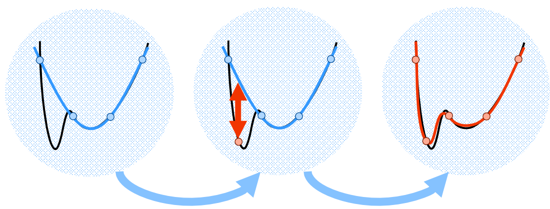
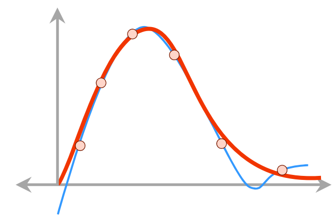




ALAMO: Machine learning from data and first principles

Nick Sahinidis

Acknowledgments:

Alison Cozad, David Miller, Zach Wilson

Carnegie Mellon University CAPD CENTER NATIONAL ENERGY TECHNOLOGY LABORATORY CCSI™ IDAES Institute for the Design of Advanced Energy Systems The Optimization Firm

MACHINE LEARNING PROBLEM

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

$$x \in \mathbb{R}^k \qquad x^l \leq x \leq x^u \qquad \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_j \\ \vdots \\ x_k \end{pmatrix} \Rightarrow \quad \Rightarrow \begin{pmatrix} z_1 \\ z_2 \\ \vdots \\ z_l \\ \vdots \\ z_m \end{pmatrix} \qquad z \in \mathbb{R}^m \qquad z = f(x)$$

Independent variables:
Operating conditions, inlet flow properties, unit geometry, molecular descriptors, etc.

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

DESIRED MODEL ATTRIBUTES

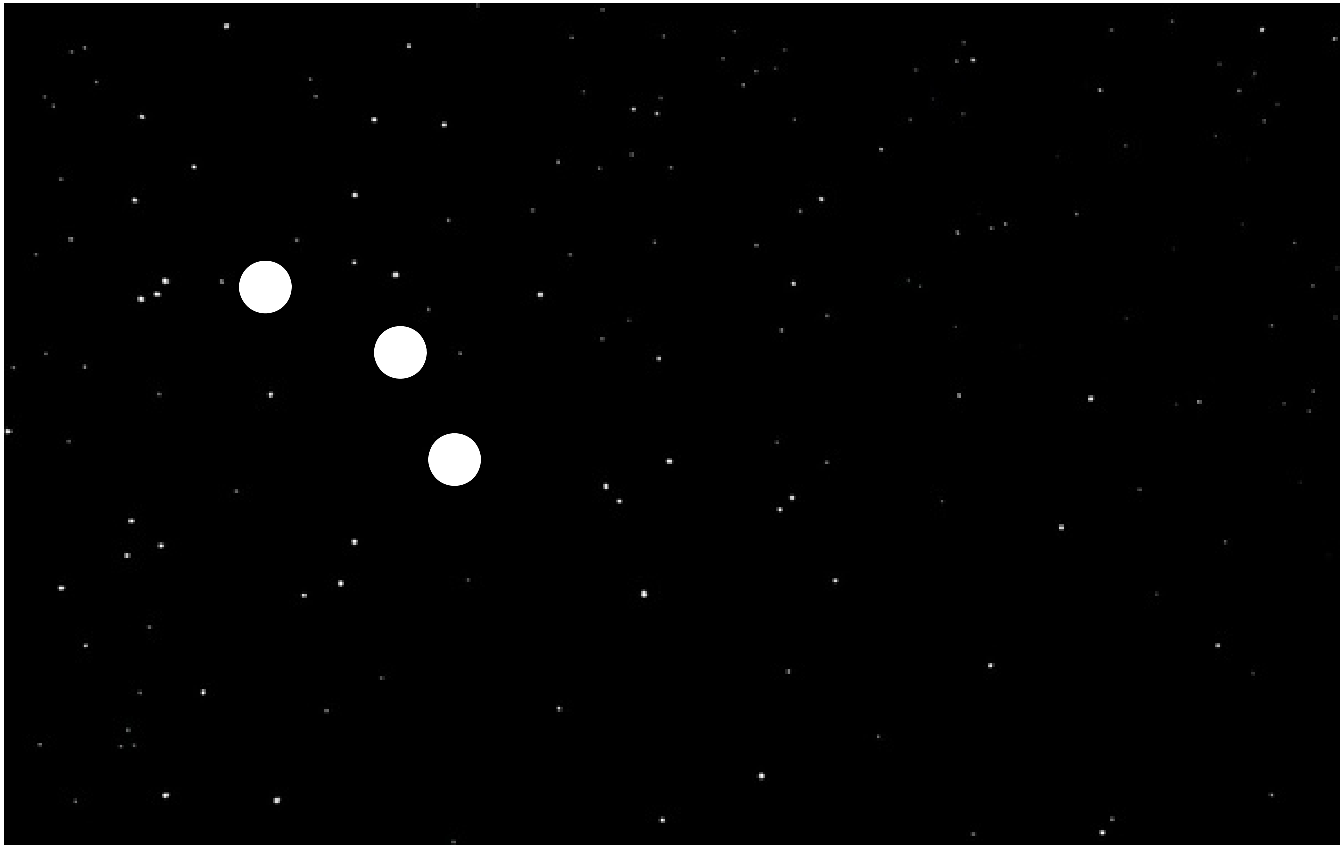
1. **Accurate**
   - We want to reflect the true nature of the system

2. **Simple**
   - Usable for algebraic optimization
   - Interpretable

3. **Generated from a minimal data set**
   - Reduce experimental and simulation requirements

4. **Obeys physics and user insights**
   - Increase fidelity and validity in regions with no measurements

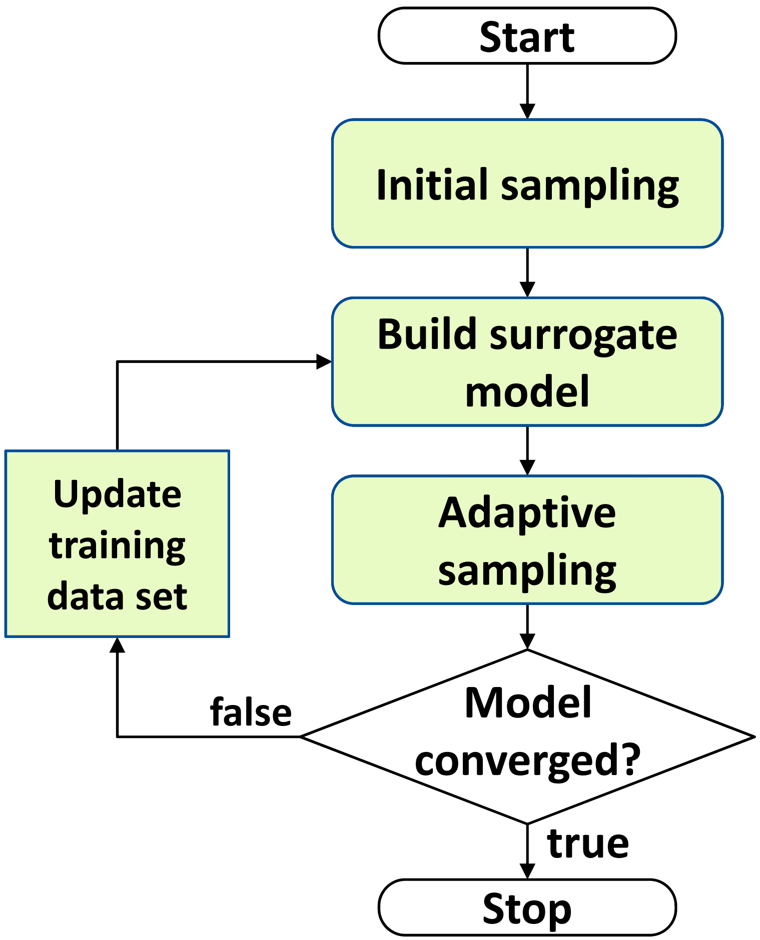
EUROPE IN 1801

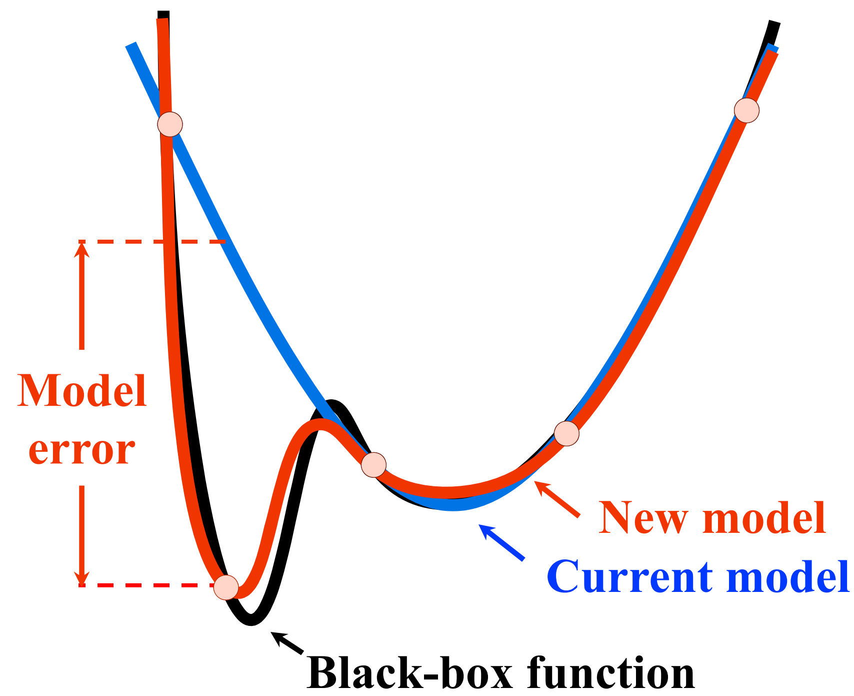


- **Piazzi observed positions of Ceres**
- **Gauss: Least squares**
  - Used observations *and* Kepler's conjecture

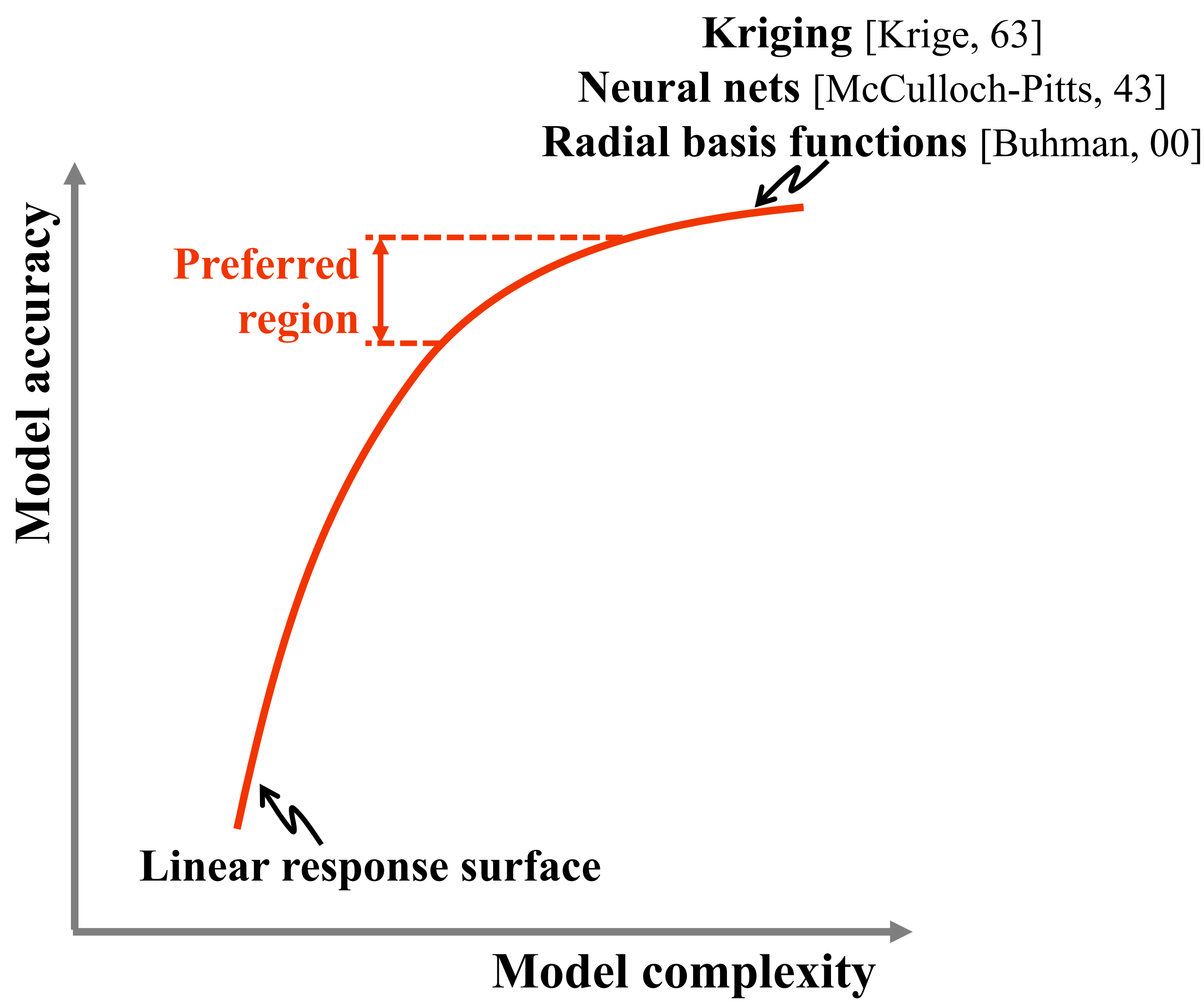
ALAMO

Automated Learning of Algebraic MOdels





MODEL COMPLEXITY TRADEOFF



MODEL IDENTIFICATION

- **Identify the functional form and complexity of the surrogate models $z = f(x)$**
- **Seek models that are linear combinations of sets of basis functions**

1. **Simple basis functions**

Category		$X_j(x)$
I.	Polynomial	$(x_d)^\alpha$
II.	Multinomial	$\prod_{d \in \mathcal{D}' \subseteq \mathcal{D}} (x_d)^{\alpha_d}$
III.	Exponential and logarithmic	$\exp\left(\frac{x_d}{\gamma}\right)^\alpha, \log\left(\frac{x_d}{\gamma}\right)^\alpha$

2. **User-specified basis functions**
3. **Radial basis functions**

OVERFITTING AND TRUE ERROR

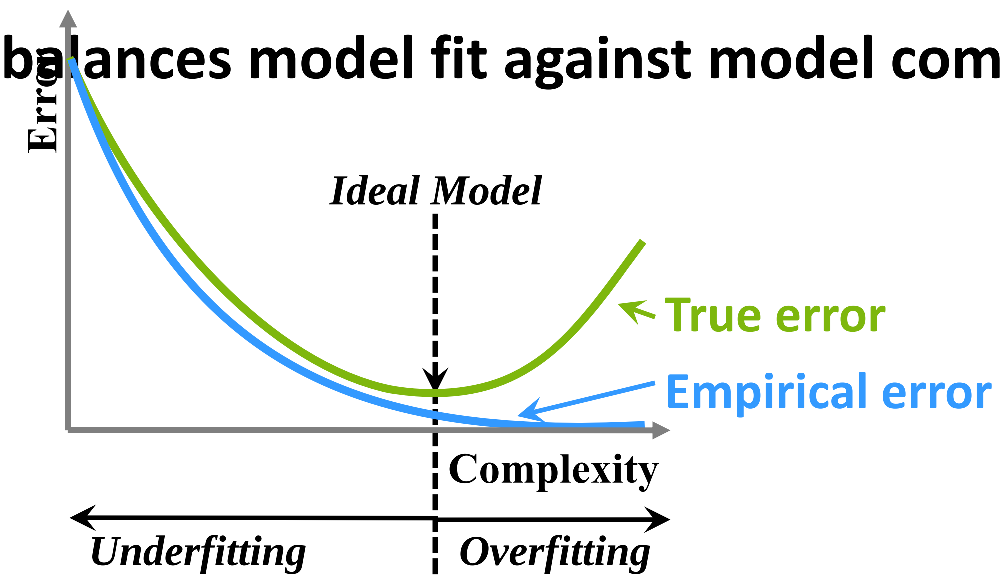
- **Step 1:** Define a large set of potential building blocks

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

- **Step 2:** Model reduction

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

Select subset that balances model fit against model complexity



MODEL SELECTION CRITERIA

- **Balance fit (sum of square errors) with model complexity (number of terms in the model; denoted by *p*)**

Corrected Akaike information criterion

$$AIC_c = N \log\left(\frac{1}{N}\sum_{i=1}^{N}(z_i - X_i\beta)^2\right) + 2\boldsymbol{p} + \frac{2\boldsymbol{p}(\boldsymbol{p}+1)}{N-\boldsymbol{p}-1}$$

Mallows' Cp

$$C_p = \frac{\sum_{i=1}^{N}(z_i - X_i\beta)^2}{\widehat{\sigma^2}} + 2\boldsymbol{p} - N$$

Hannan-Quinn information criterion

$$HQC = N \log\left(\frac{1}{N}\sum_{i=1}^{N}(z_i - X_i\beta)^2\right) + 2\boldsymbol{p}\log(\log(N))$$

Bayes information criterion

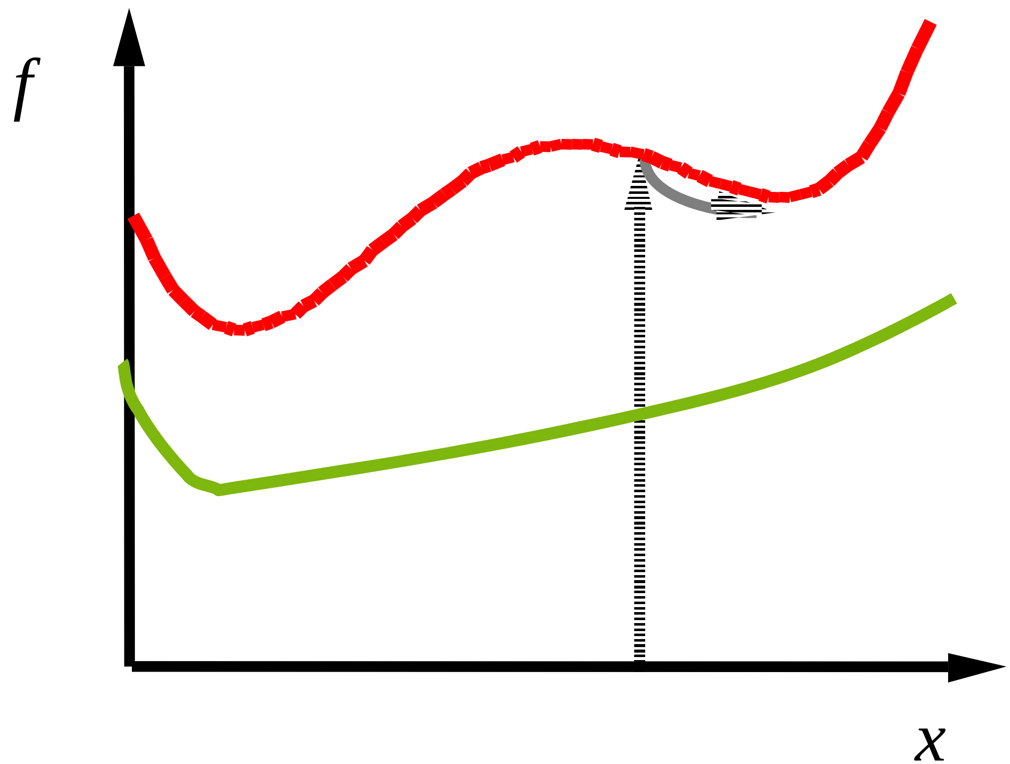
$$BIC = \frac{\sum_{i=1}^{N}(z_i - X_i\beta)^2}{\widehat{\sigma^2}} + \boldsymbol{p}\log(N)$$

Mean squared error

$$MSE = \frac{\sum_{i=1}^{N}(z_i - X_i\beta)^2}{N-\boldsymbol{p}-1}$$

- **Mixed-integer nonlinear programming models**

CONVEXIFICATION AND GLOBAL OPTIMIZATION

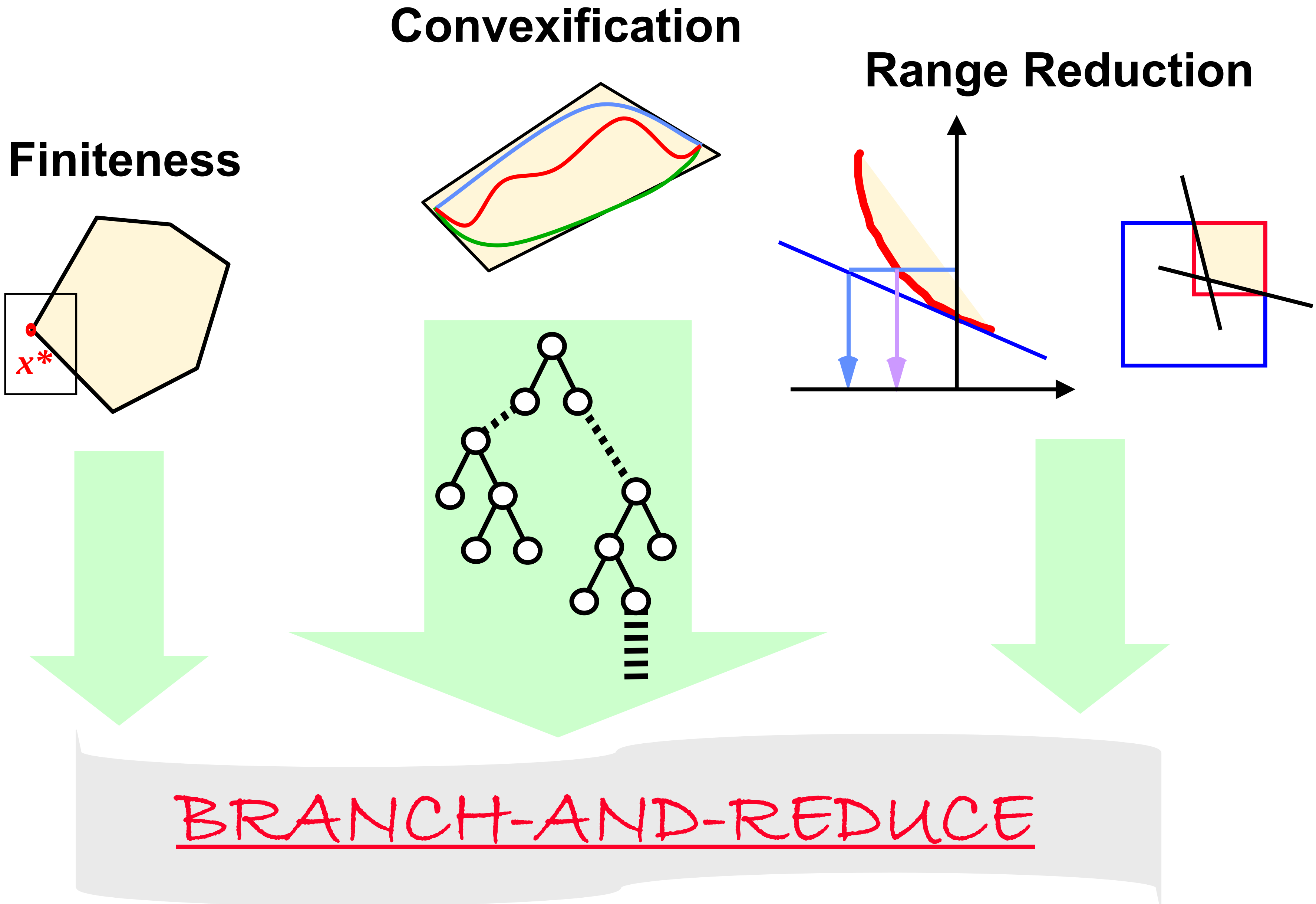


Classical optimization algorithms provide a local minimum "closest" to the starting point used

CONVEX ENVELOPES

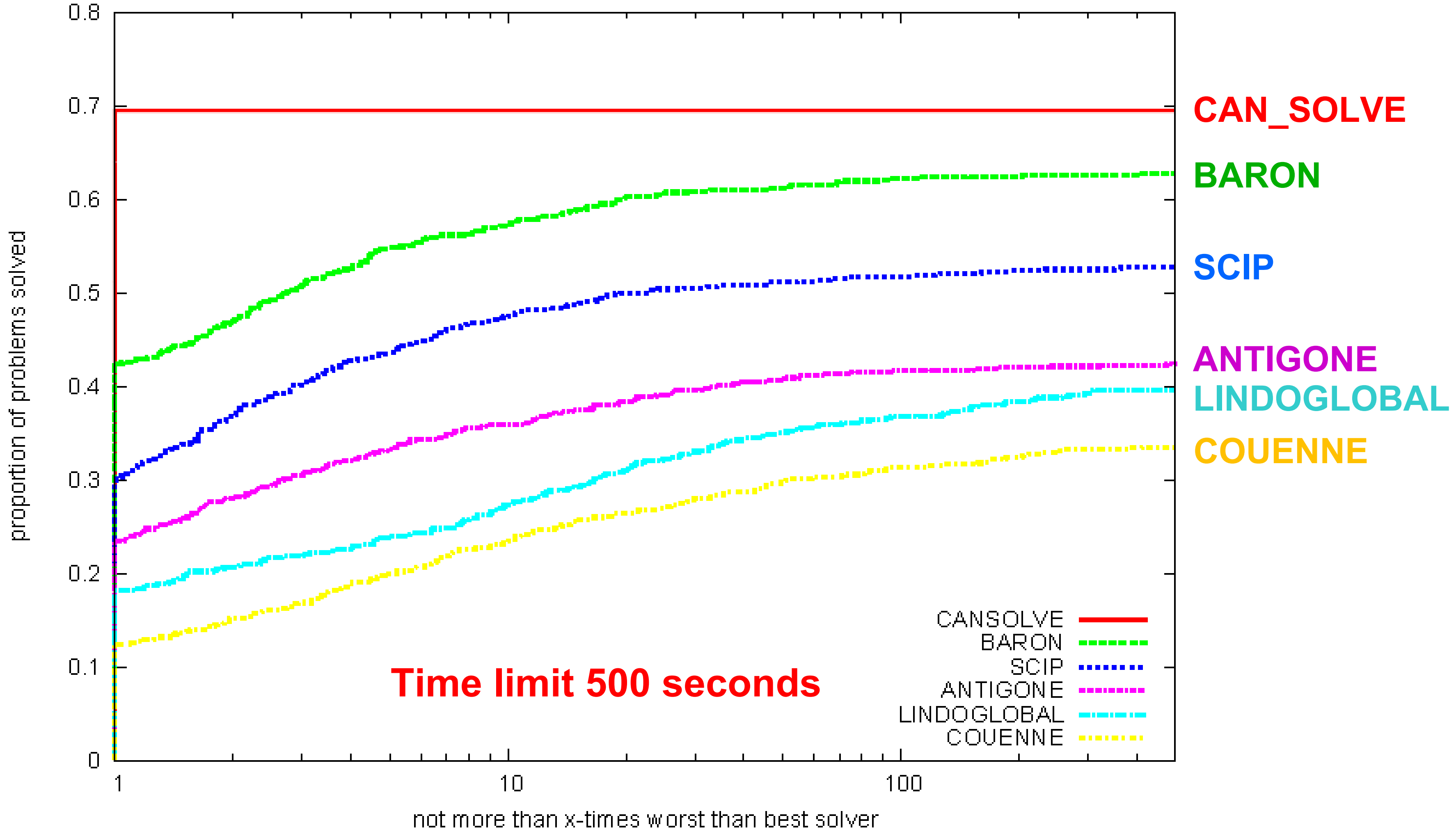
Function	Domain		
$\sqrt{y}/x^2$	$x \in [-2,-1]$	$y \in [1,4]$	
$y/(x_1x_2)$	$x_1 \in [0.1,1]$	$x_2 \in [1.5,2]$	$y \in [0.5,2]$
$y\exp(-x)$	$x \in [-1,1]$	$y \in [1,3]$	
$\log_{10} y/x^2$	$x \in [0.1,2]$	$y \in [0.1,10^2]$	
$y\exp(x_1 - x_2)$	$x_1 \in [0,1]$	$x_2 \in [0,1]$	$y \in [-1,1]$
$x^2 \log_{10} y$	$x \in [-1,2]$	$y \in [0.1,10]$	
y_1y_2/x	$x \in [0.1,1]$	$y_1 \in [0.1,1]$	$y_2 \in [0.5,1.5]$
$x^2\sqrt{y_1+y_2}$	$x \in [0.1,0.5]$	$y_1 \in [0,1]$	$y_2 \in [0.5,1.5]$
$(2y_1 - y_2)\exp(-x)$	$x \in [-0.5,1.0]$	$y_1 \in [0.6,1.5]$	$y_2 \in [0.1,1.0]$
$(y_1+y_2)/x$	$x \in [1,5]$	$y_1 \in [-2,1]$	$y_2 \in [1,3]$
y_1y_2/x	$x \in [0.1,1]$	$y_1 \in [-1,1]$	$y_2 \in [0.1,1]$
$(\sqrt{y_1} - y_2)\exp(-x)$	$x \in [0,1]$	$y_1 \in [0,1]$	$y_2 \in [0.1,2]$
$(y_1y_2 - 2)/\log x$	$x \in [10,100]$	$y_1 \in [0,1]$	$y_2 \in [1,2]$

Khajavirad and Sahinidis, 2013, 2014



- **Implemented in BARON**
  - **First deterministic global optimization solver for NLP and MINLP**

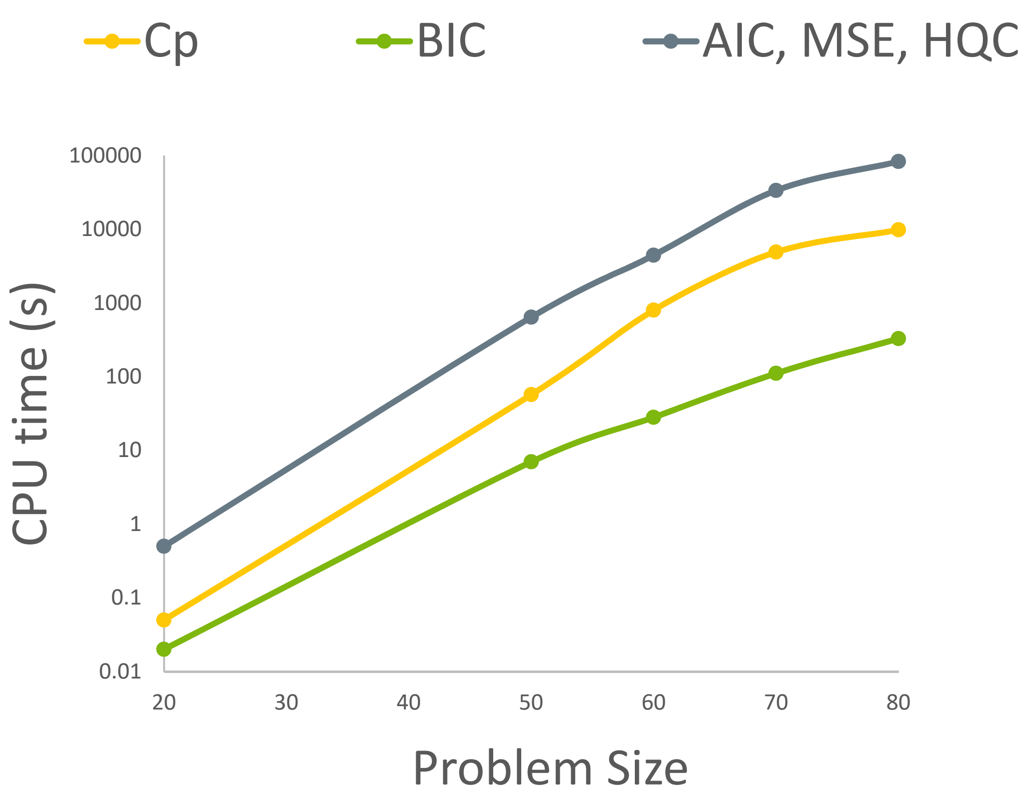
GLOBAL MINLP SOLVERS ON MINLPLIB2



Con: 1893 (1—164,321), Var: 1027 (3—107,223), Disc: 137 (1—31,824)

CPU TIME COMPARISON OF METRICS

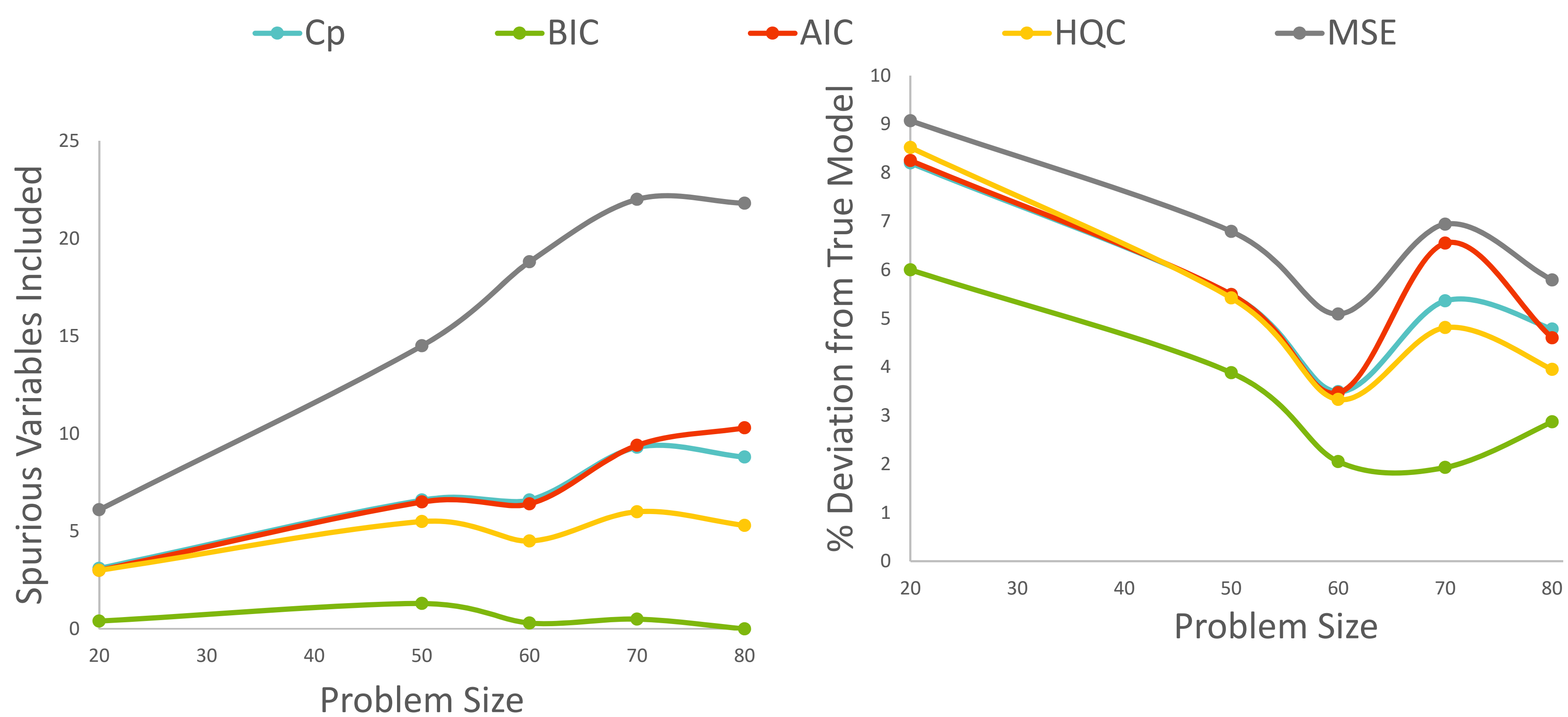
- Eight benchmarks from the UC-Irvine data set
- Seventy noisy data sets were generated with multicolinearity and increasing problem size (number of bases)



BIC solves more than two orders of magnitude faster than AIC, MSE and HQC

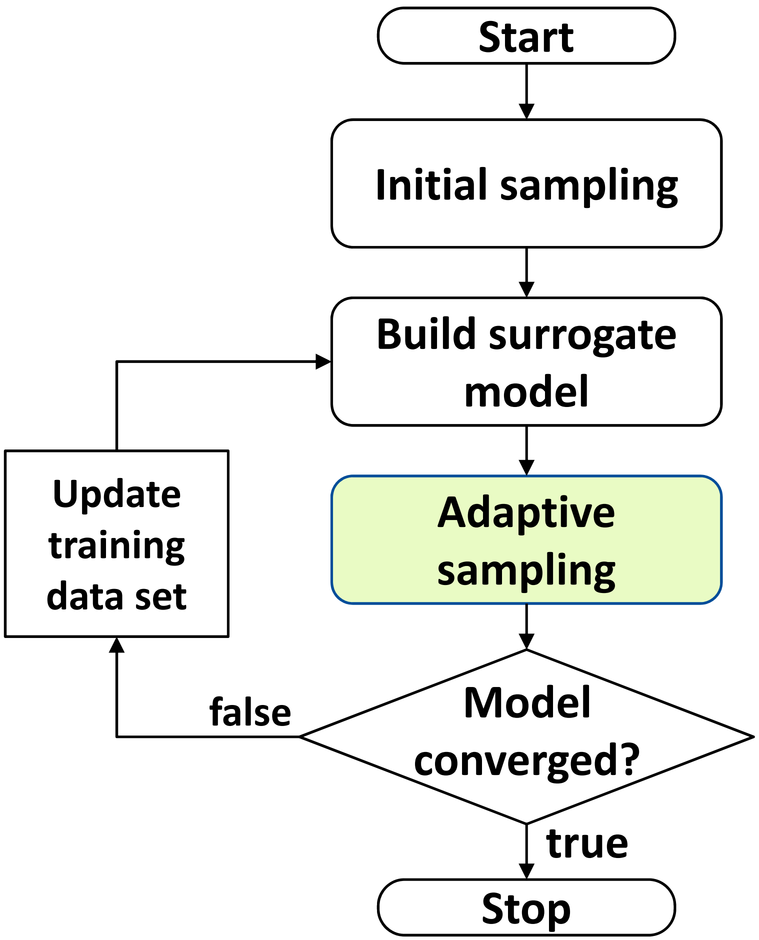
MODEL QUALITY COMPARISON

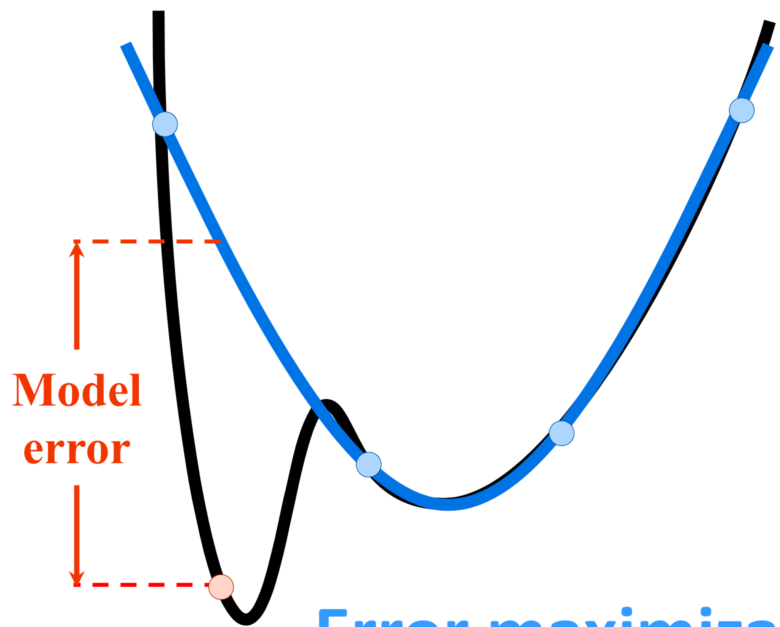
- **BIC leads to smaller, more accurate models**
  - Larger penalty for model complexity



ALAMO

Automated Learning of Algebraic MOdels





Error maximization sampling

ERROR MAXIMIZATION SAMPLING

- **Search the problem space for areas of model inconsistency or model mismatch**

- **Find points that maximize the model error with respect to the independent variables**

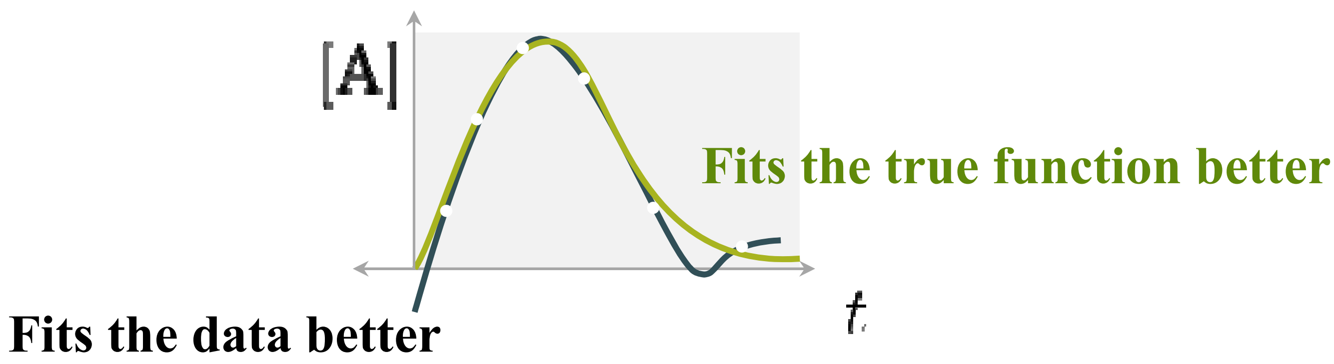
Surrogate model

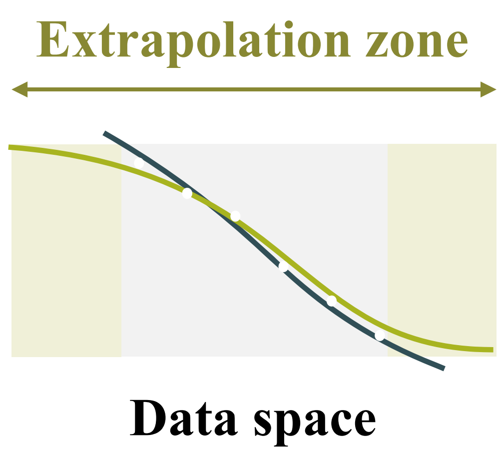
$$\max_{x} \left(z(x) - \hat{z}(x)\right)^2$$

  - Optimized using derivative-free solver SNOBFIT (Huyer and Neumaier, 2008)
  - SNOBFIT outperforms most derivative-free solvers (Rios and Sahinidis, 2013)

CONSTRAINED REGRESSION

$$0 < [A]_t < [A]^{max}$$





Safe extrapolation

CONSTRAINED REGRESSION

Standard regression

$$\min_{\beta_1,\beta_2} \sum_{i=1}^{4} (z_i - \hat{z}(x_i;\beta_1,\beta_2))^2$$

Surrogate model

easy

tough

Constrained regression

$$\min_{\beta_1,\beta_2} \sum_{i=1}^{4} (z_i - \hat{z}(x_i;\beta_1,\beta_2))^2 \quad \text{s.t.} \quad \beta_1 \geq \beta_2$$

$$\min_{\beta_1,\beta_2} \sum_{i=1}^{4} (z_i - \hat{z}(x_i;\beta_1,\beta_2))^2 \quad \text{s.t.} \quad \hat{z}(x_i;\beta_1,\beta_2) \geq 0 \quad \boxed{\forall x}$$

- **Challenging due to the semi-infinite nature of the regression constraints**
- **Use intuitive restrictions among predictor and response variables to infer nonintuitive relationships between regression parameters**

IMPLIED PARAMETER RESTRICTIONS

Find a model $\hat{z}$ such that $\hat{z}(x) \geq 0$ with a fixed model form:

$$\hat{z}(x) = \beta_1 x + \beta_2 x^3$$

Step 1: Formulate constraint in z- and x-space

$$\min_{\beta_1,\beta_2} \sum_{i=1}^{4} \left(z_i - [\beta_1 x + \beta_2 x^3]\right)^2$$

$$\text{s.t.} \quad \beta_1 x + \beta_2 x^3 \geq 0 \quad x \in [0,1]$$

1 parametric constraint

4 β-constraints

Step 2: Identify a sufficient set of β-space constraints

$$\min_{\beta_1,\beta_2} \sum_{i=1}^{4} \left(z_i - [\beta_1 x + \beta_2 x^3]\right)^2$$

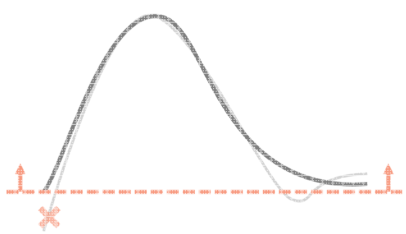
$$\text{s.t.} \quad \begin{cases} 0.240\,\beta_1 + 0.0138\,\beta_2 \geq 0 \\ 0.281\,\beta_1 + 0.0223\,\beta_2 \geq 0 \\ 0.120\,\beta_1 + 0.00173\,\beta_2 \geq 0 \\ 0.138\,\beta_1 + 0.00263\,\beta_2 \geq 0 \end{cases}$$

Global optimization problems solved with BARON

TYPES OF RESTRICTIONS

Response bounds

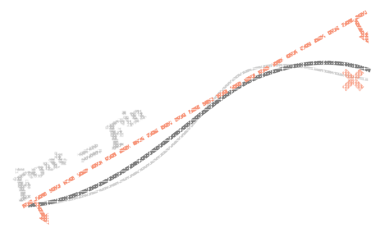
$$[\hat{A}]_t \geq 0$$



pressure, temperature, compositions

Individual responses

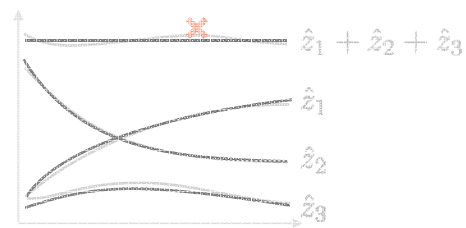
$$\hat{F}^{\mathrm{out}}(x) \leq F^{\mathrm{in}}$$



mass and energy balances, physical limitations

Multiple responses

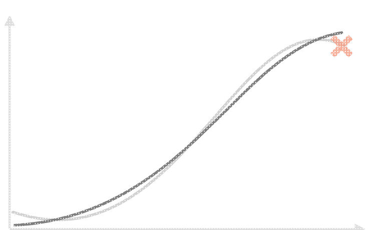
$$\hat{z}_1 + \hat{z}_2 + \hat{z}_3 = 1$$



mass balances, sum-to-one, state variables

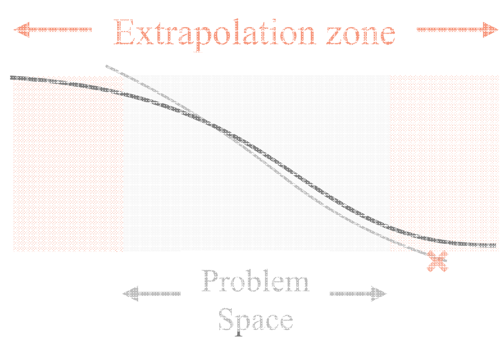
Response derivatives

$$\frac{dT}{dx} \geq 0$$



monotonicity, numerical properties, convexity

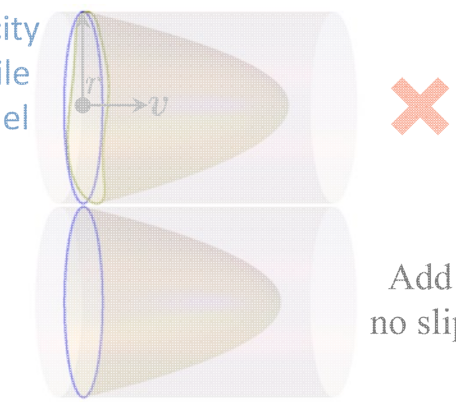
Alternative domains



safe extrapolation, boundary conditions

Boundary conditions

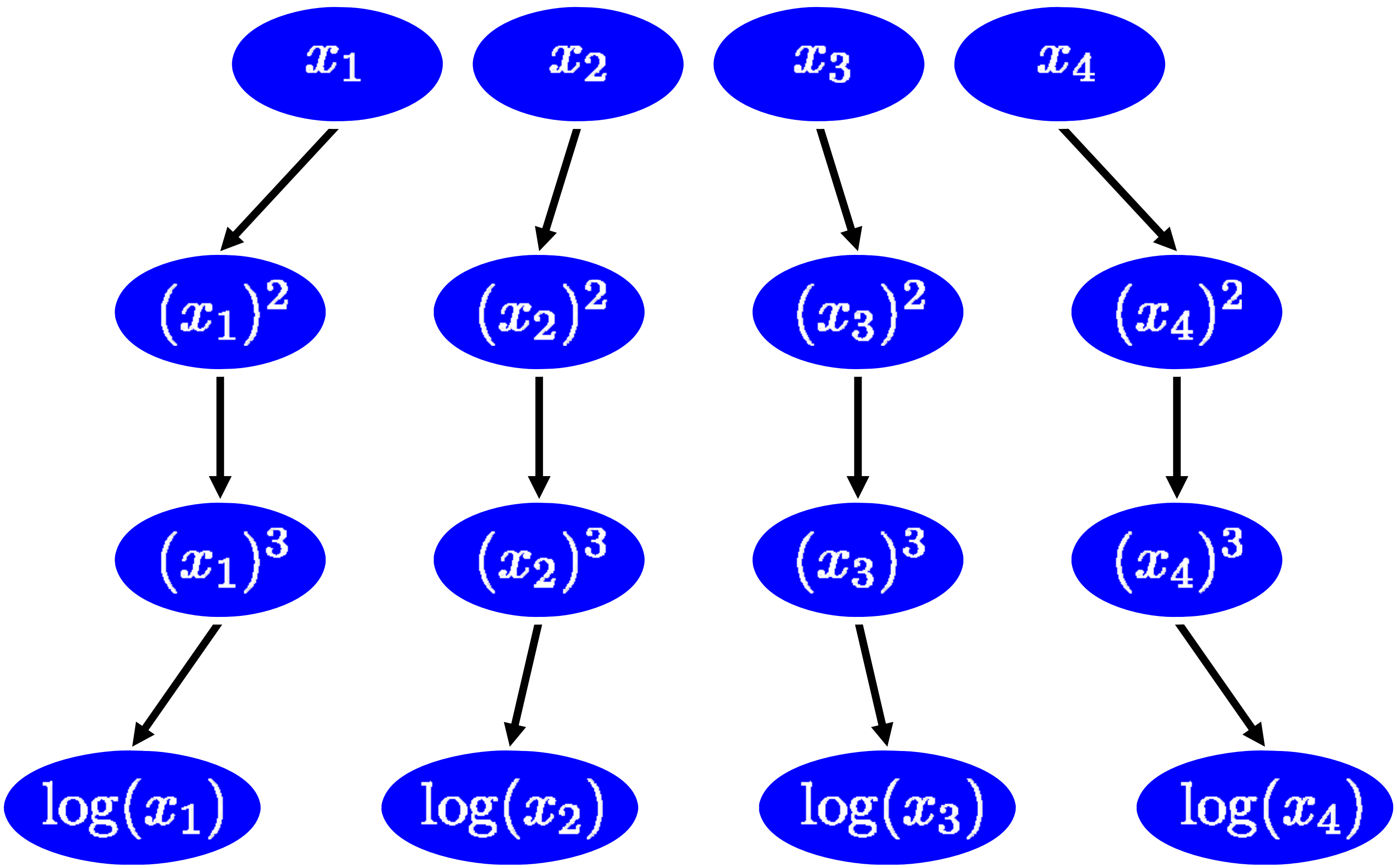
velocity profile model



Add no slip

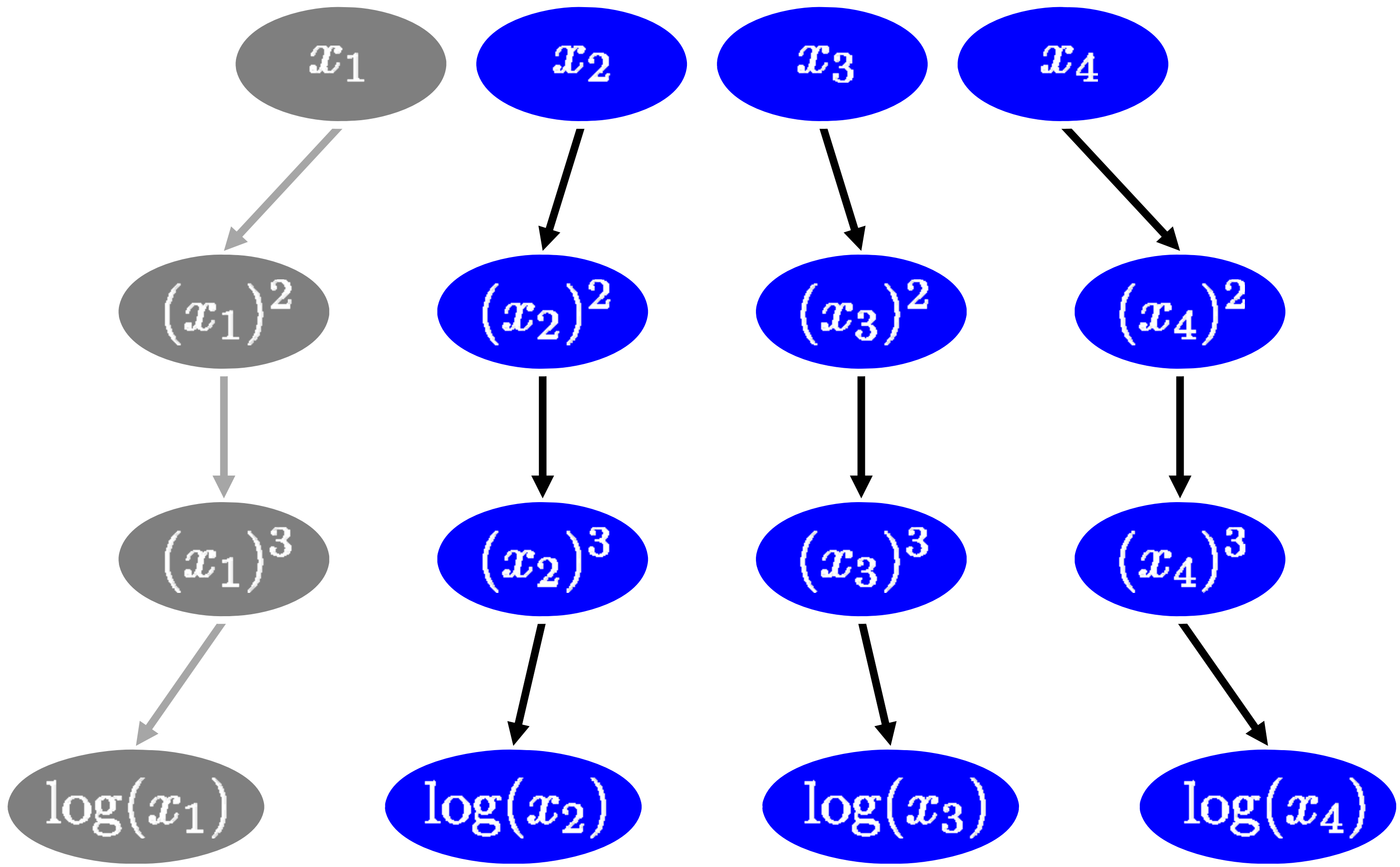
$$\hat{v}(R, \theta) = 0 \qquad \forall \theta$$

CATEGORICAL CONSTRAINTS

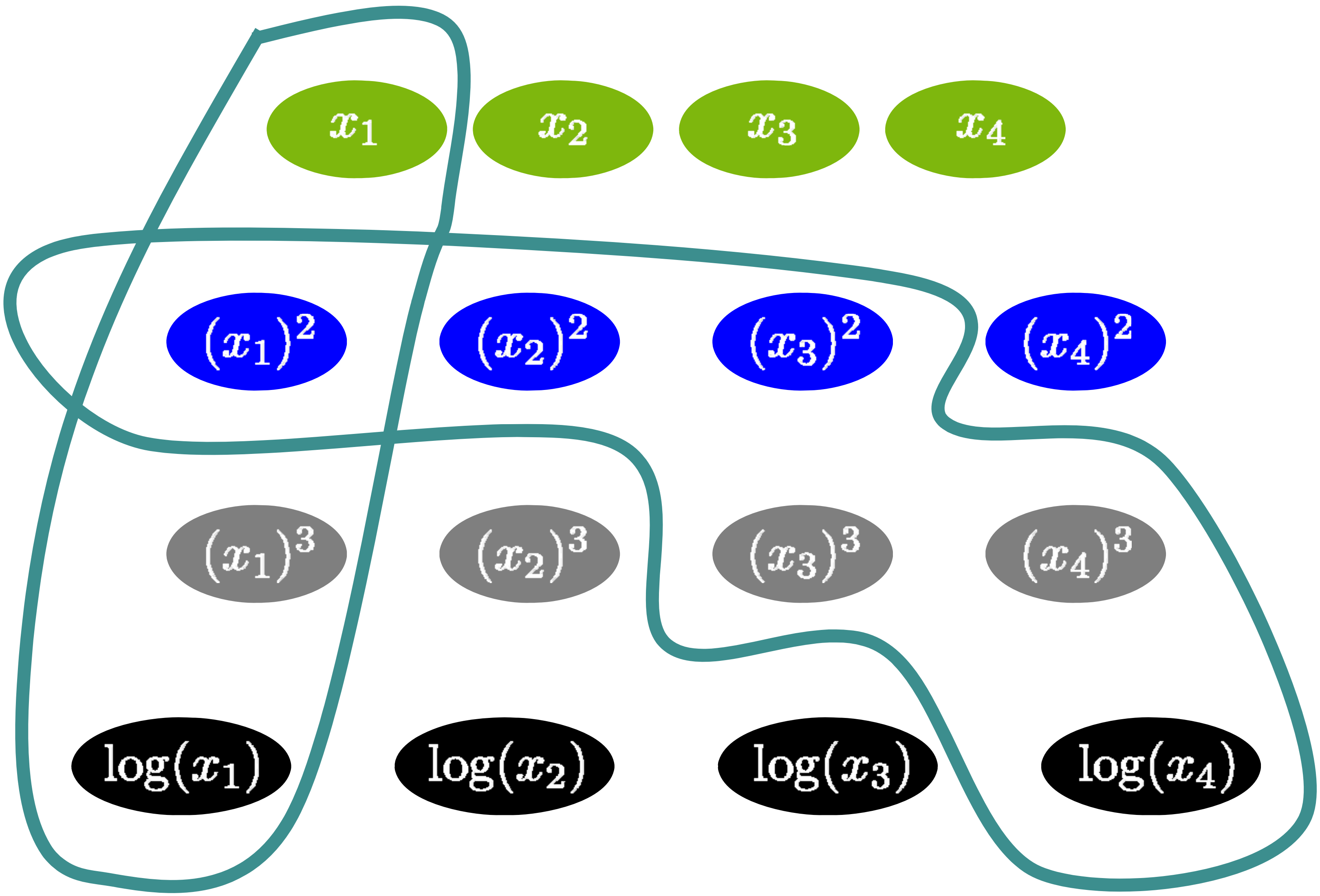


CATEGORICAL CONSTRAINTS

x_1 is shown not to be a significant predictor



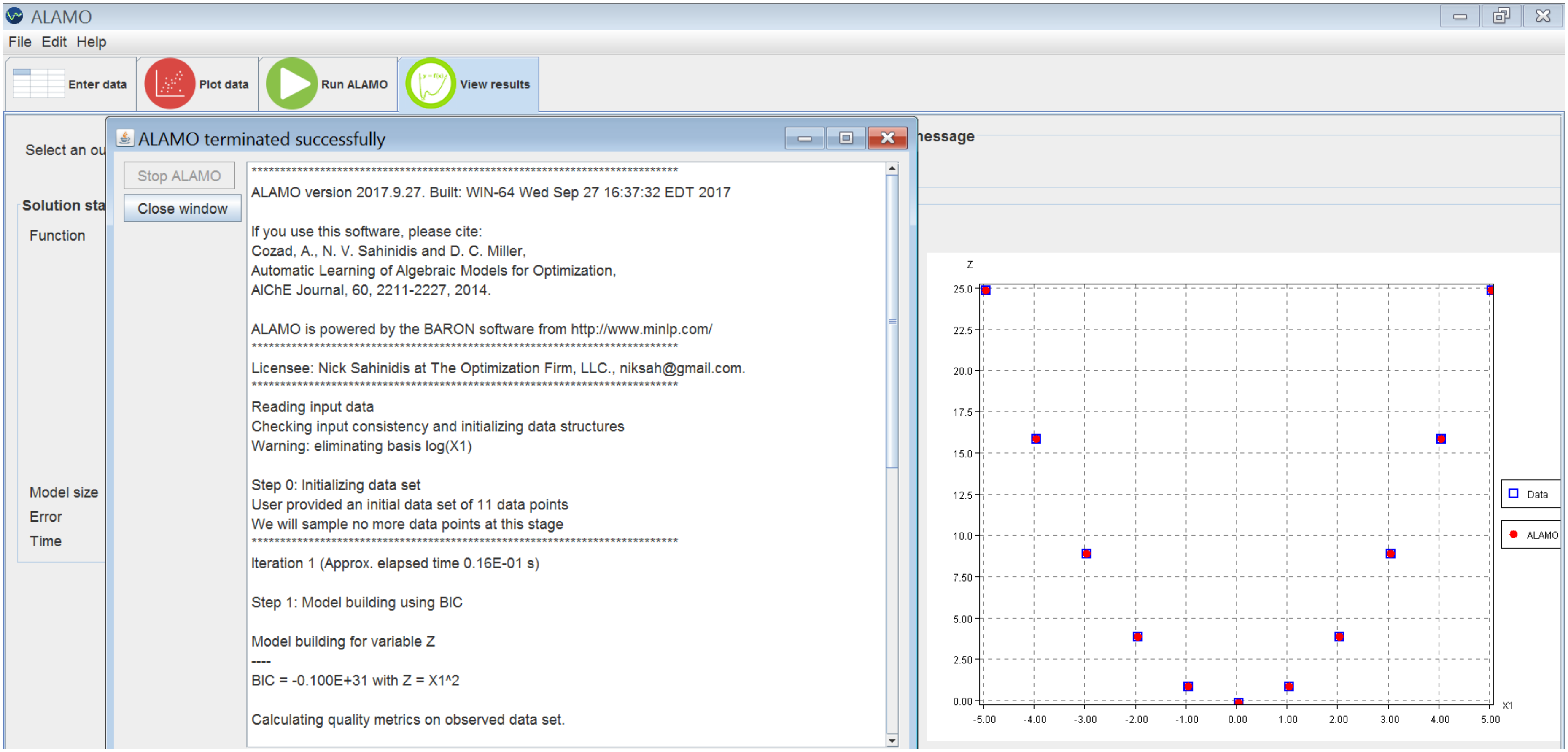
GENERAL GROUP CONSTRAINTS



No more than – At least – Requires – Excludes

SOFTWARE AVAILABILITY

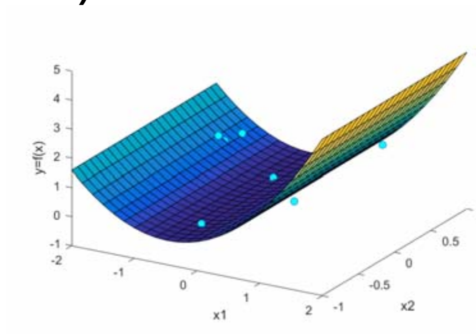
- From The Optimization Firm at http://minlp.com
- Windows, Linux, and OSX versions
- Free licenses for academics, DOE, and CAPD companies



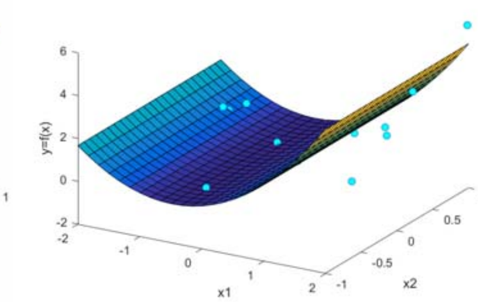
LEARNING THE SIX-HUMP CAMEL FUNCTION

$$f(x_1, x_2) = \left(4 - 2.1x_1^2 + \frac{x_1^4}{3}\right)x_1^2 + x_1x_2 + x_2^2(4x_2^2 - 4) + \epsilon$$

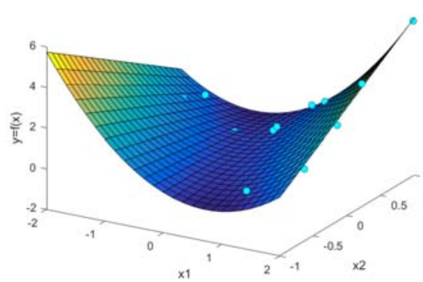
Iteration	N	R^2_{val}	$\|\beta\|_0$
1	10	< 0	2
2	16	< 0	2
3	19	< 0	2
4	27	0.98	7



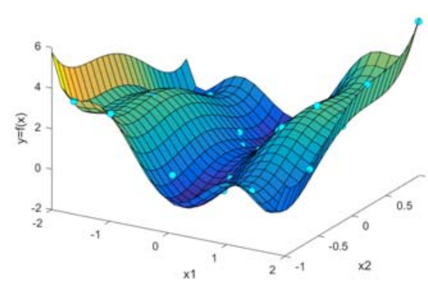
First iteration



Second iteration



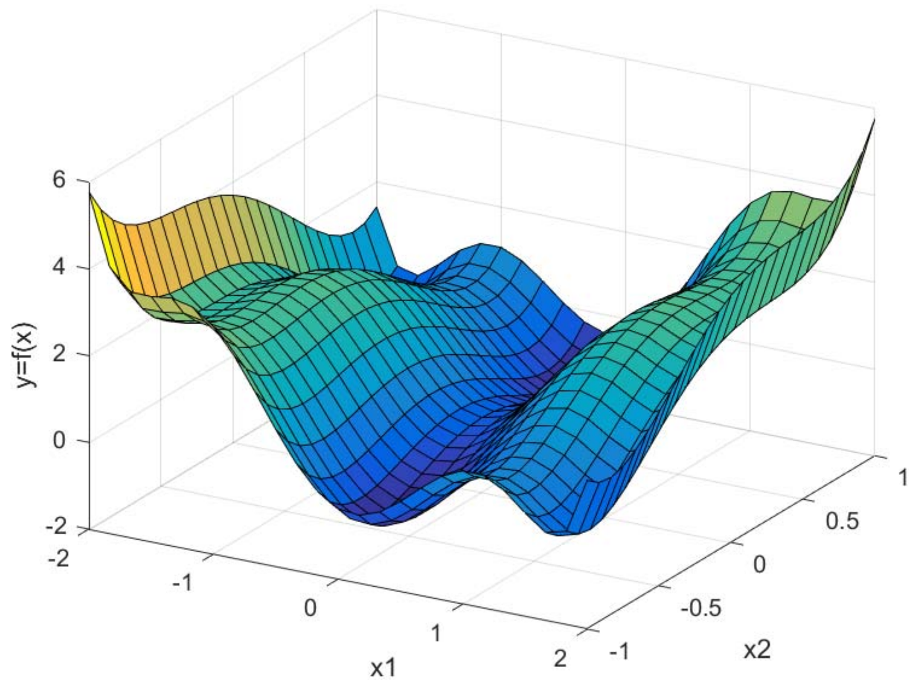
Third iteration



Final iteration

$$f = 4.56x_1^2 - 3.16x_2^2 - 2.41x_1^4 + 3.07x_2^4 + 0.38x_1^6 + 1.09x_1x_2 - 0.28$$

OPTIMIZATION WITH THE SURROGATE



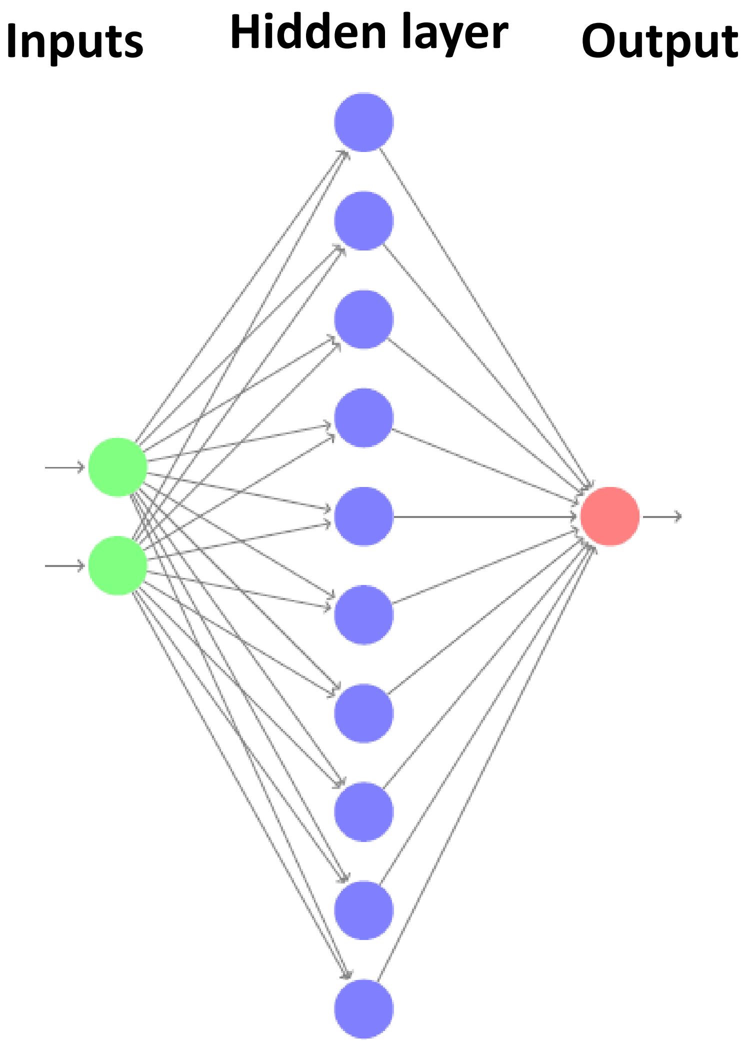
True minimum

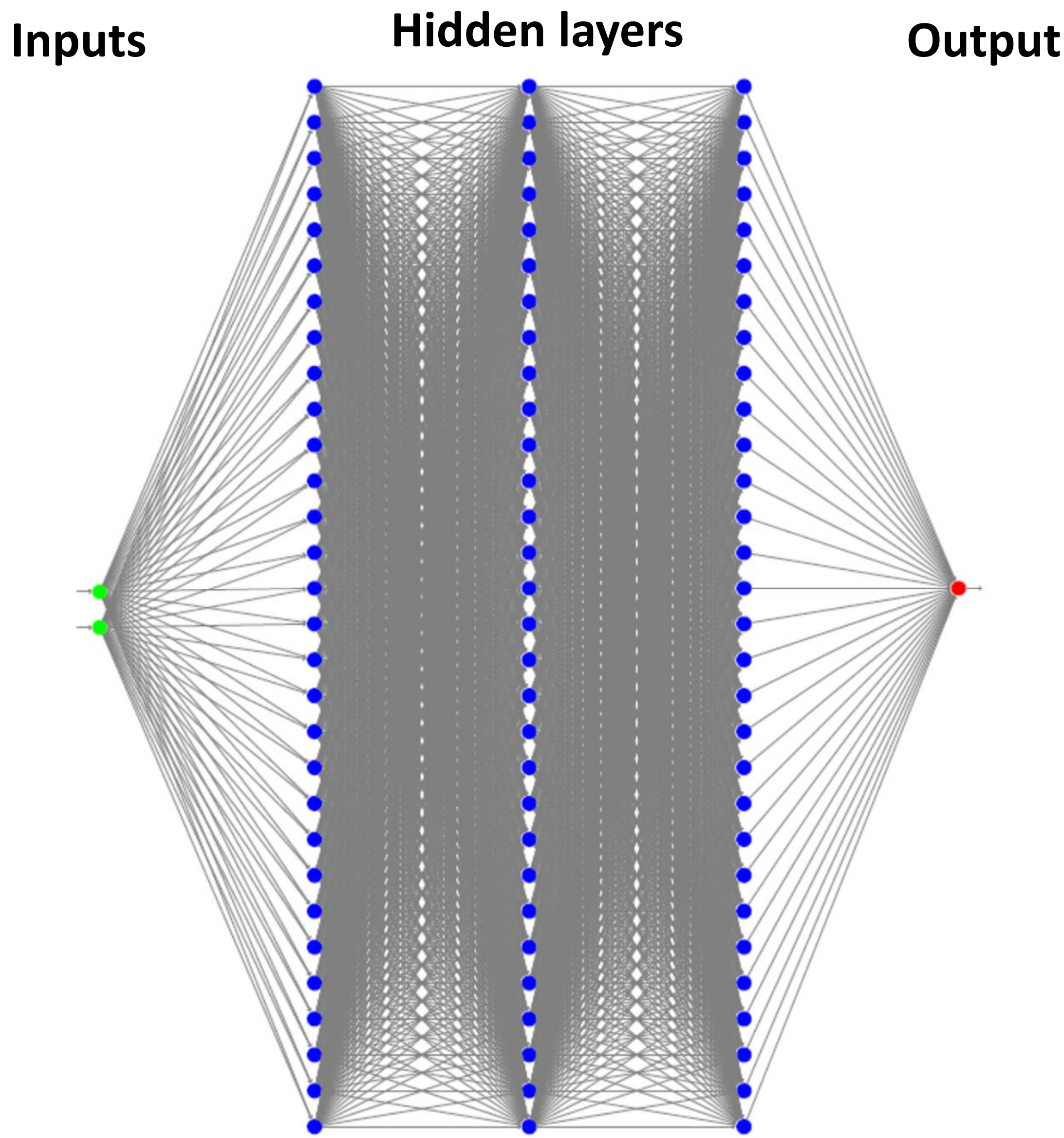
$$\boldsymbol{f(0.0898, -0.7127) = -1.0316}$$

ALAMO surrogate minimum

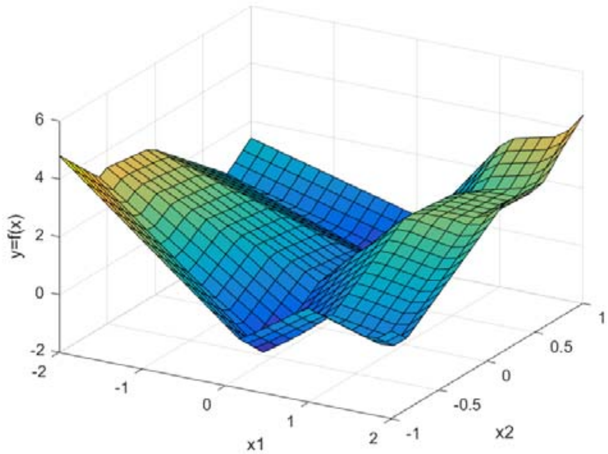
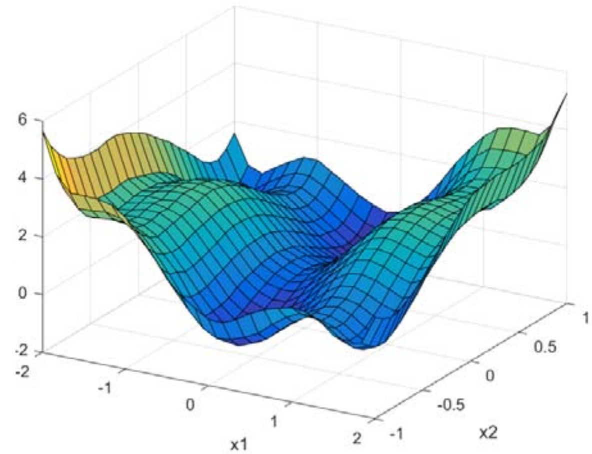
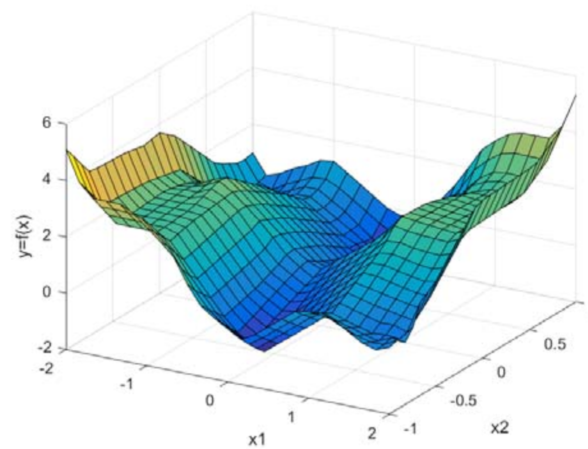
$$\boldsymbol{f(0.0871, -0.7251) = -1.1248}$$

NEURAL NETWORK SURROGATES





RELU NEURAL NETWORK SURROGATES

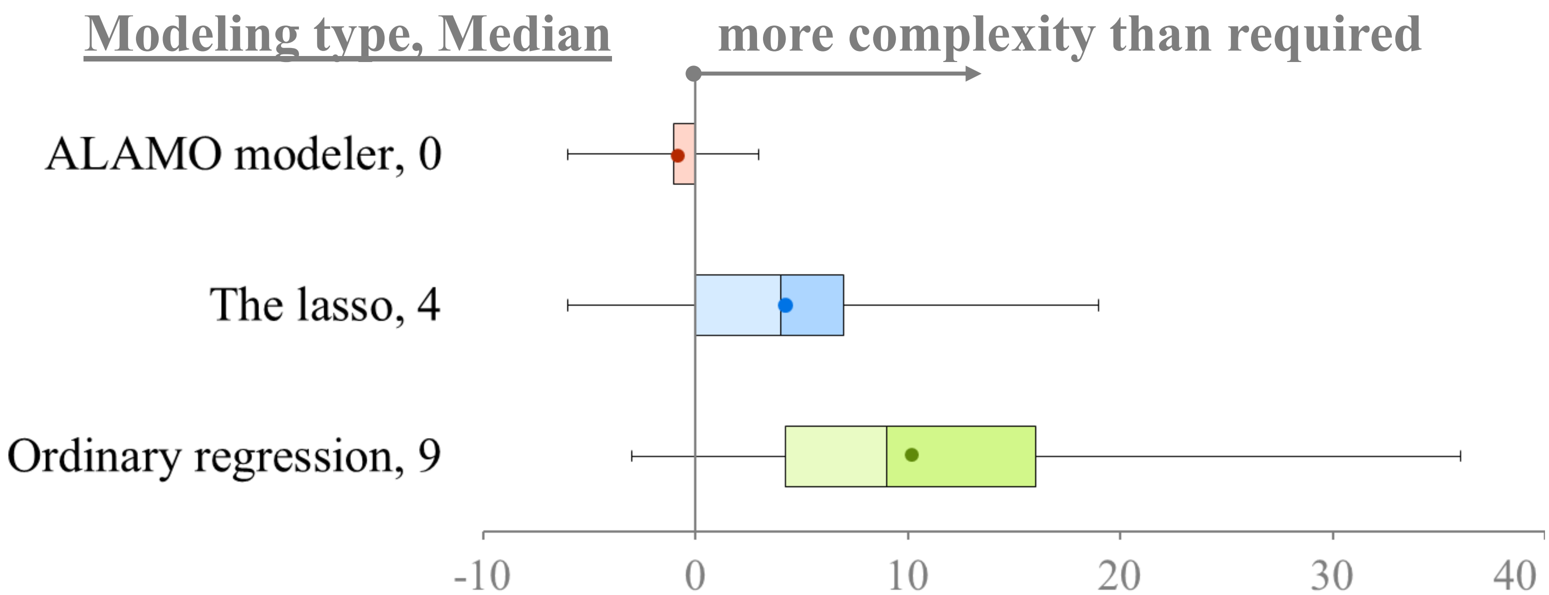
1 hidden layer 10 nodes	1 hidden layer 200 nodes	3 hidden layer 30 nodes
		

	1 hidden layer 10 nodes	1 hidden layer 200 nodes	3 hidden layer 30 nodes
f	-0.919	-1.22	-1.194
x_1	0.064	-0.134	-0.016
x_2	-0.596	0.683	0.639

True minima

$$f(0.0898, -0.7126) = -1.0316$$
$$f(-0.0898, 0.7126) = -1.0316$$

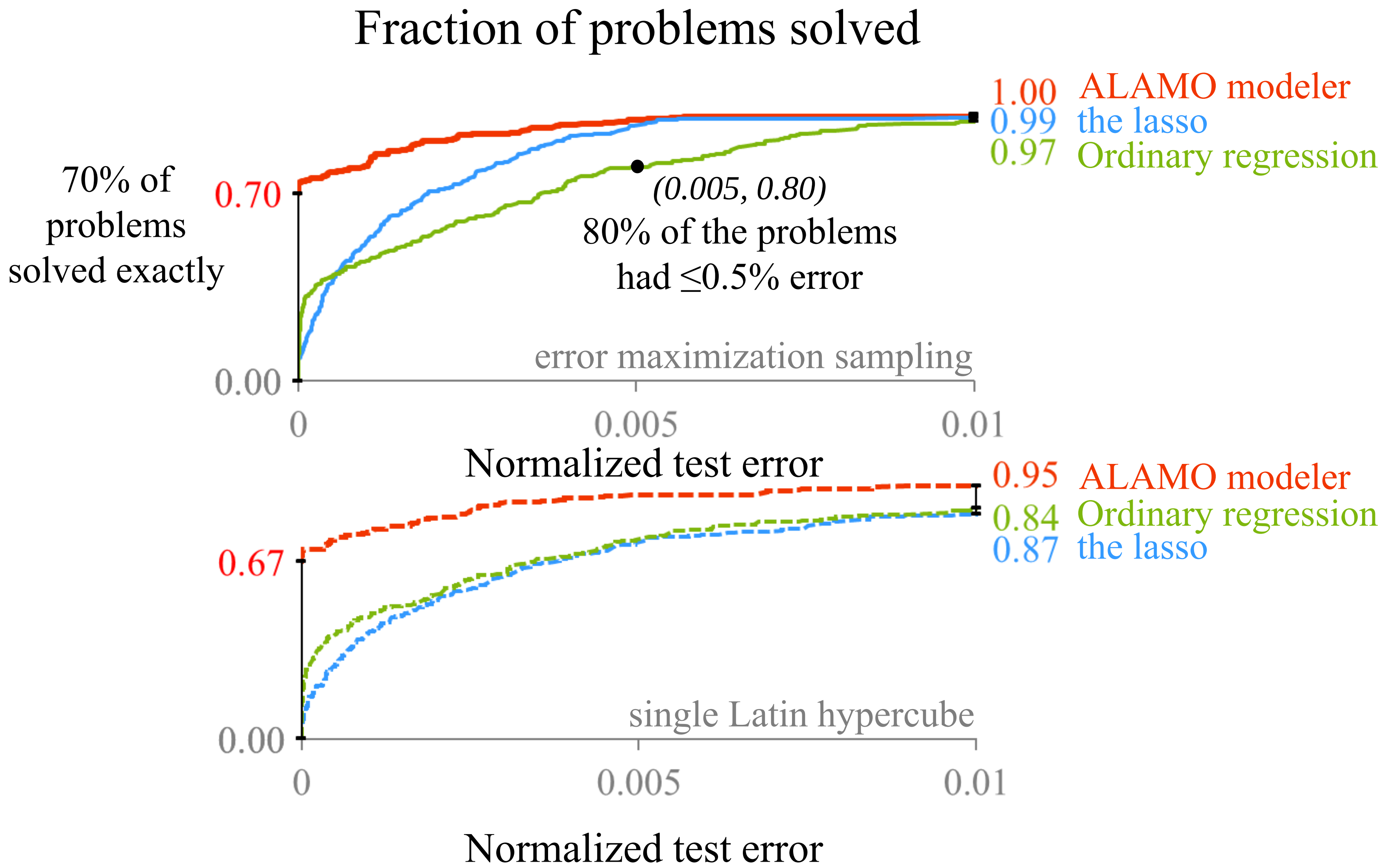
SIMPLE AND ACCURATE MODELS



Number of terms in the surrogate model – **Number of terms in the true function**

Results over a test set of 45 known functions treated as black boxes with bases that are available to all modeling methods.

SAMPLING EFFICIENCY

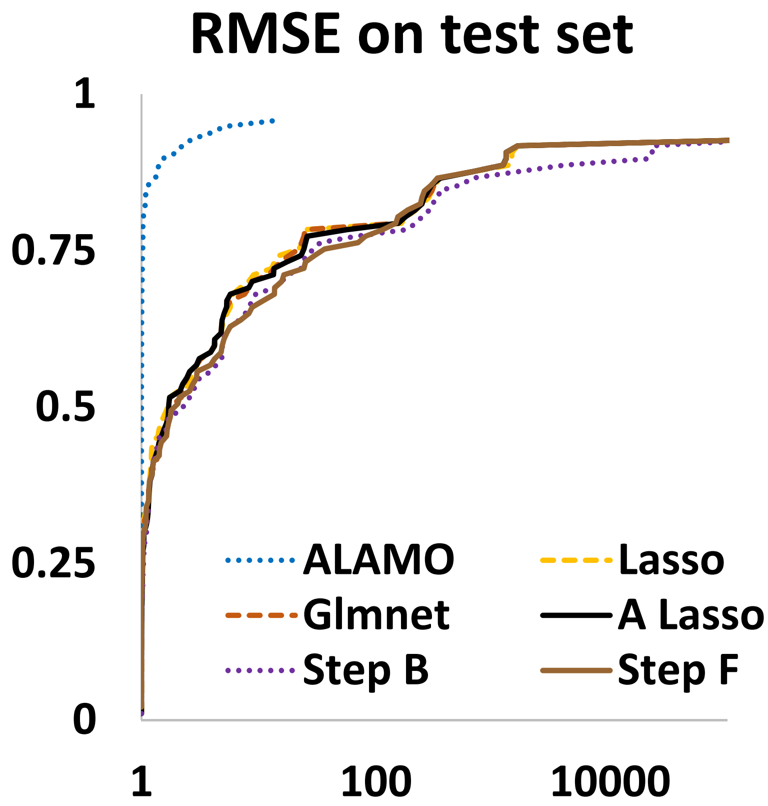


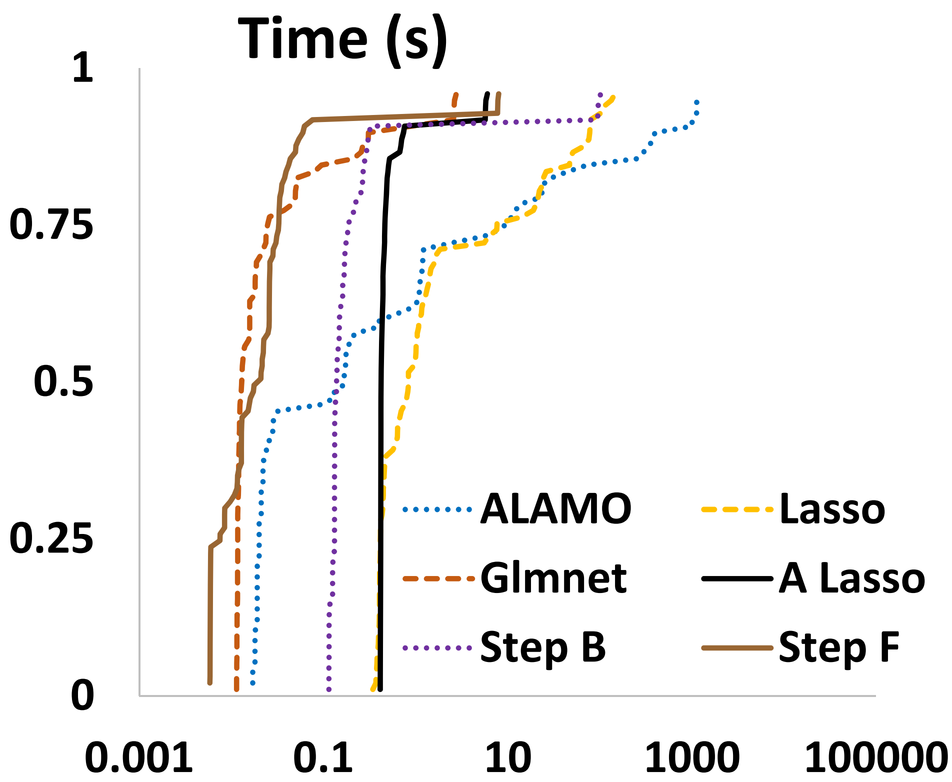
Results with 45 known functions with bases that are available to all modeling methods

COMPARISONS ON BENCHMARKS

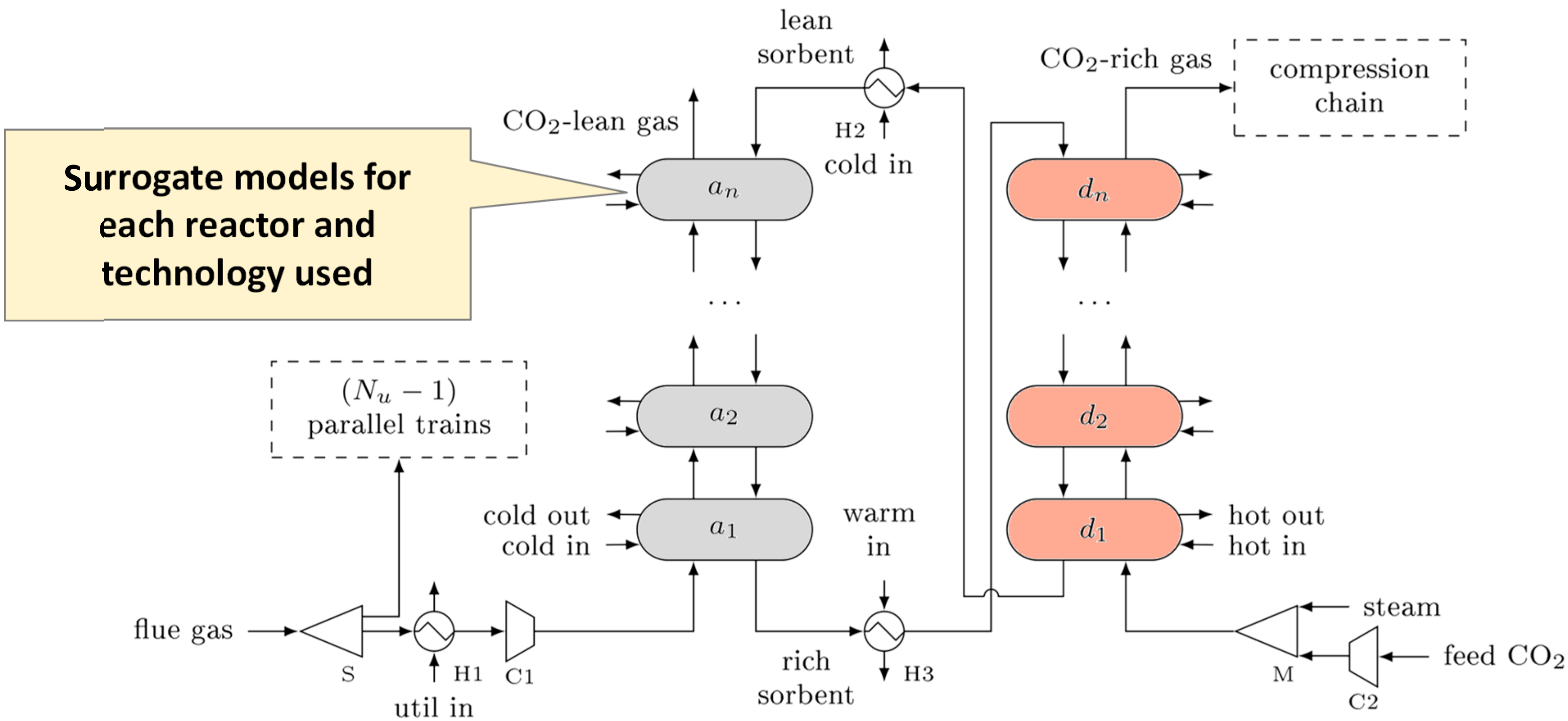
- **98 problems**
  - 30 from the UC-Irvine ML repository
  - 37 from the NIST standard regression database
  - 31 from the virtual library of simulated experiments
- **Number of inputs: 1—105 (average 11)**
- **Number of features: 6—735 (average 90)**
- **Number of measurements: 6—32561 (average 2144)**
- **Algorithms compared**
  - Lasso (Matlab)
  - Glmnet (lasso in R)
  - A lasso (adaptive lasso option in Glmnet)
  - Step F/B (Matlab)
  - ALAMO with BIC solved to optimality

TIME AND QUALITY COMPARISONS





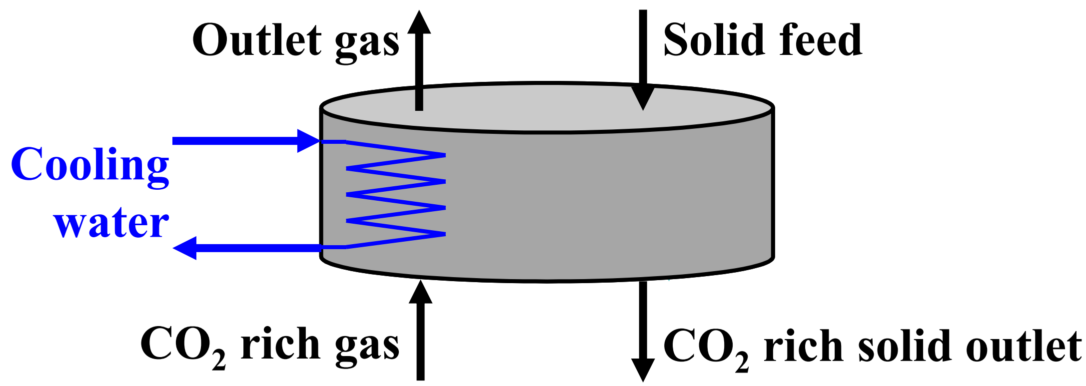
CARBON CAPTURE SYSTEM DESIGN



- **Discrete decisions:** How many units? Parallel trains?
  What technology used for each reactor?
- **Continuous decisions:** Unit geometries
- **Operating conditions:** Vessel temperature and pressure, flow rates, compositions

BUBBLING FLUIDIZED BED

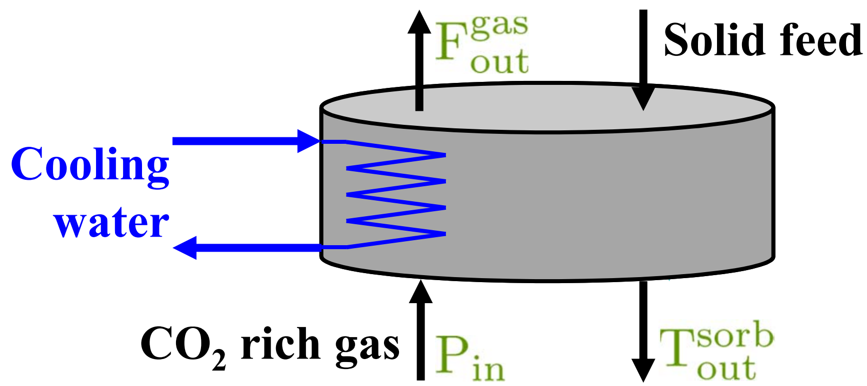
Bubbling fluidized bed adsorber diagram



- **Model inputs (16 total)**
  - Geometry (3)
  - Operating conditions (5)
  - Gas mole fractions (2)
  - Solid compositions (2)
  - Flow rates (4)
- **Model outputs (14 total)**
  - Geometry required (2)
  - Operating condition required (1)
  - Gas mole fractions (3)
  - Solid compositions (3)
  - Flow rates (2)
  - Outlet temperatures (3)

Model created by Andrew Lee at the National Energy Technology Laboratory

EXAMPLE MODELS - ADSORBER

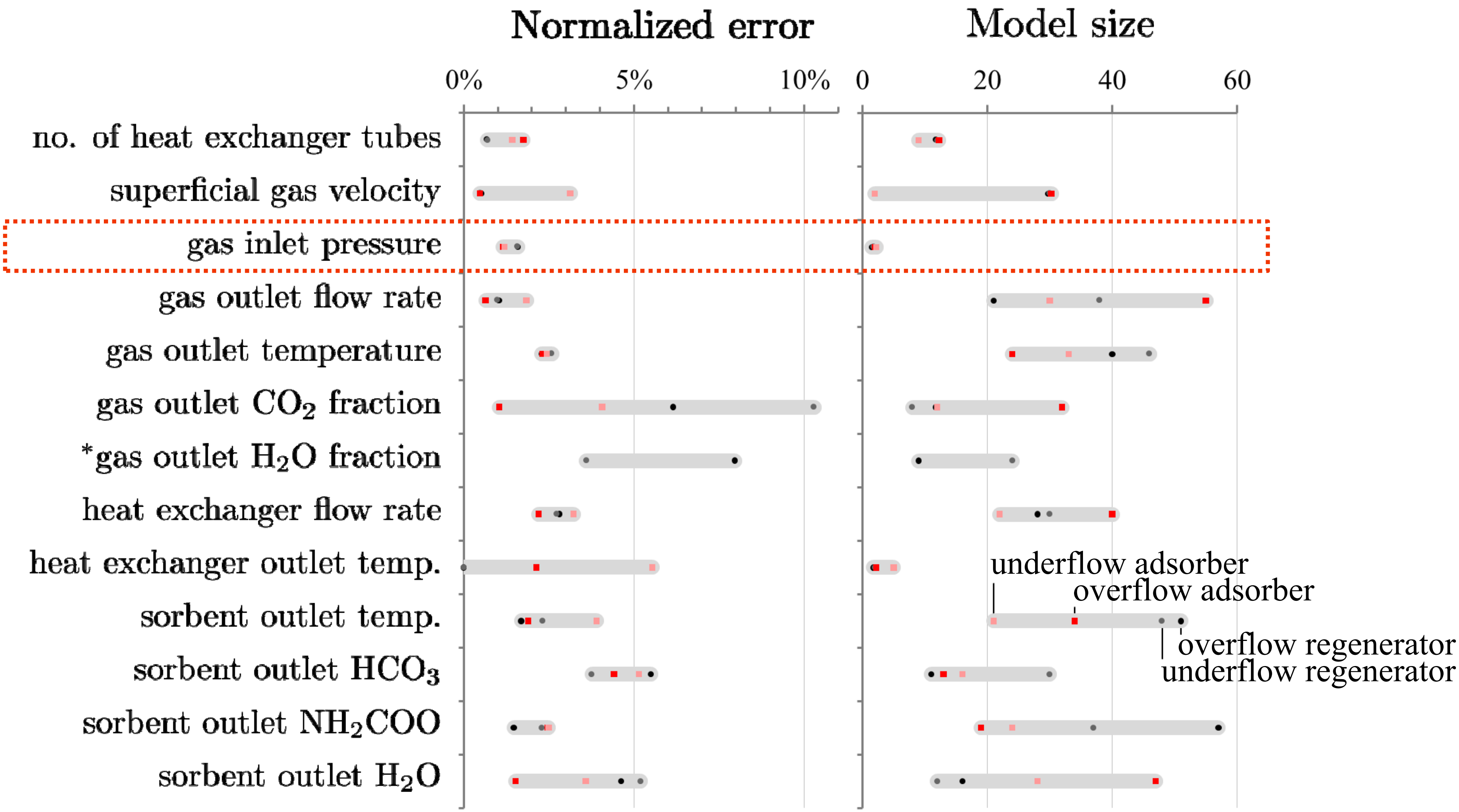


$$\mathrm{P}_{\mathrm{in}} = 1.0\,\mathrm{P}_{\mathrm{out}} + 0.0231\,L_b - 0.0187\,\ln(0.167\,L_b) - 0.00626\,\ln(0.667\,\mathrm{v}_{\mathrm{gi}}) - \frac{51.1\,\mathrm{xHCO3}^{\mathrm{ads}}_{\mathrm{in}}}{\mathrm{F}^{\mathrm{gas}}_{\mathrm{in}}}$$

$$T^{\mathrm{sorb}}_{\mathrm{out}} = 1.0\,\mathrm{T}^{\mathrm{gas}}_{\mathrm{in}} - \frac{\left(1.77\cdot 10^{-10}\right)\,\mathrm{NX}^2}{\gamma^2} - \frac{3.46}{\mathrm{NX}\,\mathrm{T}^{\mathrm{gas}}_{\mathrm{in}}\,\mathrm{T}^{\mathrm{sorb}}_{\mathrm{in}}} + \frac{1.17\cdot 10^4}{\mathrm{F}^{\mathrm{sorb}}\,\mathrm{NX}\,\mathrm{xH2O}^{\mathrm{ads}}_{\mathrm{in}}}$$

$$F^{\mathrm{gas}}_{\mathrm{out}} = 0.797\,\mathrm{F}^{\mathrm{gas}}_{\mathrm{in}} - \frac{9.75\,\mathrm{T}^{\mathrm{sorb}}_{\mathrm{in}}}{\gamma} - 0.77\,\mathrm{F}^{\mathrm{gas}}_{\mathrm{in}}\,\mathrm{xCO2}^{\mathrm{gas}}_{\mathrm{in}} + 0.00465\,\mathrm{F}^{\mathrm{gas}}_{\mathrm{in}}\,\mathrm{T}^{\mathrm{sorb}}_{\mathrm{in}} - 0.0181\,\mathrm{F}^{\mathrm{gas}}_{\mathrm{in}}\,\mathrm{T}^{\mathrm{sorb}}_{\mathrm{in}}\,\mathrm{xH2O}^{\mathrm{gas}}_{\mathrm{in}}$$

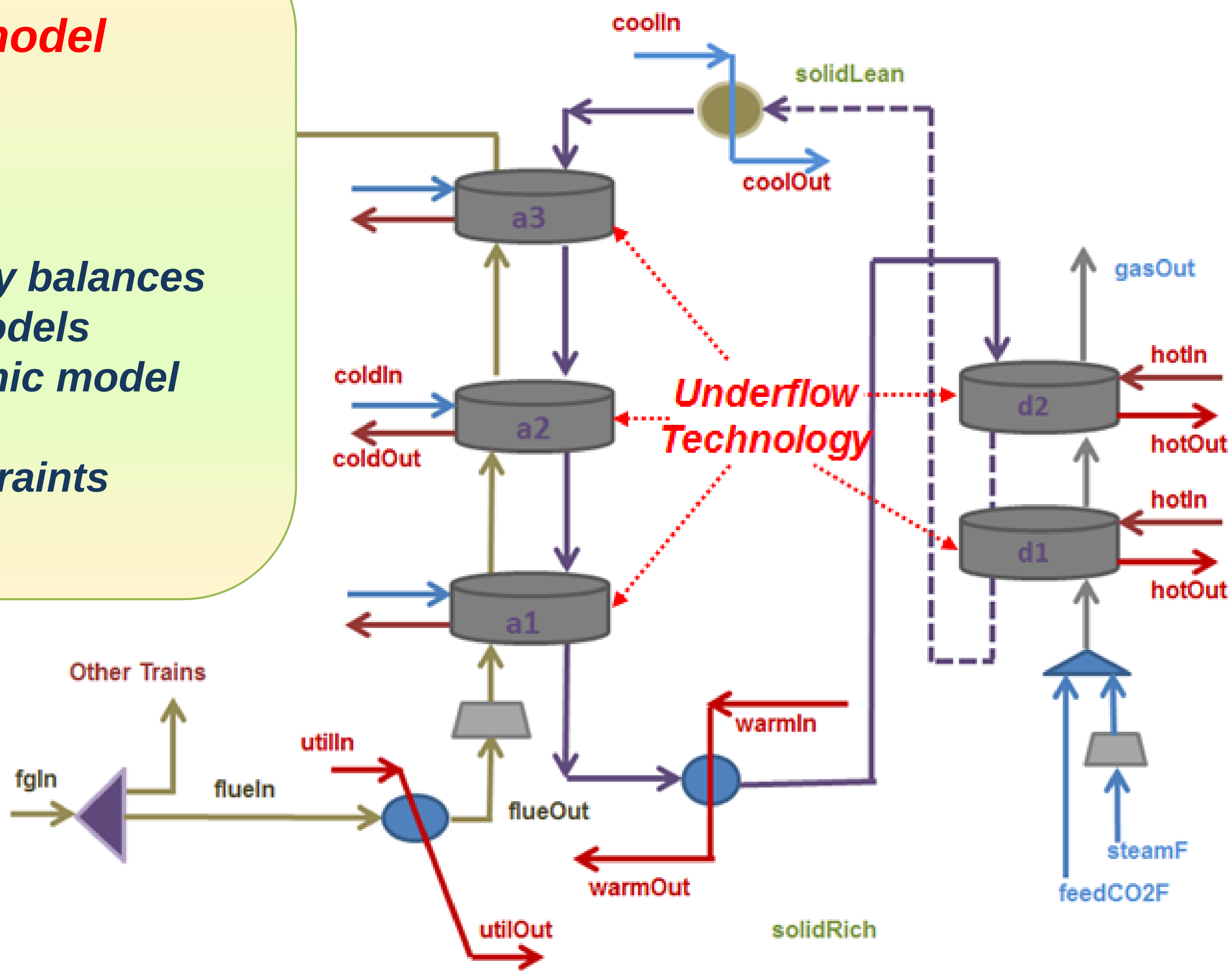
SURROGATE RESULTS



SUPERSTRUCTURE OPTIMIZATION

Mixed-integer nonlinear programming model

- *Economic model*
- *Process model*
- *Material balances*
- *Hydrodynamic/Energy balances*
- *Reactor surrogate models*
- *Link between economic model and process model*
- *Binary variable constraints*
- *Bounds for variables*

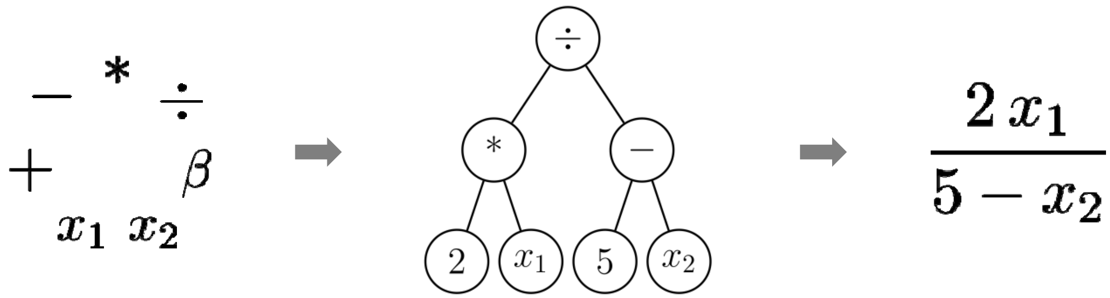


MINLP solved with BARON

SYMBOLIC REGRESSION

- **Symbolic regression**

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



- **Current practice: genetic programming**
- **Modeled as MINLP**
  - **Binary variables to select functional operators**
  - **Symmetry-breaking constraints**
- **Not currently implemented in ALAMO**

CONCLUSIONS

- **ALAMO provides algebraic models that are**
  - ✓ Accurate
  - ✓ Simple
  - ✓ Generated from a minimal number of data points
- **ALAMO's constrained regression facility allows modeling of**
  - ✓ Bounds on response variables
  - ✓ Variable groups
  - ✓ Forthcoming: constraints on gradient of response variables
- **Built on top of state-of-the-art optimization solvers**
- **Available from www.minlp.com**