Symbolic Regression via Control Variable Genetic Programming

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Symbolic Regression for Scientific Discovery

Learning an explicit symbolic expression (rather than black-box neural net) from data.

Given a dataset $\mathcal{D} = (x_1, y_1), \ldots, (x_n, y_n)$ ($x_i \in \mathbb{R}^m$ and $y_i \in \mathbb{R}$) and a loss function $\mathcal{L}$. The objective of symbolic regression is to search for the optimal symbolic expression ϕ^* within the space of all candidate expressions Π that minimizes the average loss:

$$\phi^* = \operatorname{argmin}_{\phi \in \Pi} \frac{1}{n} \sum_{\{i=1\}}^{n} \mathcal{L}(x_i, y_i)$$

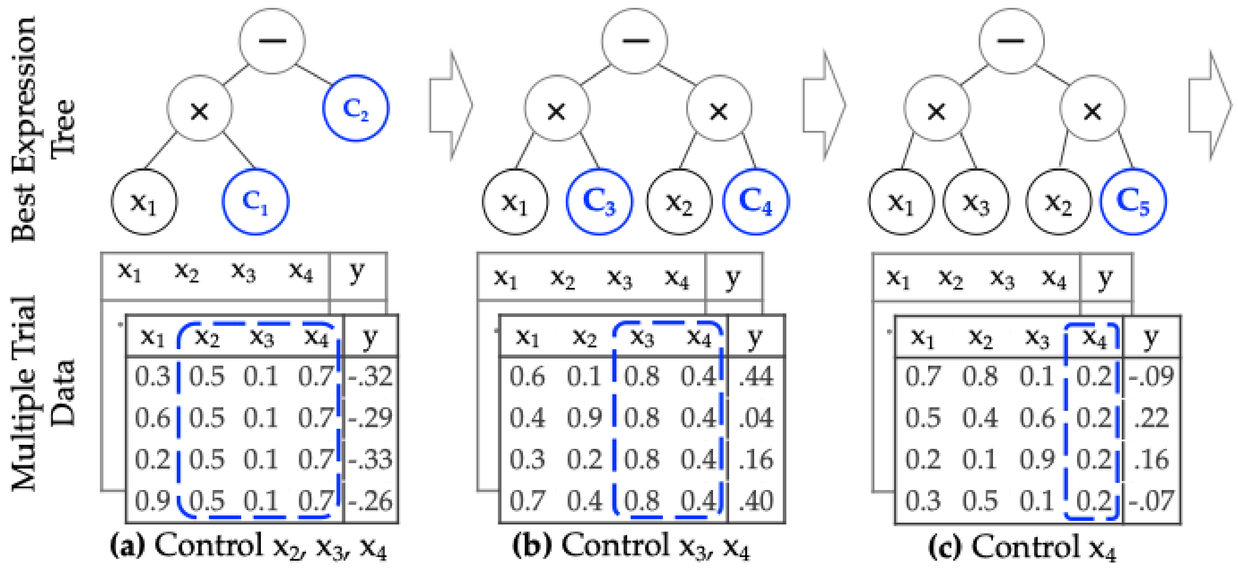
Current Challenges:

- Incredibly difficult because of the large search space of all possible expressions Π.
- Current methods are too slow to find expressions with ***Multiple variables.***
- **Our Solution**: We propose to use "***Control Variable Experiments***" (a classical scientific approach) to ***expedites*** scientific machine learning.

Method: Control Variable Genetic Programming

Found by GP

Extended from previous reduced-form equations using GP



The data are generated from a data Oracle. The constants are identified using BFGS optimizer on batches of data

Motivation: Control Variable Experiments

Can you guess which equation $y = f(x_1, x_2, x_3)$ generate the data shown in the left table?

X_1	X_2	X_3	Y
2.5	**1.0**	**9.5**	**12**
5.8	**1.0**	**7.2**	**13**
1.8	**1.0**	**3.2**	**5**
4.2	**-1.0**	**2.2**	**-2**
9.7	**-1.0**	**1.7**	**-8**
3.0	**-1.0**	**4.0**	**1**
7.1	8.6	3.8	64.9
2.5	2.6	3.1	9.6
8.9	1.1	2.0	11.8

X_2 is controlled!

How about if I only ask you to look into these rows?

$$y = x_1 + x_3$$

How about these rows?

$$y = -x_1 + x_3?$$

Maybe the WHOLE equation is:

$$y = x_2 x_1 + x_3?$$

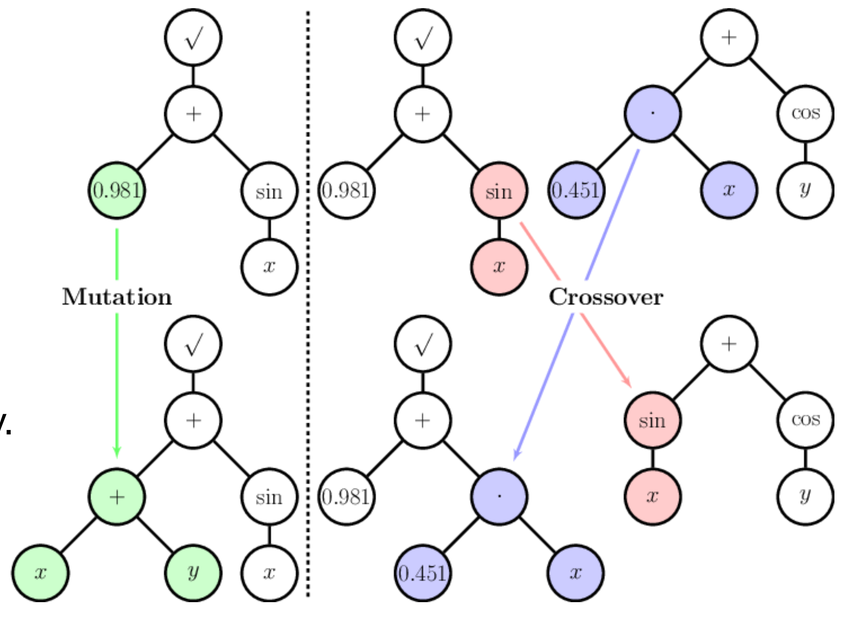
Orange and blue data are two control variable experiment trials. Control variable experiments simplify symbolic regression!

Background: Genetic Programming for Symbolic Regression

Maintain a pool of candidate expressions.

In each generation, candidate expressions are *mutated* and *crossover* randomly.

Top fitness scores expressions are selected as for the next generation.



Experiments

Table 1: Median (50%) and 75%-quantile NMSE values of the symbolic expressions found by all the algorithms on several noisy benchmark datasets. NMSE is normalized mean square errors.

Dataset	CVGP (ours)		GP		DSR		PQT		VPG		GPMeld		Eureqa	
configs	50%	75%	50%	75%	50%	75%	50%	75%	50%	75%	50%	75%	50%	75%
(3,2,2)	0.001	0.004	0.015	0.135	1.53	43.09	0.58	1.13	0.83	1.32	1.06	2.18	**<1e-6**	**<1e-6**
(4,4,6)	**0.008**	0.059	0.012	**0.054**	1.006	1.249	1.006	2.459	1.221	2.322	1.127	2.286	1.191	6.001
(5,5,5)	**0.011**	**0.019**	0.025	0.177	1.038	8.805	1.048	4.736	1.401	38.26	1.008	1.969	0.996	6.340
(5,5,8)	**0.007**	**0.013**	0.010	0.017	1.403	5.161	1.530	41.27	4.133	27.42	1.386	8.092	1.002	1.495
(6,6,8)	**0.044**	**0.074**	0.058	0.200	1.963	90.53	4.212	8.194	4.425	22.91	15.58	269.6	1.005	1.150
(6,6,10)	**0.012**	**0.027**	0.381	0.820	1.021	1.036	1.006	1.048	1.003	1.020	1.022	1.689	1.764	49.041
(a) Datasets containing operators $\{\texttt{inv}, +, -, \times\}$														
(3,2,2)	0.005	0.123	0.023	0.374	0.087	0.392	0.161	0.469	0.277	0.493	0.112	0.183	**<1e-6**	**<1e-6**
(4,4,6)	**0.028**	0.132	0.044	**0.106**	2.815	9.958	2.381	13.844	2.990	11.316	1.670	2.697	0.024	0.122
(5,5,5)	0.086	0.402	**0.063**	**0.232**	2.558	3.313	2.168	2.679	1.903	2.780	1.501	2.295	0.158	0.377
(5,5,8)	**0.014**	**0.066**	0.102	0.683	2.535	2.933	2.482	2.773	2.440	3.062	2.422	3.853	0.284	0.514
(6,6,8)	**0.066**	**0.166**	0.127	0.591	0.936	1.079	0.983	1.053	0.900	1.018	0.964	1.428	0.433	1.564
(6,6,10)	**0.104**	**0.177**	0.159	0.230	6.121	16.32	5.750	16.29	3.857	19.82	7.393	21.709	0.910	1.927
(b) Datasets containing operators $\{\sin, \cos, +, -, \times\}$.														
(3,2,2)	0.039	0.083	0.043	0.551	0.227	7.856	0.855	2.885	0.233	0.400	0.944	1.263	**<1e-6**	**<1e-6**
(4,4,6)	**0.015**	**0.121**	0.042	0.347	1.040	1.155	1.039	1.055	1.049	1.068	1.886	4.104	0.984	1.196
(5,5,5)	**0.038**	**0.097**	0.197	0.514	3.892	69.98	4.311	23.66	5.542	8.839	9.553	16.92	0.901	1.007
(5,5,8)	**0.050**	**0.102**	0.111	0.177	2.379	2.526	1.205	2.336	1.824	2.481	1.142	1.874	1.002	2.445
(6,6,8)	**0.029**	**0.038**	0.091	0.151	1.605	8.005	1.718	7.783	4.691	39.03	1.398	16.60	1.001	1.008
(6,6,10)	**0.018**	**0.113**	.087	0.194	2.083	23.57	1.797	4.521	1.888	35.45	2.590	8.784	1.001	1.008
(c) Datasets containing opeartors $\{\sin, \cos, \texttt{inv}, +, -, \times\}$.														

Our CVGP finds symbolic expressions with the smallest NMSEs.

Table 2: Ground-truth expression recovery rate.

Operator set	Dataset configs	CVGP (ours)	GP
$\{\texttt{inv}, +, -, \times\}$	(2,1,1)	**64%**	44%
$\{\sin, \cos, +, -, \times\}$		**46%**	22%
$\{\sin, \cos, \texttt{inv}, +, -, \times\}$		**44%**	32%

Our CVGP finds more correct expressions.

Acknowledgement

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