Solving Symbolic Regression Problems with Formal Constraints

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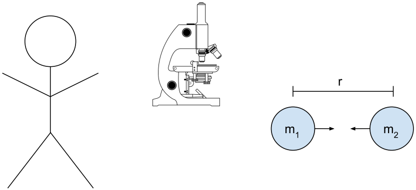
Outline

Motivation

Jane the Physicist wants to devise a formula for the force of gravity.

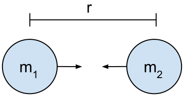


- Jane has a set of observations $(m_1, m_2, r) \mapsto F$.
- Other laws of physics tell her that:
  1. Swapping the masses does not change the force
  2. A force cannot be negative
  3. Increasing one of the masses increases the force

Example problems

Benchmark: gravity

$$f(m_1, m_2, r) = 6.67408 \cdot 10^{-11} \cdot \frac{m_1 m_2}{r^2}$$



Constraints:

- *s*: $f(m_1, m_2, r) = f(m_2, m_1, r)$
- *b*: $f(m_1, m_2, r) \geq 0$
- *m*: strict monotonicity w.r.t. both m_1 and m_2.

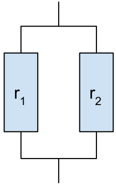
Test cases:

m1	m2	r	out
10.88386	11.36099	15.74871	0.000000000033273260096895905
11.1782	3.21214	7.67932	0.000000000040635631498539907
7.22322	0.10104	11.48446	0.000000000000369308431952941

Example problems

Benchmark: resistance2

$$f(r_1, r_2) = \frac{r_1 r_2}{r_1 + r_2}$$



Constraints:

- s**:** $f(r_1, r_2) = f(r_2, r_1)$
- c_1**:** $r_1 = r_2 \implies f(r_1, r_2) = \frac{r_1}{2}$
- c_2**:** $f(r_1, r_2) \leq r_1 \quad \wedge \quad f(r_1, r_2) \leq r_2$

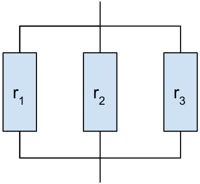
Test cases:

r1	r2	out
10.09611	17.39521	6.388341979690316
0.68719	4.75438	0.600408042568597
1.42871	17.19419	1.319102352206155

Example problems

Benchmark: resistance3

$$f(r_1, r_2, r_3) = \frac{r_1 r_2 r_3}{r_1 r_2 + r_1 r_3 + r_2 r_3}$$



Constraints:

- s: $f(r_1, r_2, r_3) = \ldots = f(r_3, r_2, r_1)$
- c_1: $r_1 = r_2 = r_3 \implies f(r_1, r_2, r_3) = \frac{r_1}{3}$
- c_2: $f(r_1, r_2, r_3) \leq r_1 \quad \wedge \quad f(r_1, r_2, r_3) \leq r_2 \quad \wedge \quad f(r_1, r_2, r_3) \leq r_3$

Test cases:

r1	r2	r3	out
9.31772	8.88437	2.90062	1.77106036258303l
19.09801	17.08167	3.09636	2.3048717244360835
17.71372	11.53495	6.26835	3.3038401592739173

Problem

Symbolic Regression with Formal Constraints (SRFC)

Given a set of *test cases* (examples) T, a set of *formal constraints* C, and a (possibly infinite) set of functions $\mathcal{F}$, find a function $f : \mathbb{R}^n \to \mathbb{R}$, $f \in \mathcal{F}$, that minimizes the approximation error on T, while satisfying all constraints in C.

Examples of formal constraints:

- Symmetry with respect to arguments: $f(x, y) = f(y, x)$
- Symmetry with respect to domain: $f(x) = f(-x)$
- Range: $f(x, y) \in [0, 1]$
- Monotonicity: $\forall_{x,y}\ x > y \implies f(x) > f(y)$
- Convexity/concavity
- Value of derivative in a given point: $f'(3.7) > 2.5$

Advantages and challenges

Advantages:

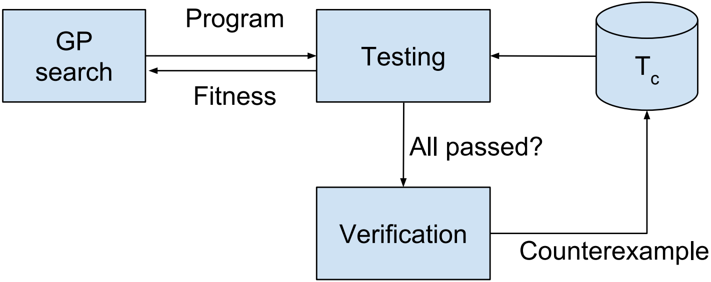
- Resulting model is guaranteed to have the requested properties.
- Arbitrary constraints can be used.
- Models can be induced from fewer examples.

Challenges:

- **Feedback bottleneck**
  A constraint is either satisfied or not; not much information for guiding search.
- **Necessity of logical proof**
  A constraint may be specified over an infinite number of points.

Outline

Counterexample-Driven Genetic Programming (CDGP)[1] [2] [3]



[1] I.Błądek, K.Krawiec, J.Swan, J.Drake, "Counterexample-Driven Genetic Programming: Stochastic Synthesis of Provably Correct Programs", IJCAI, 2018.

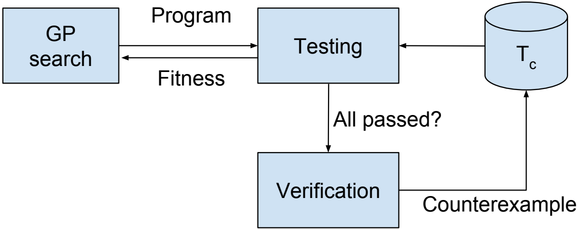
[2] I.Błądek, K.Krawiec, J.Swan, "Counterexample-Driven Genetic Programming: Heuristic Program Synthesis from Formal Specifications", ECJ, 2017.

[3] K.Krawiec, I.Błądek, J.Swan, "Counterexample-Driven Genetic Programming", GECCO, 2017.

Counterexample-Driven Genetic Programming (CDGP)

Module: **Testing**

- Fitness is computed based on the set of test cases T_c.
- T_c may initially be empty or seeded with test cases provided by the user.
- During verification phase, a new test may be added to T_c.



Counterexample-Driven Genetic Programming (CDGP)

Module: **Verification**

- Checks if a candidate solution satisfies the formal constraints.
- Involves a *Satisfiability Modulo Theories (SMT) solver*.

Formal verification

Proving for a candidate solution p that:

$$\forall_{in} \ Pre(in) \implies Post(in, p(in)), \tag{1}$$

where $p(in)$ is the output returned by p for input in, $Pre(in)$ is a precondition, and $Post(in)$ is a postcondition. In practice, often the negated form is disproved:

$$\exists_{in} \ Pre(in) \not\Longrightarrow Post(in, p(in)). \tag{2}$$

An example of SMT verification

Incorrect program (MAX):

```
if x < y:
  res = x
else:
  res = y
```

Formal specification:

$$\begin{gathered} max(x,y) \geq x \quad \wedge \\ max(x,y) \geq y \quad \wedge \\ (max(x,y) = x \ \vee \ max(x,y) = y) \end{gathered}$$

Solver result:

```
SAT
x = -1
y = 0
```

SAT means that the program is incorrect and solver provides us a counterexample (-1, 0).

An example of SMT verification

Correct program (MAX):

```
if x > y:
  res = x
else:
  res = y
```

Formal specification:

$$\begin{gathered} max(x,y) \geq x \quad \wedge \\ max(x,y) \geq y \quad \wedge \\ (max(x,y) = x \;\vee\; max(x,y) = y) \end{gathered}$$

Solver result:

```
UNSAT
```

UNSAT means that the program is correct with respect to the specification. No counterexample was found.

Complete and incomplete tests

Two types of tests may be created from counterexamples:

- **Complete tests**
  Conventional tests of the form (*input, desired output*).
- **Incomplete tests**
  Tests without a specified desired output.
  Evaluated using the SMT solver.

Example 1: $f(x) = \sqrt{x}$

x	$f(x)$
4	2 or -2
9	3 or -3
...	...

$\leftarrow$ There is no single desired output for easy testing

Complete and incomplete tests

Two types of tests may be created from counterexamples:

- **Complete tests**
  Conventional tests of the form (*input, desired output*).
- **Incomplete tests**
  Tests without a specified desired output.
  Evaluated using the SMT solver.

Example 2: $f(x) > 2x$

x	$f(x)$
4	9, 10, ...
9	19, 20, ...
...	...

$\leftarrow$ There is no single desired output for easy testing

Outline

Counterexample-Driven Symbolic Regression (CDSR)

Changes introduced in CDGP to handle SR problems:

1. **Definition of "All passed?"**
   A program is sent to verification if it passes α percent of incomplete tests.

   Why: complete tests are ignored in order to avoid arbitrary thresholds on the difference between function's output and the expected output of the test.

Counterexample-Driven Symbolic Regression (CDSR)

Changes introduced in CDGP to handle SR problems:

2. **Definition of termination condition**
   Search process terminates when both (i) its aggregated error (MSE) on *complete* tests is below the automatically computed error threshold; (ii) it meets the formal constraints.

   Why: solution needs to both have low error on tests and satisfy all the constraints. Absolute threshold leads to problems.

   The error threshold for MSE:

   $$\epsilon = (t \cdot \sigma_Y)^2$$

   where t is called **tolerance**, and σ_Y is standard deviation of the output variable in the data.

Counterexample-Driven Symbolic Regression (CDSR)

CDSR with tests for properties ($CDSR_{props}$)

- Extends the initial set of tests T_c with incomplete tests, one for each constraint.
- These additional tests are verified by SMT solver, and they are always evaluated either to 0 or 1.
- Uses ϵ-Lexicase[4] selection on both complete and incomplete tests.

#	r1	r2	out
1	10.09611	17.39521	6.388341979690316
2	0.68719	4.75438	0.600408042568597
3	1.42871	17.19419	1.319102352206155
4	$f(r_1, r_2) = f(r_2, r_1)$		-
5	$r_1 = r_2 \implies f(r_1, r_2) = \frac{r_1}{2}$		-
6	$f(r_1, r_2) \leq r_1 \quad \wedge \quad f(r_1, r_2) \leq r_2$		-

[4] W.L. Cava, L. Spector, K. Danai, "Epsilon-lexicase Selection for Regression", GECCO, 2016.

State of the art

There are only a handful of approaches which allow GP to synthesize provably-correct programs.

Approaches to provably-correct synthesis in GP

Fitness based on satisfying subconstraints

- (2007) C.G. Johnson, *Genetic Programming with Fitness Based on Model Checking*
- (2008) G. Katz, D. Peled, *Genetic Programming and Model Checking: Synthesizing New Mutual Exclusion Algorithms*
- (2011) P. He, L. Kang, C.G. Johnson, S. Ying, *Hoare logic-based genetic programming*
- (2016) G. Katz, D. Peled, *Synthesizing, correcting and improving code, using model checking-based genetic programming*

Generating counterexamples

- (2017) I.Błądek, K.Krawiec, J.Swan, *Counterexample-Driven Genetic Programming: Heuristic Program Synthesis from Formal Specifications*

Outline

1. Introduction

2. CDGP

3. CDGP for regression

4. Experiments

Experiment dimensions

Dimension 1: **synthesis method**

- **GP** – baseline
- **CDSR** – our approach
- **CDSR**$_{props}$ – our approach with added tests for individual constraints

Dimension 2: **number of test cases**

- **3 tests**
- **5 tests**
- **10 tests**

Dimension 3: **tolerance**

- **0.01**
- **0.1**

Total # tested configurations: $3 \cdot 3 \cdot 2 = 18$

Benchmarks

- **Gravity**
- **Resistance 2**
- **Resistance 3**

With variants:

- b: bound
- m: monotonicity
- s: symmetry
- c1: custom constraint – equal arguments
- c2: custom constraint – output always smaller than any of the arguments

Total # benchmark variants: $8 + 4 + 4 = 16$

Noise

- To make benchmarks more realistic, noise was introduced to both the inputs and the output of the function.

- Noise is calculated according to the formula:

$$\widetilde{X} = X + \mathcal{N}(0, \beta \cdot \sigma_X)$$

and in our experiments we assumed $\beta = 0.1$, and σ_X is a standard deviation of the variable X in the data.

Evolution parameters

Parameter	Value
Number of runs	25
Population size	500
Maximum number of generations	∞
Maximum runtime in seconds	1800
Probability of mutation	0.5
Probability of crossover	0.5
Maximum height of initial programs	4
Maximum height of trees inserted by mutation	4
Maximum height of programs in population	12
Selection method	ϵ-Lexicase[5]

https://github.com/kkrawiec/CDGP

[5] W.L. Cava, L. Spector, K. Danai, "Epsilon-lexicase Selection for Regression", GECCO, 2016.

Results – success rates

Properties and MSE

	GP	CDSR	$CDSR_{props}$
gr_b	0.07	0.03	0.04
gr_m	0.00	0.01	0.01
gr_s	0.10	0.13	0.15
gr_bm	0.00	0.01	0.04
gr_bs	0.11	0.05	0.11
gr_ms	0.00	0.04	0.07
gr_bms	0.00	0.01	0.15
res2_c1	0.01	0.43	0.45
res2_c2	0.04	0.25	0.36
res2_s	0.00	0.22	0.29
res2_sc	0.03	0.17	0.35
res3_c1	0.00	0.07	0.21
res3_c2	0.01	0.02	0.01
res3_s	0.00	0.03	0.02
res3_sc	0.00	0.00	0.01
mean	0.02	0.10	0.15

Properties

	GP	CDSR	$CDSR_{props}$
gr_b	0.14	0.79	1.00
gr_m	0.00	0.02	0.91
gr_s	0.13	0.86	0.99
gr_bm	0.00	0.01	0.83
gr_bs	0.19	0.91	0.98
gr_ms	0.00	0.05	0.91
gr_bms	0.00	0.02	0.97
res2_c1	0.01	0.55	0.75
res2_c2	0.04	0.33	0.83
res2_s	0.00	0.60	0.99
res2_sc	0.03	0.22	0.83
res3_c1	0.00	0.07	0.26
res3_c2	0.01	0.02	0.11
res3_s	0.00	0.31	0.50
res3_sc	0.00	0.01	0.13
mean	0.04	0.32	0.73

- b: bound
- m: monotonicity
- s: symmetry
- c1: custom constraint – equal input arguments
- c2: custom constraint – output smaller than any of the inputs
- c: conjunction of c1 and c2

Statistical analysis

Friedman statistical test was used to analyze the findings.

MSE below threshold and properties met (Friedman's test $p = 7.1 \cdot 10^{-25}$).

method	rank
CDSR_{props} _0.1	1.6
CDSR _0.1	2.5
GP_0.1	4.0
CDSR_{props} _0.01	4.2
CDSR _0.01	4.3
GP_0.01	4.4

Fraction of models that meet the formal properties ($p = 1.6 \cdot 10^{-40}$).

method	rank
CDSR_{props} _0.1	1.5
CDSR_{props} _0.01	1.6
CDSR _0.1	3.3
CDSR _0.01	4.1
GP_0.1	5.1
GP_0.01	5.4

Observations

Pros:

- CDSR systematically outperforms GP.
- Much lower risk of overfitting.
- Valid models induced from as few as three examples.

Cons:

- Significant computational overhead.
- Limitations of the theorem prover – SMT solvers do not handle well transcendental functions like *cos*, *log*, etc.

Summary

Main points:

- CDSR, a method for solving the task of symbolic regression with formal constraints by finding counterexamples.
- Solutions produced by CDSR generalize well in terms of expected properties.
- $CDSR_{props}$ was best at that, thanks to treating individual constraints as incomplete tests.

Thank you for your attention!

Questions.