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PROMMIS
Process Optimization and Modeling for Minerals Sustainability

MINLP for regularized symbolic regression

with applications to data-driven discovery of physical laws

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MODELS FROM DATA

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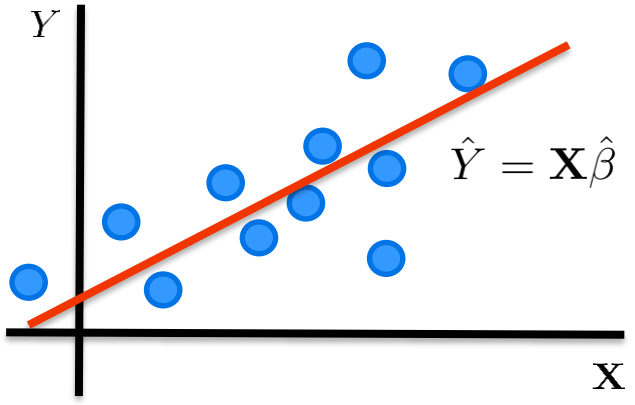
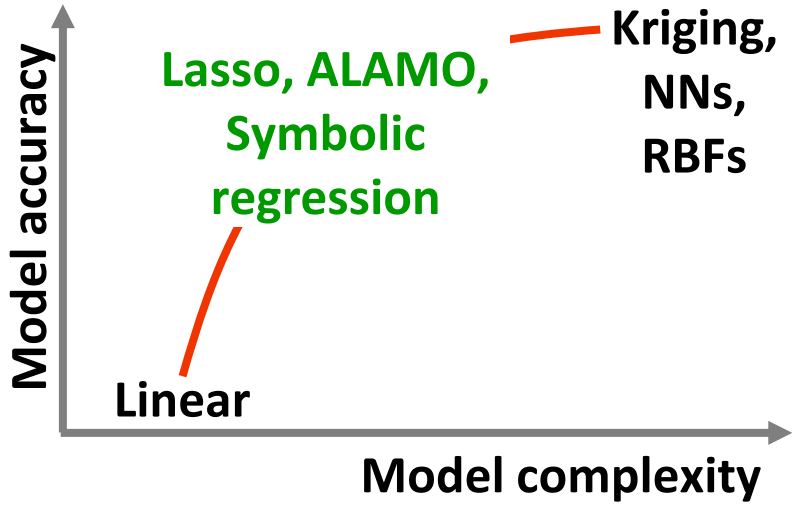
- **(Ordinary) Least Squares method[1]**
- **Polynomial models: simple and interpretable**
  - Can be built quickly, necessary for real-time use
  - Not always accurate: too simple or overfitted
- **L1 regularization (Lasso[2]), best subset selection (e.g. ALAMO[3])**



$$\beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1 x_2$$

- **Neural Networks[4,5], kriging[6,7], radial basis functions[8]**
- **Model complexity-accuracy tradeoff**



[1]Hastie et al., 2009; [2]Tibshirani, 1996; [3]Cozad et al., 2013; [4]McCulloch and Pitts, 1943; [5]Rosenblatt, 1958; [6]Krige, 1951; [7]Matheron, 1963; [8]Hardy, 1971

TREES AND SYMBOLIC REGRESSION

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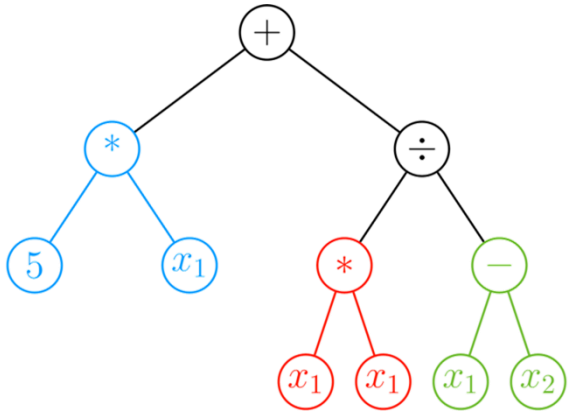
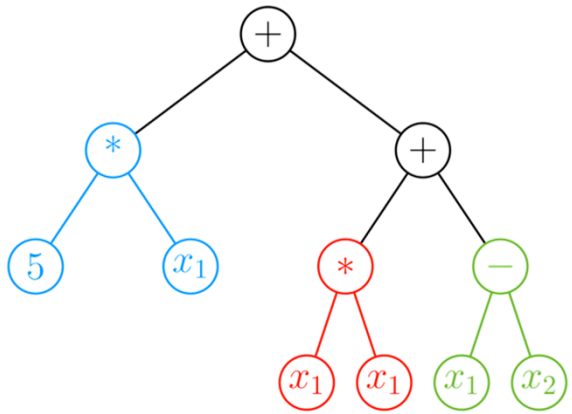
- **Any closed-form expression can be represented as a binary tree**
  - Leaves: variables and constants
  - Non-terminal nodes: operators

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



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



SYMBOLIC REGRESSION

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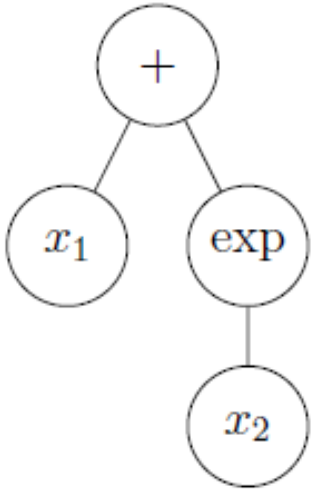
- **Supervised machine learning (ML) technique that determines simultaneously**
  - **The functional form of a model**
  - **The values of the regression parameters that best fit the data**
- **Symbolic regression (SR) models are parameterized using a set of operators**
  - **Usual operators are** $+, -, *, \div, \mathrm{sqrt}(\cdot), \exp(\cdot), \log(\cdot), \sin(\cdot), (\cdot)^2$
- **Data-driven modeling with SR**

$$\hat{y} = x_1 + e^{(x_2)}$$



- **Symbolic regression is an emerging field on its own[1,2,3,4]**

Kronberger et al., 2024; Angelis et al., 2023; Makke and Chawla, 2024 ; Dong and Zhong, 2025

GENETIC PROGRAMMING

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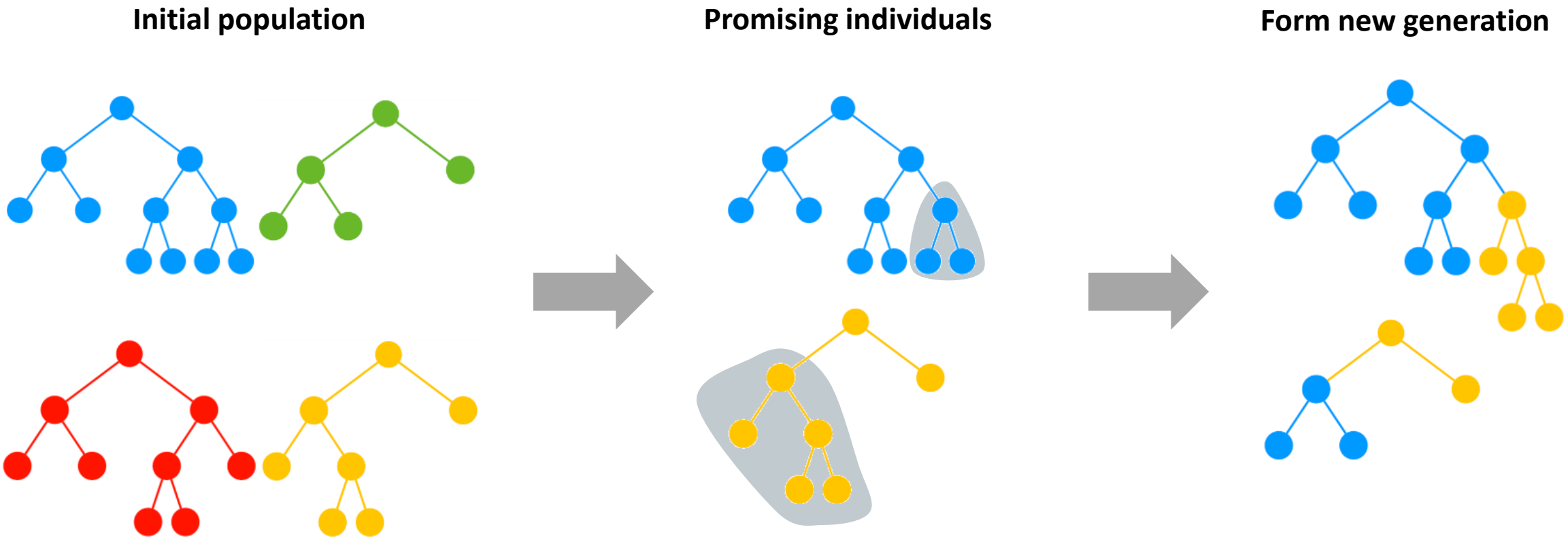

GP (Koza, 1992); Eureqa (Lipson et al., 2009); SRBench (Cava et al., 2021); gplearn (Stephens, 2015); Operon (Burlacu et al., 2020); AIFeynman (Udrescu et al., 2020); PySR (Cranmer, 2023); GP inefficient for SR (Kronberger et al., 2024)

MINLP FOR SYMBOLIC REGRESSION

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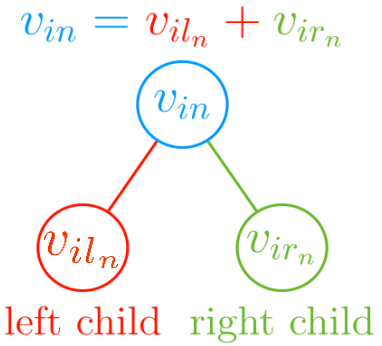
- **SR as a Generalized Disjunctive Program[1,2]**

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



- **Binary variables represent the choice of operators/operands at each node**

$$z_n^+,\ z_n^{\log},\ z_n^{\exp},\ z_n^*,\ z_n^{\text{cst}},\ z_n^{x_1}$$

- **Value-defining constraints formulate operations using big-M constraints**
  - **Defining operation at each non-terminal node, data point, and operator**
  - **Example: Addition operator**

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

[1]Cozad, 2014; [2]Cozad and Sahinidis, 2018; Austel et al., 2017, 2020; Kim et al., 2023

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CONSTRAINTS AND OBJECTIVE

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- **Tree-defining constraints formulate logical conditions about the structure of tree**
  - Example: Only one operator/operand can be assigned to a node

$$\sum_{o \in O} z_n^o \leq 1$$

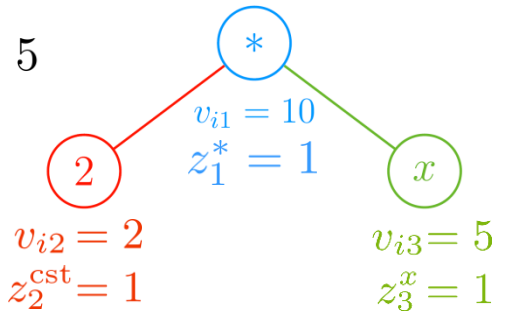
- **Redundancy-eliminating constraints eliminate similar trees**
  - Example: Do not make operations between constants

$$z_{2n}^{cst} + z_{2n+1}^{cst} \leq 1$$

- **The loss function is the SSR in existing MINLP approaches**

$$\text{Loss} = \sum_{i=1}^{n_{data}} (y_i - \hat{y}_i)^2 \quad where \quad \hat{y}_i = v_{i1}$$

Function: $y(x) = 2\,x$
$y = 10$ at point i, $x_i = 5$



RANDOMIZED ROUNDING ALGORITHM

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- **STAR (Symbolic regression Through Algebraic Representations) algorithm[1]**
  - Solve a continuous relaxation of the MINLP
  - Obtain probabilities of assigning operands and operators to trees' nodes
  - Use randomized rounding to generate a number of expression trees
  - Enhance trees: multiply each input variable with a constant slope and add an intercept
  - Optimize parameters of each tree
  - Evaluate trees

- **PySTAR[2,3] has superior overall predictive performance compared to the state-of-the-art GP methods gplearn, Operon, and PySR**

[1]Sarwar, 2022; [2]Kim et. al, 2025; [3]https://github.com/IDAES/idaes-pySTAR

REGULARIZED SYMBOLIC REGRESSION

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- **Model selection criteria that penalize complexity**
  - Complexity as the depth L of the expression tree

- **Bayesian Information Criterion (BIC):** $$\mathrm{BIC} = n_{data} \ln \frac{\mathrm{SSR}}{n_{data}} + L \ln n_{data}$$

- **The level l_n for node n in the tree is:** $$l_n = \lceil \log_2(n+1) \rceil - 1$$

- **Let z_{no} is the binary variable of assigning the operator or operand $o \in O$ to node $n \in N$. The depth of the tree L is:**

$$L = \max_{n \in \mathcal{N}} l_n \sum_{o \in \mathcal{O}} z_{no}$$

PENALIZE COMPLEXITY USING THE BIC

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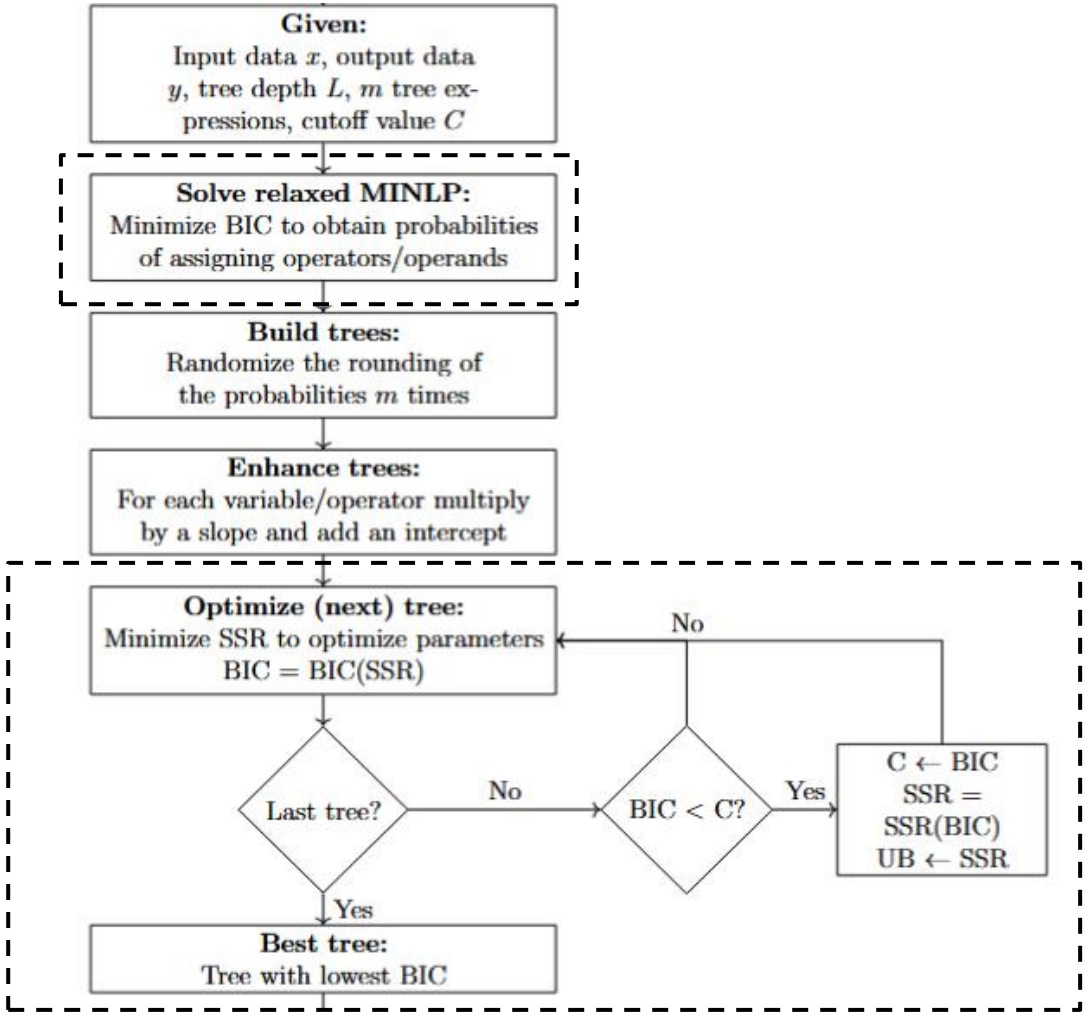

$$\mathrm{BIC} = n_{data} \ln \frac{\mathrm{SSR}}{n_{data}} + k \ln n_{data}$$

$$\mathrm{SSR} = n_{data} \exp\left(\frac{\mathrm{BIC} - k \ln n_{data}}{n}\right)$$

SR FOR CRITICAL MINERALS RECOVERY

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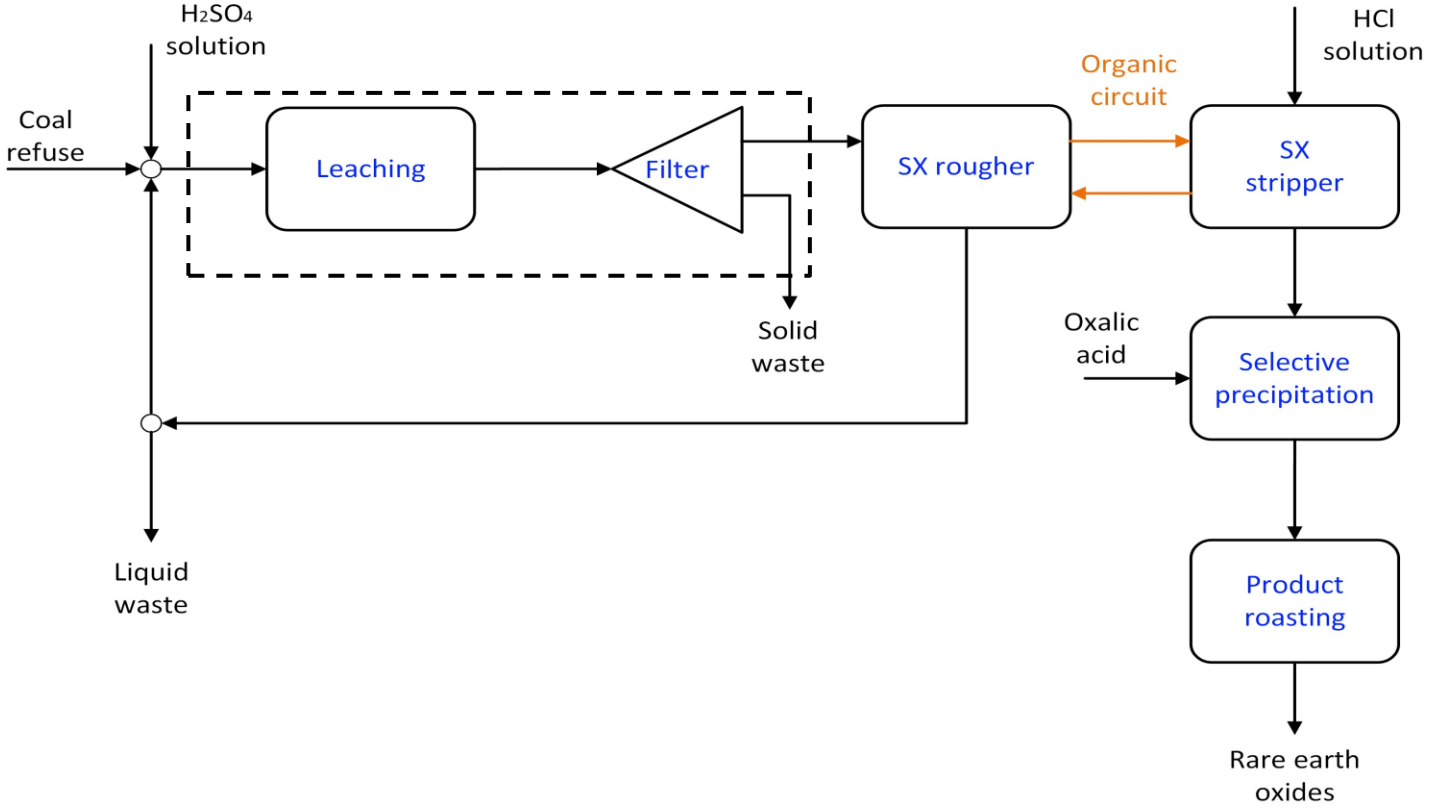
- **Modeling, simulation and optimization of critical mineral processes**
  - Goal: simplify modeling and optimization of leaching using SR models



- **Input variables of leaching**
  - Solid feed ranging in [50, 100] lb/hr
  - Concentration of sulfuric acid ranging in [0.025, 0.075] mol/L
- **30 outputs in the liquid and solid outlets**

MODELING AND OPTIMIZATION

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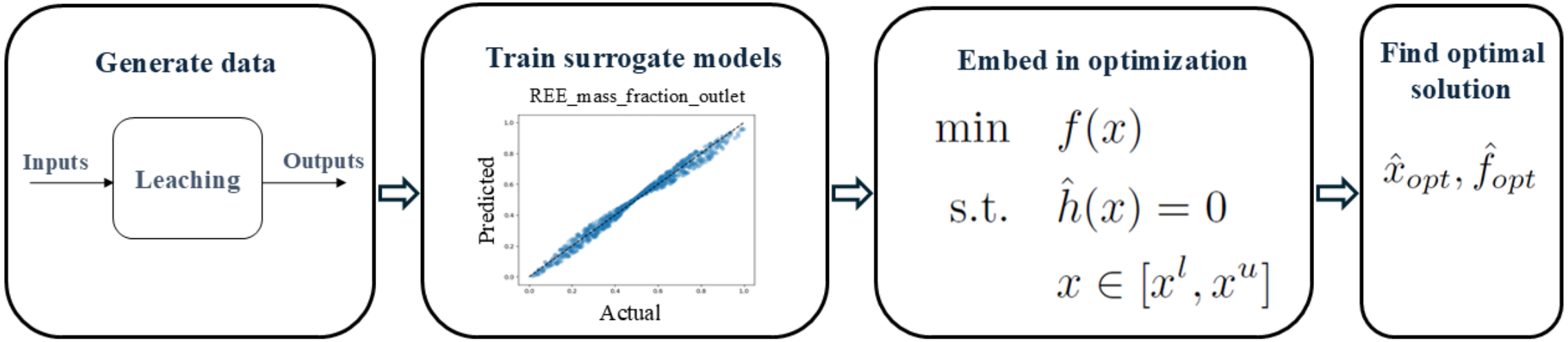
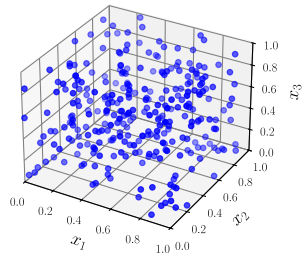
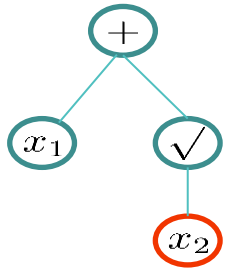
- **Build STAR models for a chemical process**
  - Leaching process of a flowsheet for the recovery of critical minerals[1]







[1]Fardis et al., 2025

EVALUATION OF DATA-DRIVEN MODELS

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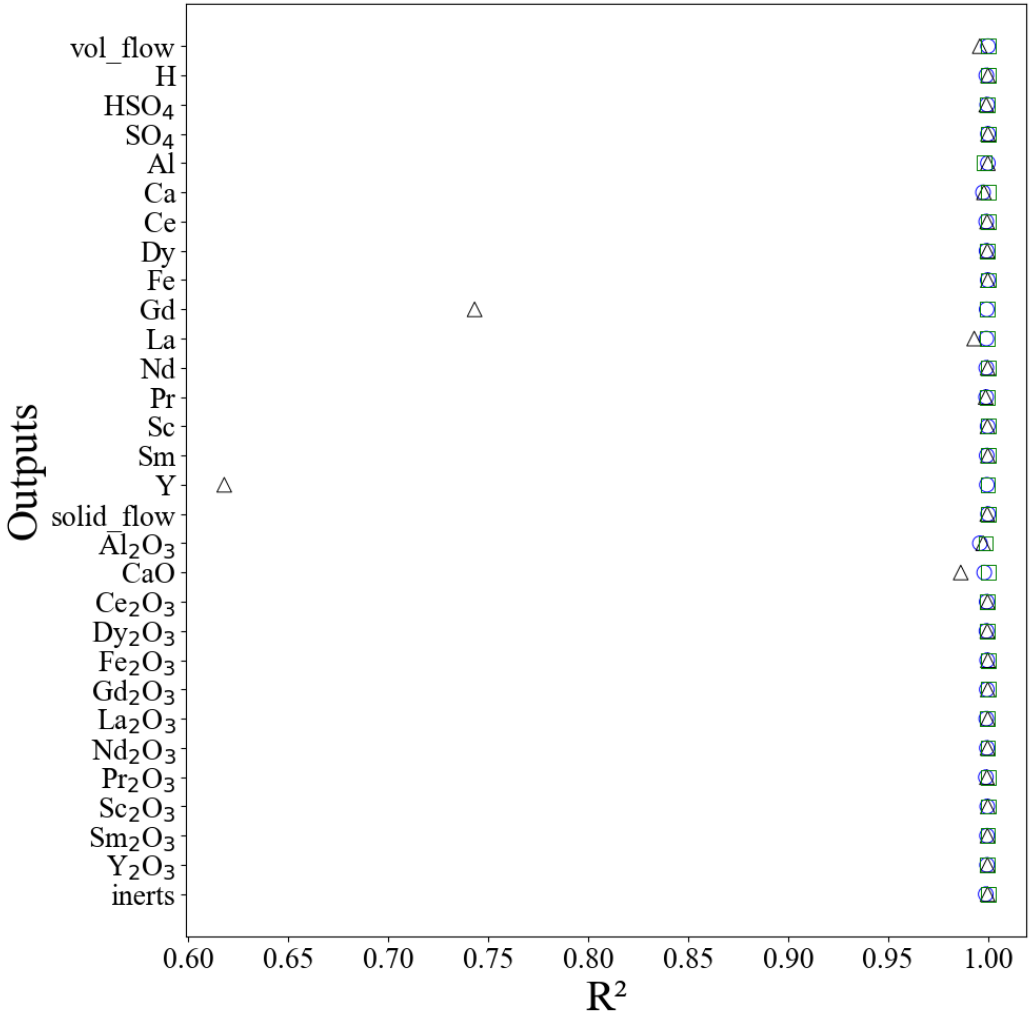

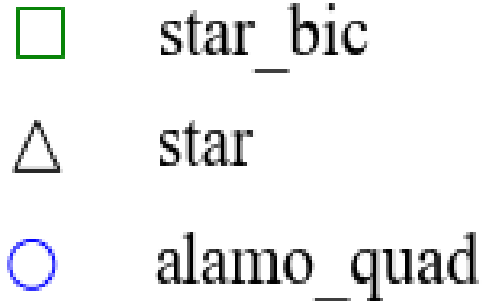

- **ALAMO sparse quadratics balanced accuracy and efficiency in the best way compared to lasso, ANN, kriging, RBF[1]**
- **Regularized SR models are accurate, even when trained with 10 points**

[1]Fardis et al., 2025

REGULARIZED SR MODELS

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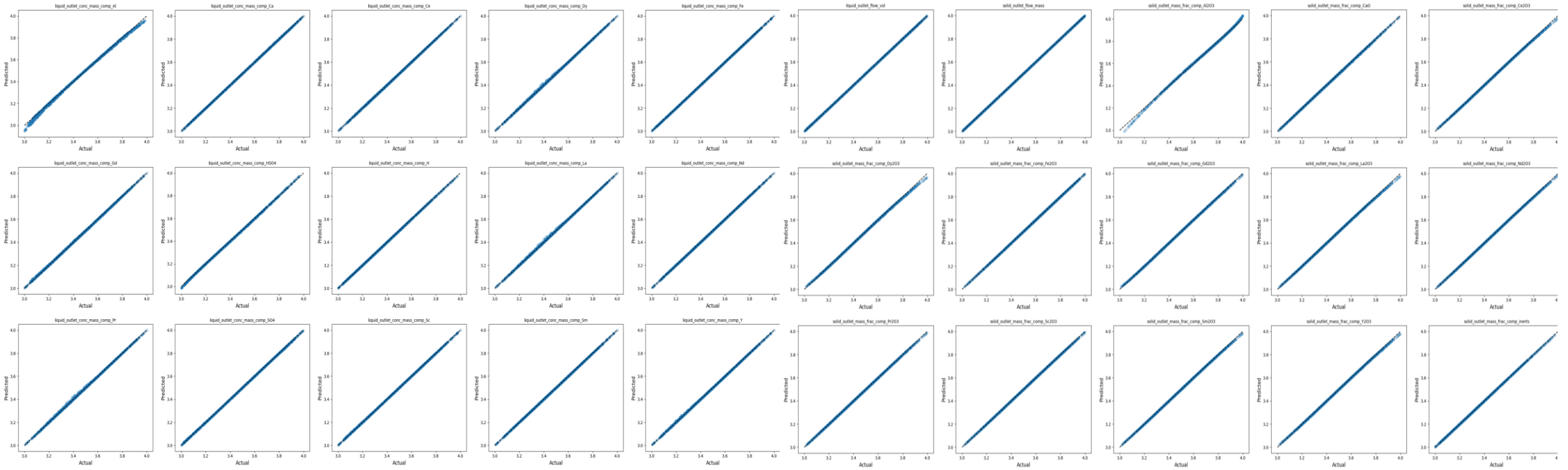

Regularized SR models trained with 10 points achieve

- **Excellent predictive performance**
- **Low model complexity**

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TRAINING TIMES

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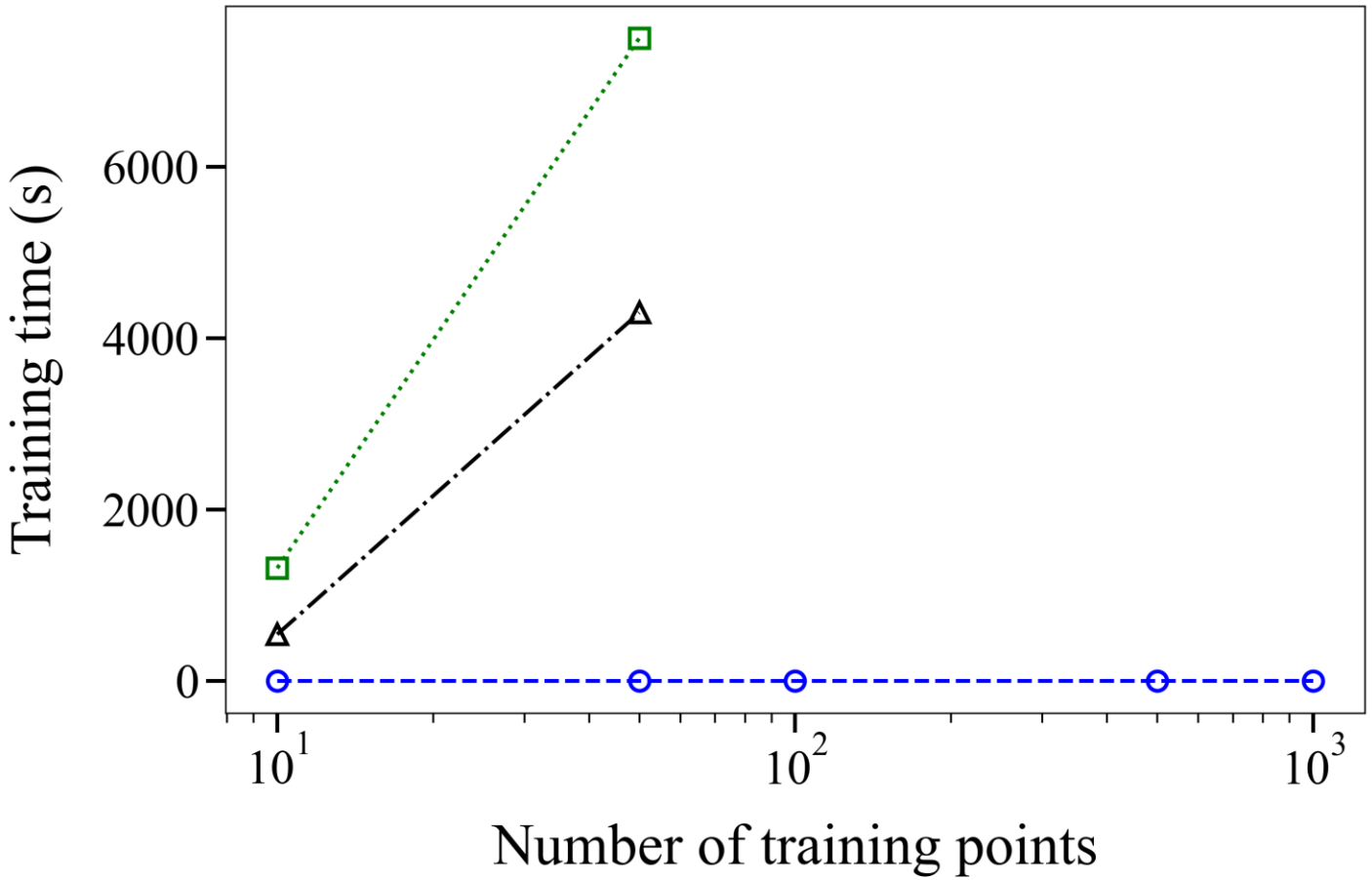

alamo_quad
star
star_bic

- **Training times are 4-5 orders of magnitude larger for SR models**
- **Regularization with BIC doubles the training time for SR**

SURROGATE-BASED OPTIMIZATION

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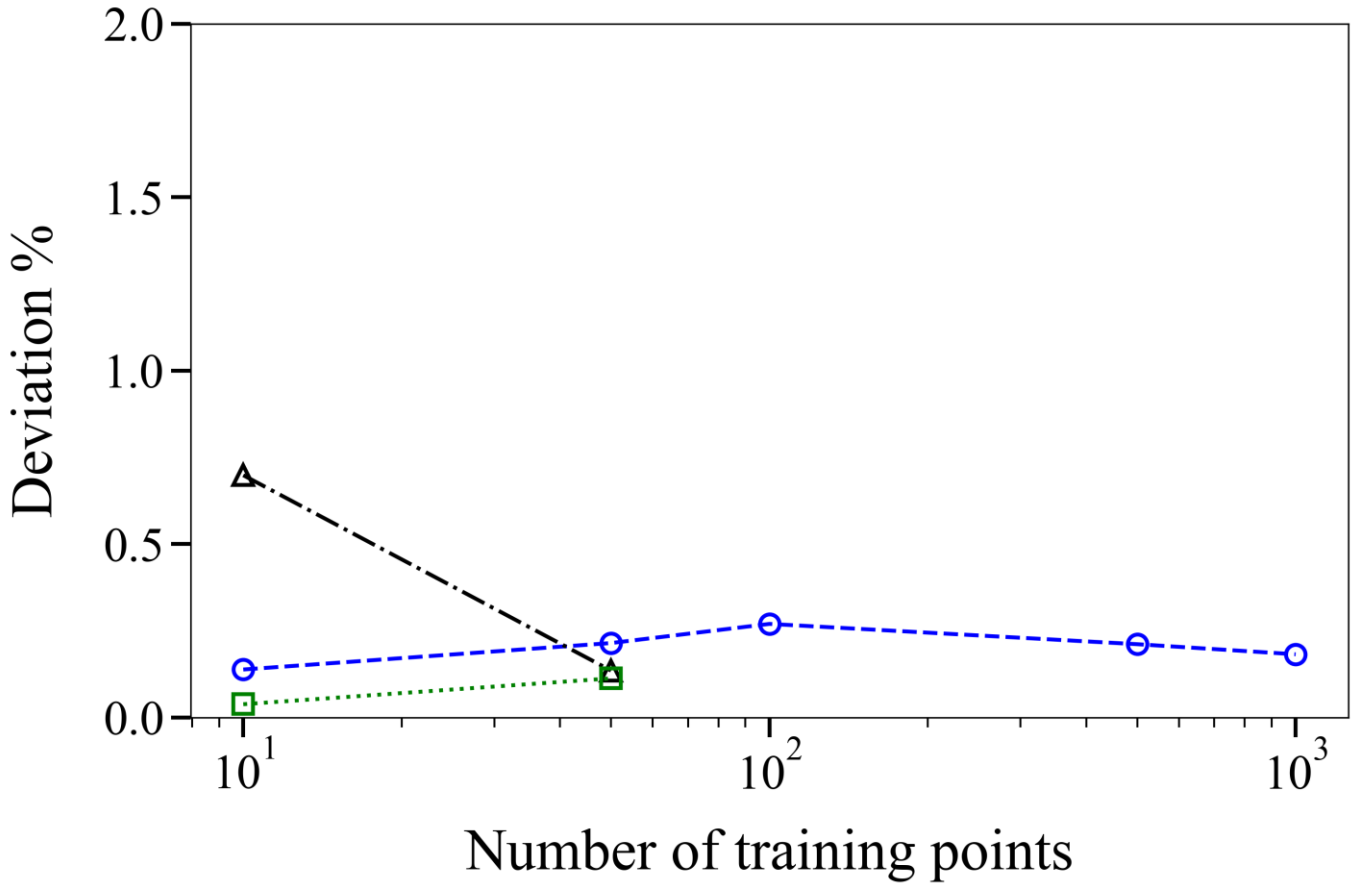

- **Correct solution point**
  - 45.36 kg/h solid feed
  - 0.075 M sulfuric acid
- **Little deviation in the objective across methods**
  - EO optimal objective value is 5128.2 mg rare earths per hour
- **Regularized SR models trained with 10 points provide the lowest deviation**

CONCLUSIONS AND FUTURE WORK

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- **SR is attractive**
  - It provides simple data-driven models
  - It makes no prior assumptions about their functional forms (useful for law discovery)
- **SR efficient for moderate numbers of training points**
- **Regularization can expand the applicability of SR**
  - No overfitting
  - Simple and interpretable models
- **Compare various complexity metrics**
  - Depth, number of nodes, number of operators, number of complexity-weighted nodes
- **Compare various model selection criteria**
  - BIC, AIC, HQIC, etc.

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For questions and comments, please contact our Technical Director, Thomas Tarka (Thomas.Tarka@netl.doe.gov).

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