A Reduced-Order Building Approach to Simulation-Based Optimization of Complex Energy Systems

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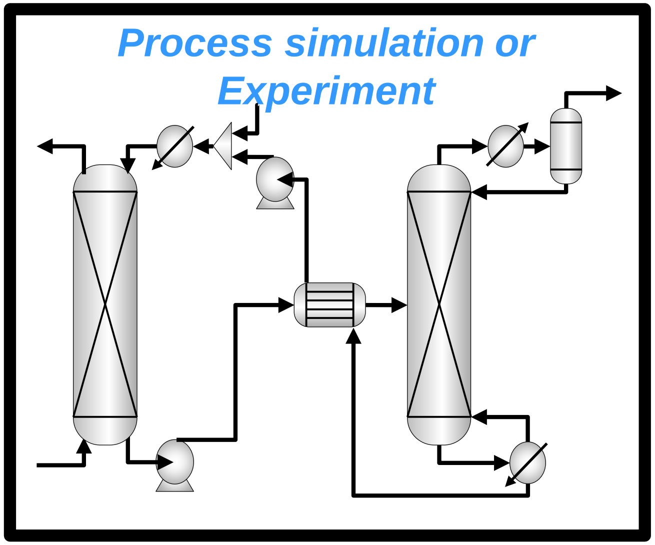
LEARNING PROBLEM

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.

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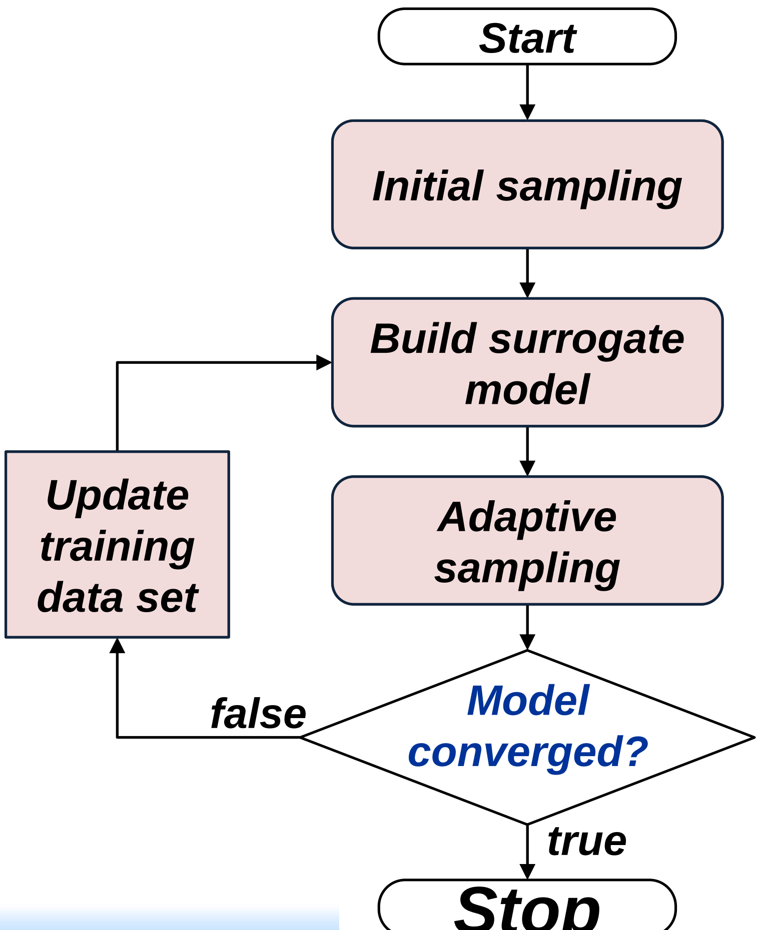
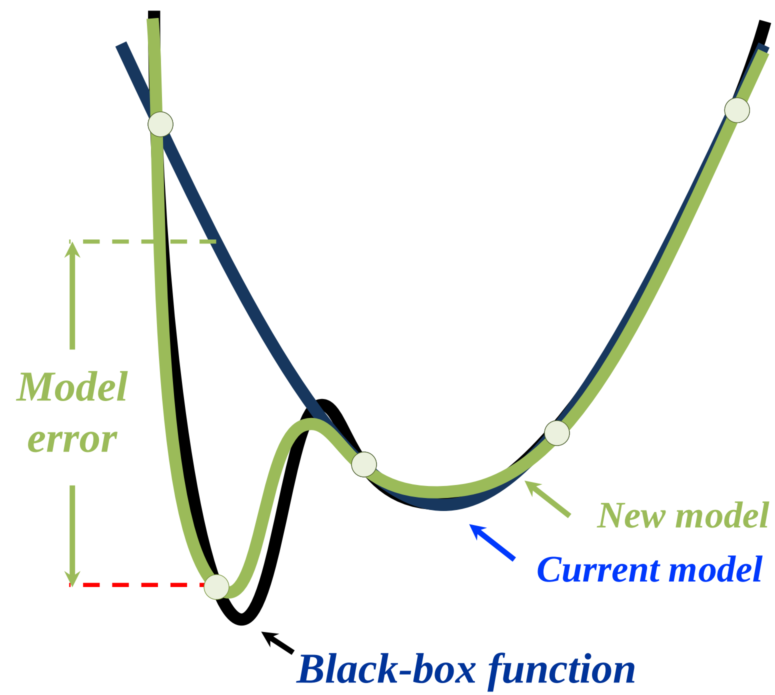
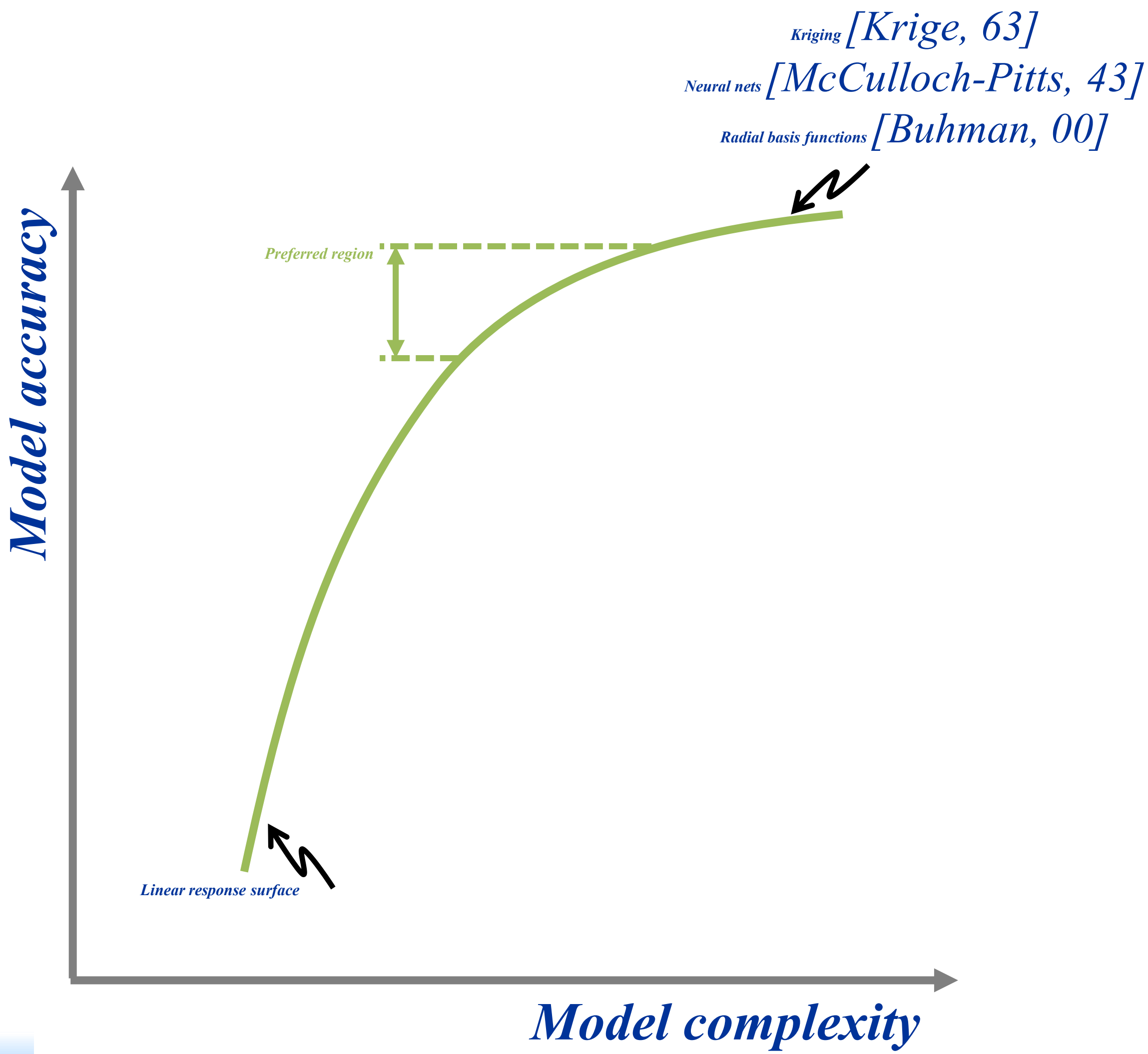
ALAMO

Automated Learning of Algebraic Models using Optimization



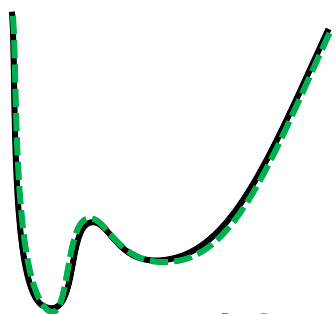


Model complexity tradeoff



DESIRED MODEL ATTRIBUTES

- We aim to build surrogate models that are
  - Accurate
    - We want to reflect the true nature of the simulation
  - Simple
    - Interpretable; 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

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.

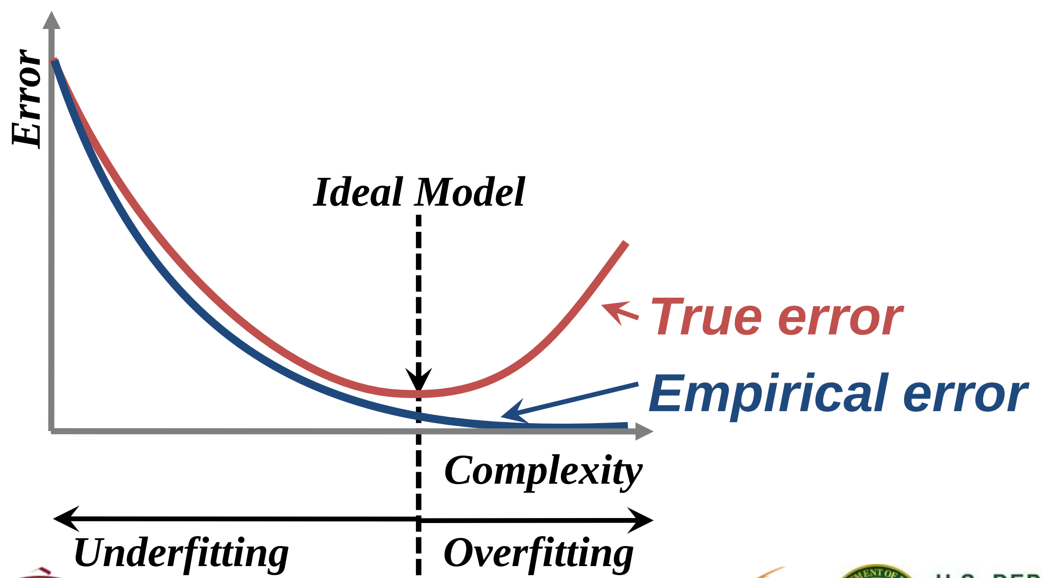
Overfitting and true error

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

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

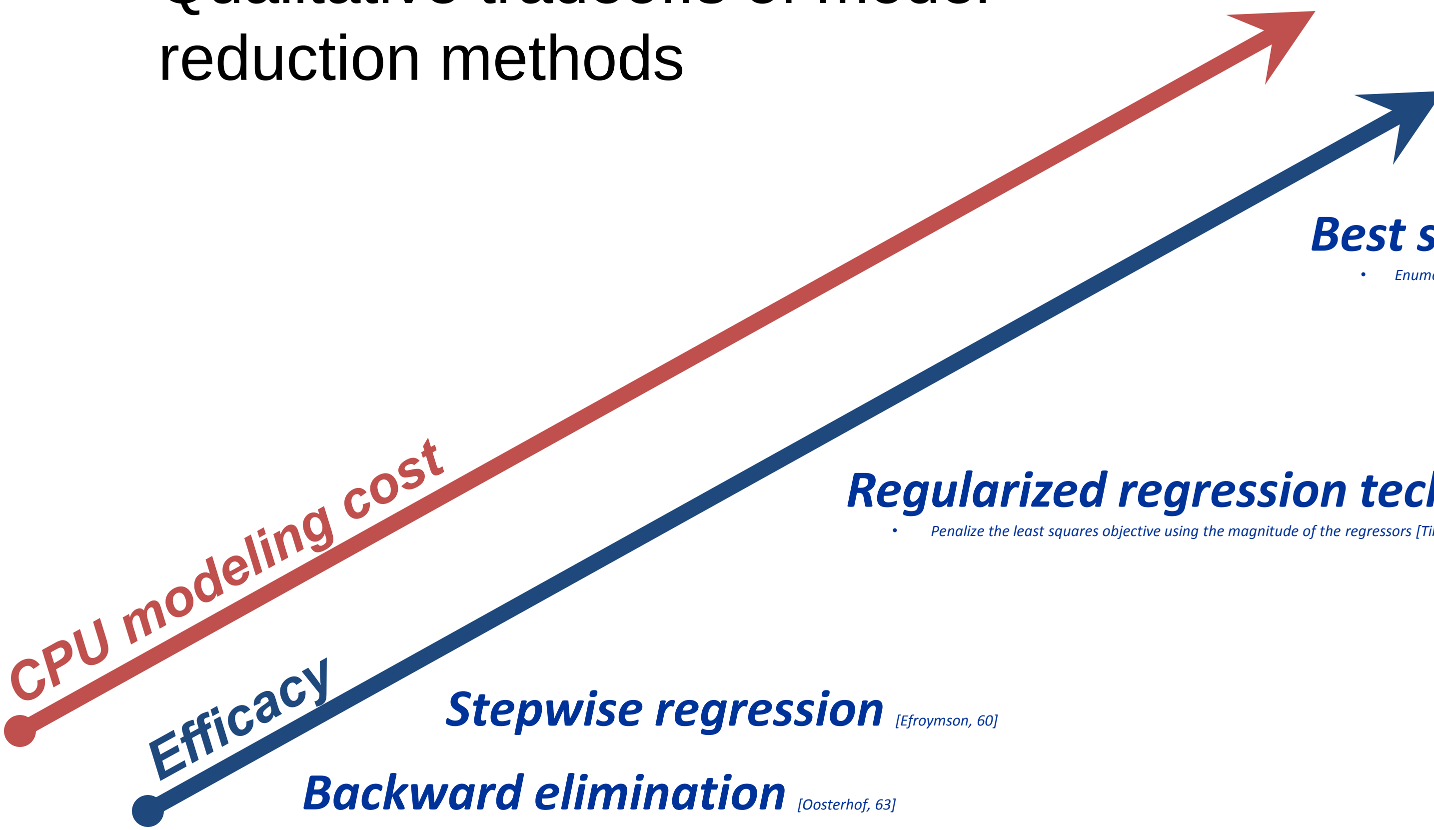
- Step 2: Model reduction

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



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]*

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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

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

Direct optimization via miqp

- ***Convex metrics can be optimized directly***

$$\begin{aligned} \min \quad & C_p = \frac{\sum_{i=1}^{N} \left(z_i - X_{i,j}\beta_j\right)^2}{\hat{\sigma}^2} + 2\sum_{j=1}^{k} y_j - N \\ \text{s.t.} \quad & -My_j \leq \beta_j \leq My_j \qquad j = 1, \ldots, k \\ & y_j \in \{0, 1\} \end{aligned}$$

- ***Exclusion of variables modeled with big-M constraints***
  - *Value of M selected using lasso based logic*

$$M = \sum_{j=1}^{k} |\hat{\beta}_{ols}|$$

Direct optimization via CCmiqp

- ***Nonconvex metrics are optimized by solving a series of cardinality constrained MIQPs***

$$\min \quad AIC_c = \left(N\log\left(\frac{1}{N}SSR\right)\right)\Big|_T + 2T + \frac{2T(T+1)}{N-T-1} \qquad T = 1, \ldots, k$$

$$\min \quad SSR = \sum_{i=1}^{N}(z_i - X_{i,j}\beta_j)^2$$

$$\text{s.t.} \quad \sum_{j=1}^{k} y_j \leq T$$

$$-My_j \leq \beta_j \leq My_j \qquad j = 1, \ldots, k$$

$$y_j \in \{0, 1\}$$

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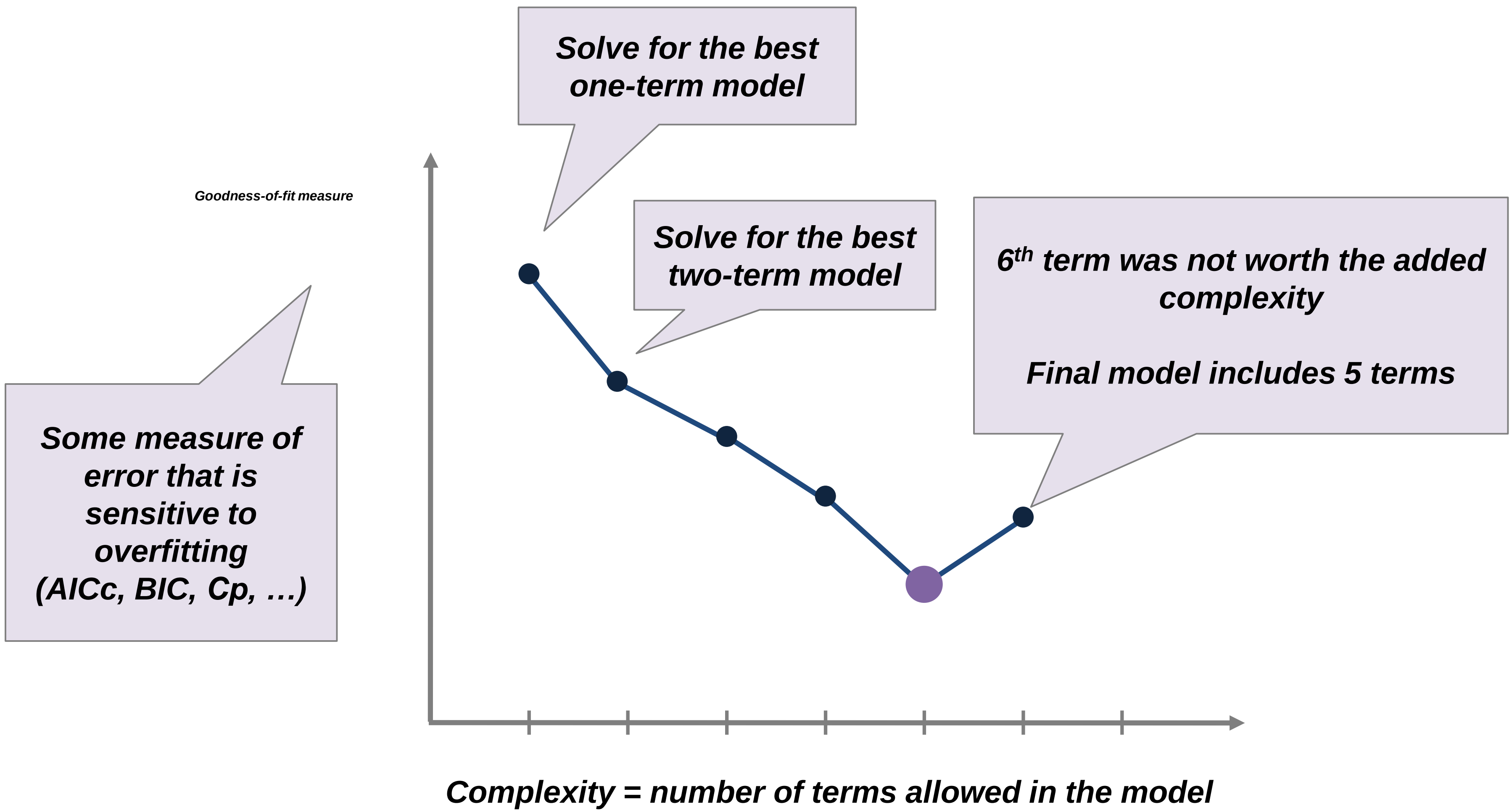
Model sizing



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ALAMO

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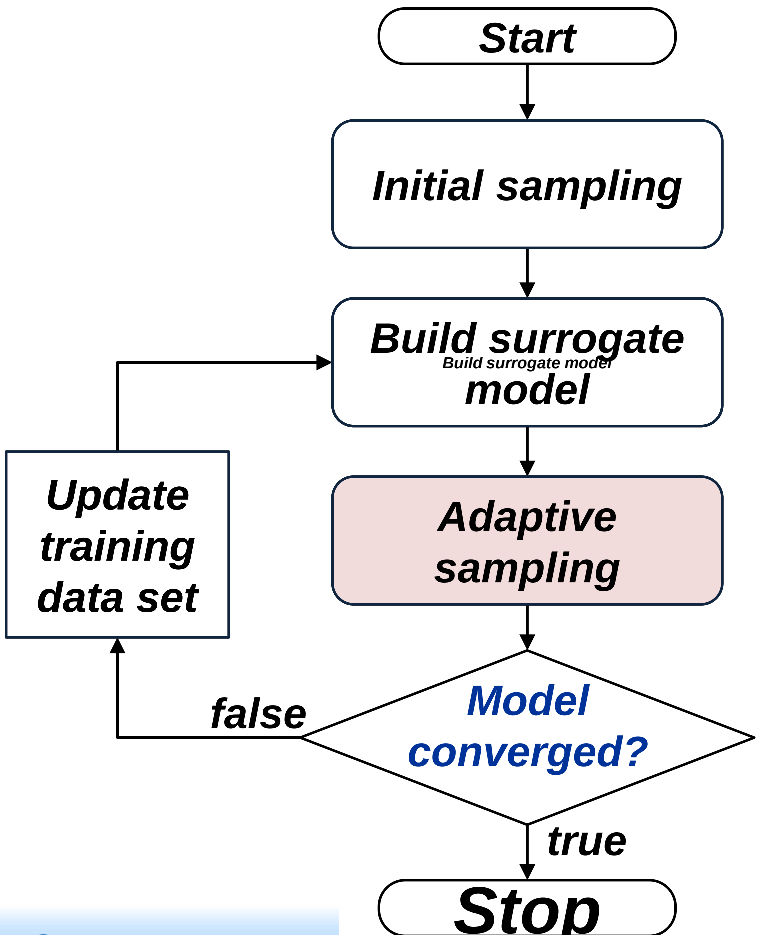
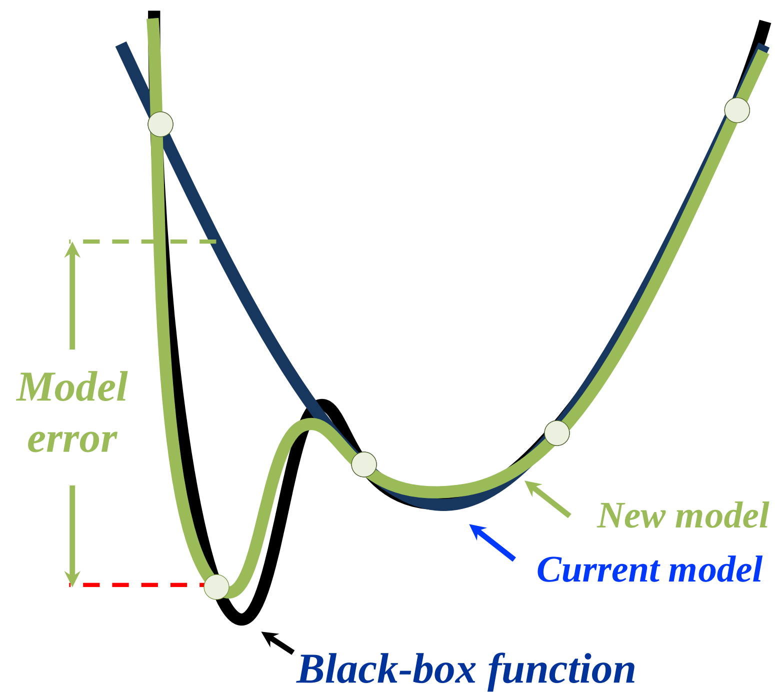
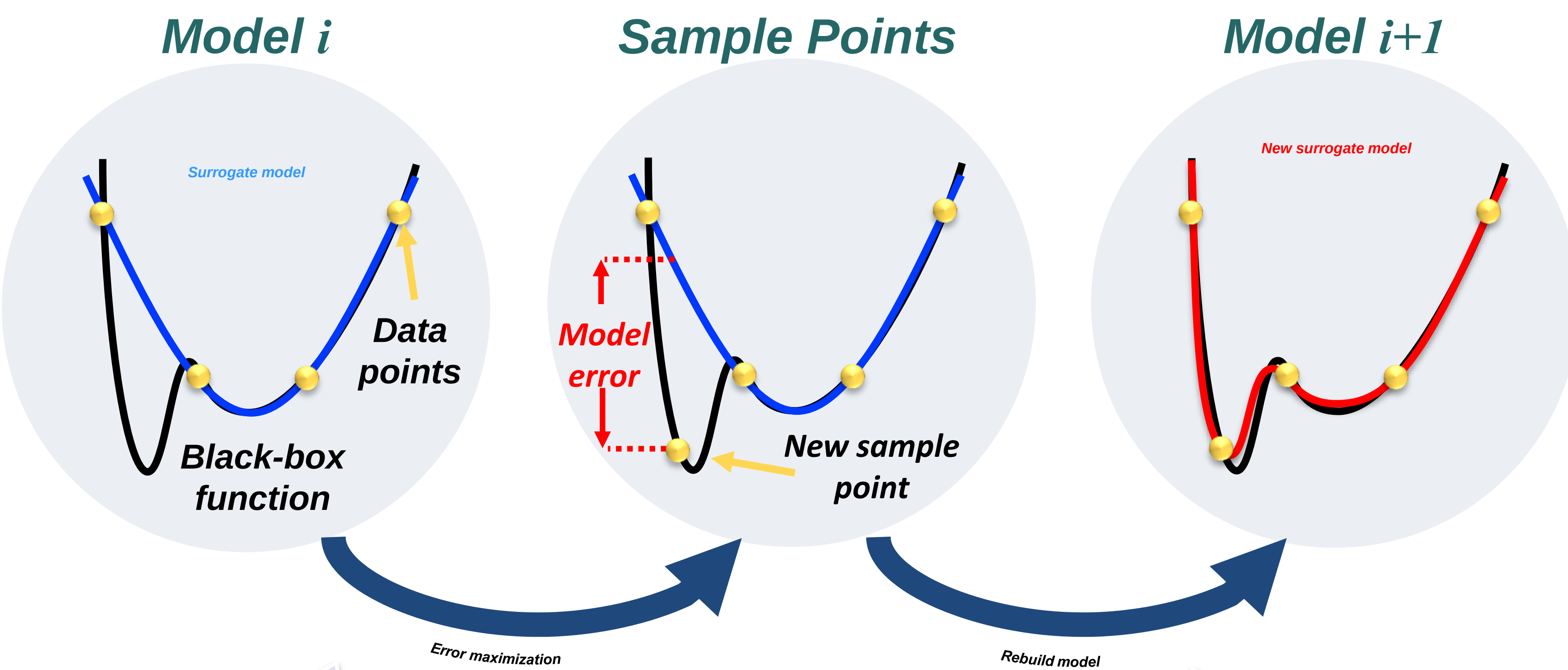




SYNOPSIS



Derivative-free optimization
In low dimensions

Mixed-integer programming for best simple model

Error maximization sampling

- New Goal: Search the problem space for areas of model inconsistency or model mismatch

- More succinctly, we are trying to find points that maximizes the model error with respect to the independent variables

Surrogate model

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

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

Computational results

- Goal – Compare methods on three target metrics

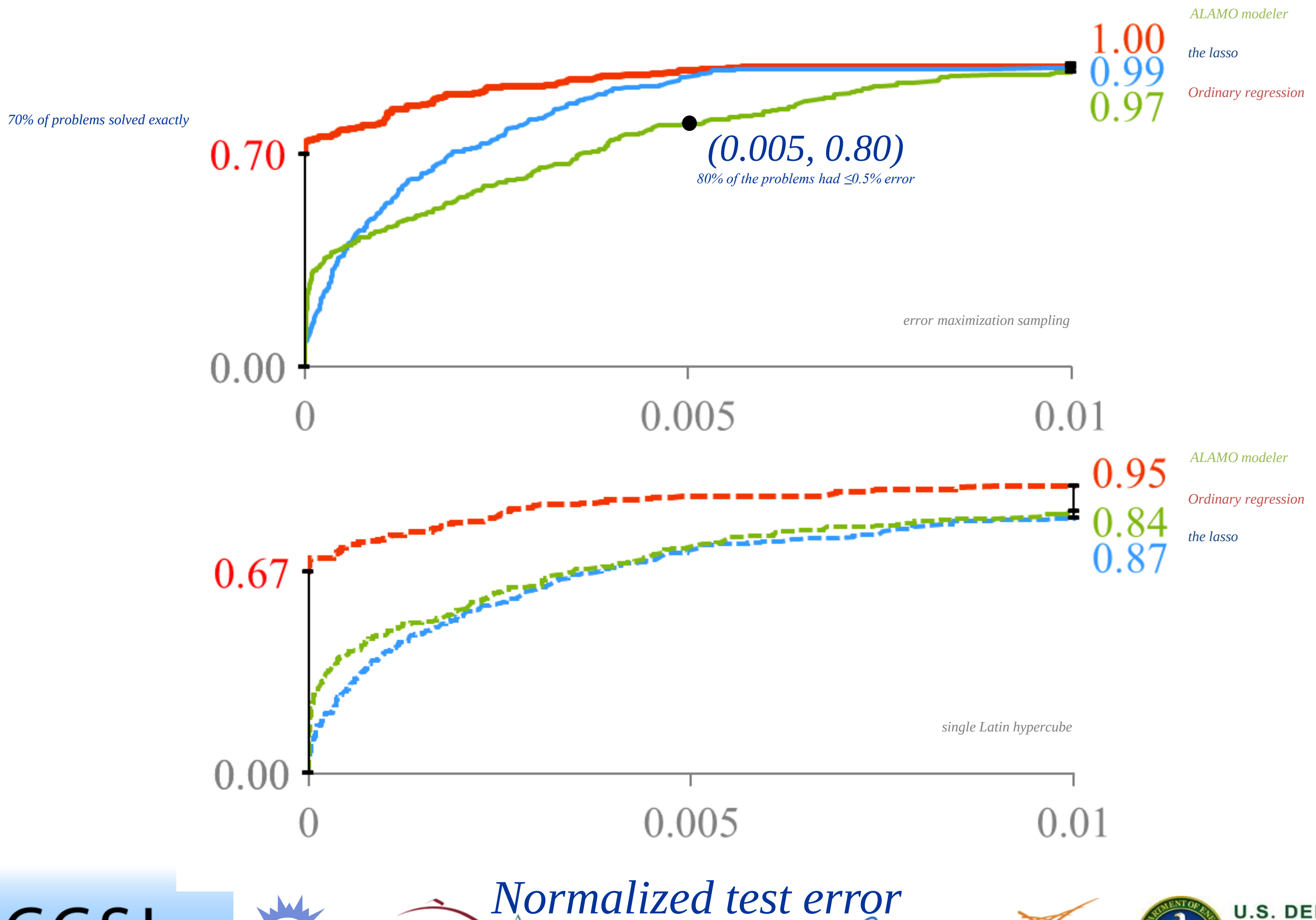
1 Model accuracy	2 Data efficiency	3 Model simplicity

- Modeling methods compared
  - ALAMO modeler – Proposed best subset 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)

1 **Model accuracy** | 2 **Data efficiency** | 3 **Model simplicity**

Fraction of problems solved



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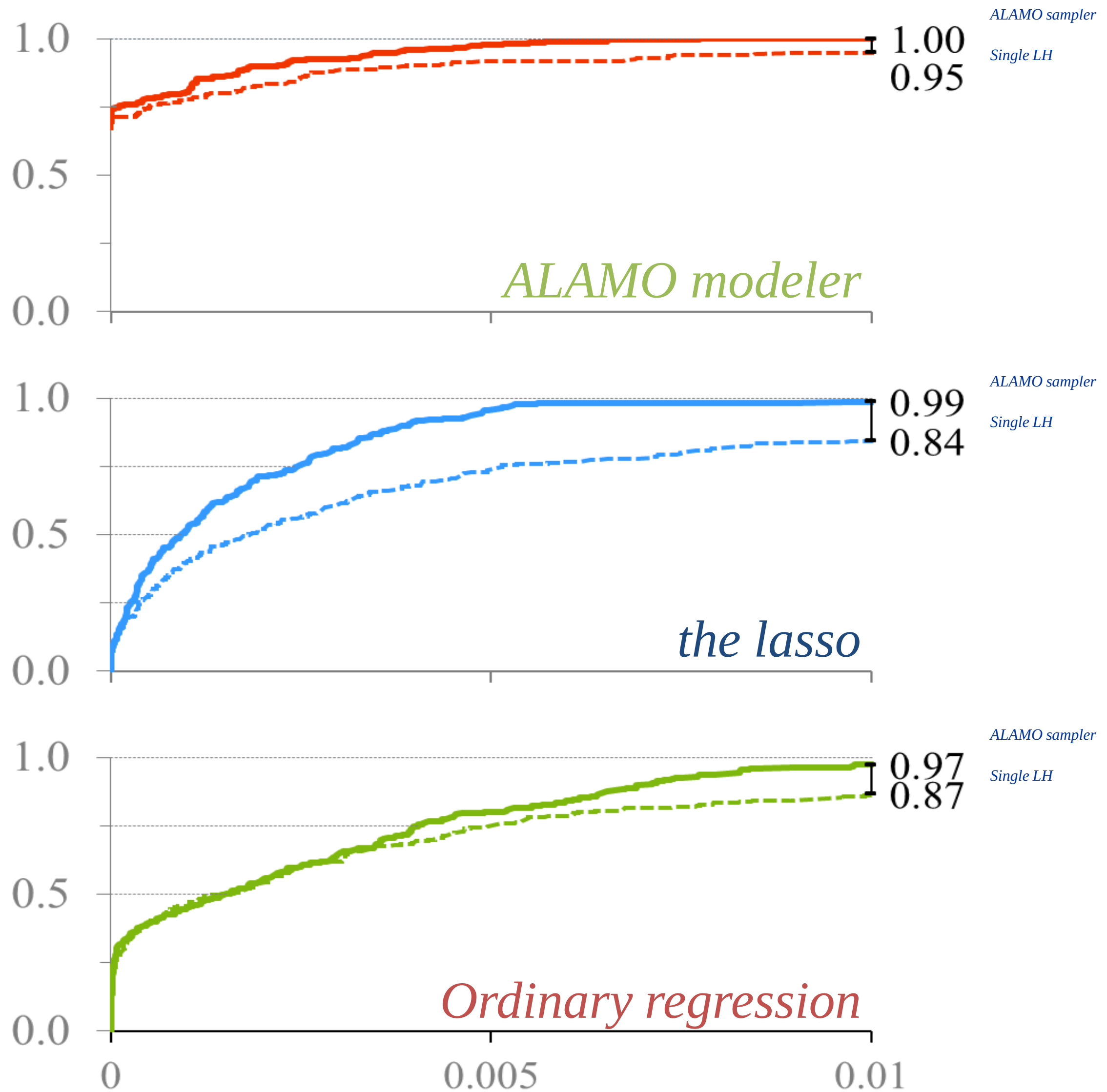
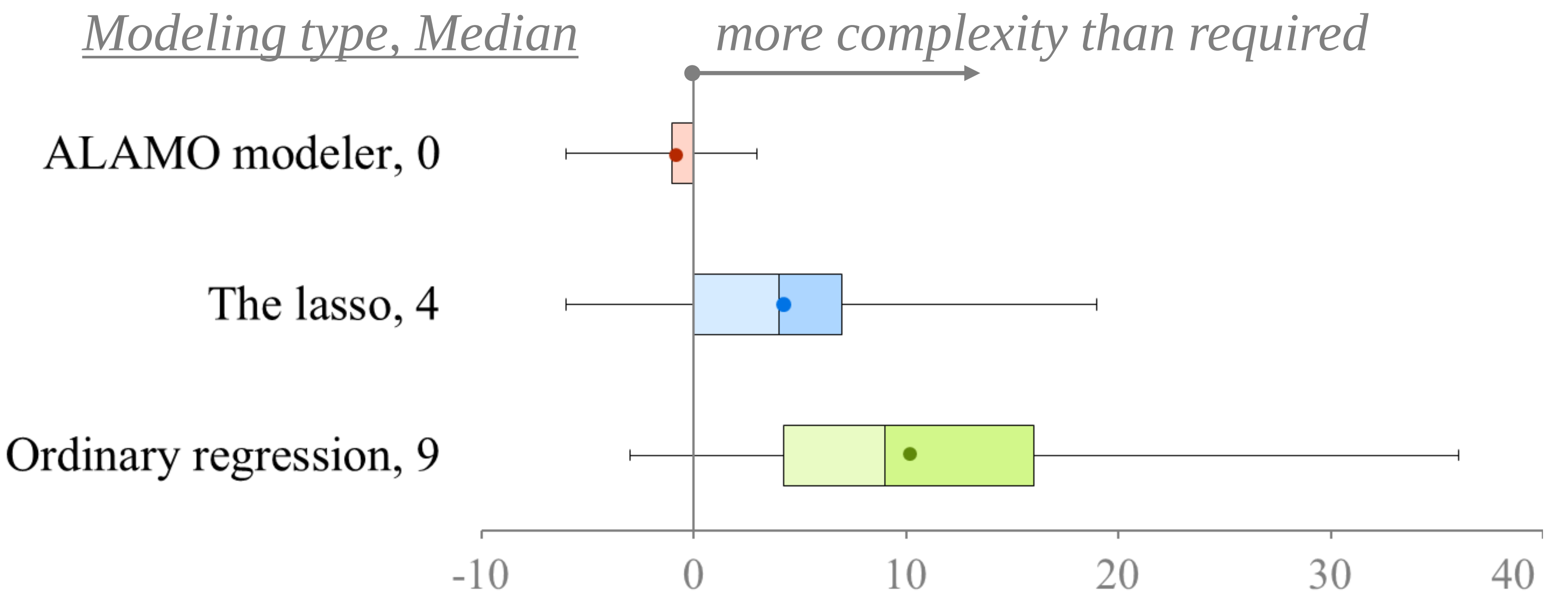
1 Model accuracy | **2 Data efficiency** | 3 Model simplicity

Fraction of problems solved



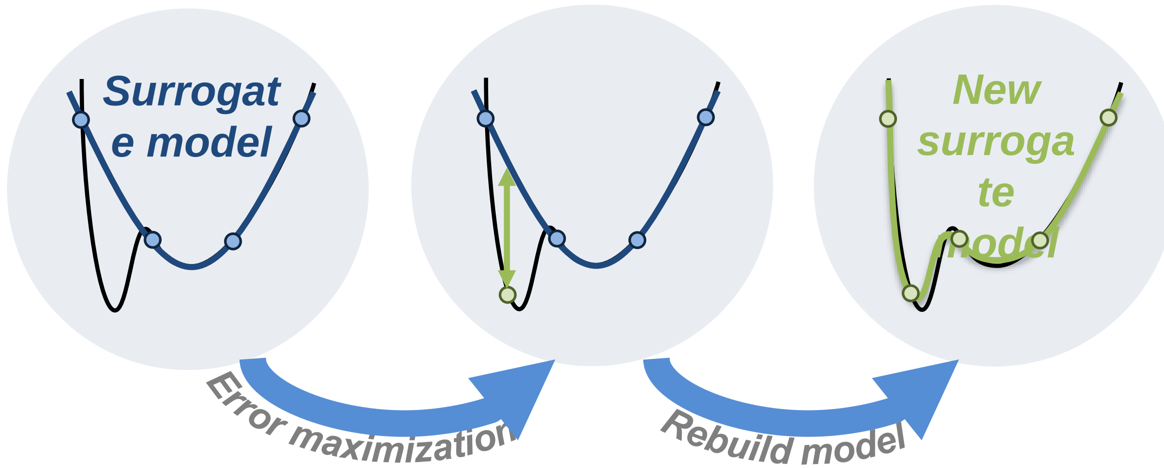
Normalized test error



$$\begin{bmatrix} \text{Number of} \\ \text{terms in model} \end{bmatrix} - \begin{bmatrix} \text{True number} \\ \text{of terms} \end{bmatrix}$$

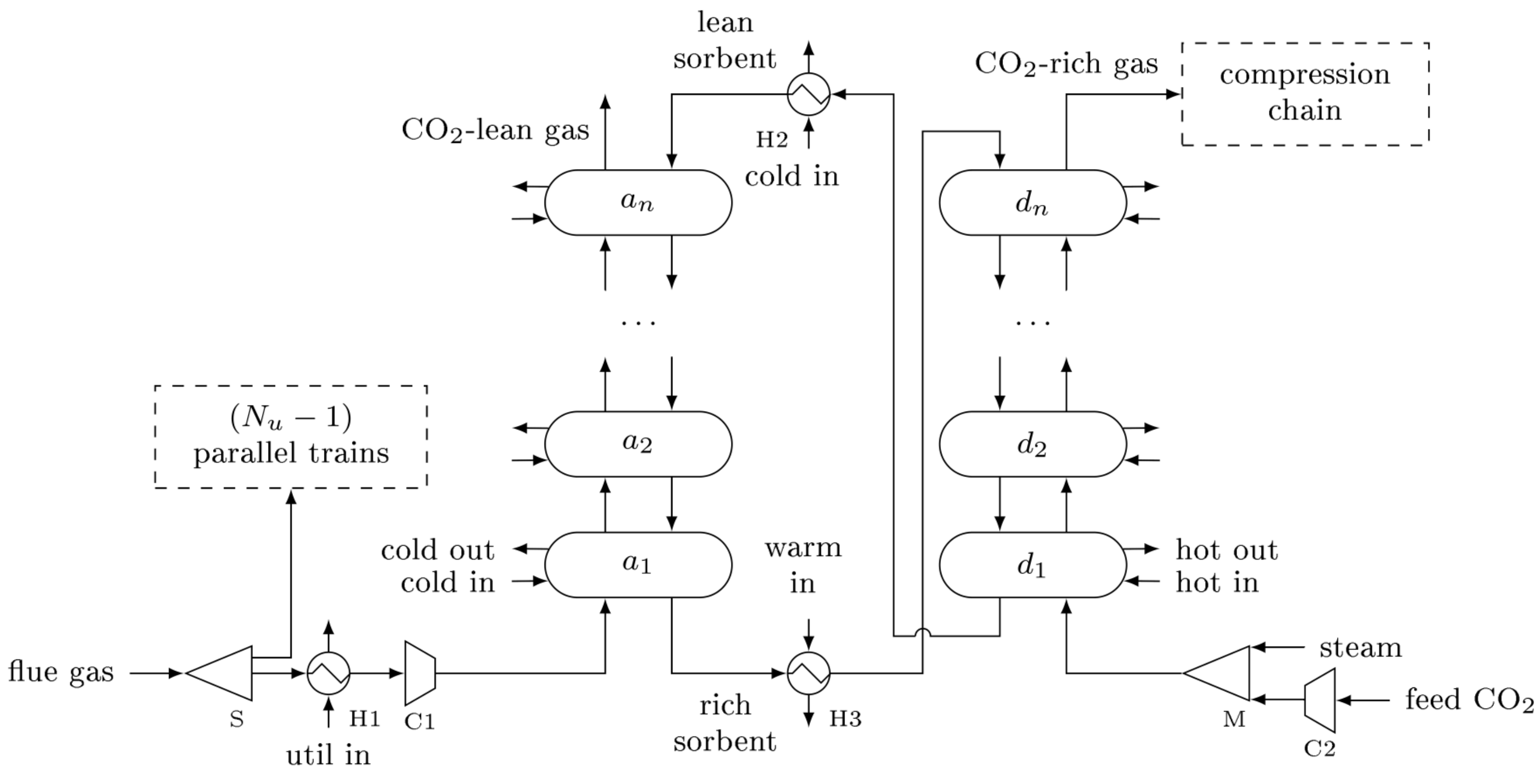
Results over a test set of 45 known functions treated as black boxes with bases that are available to all modeling methods.

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

Carbon capture system design

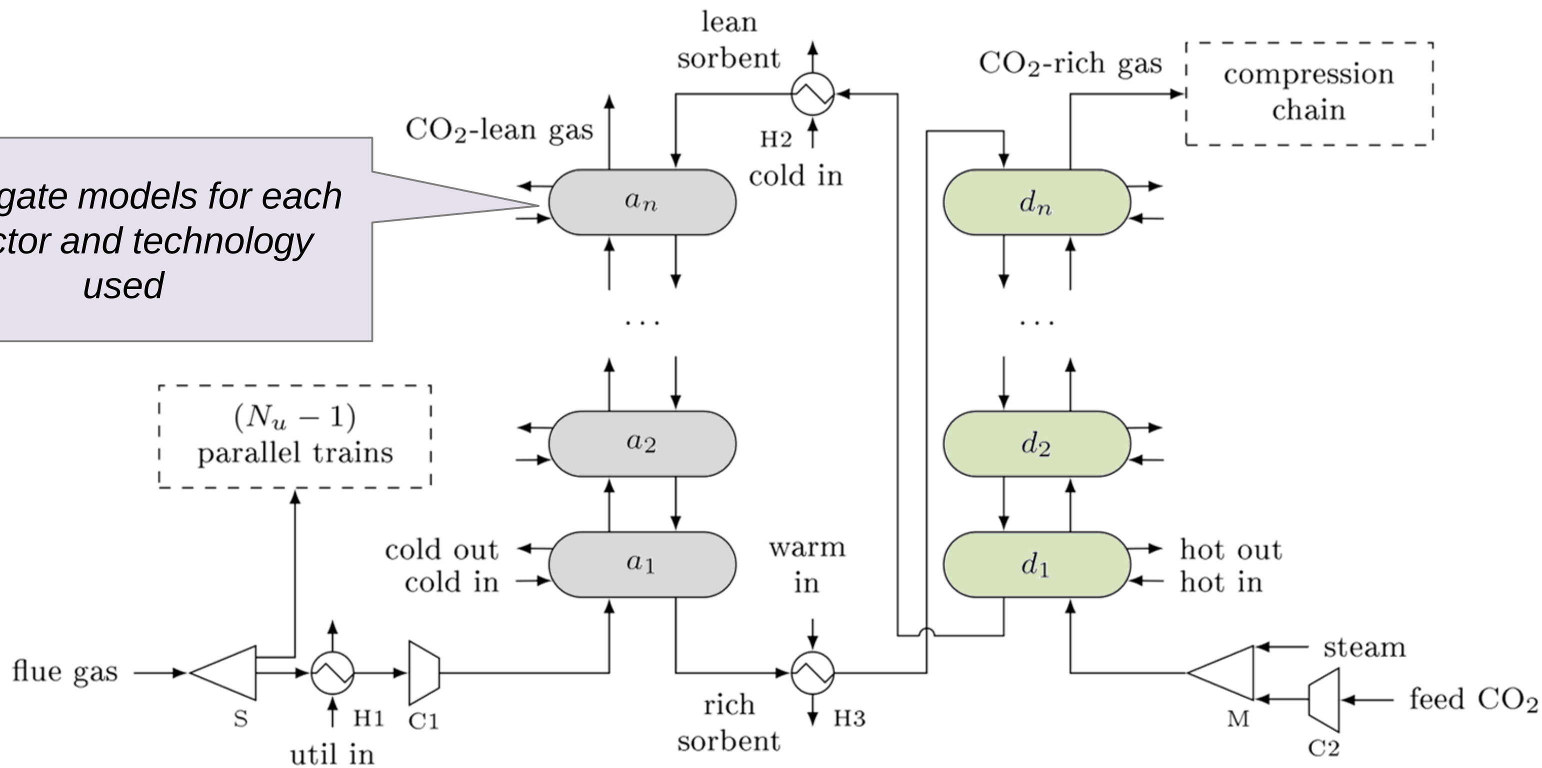


- Post combustion carbon capture design and optimization
- Minimize increased cost of electricity [Black et al., 11]
  - Subject to 90% carbon capture

Simulations, cost models, superstructure, and surrogate models were developed as part of the DOE Carbon Capture Simulation Initiative

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

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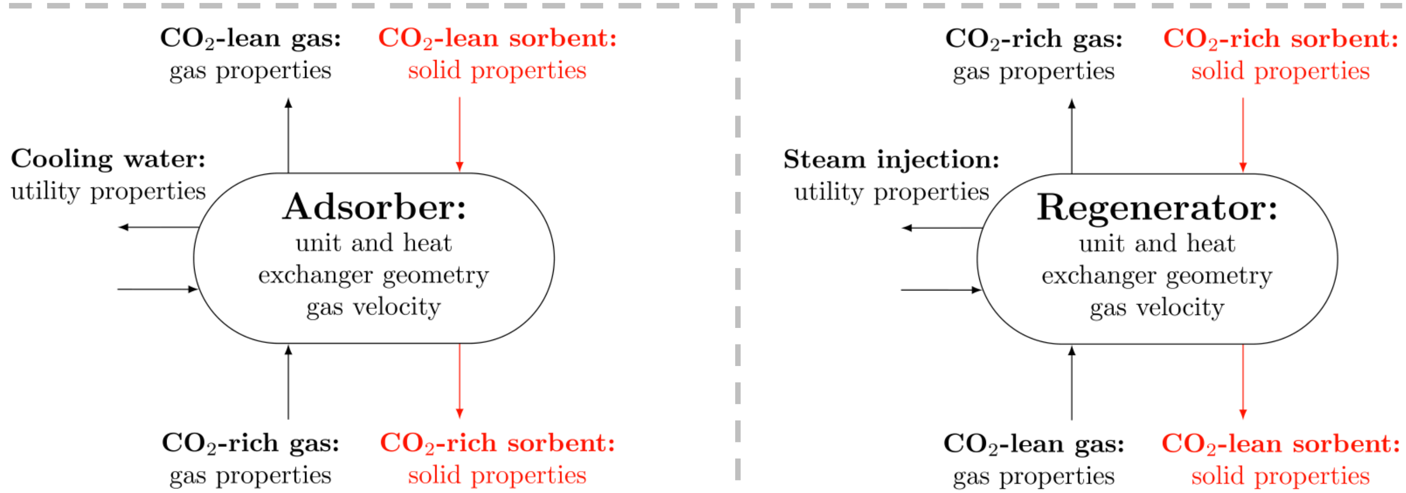
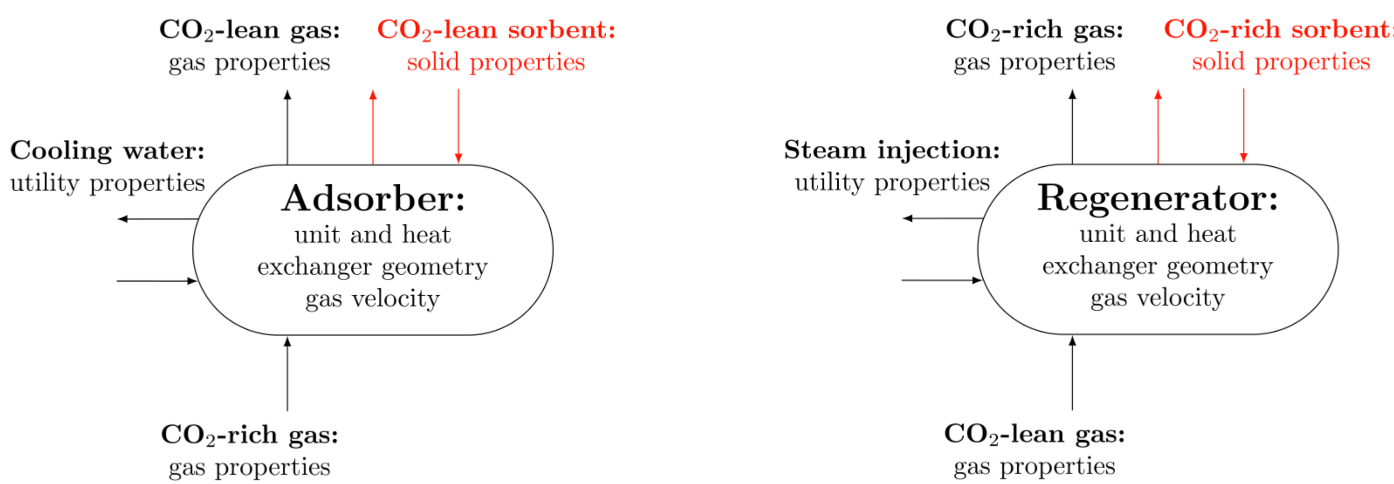
Carbon Capture Reactors

Adsorber | Regenerator

Underflow configuration



Overflow configuration



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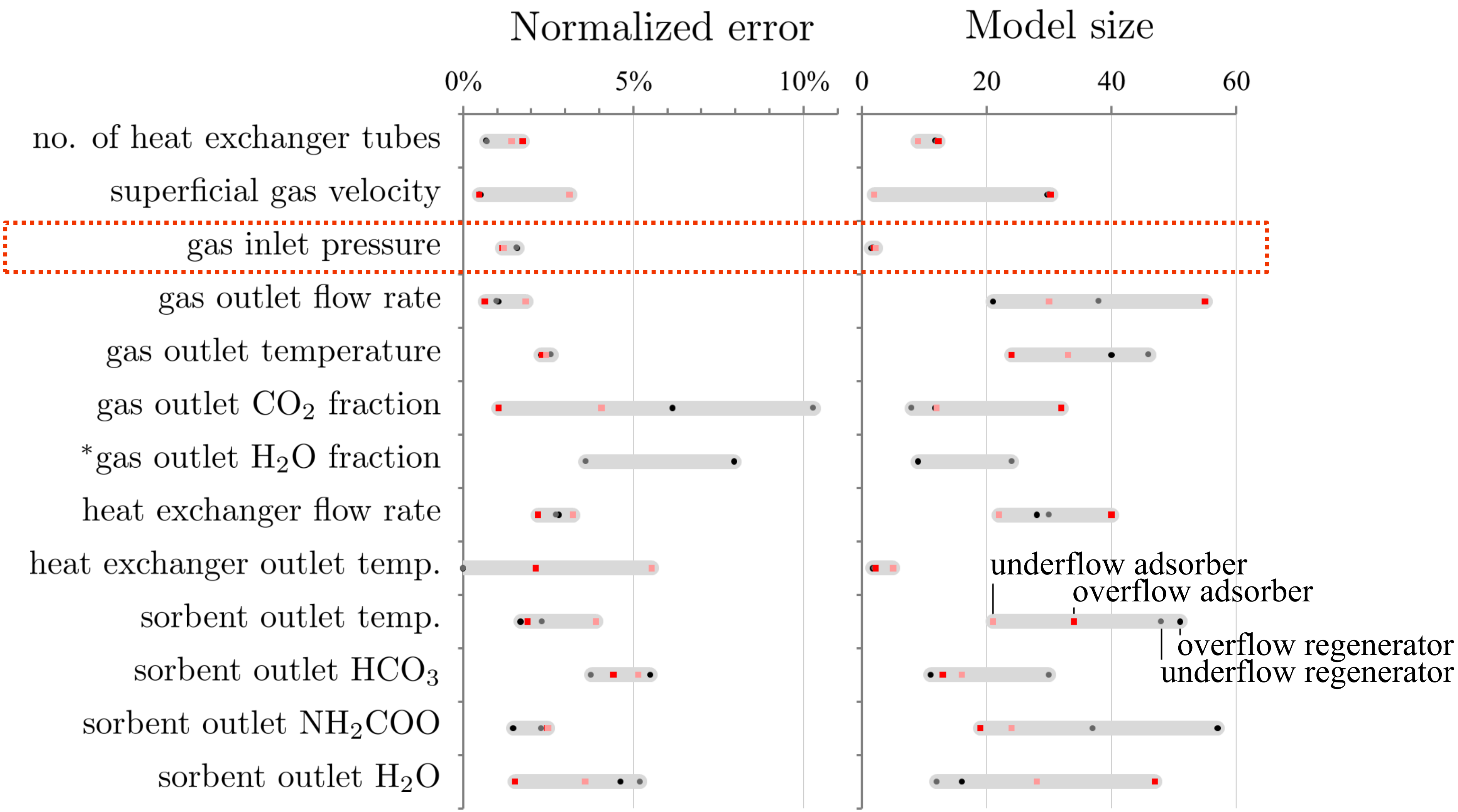
Surrogate Results



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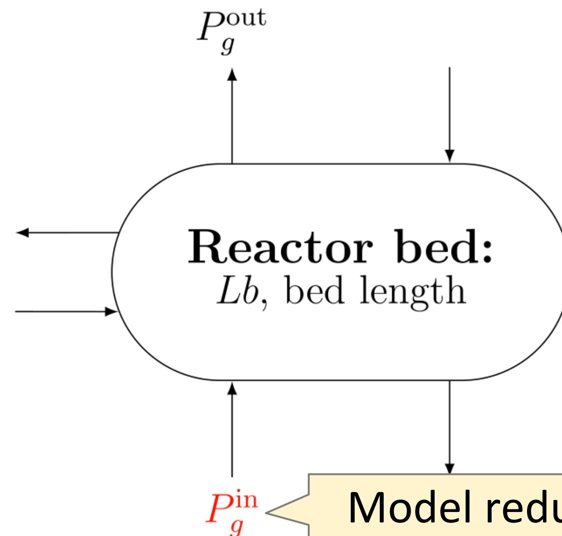
Inlet Gas Pressure Models

Example models for the inlet pressure of the gas stream.

Original input variables:
13 – 14

Potential number of terms:
1,071 – 1,140



Model reduced from 13-14 dimensions to **2 dimensions**

Flow regime	Range of P_g^{in}	Error, RMSE	Model, $\hat{P}_g^{\text{in}}$
Adsorbers:			
Overflow	[1.0784,1.5762]	0.00791	$0.5217 \exp(P_g^{\text{out}}/1.4) + 0.016063\, Lb\, P_g^{\text{out}}$
Underflow	[1.0786,1.5763]	0.00791	$0.5216 \exp(P_g^{\text{out}}/1.4) + 0.016096\, Lb\, P_g^{\text{out}}$
Regenerators:			
Overflow	[1.0996,1.4781]	0.00440	$0.4852 \exp(P_g^{\text{out}}/1.4) + 0.018412\, Lb\, P_g^{\text{out}}$
Underflow	[1.0995,1.4783]	0.00451	$0.4851 \exp(P_g^{\text{out}}/1.4) + 0.018346\, Lb\, P_g^{\text{out}}$

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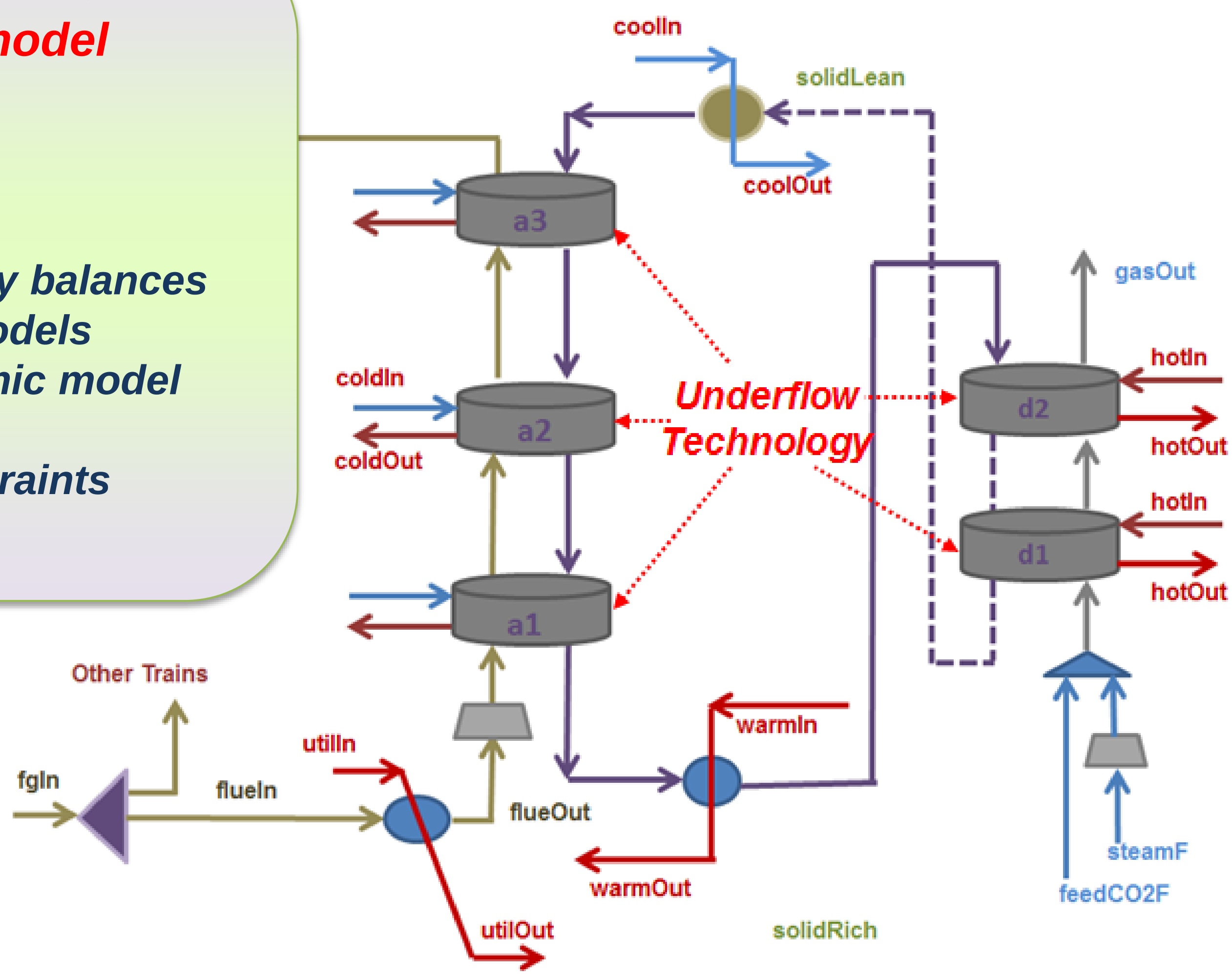
SUPERSTRUCTURE OPTIMIZATION

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

conclusions

- ALAMO generates algebraic models that are accurate and simple
  - Highly amenable to algebraic optimization
- Adaptive sampling allows models to be generated from a minimal number of function evaluations
  - Very important for high cost simulations or experiments
- Surrogate models can be incorporated into larger superstructure optimization problems to intelligently design process systems

Acknowledgements

- Nick Sahinidis
- Alison Cozad
- David Miller & CCSI