcal{U}_h^m , we can expand it in one backward transition by a non-fact linear rule $\mathcal{C}_r: \phi \wedge p(T_0) \rightarrow h(T)$ to get an expanded unsafe zone \mathcal{U}_p^{m+1} , where $\mathcal{U}_p^{m+1}(T_0) = \exists \mathcal{X}_{\varphi}, \phi \wedge \mathcal{U}_h^m$.

Major experiment settings

- 288 arithmetic instances collected by FreqHorn, including non-linear ones
- Timeout: 360s (but we also care about efficiency within this period)
- Chronosymbolic-single: one configuration (hyperparameter set and strategy)
 for all instances (Meta-Learning-liked)
- Chronosymbolic-cover: all solved instances in 13 configurations (like
 LinearArbitrary which sets specific hyperparameters for different instances)

Experiment

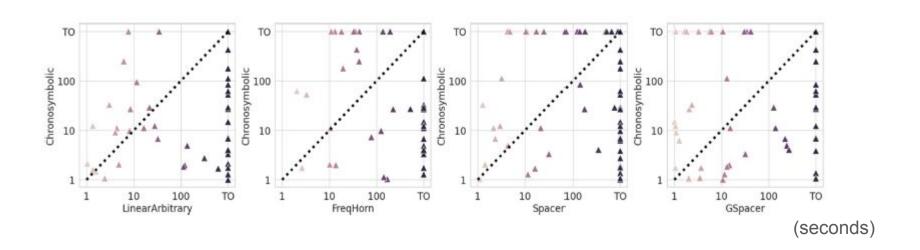
- Efficient in arithmetic benchmarks
- Meet challenges in benchmarks with many Bool vars
- On our main dataset, the average time for SVM, DT, the teacher and reasoner are 26.68s, 4.74s, 14.58s,1.29s respectively



Method	#total	percentage	#safe	#unsafe	avg-time (s)	avg-time-solved (s)
LinearArbitrary	187	64.93%	148	39	135.0	13.48
FreqHorn	191	66.32%	191	0	129.1	11.80
FreqHorn-expl	50	17.36%	0	50	299.5	13.57
Spacer	184	63.89%	132	52	132.8	15.30
GSpacer	220	76.39%	174	46	83.50	7.83
Chronosymbolic-single	237	82.29%	189	48	68.33	7.51
Chronosymbolic-cover	252	87.50%	204	48	-	_

Experiment

Below the diagonal: ours > baseline



Ablation

BMC-styled	$\tilde{\mathcal{I}}_s\left[p_i\right] = \mathcal{S}_{p_i}$	(2)
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Table 4. Different configurations of Chronosymbolic Learning.

Configuration	#total	percentage	#safe	#unsafe	avg-time (s)	avg-time-solved (s)
without safe zones (4)	228	79.17%	183	45	78.56	9.11
without unsafe zones (5)	218	75.69%	173	45	94.75	12.87
without both zones (3)	211	73.26%	166	45	93.84	10.09
without learner (2)	131	45.49%	96	35	196.3	0.16
parallel	216	75.00%	180	36	_	_
Chronosymbolic-single	237	82.29%	189	48	68.33	7.51

Parallel: learner and reasoner running individually and simultaneously for 360s

Future work and discussion

Better Learner:

- Some better symbolic classifier that can deal with zones and samples simultaneously
- Better handling a large number of Boolean variables
- Embracing the LLMs as symbolic classifiers

Better Reasoner:

- Go beyond BMC; e.g., model-based projection
- Add support for approximated zones (IC3/PDR),
- Zones induced from samples (symbolic regression)
- Better procedure to simplify complicated zones
- Currently reasoner can benefit from the learner, but learner's impact on reasoner is small

Better Teacher:

- Can produce zonal feedback / counterexample
- Better support for NL CHCs
- Beyond Integer Arithmetics

Thank you for your careful listening!

- Code is available here:
 <u>https://github.com/Chronosymbolic/Chronosymbolic-Learning</u>, with examples on how it works, and the detailed experimental results
- Slides can be downloaded from my personal website https://zyluo.netlify.app/
- Email me (<u>ziyan.luo@mail.mcgill.ca</u>) or Xujie (<u>six@cs.toronto.edu</u>) for further questions or comments

Paper:



Code:

