CCSI
Carbon Capture Simulation Initiative

Learning Models of Unspecified Functional Form through Symbolic Regression

Alison Cozad, Nick Sahinidis, Zachary Wilson

CMPD CENTER

Carnegie Mellon University

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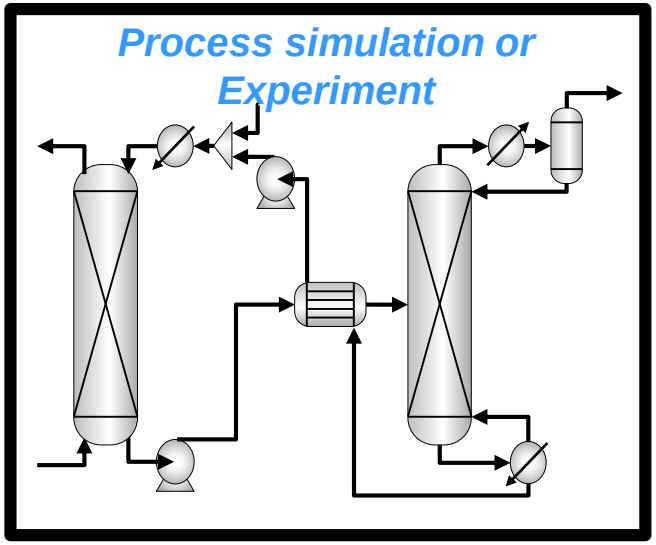
LEARNING Problem

Build a model of output variables z as a function of input variables x over a specified interval

$$x \in \mathbb{R}^k$$
$$x^l \leq x \leq x^u$$

$$\begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_j \\ \vdots \\ x_k \end{pmatrix}$$



$$\begin{pmatrix} z_1 \\ z_2 \\ \vdots \\ z_l \\ \vdots \\ z_m \end{pmatrix}$$

$$z \in \mathbb{R}^m$$
$$z = f(x)$$

Independent variables:
Operating conditions, inlet flow properties, unit geometry

Dependent variables:
Efficiency, outlet flow conditions, conversions, heat flow, etc.

PARAMETRIC REGRESSION

- Functional forms specified a priori
  - Multiple linear regression

    Model selection can compare functional forms, linear in coefficients

$$\hat{z}(x) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1 x_2 + \beta_4 e^{x_1} + \beta_5 e^{x_2} + \ldots$$

$$\hat{z}(x) = 2 + x_2 + 5\, e^{x_1}$$

  - Nonlinear regression

    Function is nonlinear in terms of regression variable

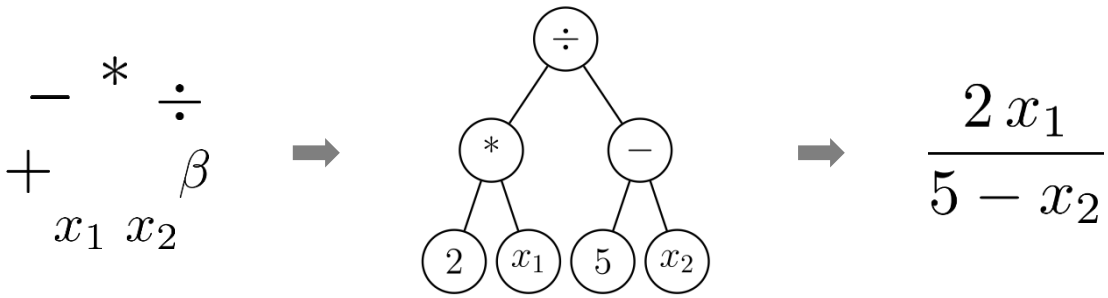
$$\hat{z}(x) = \beta_0 \exp^{\frac{\beta_1}{T}}$$

$$\hat{z}(x) = x_1^{\beta_1} + x_2^{\beta_2} + \beta_0$$

SYMBOLIC REGRESSION

- Flexible nonlinear regression
  - Symbolic regression

    Offers a source of nonlinear forms given only a set of operators addition, subtraction, multiplication, division, etc.



  - General linear models

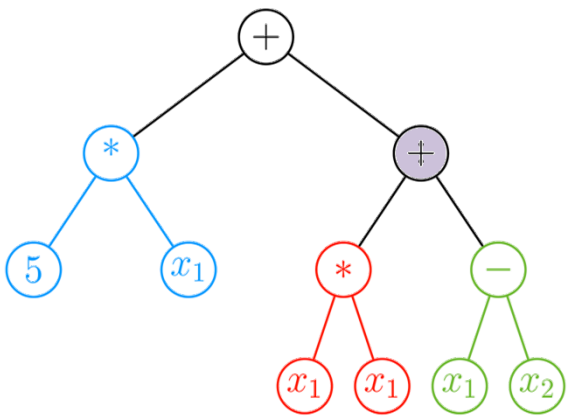
    Functional forms generated can be added to larger linear models

$$\hat{z}(x) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1 x_2 + \beta_4 \frac{2x_1}{5 - x_2}$$

EXPRESSION TREES

- Representation of nonlinear functional form
  - Can define any function using an appropriate tree

    Recursively defines the order of operations in a function using operands at leaf nodes and operators for all other nodes



$$5\,x_1 + \frac{(x_1)^2}{x_1 - x_2}$$

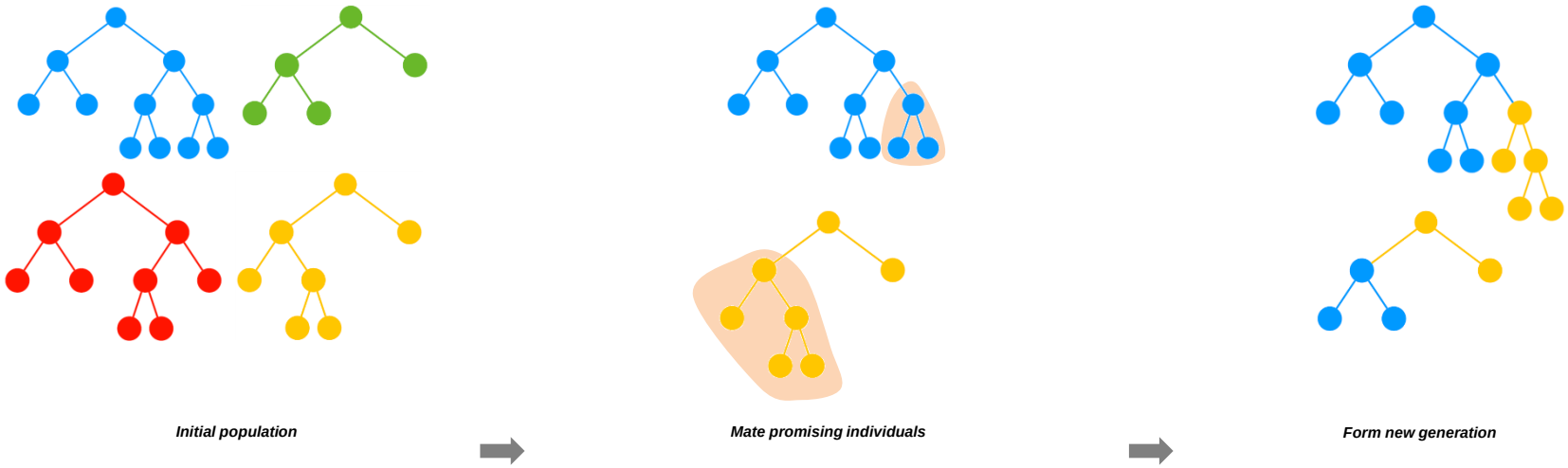
$$5\,x_1 + (x_1)^2 + x_1 - x_2$$

- Small changes drastically alter function

GENETIC PROGRAMMING

- ***Functional form learned without explicit instructions***
  - *Symbolic regression thought of as an application of genetic programming [Koza, 1992]*
  - *Stochastic nature offers no guarantees of an optimal model*

- ***Genetic algorithms are typically used to adjust and improve expression trees***



EXPRESSION TREE NOTATION

- Disjunctions modeled with binary variables $\{\boldsymbol{y_n^o}\}$

$$\{+\} \vee \{-\} \vee \{*\} \vee \{\div\} \vee \{\mathrm{cst}\} \vee \{x_d\} \vee \ldots$$

  - Nodes indexed by n
  - Sets of operators used as basis for logical constraints

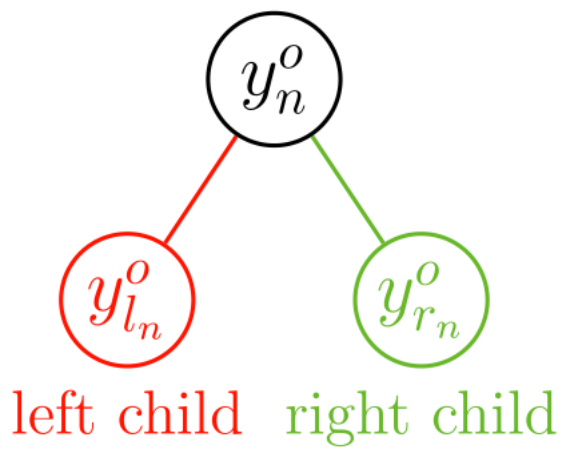
- Value at each node $\{\boldsymbol{v_{i,n}}\}$

  - Associated upper and lower bounds

- Function value at root node

$$f_i^o\left(v_{in}, v_{il_n}, v_{ir_n}, x_{id}\right)$$

  - Dependent on binary variables
  - Models constants and variables



$\mathcal{O}$	All operators and operands
$\mathcal{B}$	Binary operators
$\mathcal{U}$	Unary operators
$\mathcal{L}$	Operands or leaf nodes
$\mathcal{V}$	Variable node

RIGOROUS SYMBOLIC REGRESSION

- Benefits of the rigorous formulation include
  - Certification of the globally optimal functional form and parameter levels
  - Deterministic solutions, no run-to-run variation

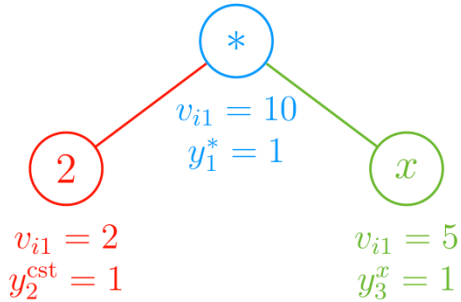
- Rigorous disjunctive mixed-integer nonlinear problem that
  - Minimizes model error
  - By relating node values using disjunctions over each node

$$\{+\} \vee \{-\} \vee \{*\} \vee \{\div\} \vee \{\text{cst}\} \vee \{x_d\} \vee \ldots$$

  - Example function

$$\text{Function: } \hat{z}(x) = 2\,x$$
$$\hat{z} = 10 \text{ at point } i,\ x_i = 5$$

$$\{*\} \text{ is active at Node 1} \Longrightarrow y_1^* = 1$$
$$\{\text{cst}\} \text{ is active at Node 2} \Longrightarrow y_2^{\text{cst}} = 1$$
$$\{x\} \text{ is active at Node 3} \Longrightarrow y_3^x = 1$$



OPTIMIZATION FORMULATION

$$
\begin{aligned}
\min \quad & [\text{error}] \\
\text{s.t.} \quad & \{+\} \vee \{-\} \vee \{*\} \vee \{\div\} \vee \{\text{cst}\} \vee \{x_d\} \vee \ldots \quad \forall \text{ nodes} \\
& [\text{logical constraints}] \\
& v_{in} \in [v_{in}^{\text{lo}}, v_{in}^{\text{up}}] \qquad \forall \text{ nodes } n \text{ and points } i
\end{aligned}
$$

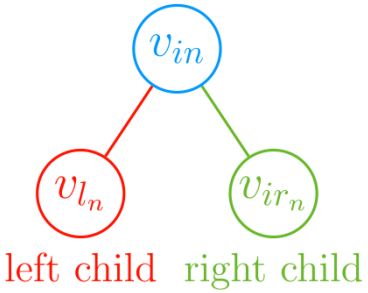
- Disjunctions formulated using big-M constraints
  - Defining operation at each non-terminal nodes, data point, and operator

$$
\begin{aligned}
f_i^o\left(v_{in}, v_{il_n}, v_{ir_n}, x_{id}\right) &\leq \overline{M}_{in}^o\left(1 - y_n^o\right) \\
f_i^o\left(v_{in}, v_{il_n}, v_{ir_n}, x_{id}\right) &\geq \underline{M}_{in}^o\left(1 - y_n^o\right)
\end{aligned}
$$

  - Example: Addition operator

$$
\begin{aligned}
y_n^+ &= 1 \\
v_{il_n} + v_{ir_n} - v_{in} &\leq \overline{M}_{in}^+\left(1 - y_n^+\right) \\
v_{il_n} + v_{ir_n} - v_{in} &\geq \underline{M}_{in}^+\left(1 - y_n^+\right)
\end{aligned}
$$

$$v_{in} = v_{il_n} + v_{ir_n}$$



OPTIMIZATION FORMULATION

$$
\begin{aligned}
\min \quad & [\text{error}] \\
\text{s.t.} \quad & \{+\} \vee \{-\} \vee \{*\} \vee \{\div\} \vee \{\text{cst}\} \vee \{x_d\} \vee \ldots \quad \forall \text{ nodes} \\
& [\text{logical constraints}] \\
& v_{in} \in [v_{in}^{\text{lo}}, v_{in}^{\text{up}}] \qquad \forall \text{ nodes } n \text{ and points } i
\end{aligned}
$$

- Disjunctions formulated using big-M constraints
  - Defining operation at each terminal nodes, data point, and operator

$$
\begin{aligned}
f_i^o\left(v_{in}, x_{id}\right) &\leq \overline{M}_{in}^o \left(1 - y_n^o\right) \\
f_i^o\left(v_{in}, x_{id}\right) &\geq \underline{M}_{in}^o \left(1 - y_n^o\right)
\end{aligned}
$$

  - Set constant term

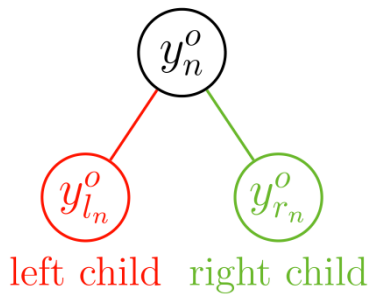
$$
\begin{aligned}
& v_{in} = v_{i'n} \\
& \text{for all data points } i \neq i'
\end{aligned}
\qquad
\begin{aligned}
& y_n^{\text{cst}} = 1 \\
& v_{in} - v_{i'n} \leq \overline{M}_{in}^{\text{cst}} \left(1 - y_n^{\text{cst}}\right) \quad \forall i \neq i' \\
& v_{in} - v_{i'n} \geq \underline{M}_{in}^{\text{cst}} \left(1 - y_n^{\text{cst}}\right) \quad \forall i \neq i'
\end{aligned}
$$

  - Set variable

$$
\begin{aligned}
& v_{in} = x_i \\
& \text{for data point } i
\end{aligned}
\qquad
\begin{aligned}
& y_n^x = 1 \\
& v_{in} - x_i \leq \overline{M}_{in}^x \left(1 - y_n^x\right) \\
& v_{in} - x_i \geq \underline{M}_{in}^x \left(1 - y_n^x\right)
\end{aligned}
$$

  - If no operator or operation is active, the nodes values are set to zero

OPTIMIZATION FORMULATION



$\mathcal{O}$	All operators and operands
$\mathcal{B}$	Binary operators
$\mathcal{U}$	Unary operators

- Logical constraints
  - Ensure only one operator per node

$$\sum_{o \in \mathcal{O}} y_n^o \leq 1 \qquad n = 1, 2, \ldots, N$$

  - If the node is a binary operator both children are active

$$\sum_{o \in \mathcal{B}} y_n^o \leq y_{l_n}^o \qquad n = 1, 2, \ldots, N$$

$$\sum_{o \in \mathcal{B}} y_n^o \leq y_{r_n}^o \qquad n = 1, 2, \ldots, N$$

  - If the node is a unary operator the left child is active

$$\sum_{o \in \mathcal{U}} y_n^o \leq 1 - y_{r_n}^o \qquad n = 1, 2, \ldots, N$$

EXAMPLE – COMPLEXITY CONTROL

Find a model for actual function:

$$z(x) = \frac{2\,x_1}{5 - x_2}$$

given 10 randomly sampled points $x_1, x_2 \in [0, 1]$

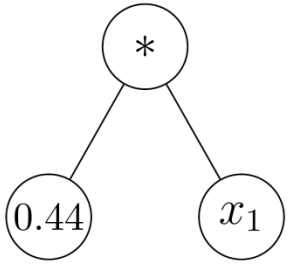
$$\sum_{i=1}^{N} \sum_{o \in O} y_n^o \leq T$$

One node

$\hat{z}(x) = 0.2405$

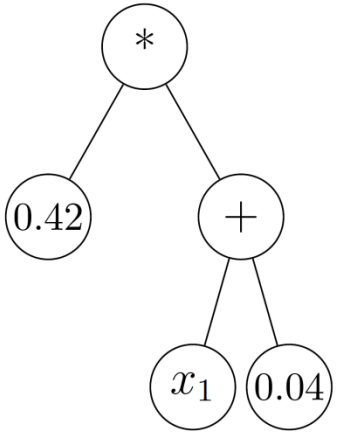
Three node

$0.4434\,x_1$



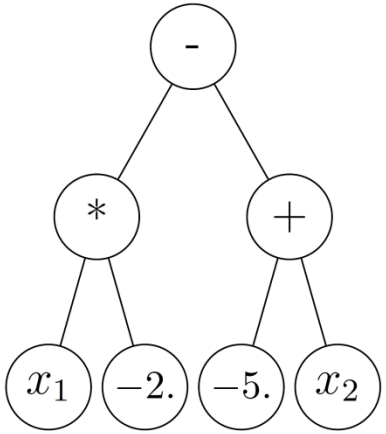
Five node

$0.42\,(\,x_1 + 0.039)$



Seven node

$-2.00\,x_1/\,(-5.00 + x_2)$



RMSE: 0.129 | 0.00360 | 0.00306 | 0.000

ILLUSTRATIVE EXAMPLE

Find a model for actual function:

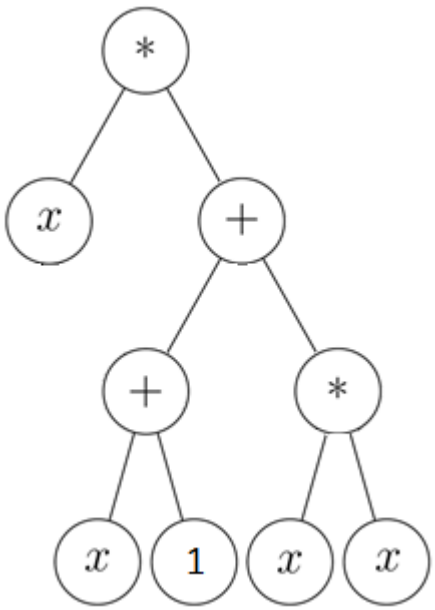
$$z(x) = x^3 + x^2 + x$$

given 20 randomly sampled points $x \in [-1, 1]$

- ***"Difficult synthetic problem" [McDermott 2014]***
  - ***50% success rate for an error tolerance of 0.01 using state-of-the-art implementations [Uy 2011]***
- ***Starts with tree depth of 4***
  - $\boldsymbol{O} \in \{+, -, *, \div, \exp, \log, \boldsymbol{x}, c\}$
  - ***MINLP formulation contains 300 continuous variables, 120 binary variables, and 9,047 constraints***
  - ***Optimal solution found in 1200s***
  - ***7 node function chosen in favor of 11 node function***

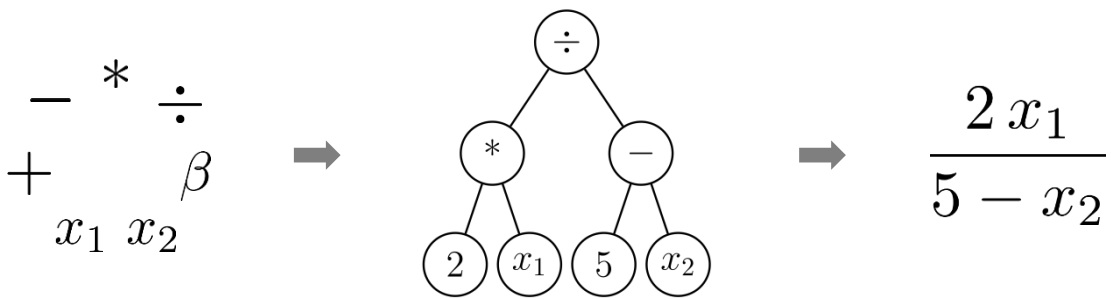
Seven node

$$z(x) = x * (x + 1 + x * x)$$



RMSE: 0.000

CONCLUSIONS



- We propose the first deterministic optimization formulation for the rigorous solution of symbolic regression problems
  - provides a certified optimal solution
  - No run-to-run variation
- We have shown exact function matches for literature problems that routinely show less that 50% success using current state-of-the-art symbolic regression methods

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