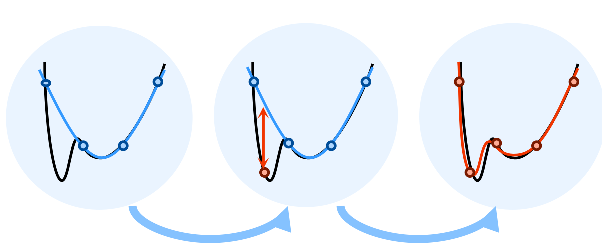
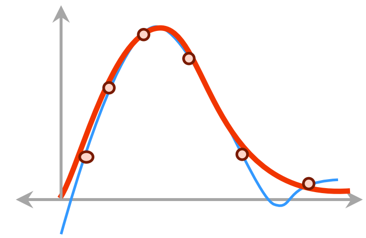




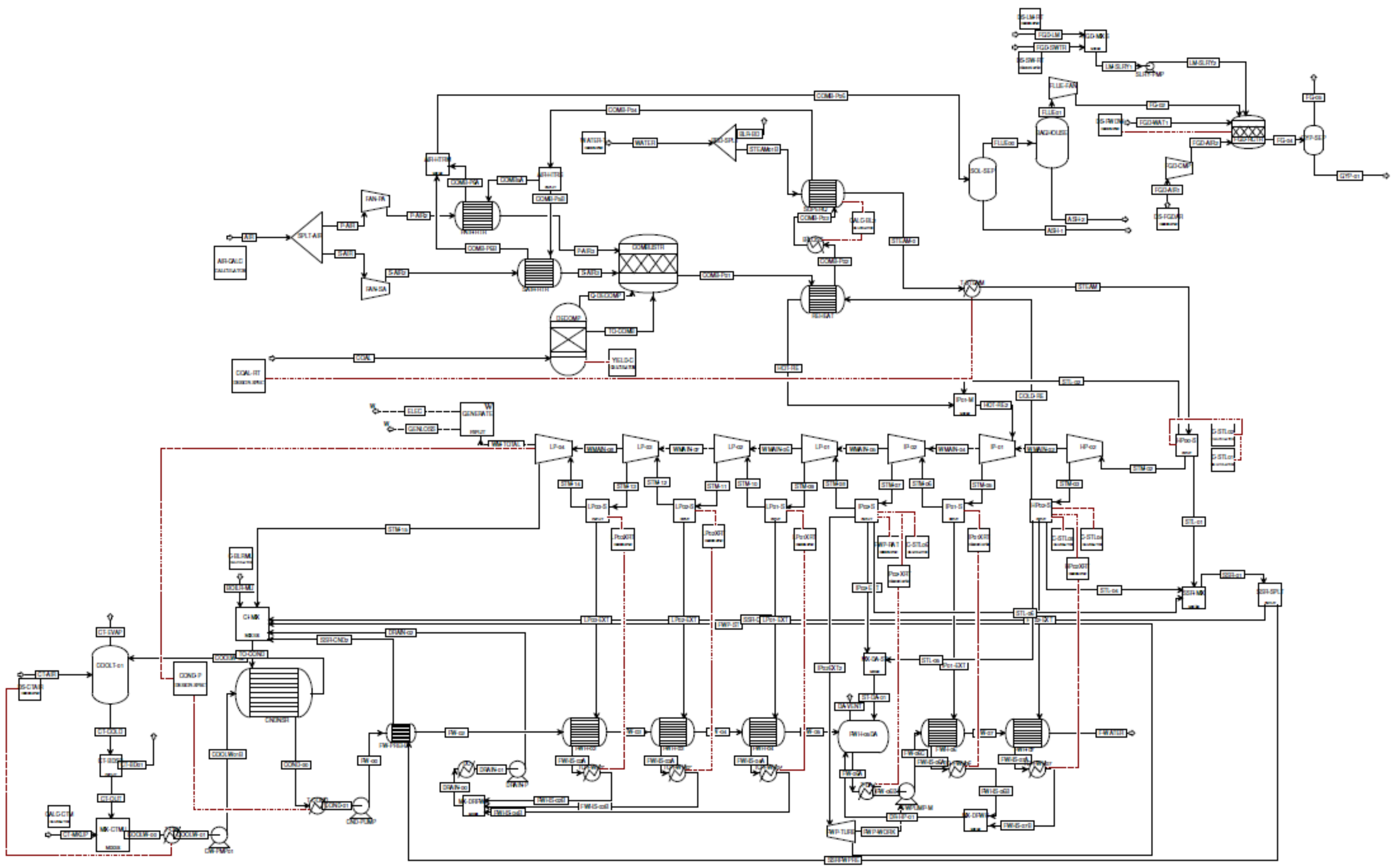
Extending the Scope of Algebraic MINLP Solvers to Black- and Grey-box Optimization

Nick Sahinidis

Acknowledgments:

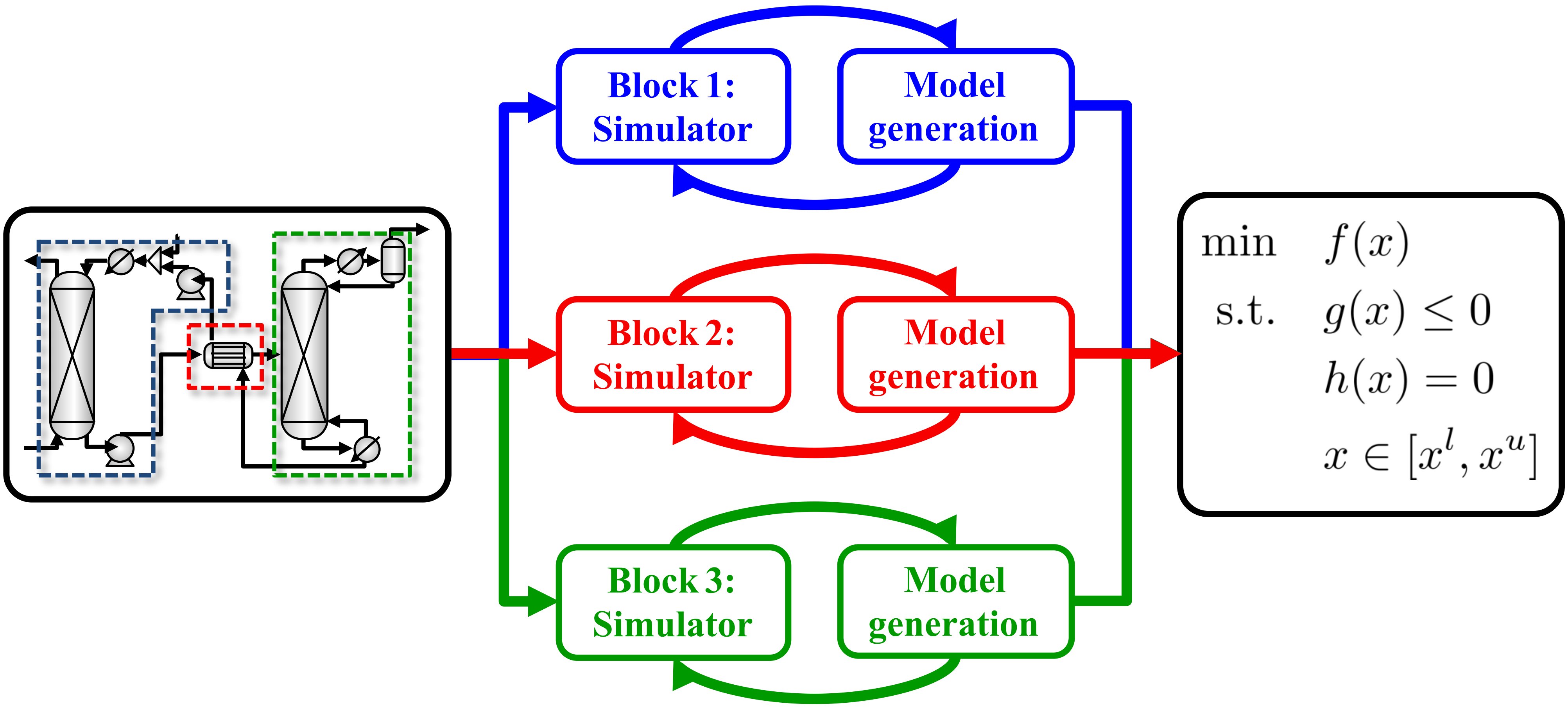
Alison Cozad, David Miller, Zach Wilson

SIMULATION OPTIMIZATION



Pulverized coal plant Aspen Plus® simulation provided by the National Energy Technology Laboratory

PROCESS DISAGGREGATION



Process Simulation

Disaggregate process into process **blocks**

Surrogate Models

Build **simple** and **accurate** models with a functional form tailored for an optimization framework

Optimization Model

Add algebraic constraints design specs, heat/mass balances, and logic constraints

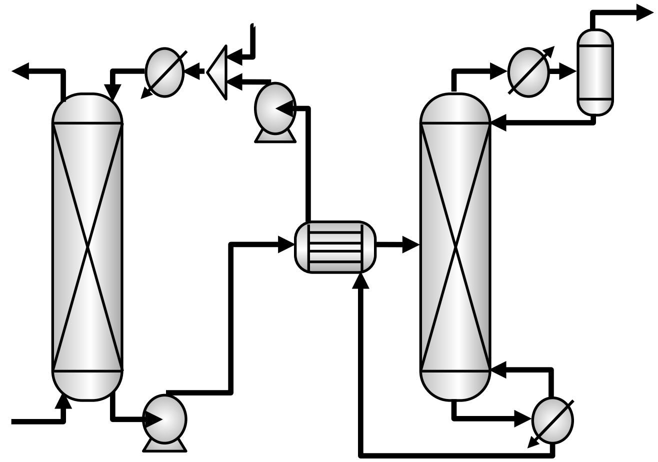
LEARNING PROBLEM

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

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

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

Process simulation or Experiment



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

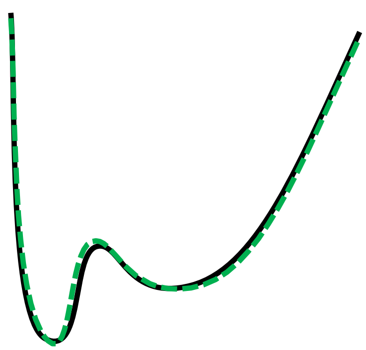
$$z \in \mathbb{R}^m$$
$$z = f(x)$$

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

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

HOW TO BUILD THE SURROGATES

- **We aim to build surrogate models that are**
  - Accurate
    - *We want to reflect the true nature of the simulation*
  - Simple
    - *Tailored for algebraic optimization*



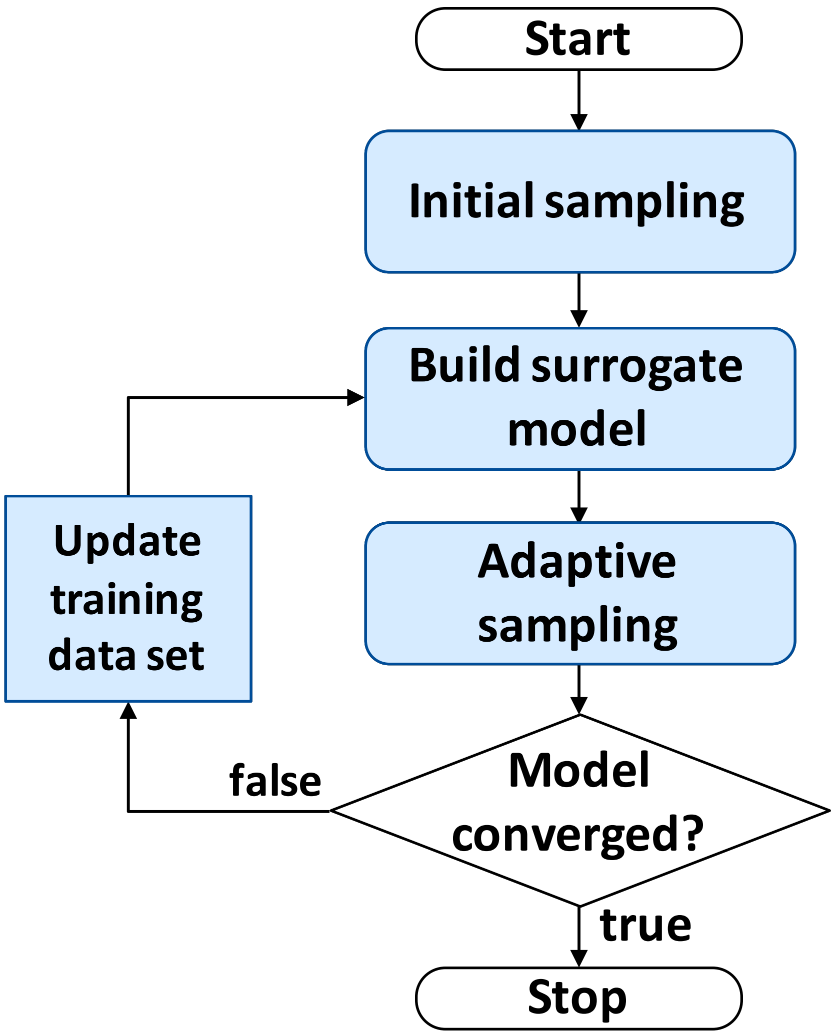
$$\hat{f}(x) = \sum_{i=1}^{n} \gamma_i \exp\left(\frac{\|x\|}{\sigma^2}\right) + \beta_0 + \beta_1\, x + \ldots$$

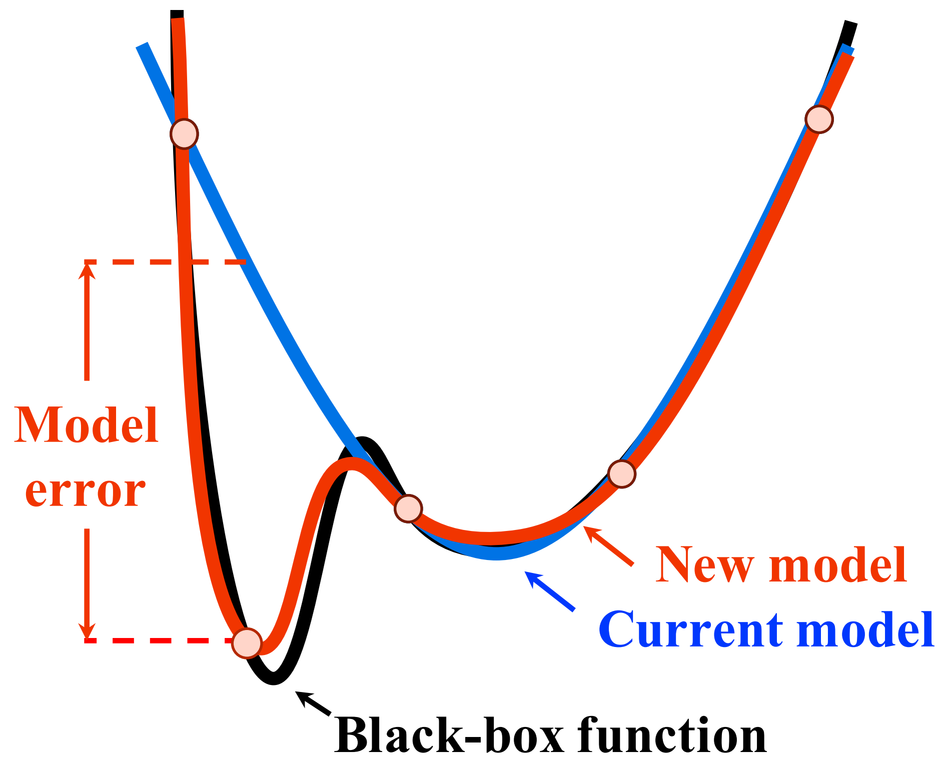
$$\hat{f}(x) = \beta_1\, x + \beta_2\, x^2 + \beta_3\, x^3 + \beta_4\, e^x$$

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

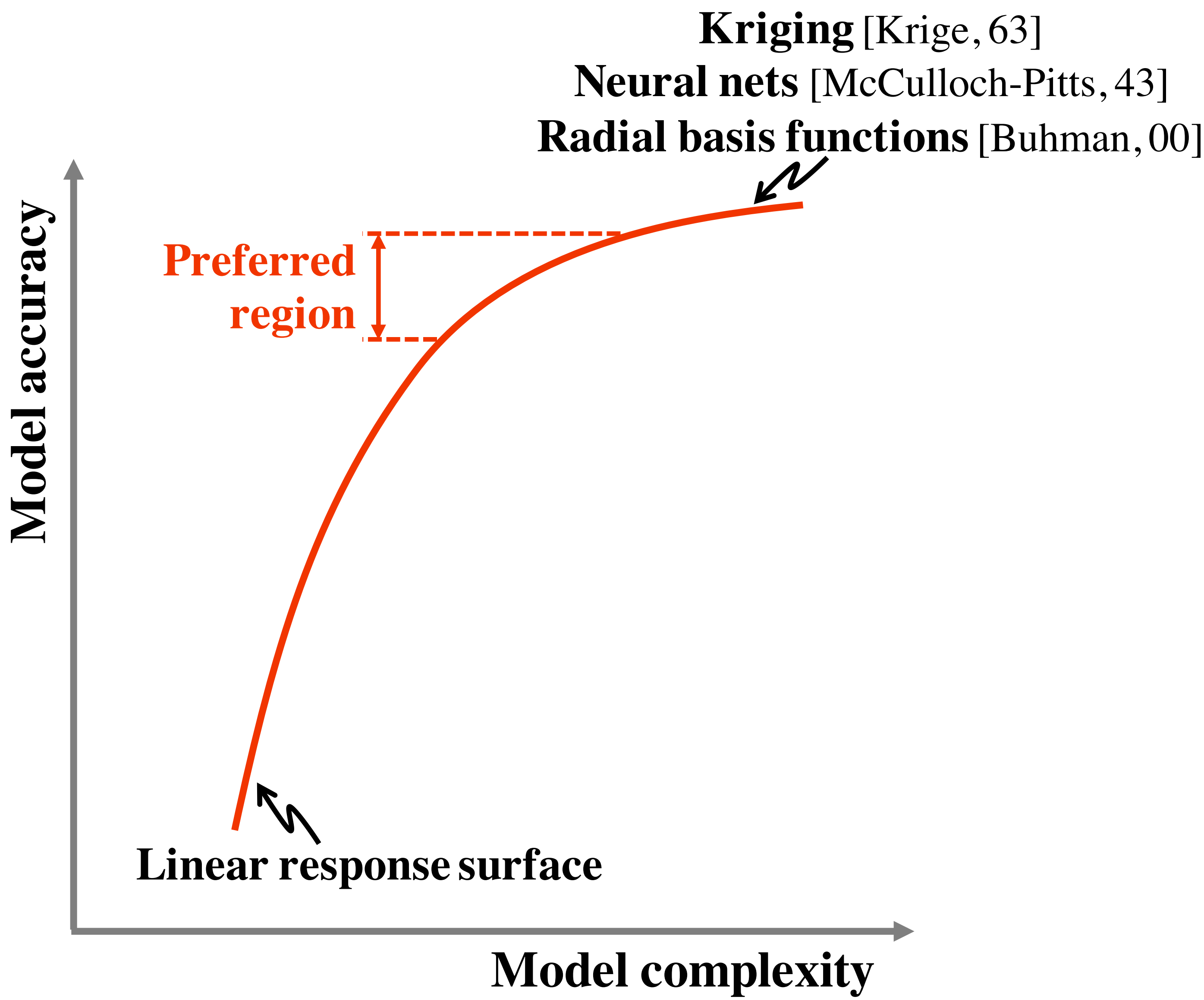
ALAMO

Automated Learning of Algebraic Models for Optimization





MODEL COMPLEXITY TRADEOFF



MODEL IDENTIFICATION

- **Goal: Identify the functional form and complexity of the surrogate models**

$$z = f(x)$$

- **Functional form:**
  - General functional form is unknown: Our method will identify models with combinations of 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	$\exp\left(\frac{x_d}{\gamma}\right)^\alpha$, $\log\left(\frac{x_d}{\gamma}\right)^\alpha$
IV.	Expected bases	From experience, simple inspection, physical phenomena, etc.

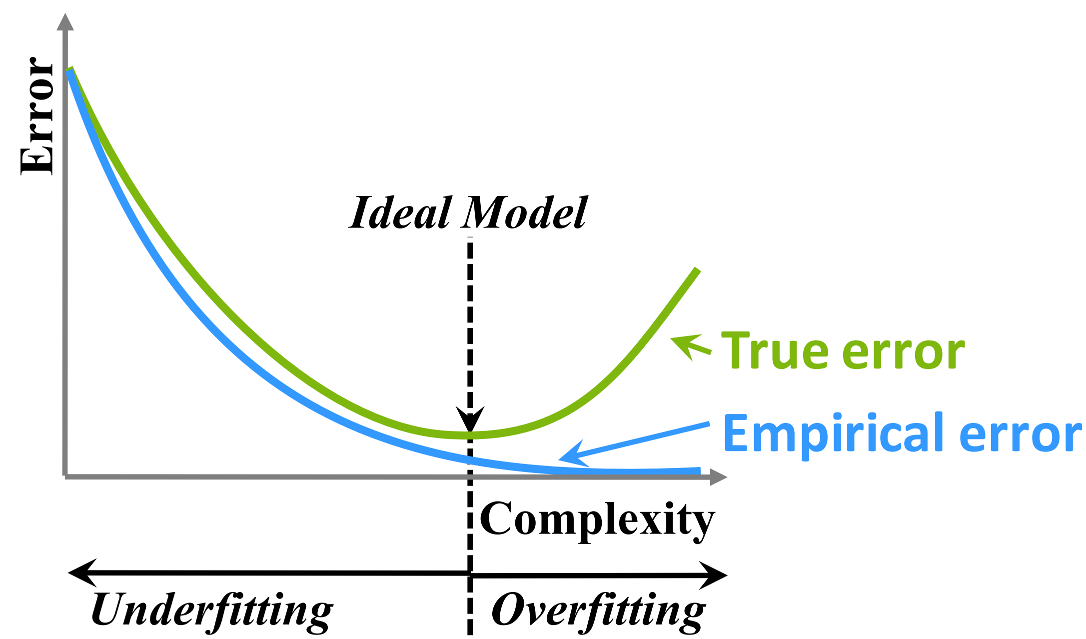
OVERFITTING AND TRUE ERROR

- **Step 1:** Define a large set of potential basis functions

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

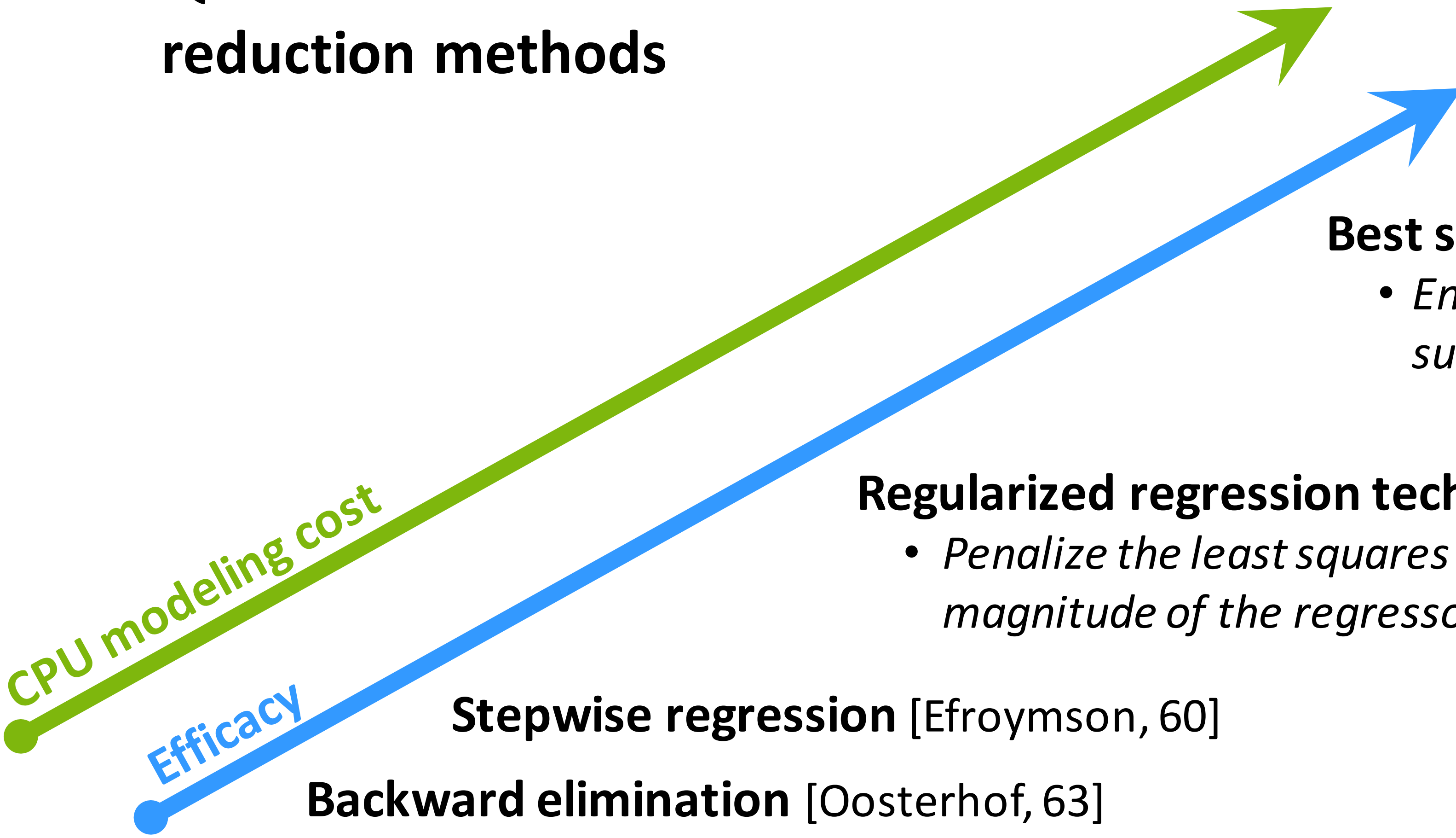
- **Step 2:** Model reduction

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



MODEL REDUCTION TECHNIQUES

- **Qualitative tradeoffs of model reduction methods**



Best subset methods

- *Enumerate all possible subsets*

Regularized regression techniques

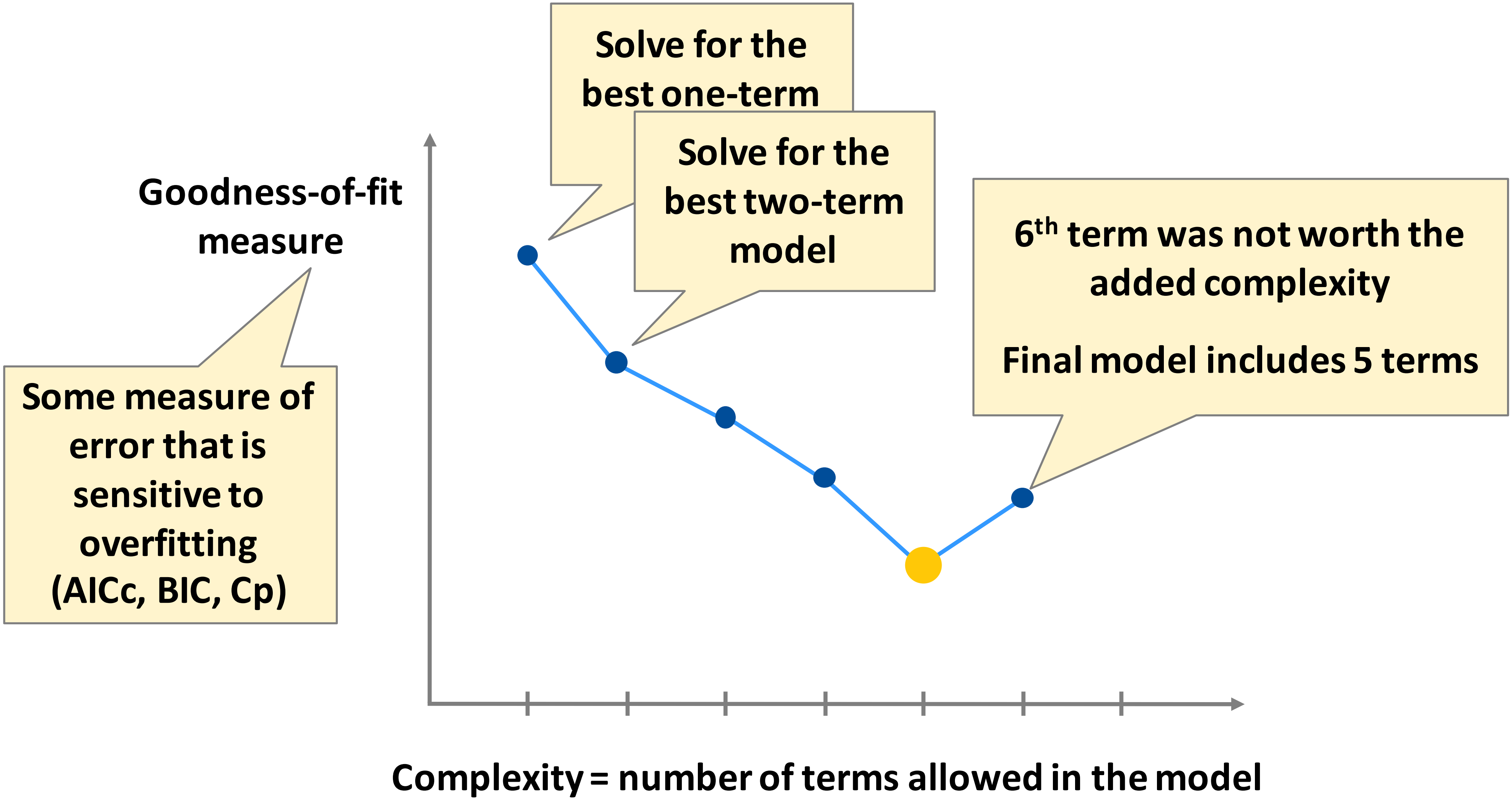
- *Penalize the least squares objective using the magnitude of the regressors* [Tibshirani, 95]

Stepwise regression [Efroymson, 60]

Backward elimination [Oosterhof, 63]

Forward selection [Hamaker, 62]

MODEL SIZING



BASIS FUNCTION SELECTION

$$\min \quad SE = \sum_{i=1}^{N} \left| z_i - \sum_{j \in \mathcal{B}} \beta_j X_{ij} \right|$$

$$\text{s.t.} \quad \sum_{j \in \mathcal{B}} y_j = T$$

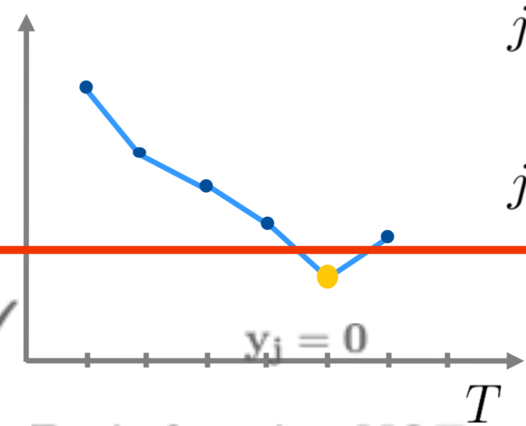
Find the model with the least error

$$-U(1-y_j) \leq \sum_{i=1}^{N} X_{ij} \left(z^i - \sum_{j \in \mathcal{B}} \beta_j X_{ij} \right) \leq U(1-y_j) \qquad j \in \mathcal{B}$$

$$\beta^l y_j \leq \beta_j \leq \beta^u y_j \qquad j \in \mathcal{B}$$

$$y_j = \{0, 1\} \qquad j \in \mathcal{B}$$

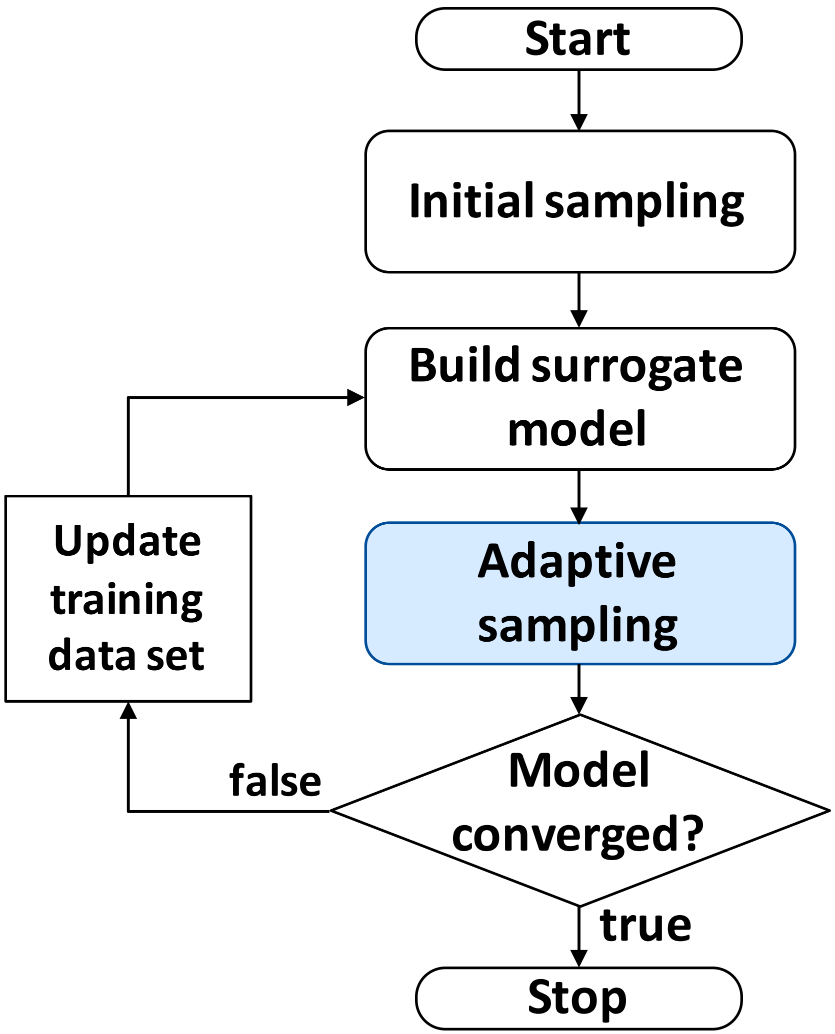
$$\left(\begin{array}{c} y_j = 1 \\ \text{Basis function used in the model} \\ \beta_j \text{ is chosen to satisfy a least} \\ \text{squares regression} \\ (\text{assumes loose bounds on } \beta_j) \end{array} \right) \vee \left(\begin{array}{c} y_j = 0 \\ \text{Basis function NOT used} \\ \text{in the model} \\ \beta_j = 0 \end{array} \right)$$

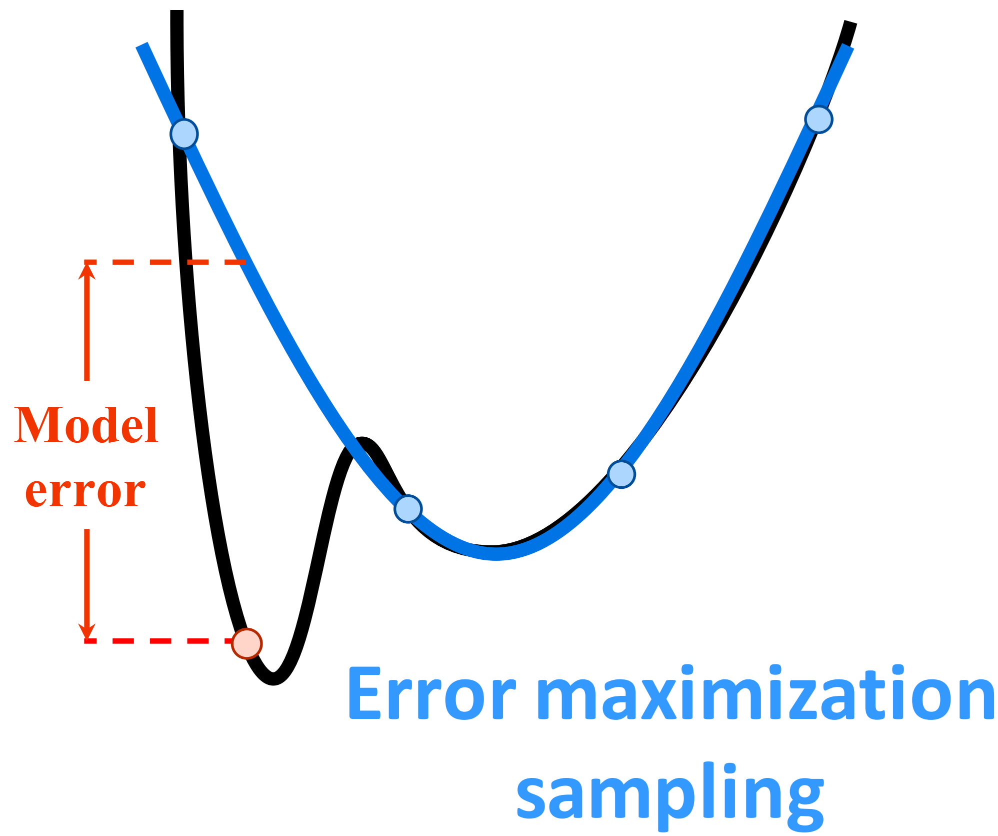


We will solve this model for increasing T until we determine a model size

ALAMO

Automated Learning of Algebraic Models for Optimization





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

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

  - **Derivative-free solvers work well in low-dimensional spaces** [Rios and Sahinidis, 12]
  - **Optimized using a black-box or derivative-free solver (SNOBFIT)** [Huyer and Neumaier, 08]

COMPUTATIONAL RESULTS

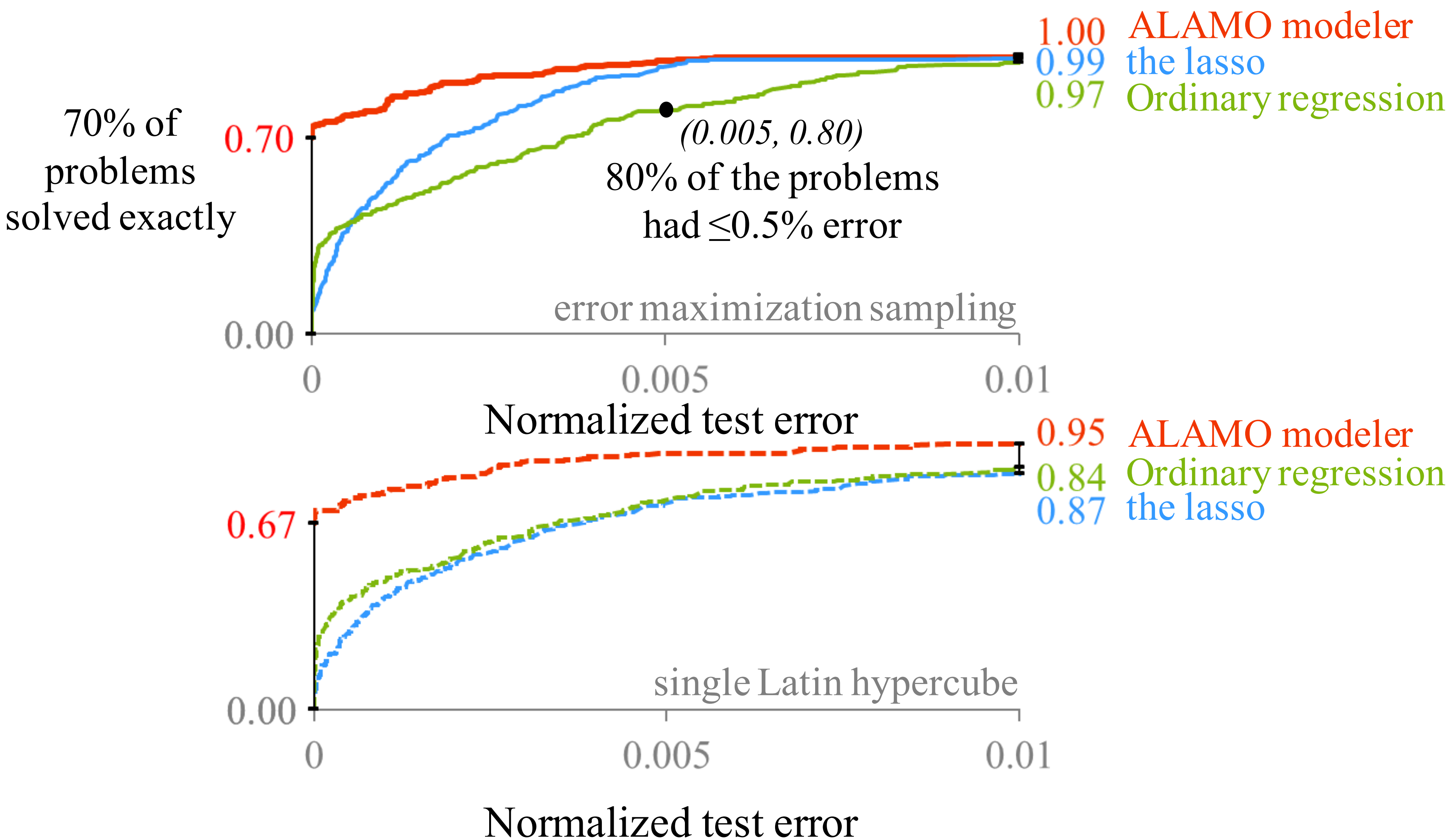
- **Goal – Compare methods on three target metrics**

1 Model accuracy	2 Data efficiency	3 Model simplicity

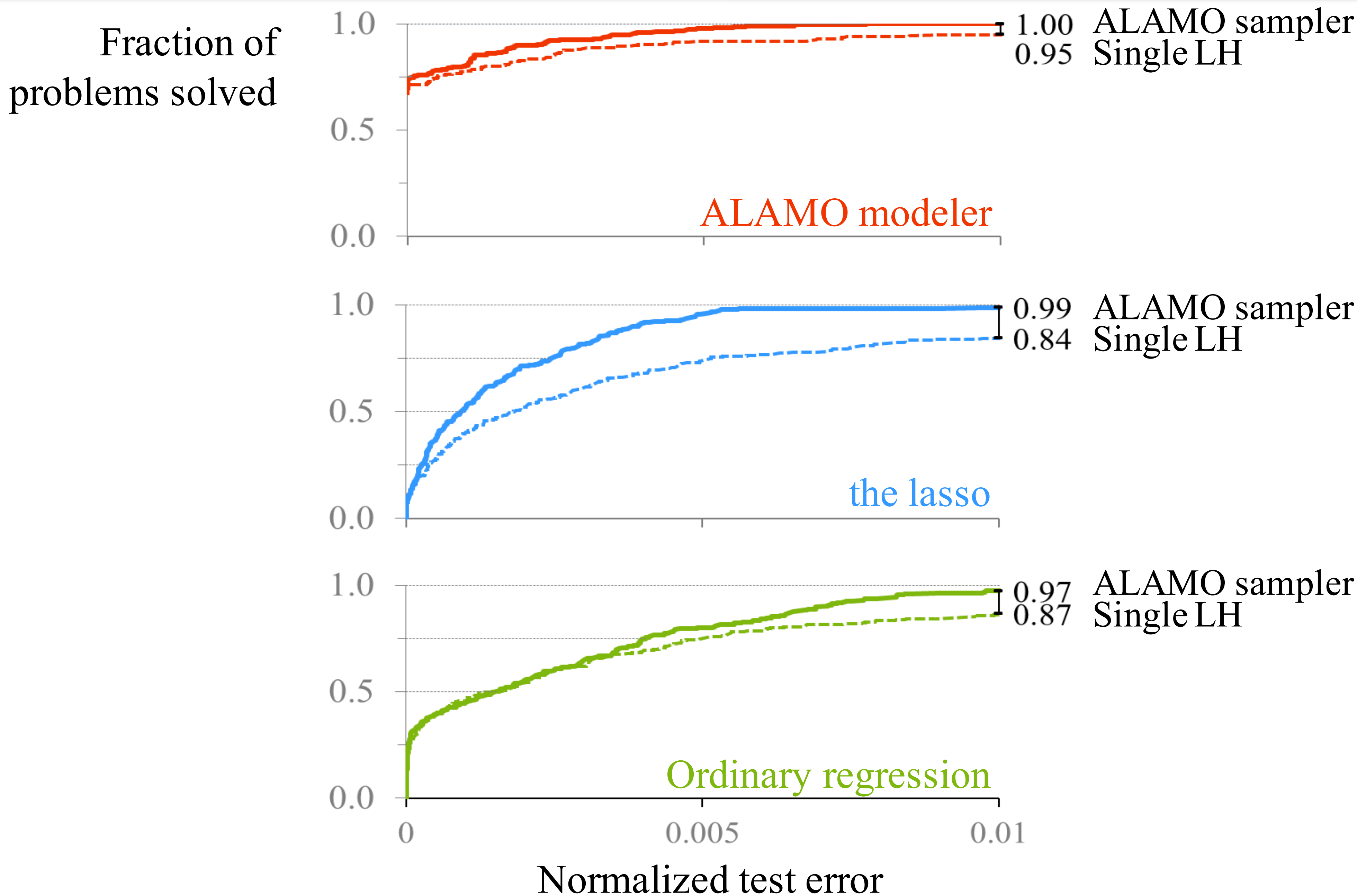
- **Modeling methods compared**
  - **ALAMO modeler – Proposed methodology**
  - **The LASSO – The lasso regularization**
  - **Ordinary regression – Ordinary least-squares regression**

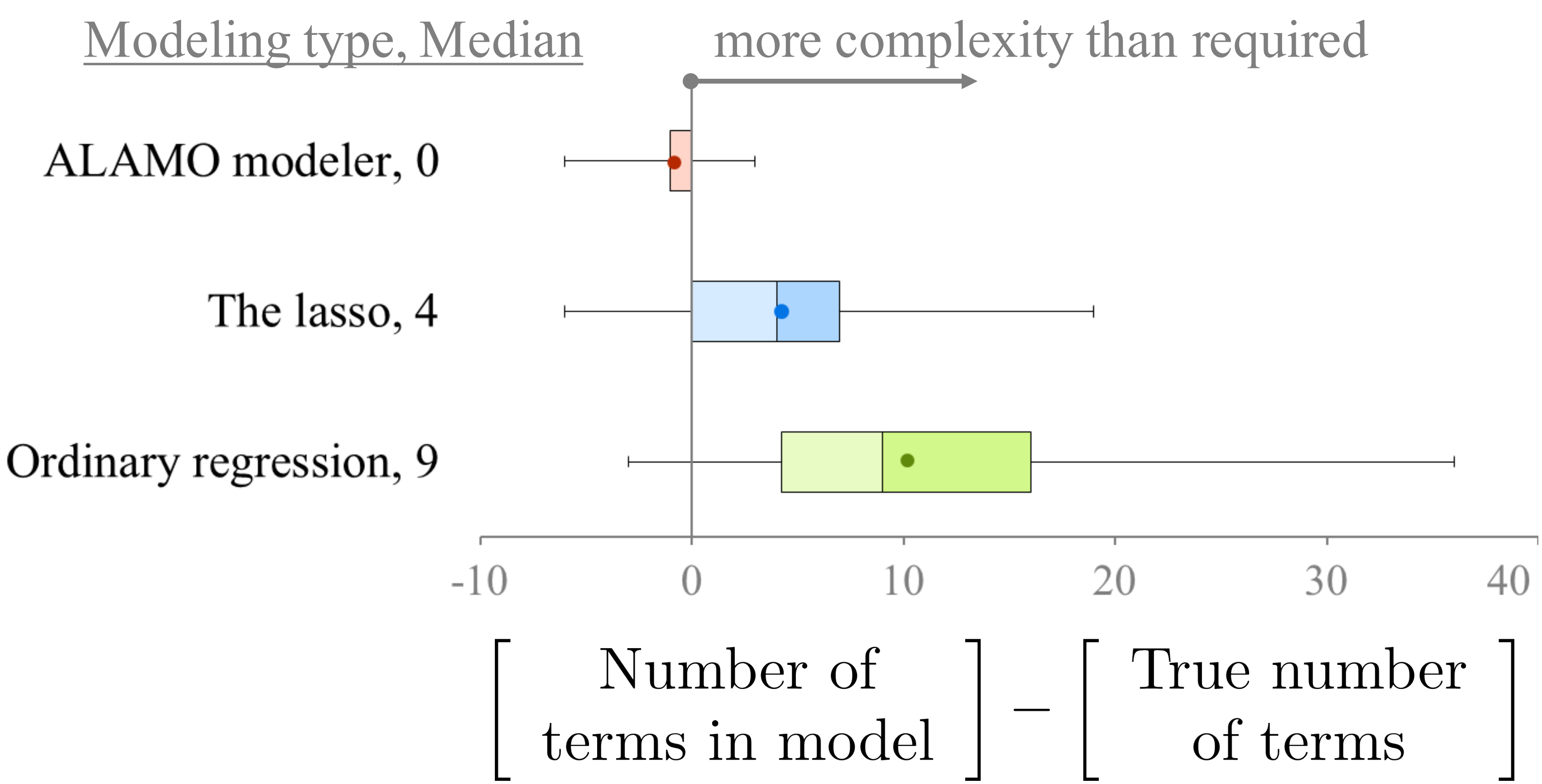
- **Sampling methods compared (over the same data set size)**
  - **ALAMO sampler – Proposed error maximization technique**
  - **Single LH – Single Latin hypercube (no feedback)**

Fraction of problems solved



1 Model accuracy | 2 Data efficiency | 3 Model simplicity





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

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

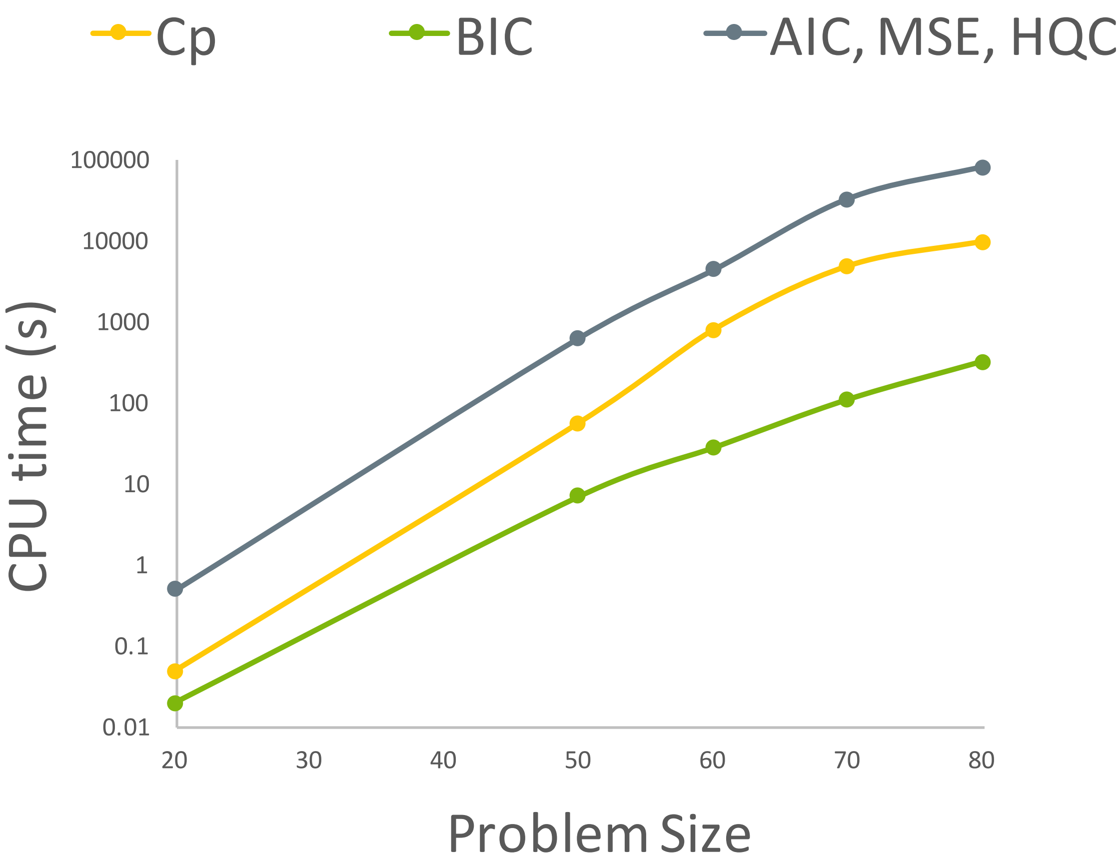
$$BIC = \frac{\sum_{i=1}^{N}(z_i - X_i\beta)^2}{\widehat{\sigma^2}} + \boldsymbol{p}\log(N)$$

Mean Squared Error

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

CPU TIME COMPARISON

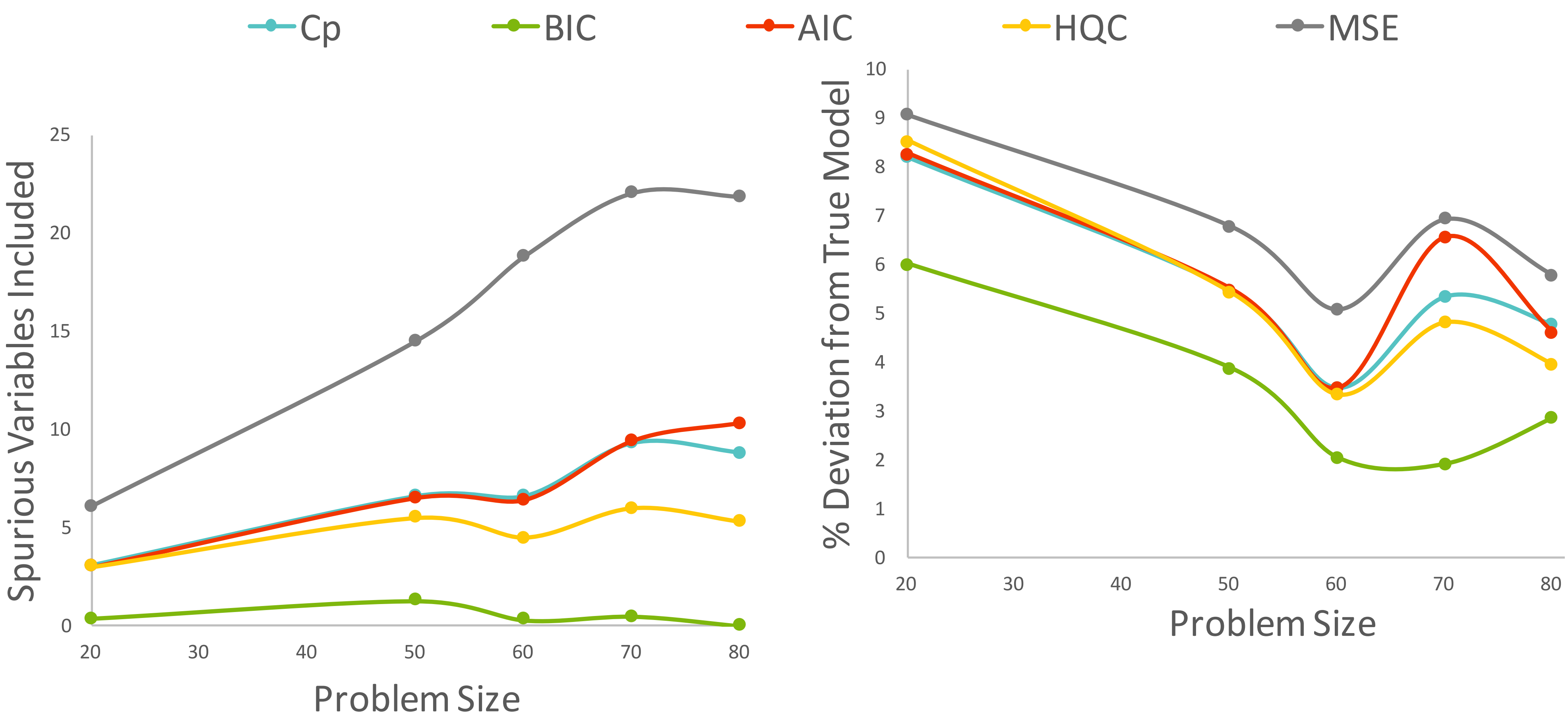
- **Eight benchmarks from the UCI and CMU data sets**
- **Seventy noisy data sets were generated with multicolinearity and increasing problem size (number of bases)**



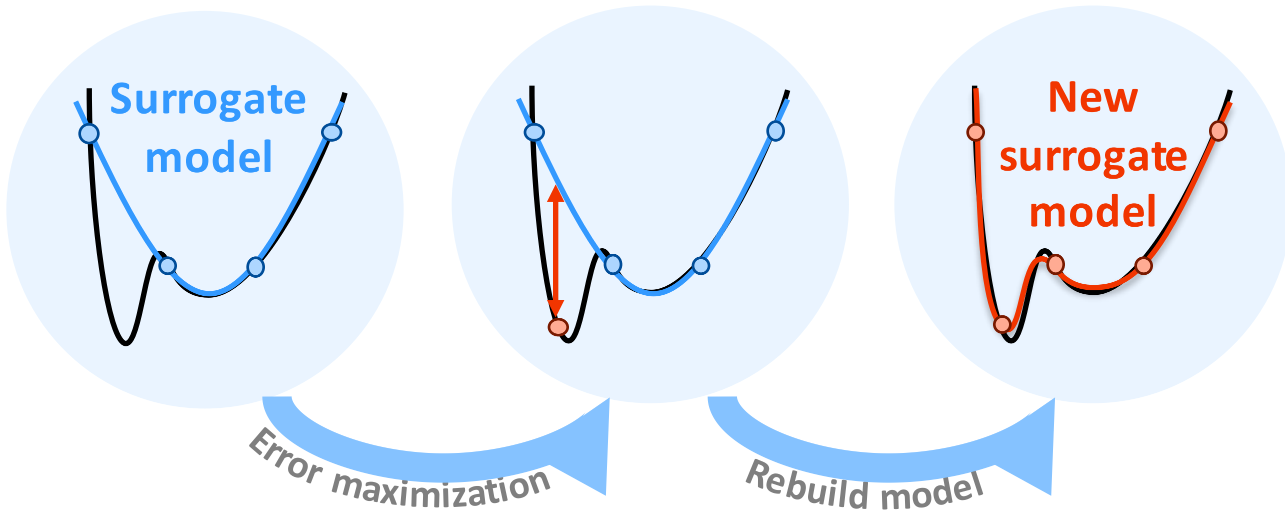
- **BIC solves more than two orders of magnitude faster than AIC, MSE and HQC**
  - Optimized directly via a single mixed-integer convex quadratic model

MODEL QUALITY COMPARISON

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

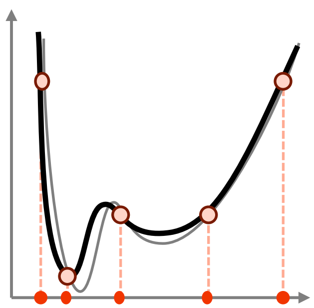


ALAMO REMARKS

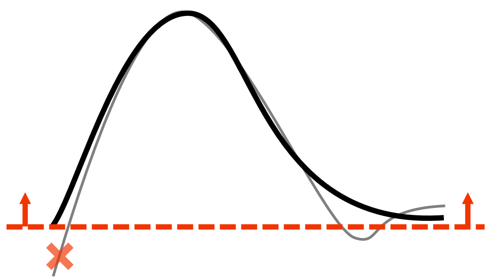


- **Expanding the scope of algebraic optimization**
  - Using low-complexity surrogate models to strike a balance between optimal decision-making and model fidelity
- **Surrogate model identification**
  - Simple, accurate model identification – Integer optimization
- **Error maximization sampling**
  - More information found per simulated data point

THEORY UTILIZATION



empirical data



non-empirical information

- **Use freely available system knowledge to strengthen model**
  - Physical limits
  - First-principles knowledge
  - Intuition
- **Non-empirical restrictions can be applied to general regression problems**

CONSTRAINED REGRESSION

- **Challenging due to the semi-infinite nature of the regression constraints**

Standard regression

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

Surrogate model

easy

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

tough

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

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

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

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

1 parametric constraint

4 β-constraints

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

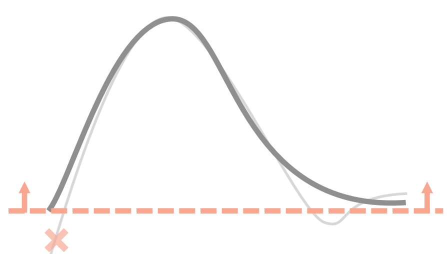
$$\min_{\beta_1,\beta_2} \sum_{i=1}^{4} \left(z_i - \left[\beta_1 x + \beta_2 x^3\right]\right)^2$$

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

TYPES OF RESTRICTIONS

Response bounds

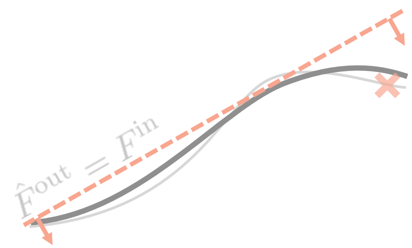
$$[\hat{A}]_t \geq 0$$



pressure, temperature, compositions

Individual responses

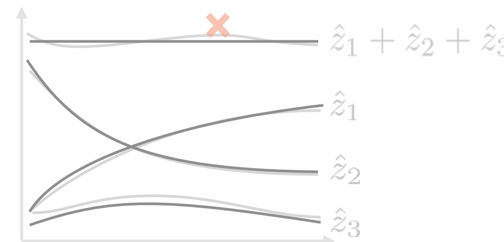
$$\hat{F}^{\text{out}}(x) \leq F^{\text{in}}$$



mass and energy balances, physical limitations

Multiple responses

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



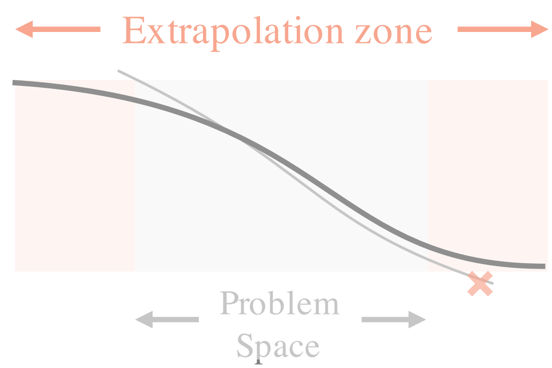
mass balances, sum-to-one, state variables

Response derivatives

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

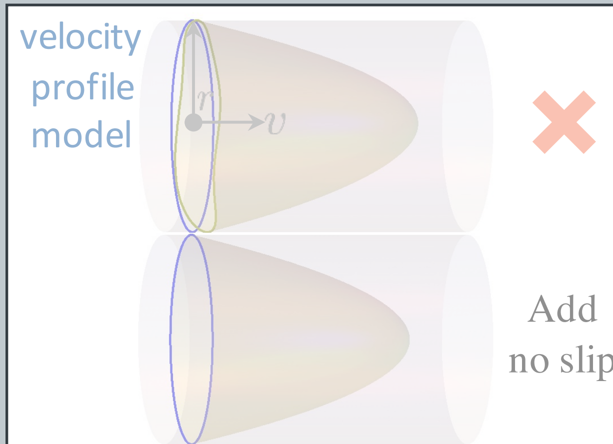
monotonicity, numerical properties, convexity

Alternative domains



safe extrapolation, boundary conditions

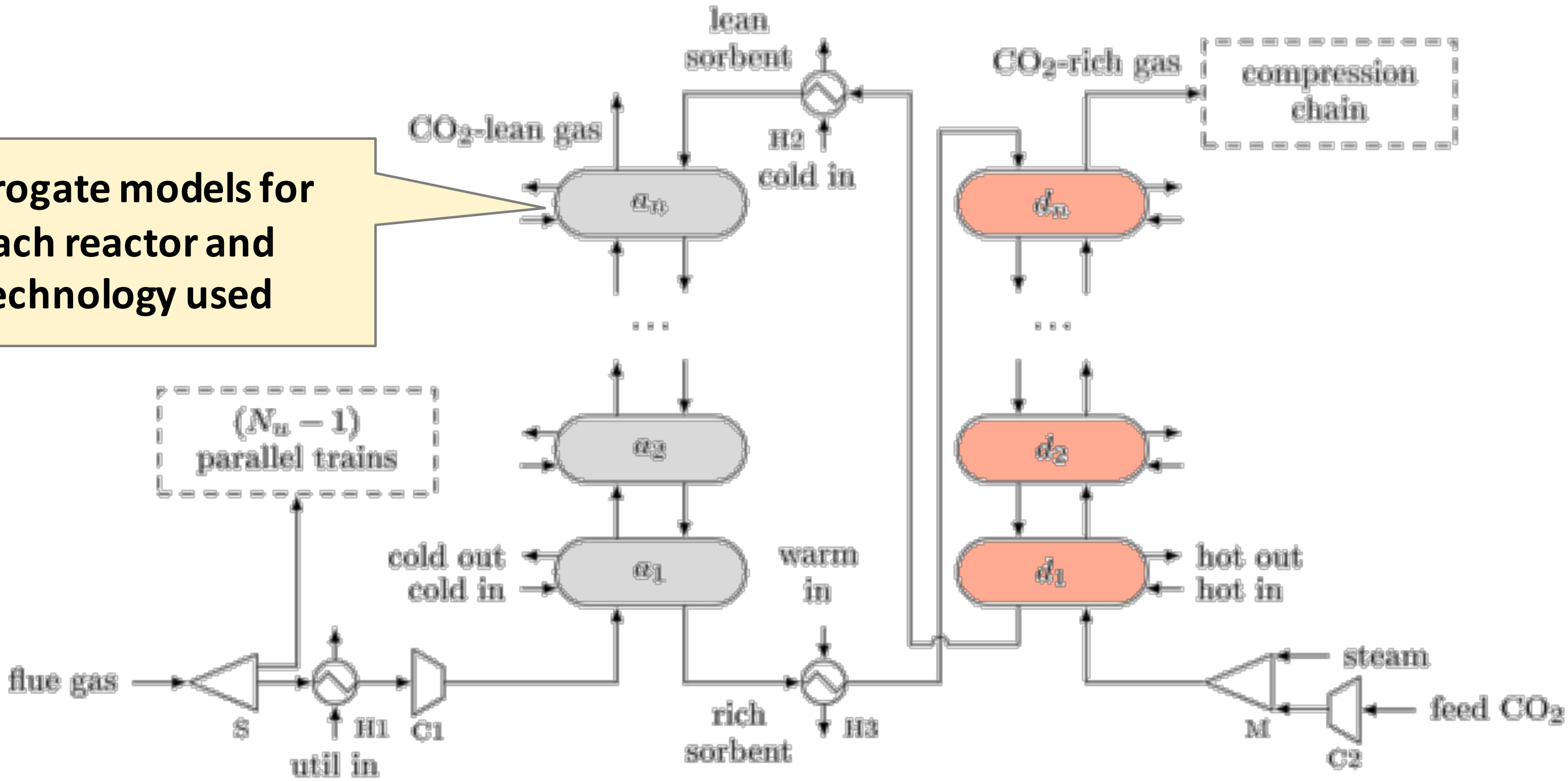
Boundary conditions



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

CARBON CAPTURE SYSTEM DESIGN

Surrogate models for each reactor and technology used

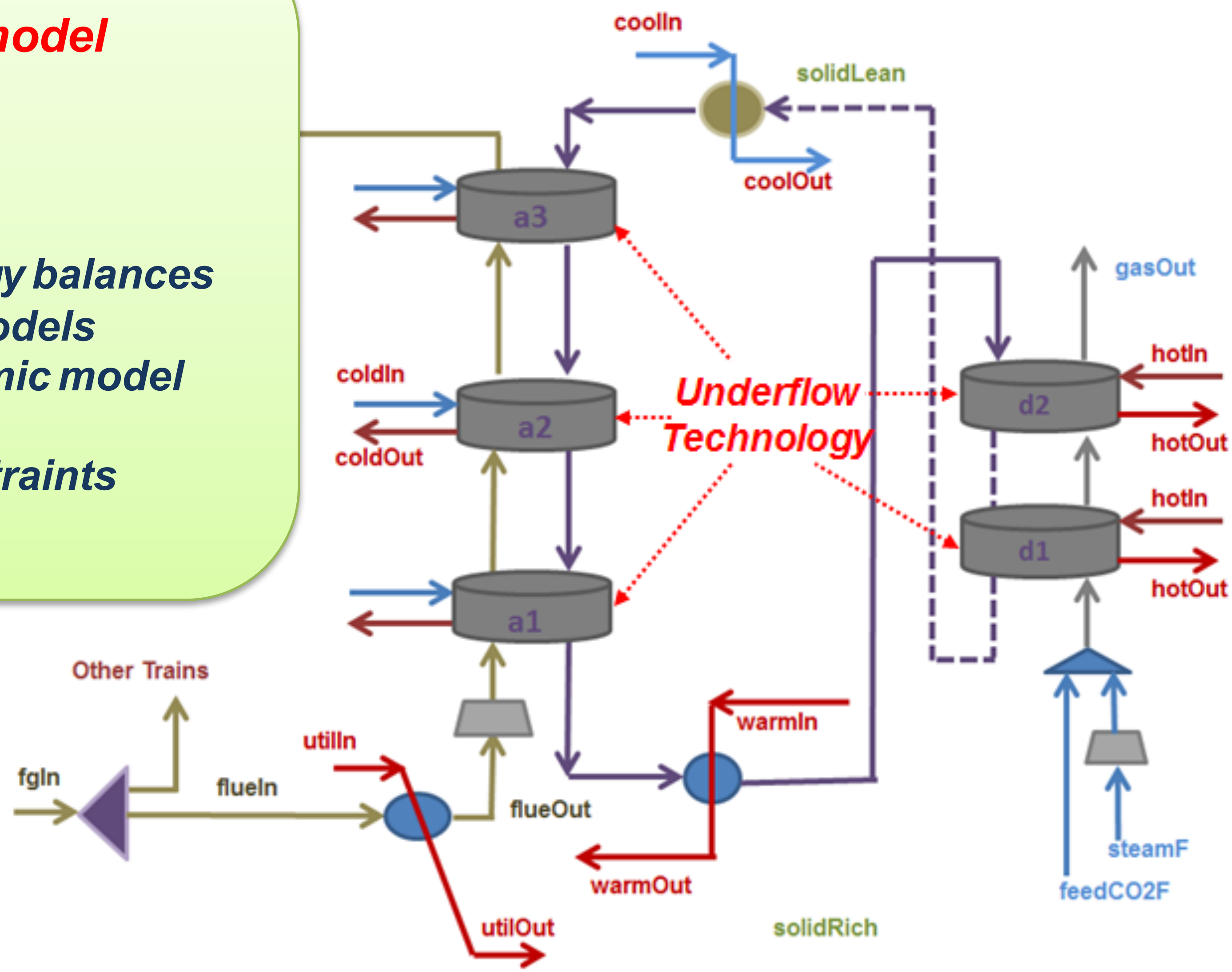


- **Discrete decisions:** How many units? Parallel trains?
  What technology used for each reactor?
- **Continuous decisions:** Unit geometries
- **Operating conditions:** Vessel temperature and pressure, flow rates, compositions

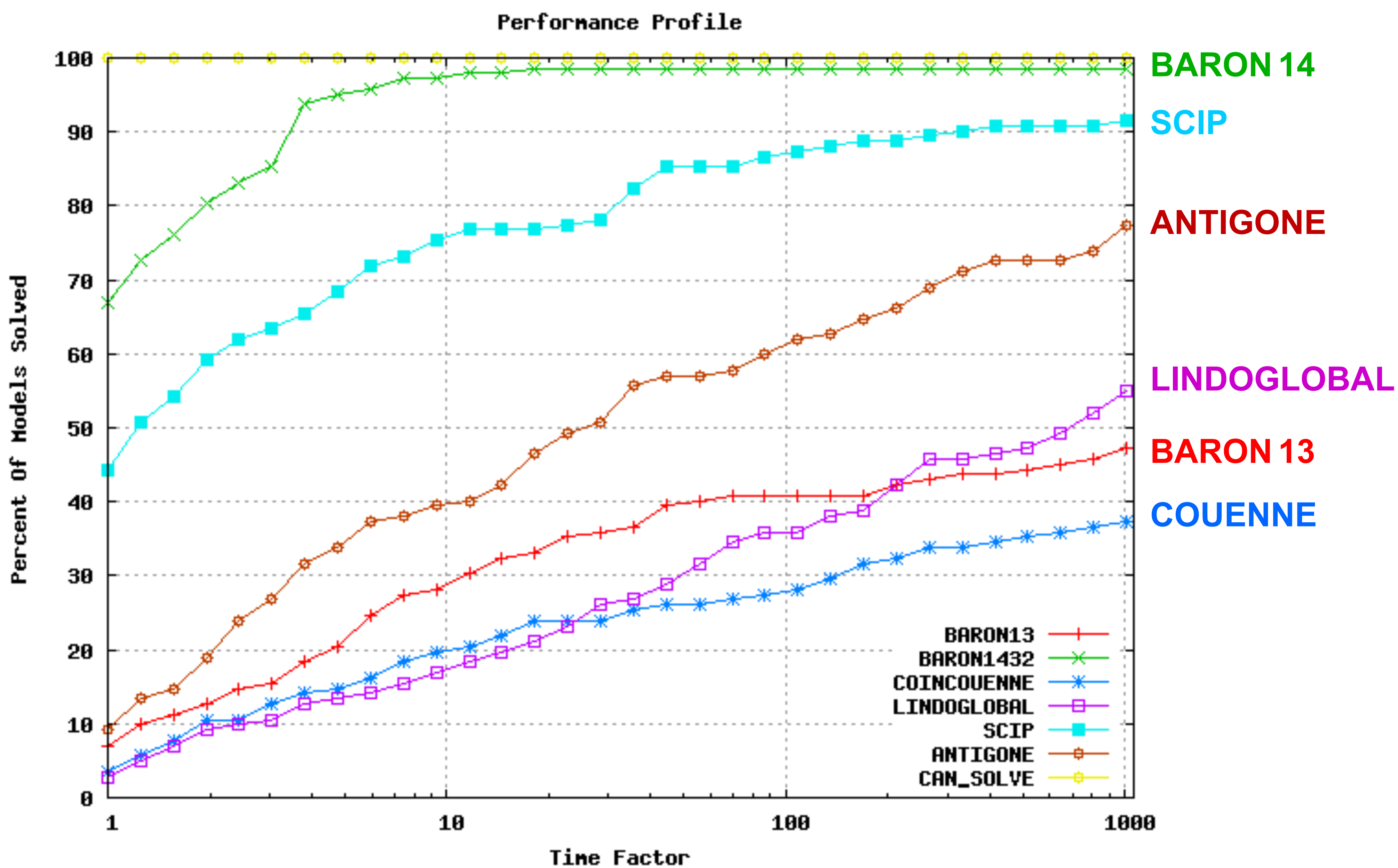
SUPERSTRUCTURE OPTIMIZATION

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*



GLOBAL MINLP SOLVERS ON CMU/IBMLIB



CONCLUSIONS

- **ALAMO provides algebraic models that are**
  - ✓ Accurate and simple
  - ✓ Generated from a minimal number of function evaluations
- **ALAMO's constrained regression facility allows modeling of**
  - ✓ Bounds on response variables
  - ✓ Convexity/monotonicity of response variables
- **On-going efforts**
  - Uncertainty quantification
  - Symbolic regression
- **ALAMO site: archimedes.cheme.cmu.edu/?q=alamo**