What's in the Box?

Systematic approaches for inferring algebraic models from experimental data or simulations

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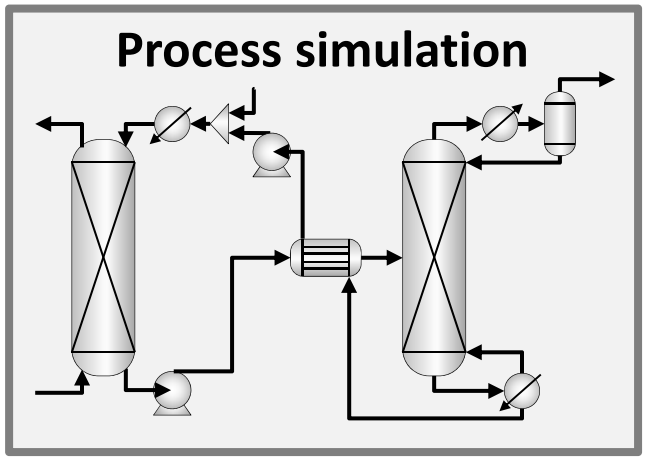
LEARNING PROBLEM

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

$$x \in \mathbb{R}^D \qquad x^l \leq x \leq x^u \qquad \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_d \\ \vdots \\ x_D \end{pmatrix}$$



$$\begin{pmatrix} z_1 \\ z_2 \\ \vdots \\ z_k \\ \vdots \\ z_K \end{pmatrix} \qquad z \in \mathbb{R}^K \qquad z = f(x)$$

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

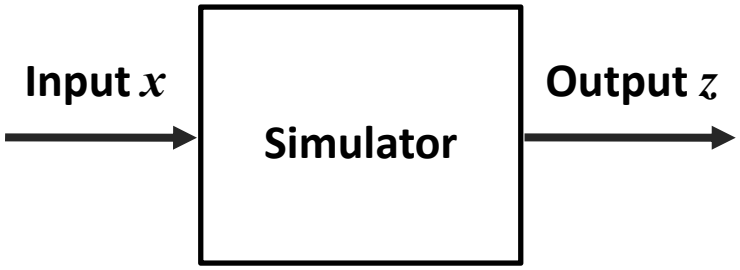
Dependent variables:
Efficiency, outlet flow conditions, conversions, heat flow, etc.

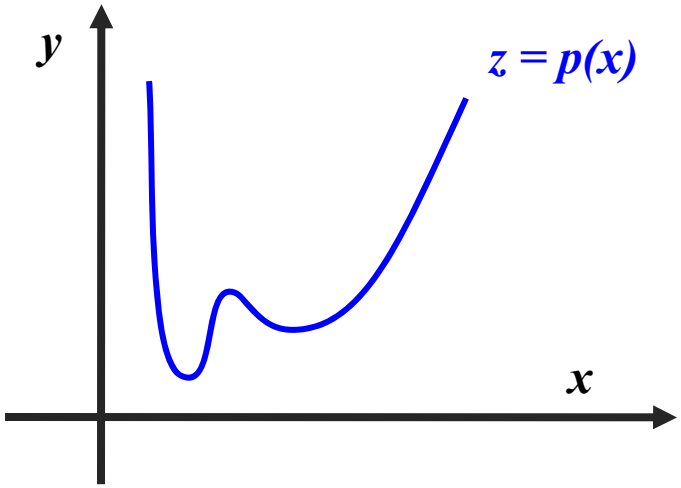
OUTLINE

- Polynomial chaos expansion
  - Best subset selection method
  - Application in risk assessment
- ALAMO: Automatic Learning of Algebraic Models for Optimization
  - Best subset selection method
  - Adaptive sampling
  - Comparisons with least squares and the lasso
  - Application in optimization

POLYNOMIAL CHAOS EXPANSION

- **Build polynomial surrogate models of a given simulator**





Polynomial chaos expansion:

$$z = P(\boldsymbol{x}) = \alpha_0 B_0 + \sum_{j=1}^{M} \alpha_j B_1(x_j) + \sum_{j=1}^{M} \sum_{k=1}^{j} \alpha_{jk} B_2(x_j, x_k) + \sum_{j=1}^{M} \sum_{k=1}^{j} \sum_{h=1}^{k} \alpha_{jkh} B_3(x_j, x_k, x_h) + \ldots$$

Key steps:

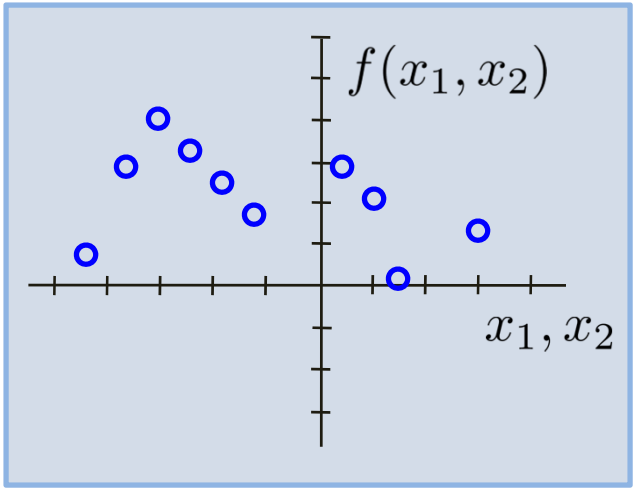
- Choose basis functions $\boldsymbol{B}$
- Determine coefficients $\boldsymbol{\alpha}$

OVERVIEW OF PCE METHODS

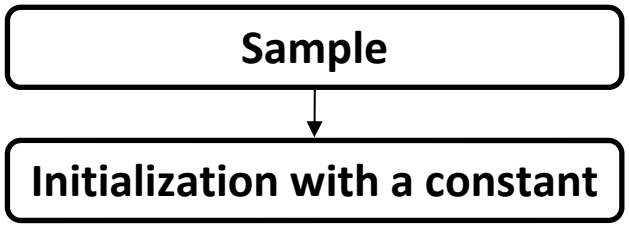
- **Intrusive PCE methods (Xiu and Karniadakis, 2003)**
  - **Substitute PCE's into partial differential equations**
  - **Solve new equations for coefficients**
- **Nonintrusive PCE methods (Webster *et al.,* 1996, Isukapalli *et al.,* 1998, Ghiocel and Ghanem, 2002, Li and Zhang, 2007, Eldred and Burkardt, 2009, Blatman and Sudret, 2010, Oladyshkin *et al.,* 2011)**
  - **No manipulation of partial differential equations**
  - **Estimate coefficients by projection**
  - **Estimate coefficients by fitting curves**

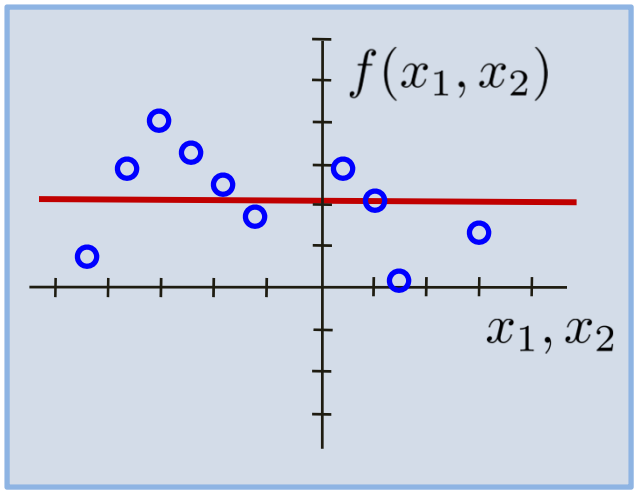
PROPOSED PCE ALGORITHM

Sample



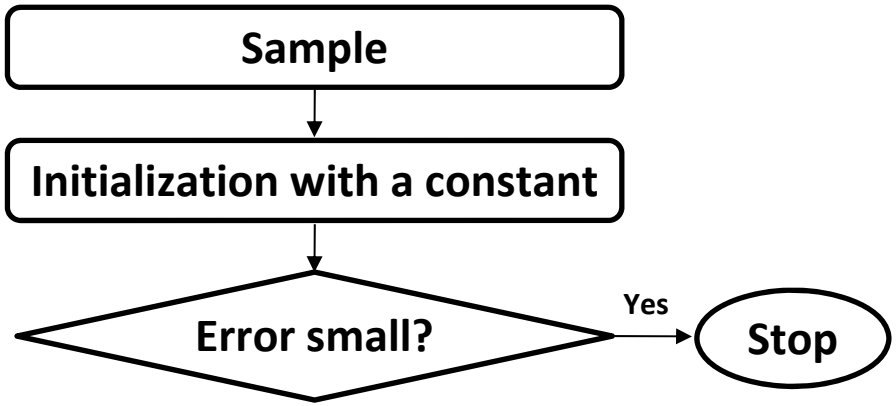
PROPOSED PCE ALGORITHM

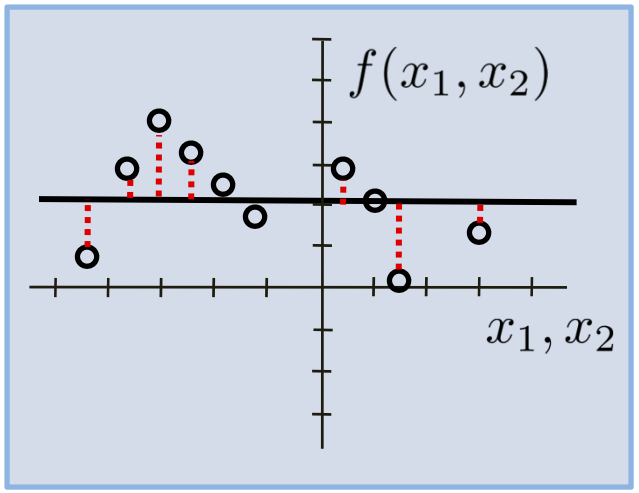




z = constant

PROPOSED PCE ALGORITHM

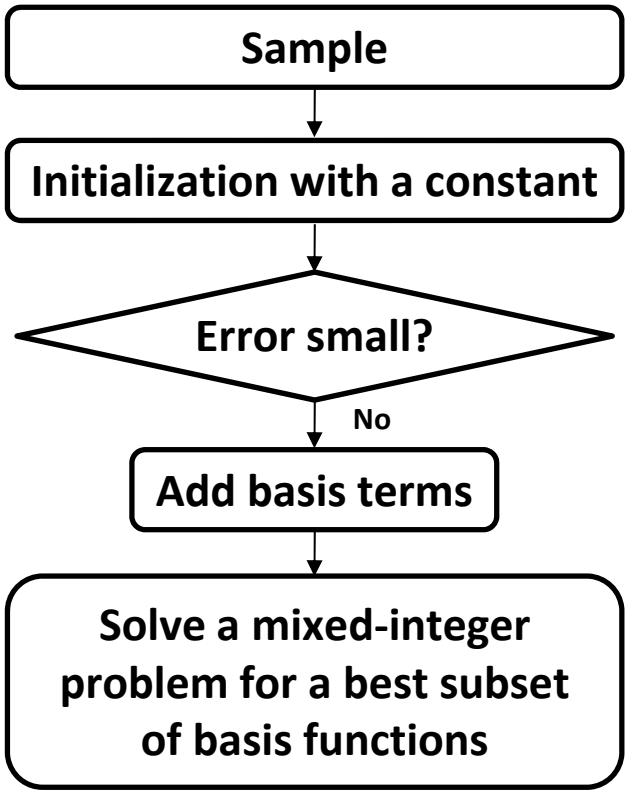




z = constant

Error = ($z_{surrogate} - z_{simulation}$)^2

PROPOSED PCE ALGORITHM



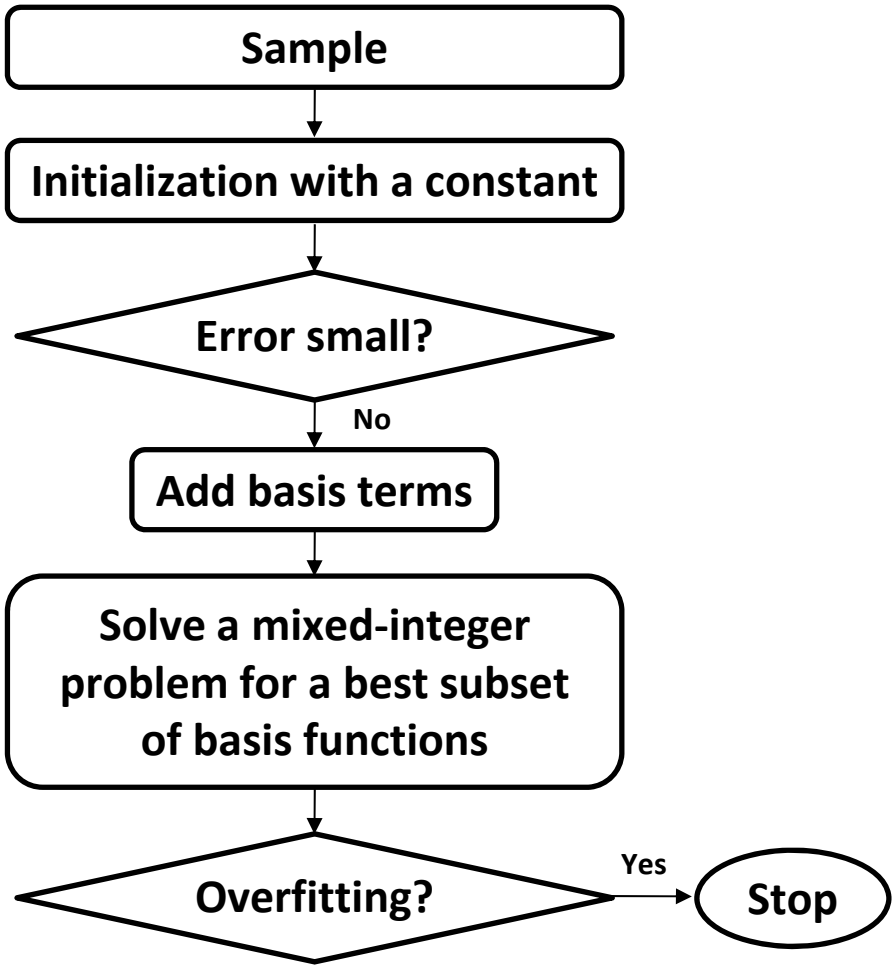
Add higher-order terms to current PCE:

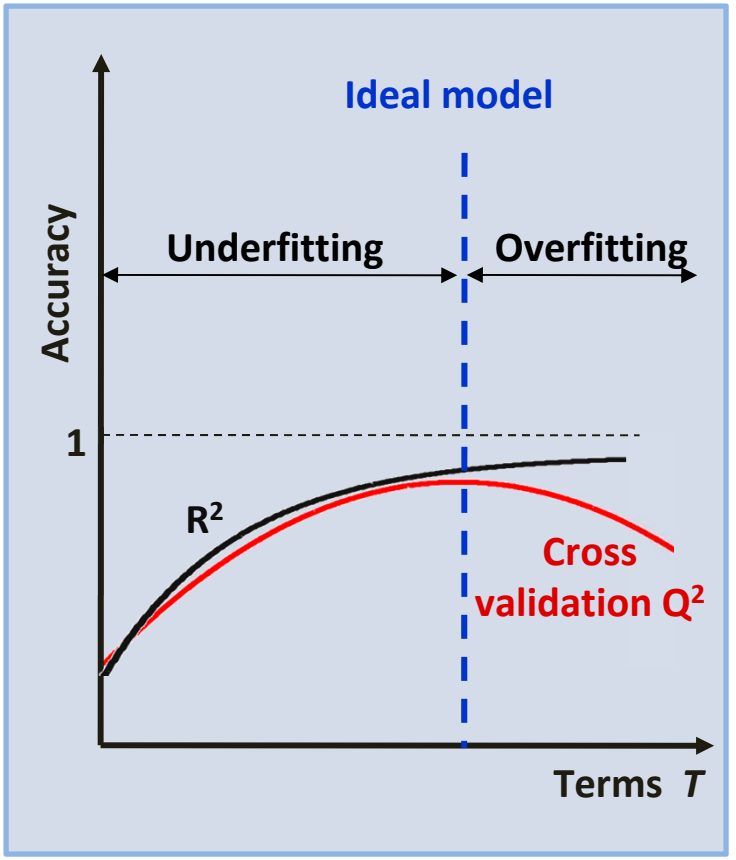
$$z = \alpha_0 + \alpha_1 x_1 + \alpha_2 x_2$$

Best subset selected by MIP:

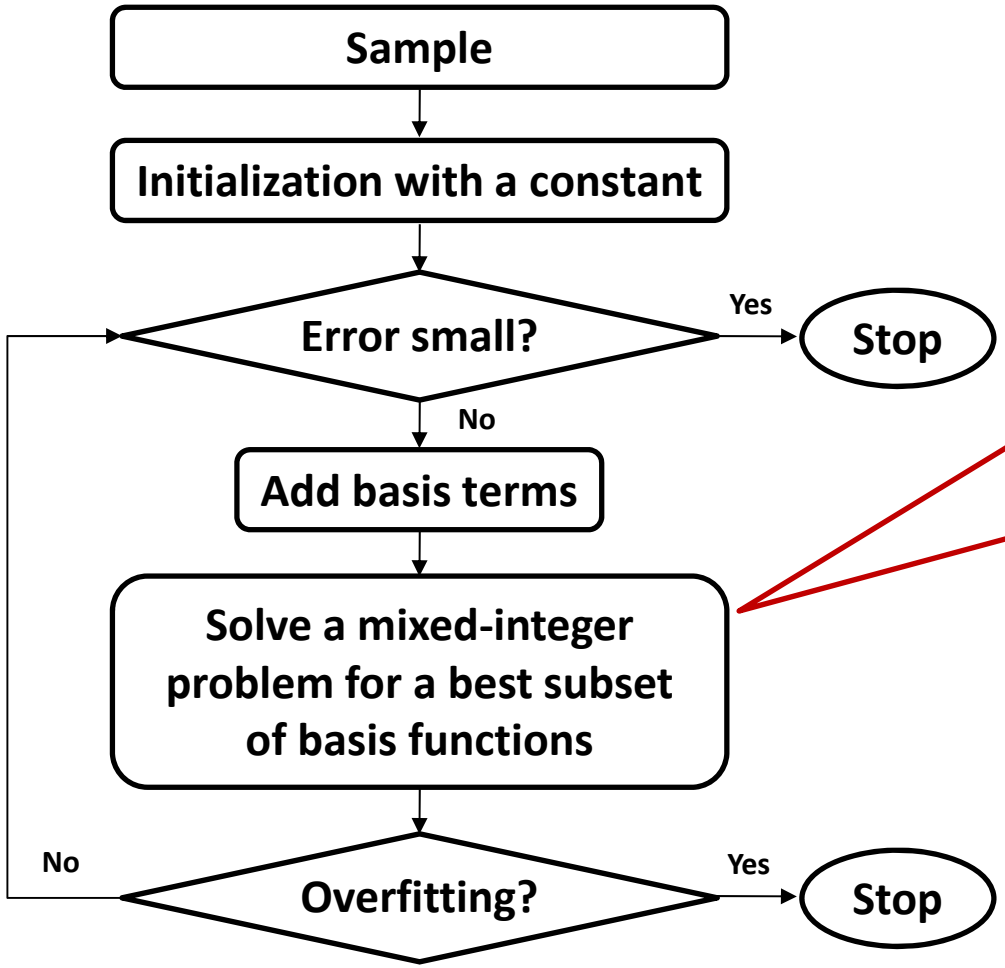
$$z = \alpha_0 + \alpha_2 x_2$$

PROPOSED PCE ALGORITHM





PROPOSED PCE ALGORITHM



Novelty of proposed method:

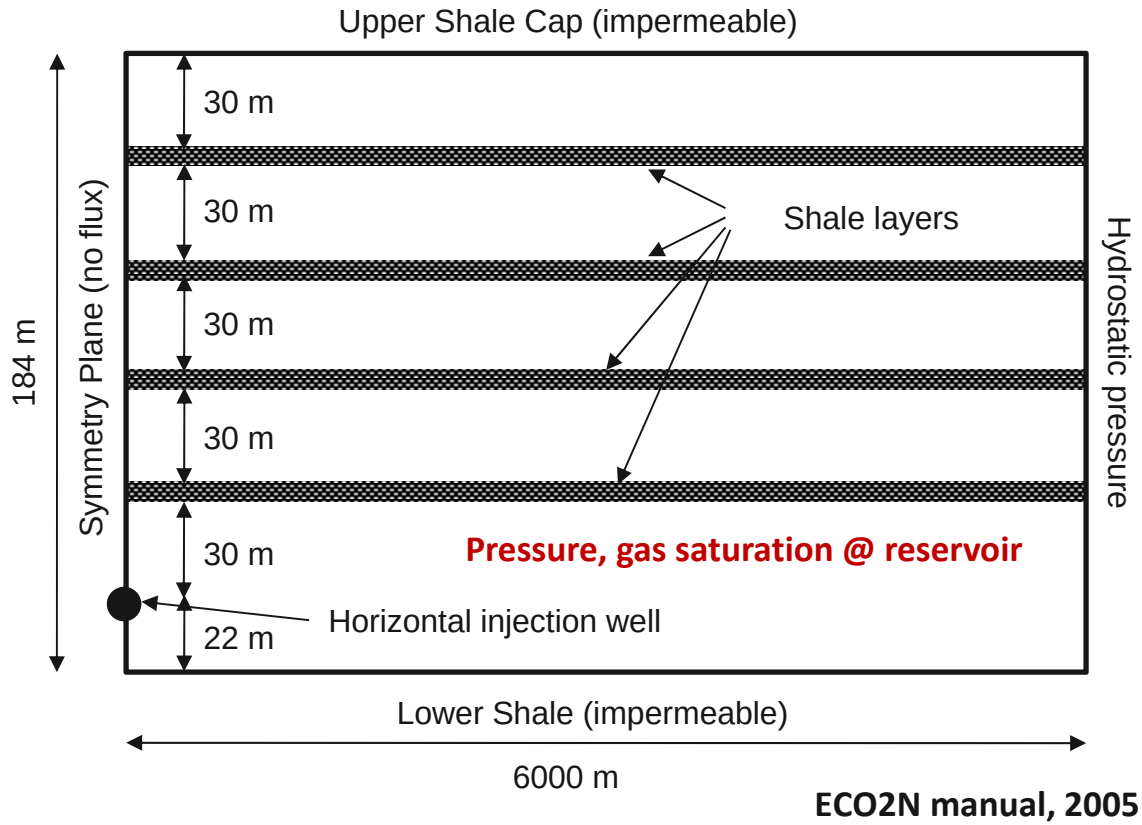
Math programming for basis selection

- **Global optimal subset**
- **Obtains more accurate models**

TESTING ON A BENCHMARK PROBLEM

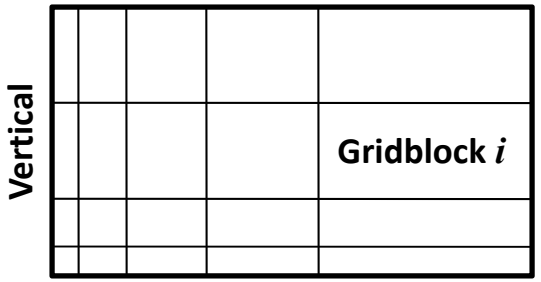
- **CO_2 injection into a deep saline aquifer**
- **Simulated using TOUGH2**

$$\text{mass/pressure/gas saturation} = f\ (\text{porosity, permeability, injection rate})$$

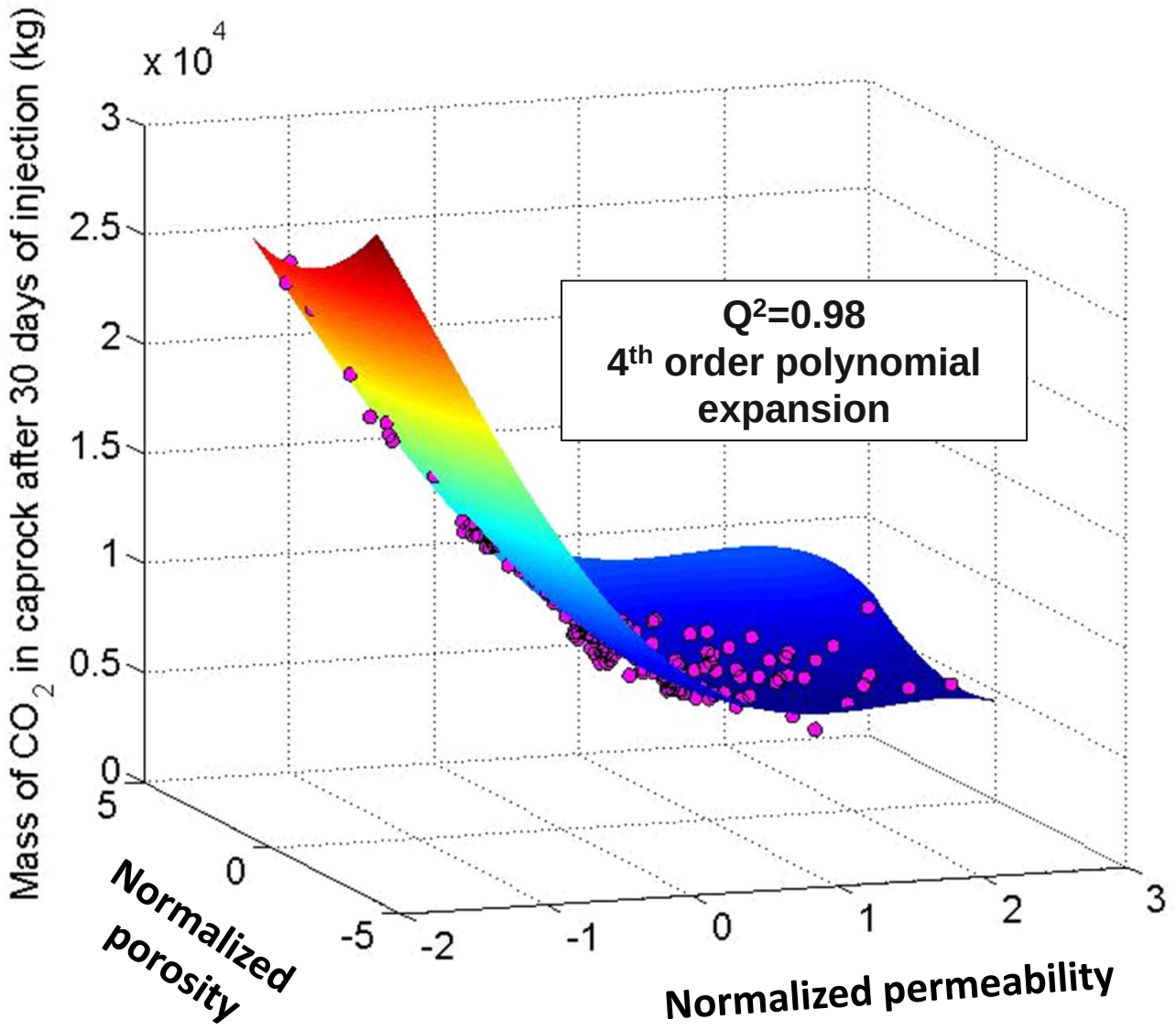


ECO2N manual, 2005

986 gridblocks
986 surrogate models for each output



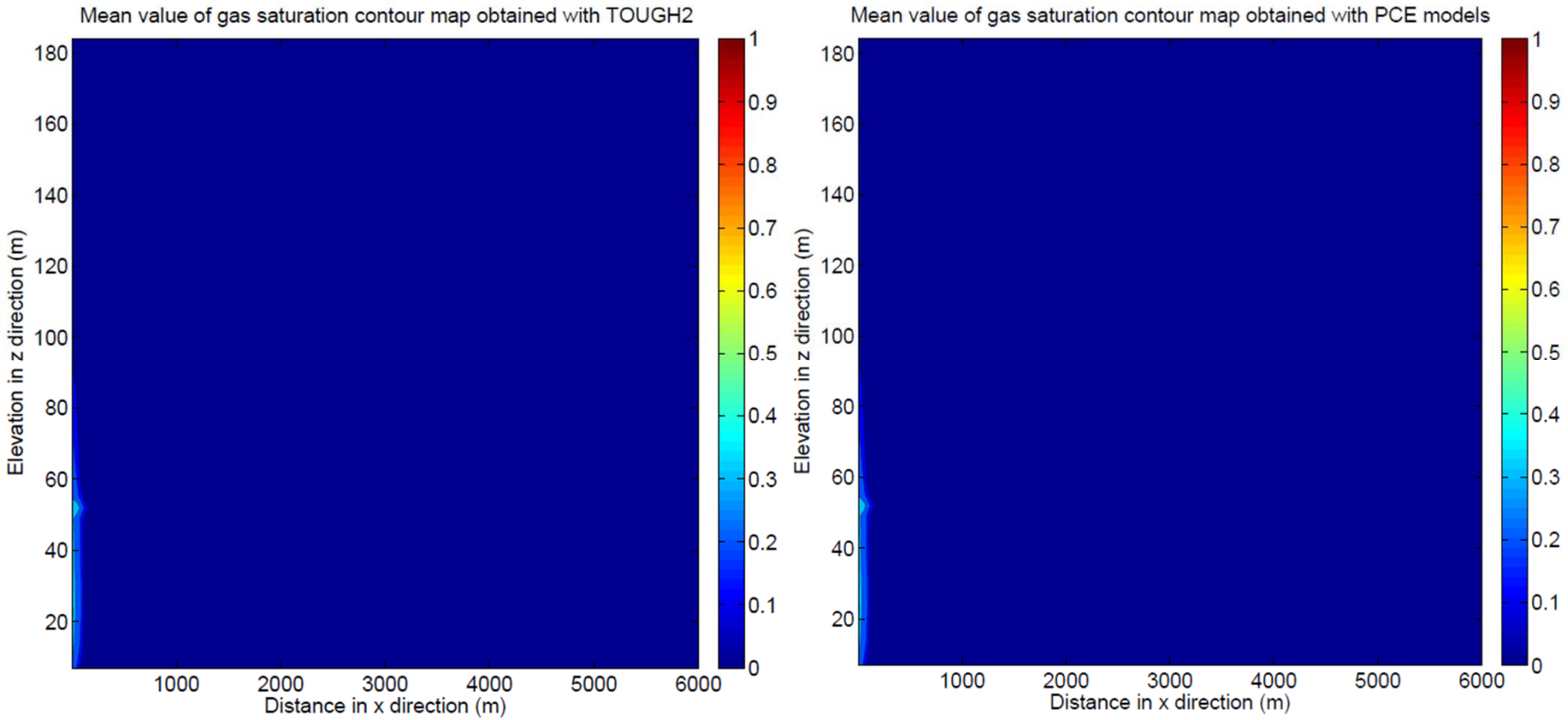
POLYNOMIAL SURROGATE MODEL



COMPARISON AGAINST TOUGH2

For every gridblock i, $i = 1, \ldots, 986$

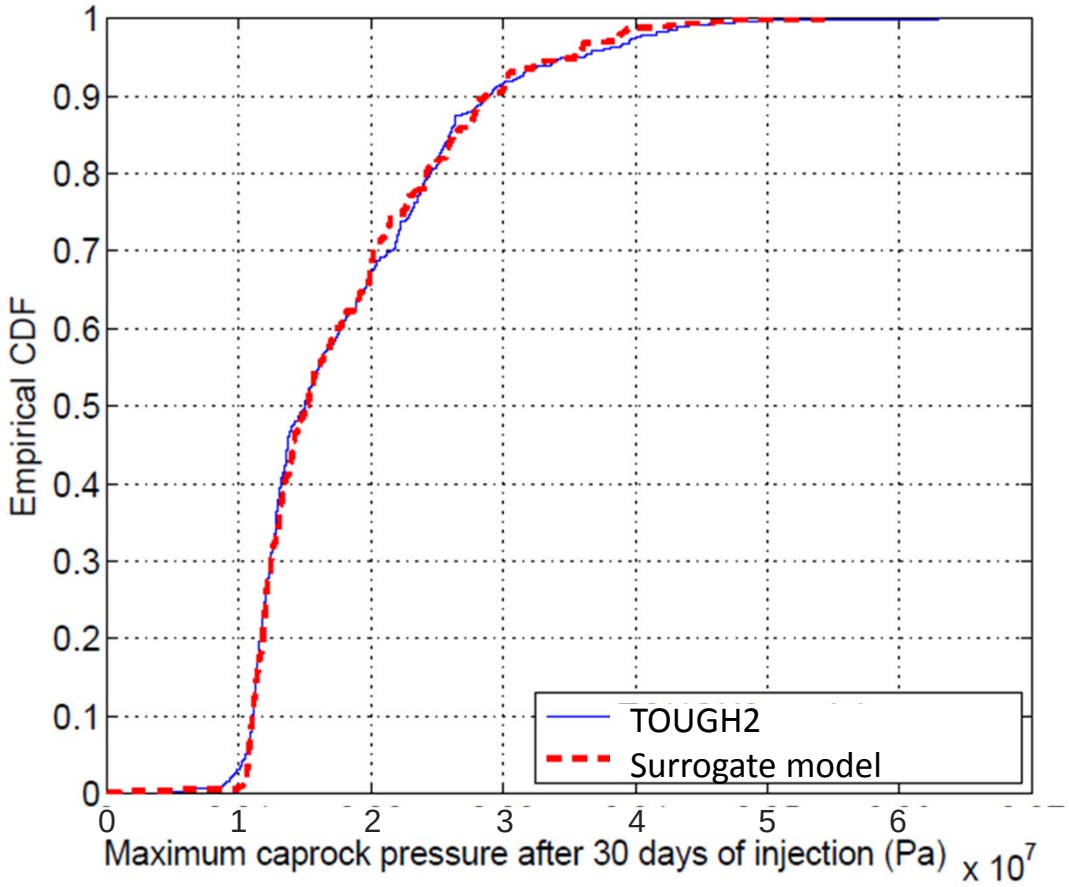
$\mathrm{CO_2}$ saturation in brine $= f_i$ (porosity, permeability, injection rate)



Maximum relative error = 6%

MONTE CARLO SIMULATION

Cumulative probability distribution obtained with 4000 simulations of surrogate models



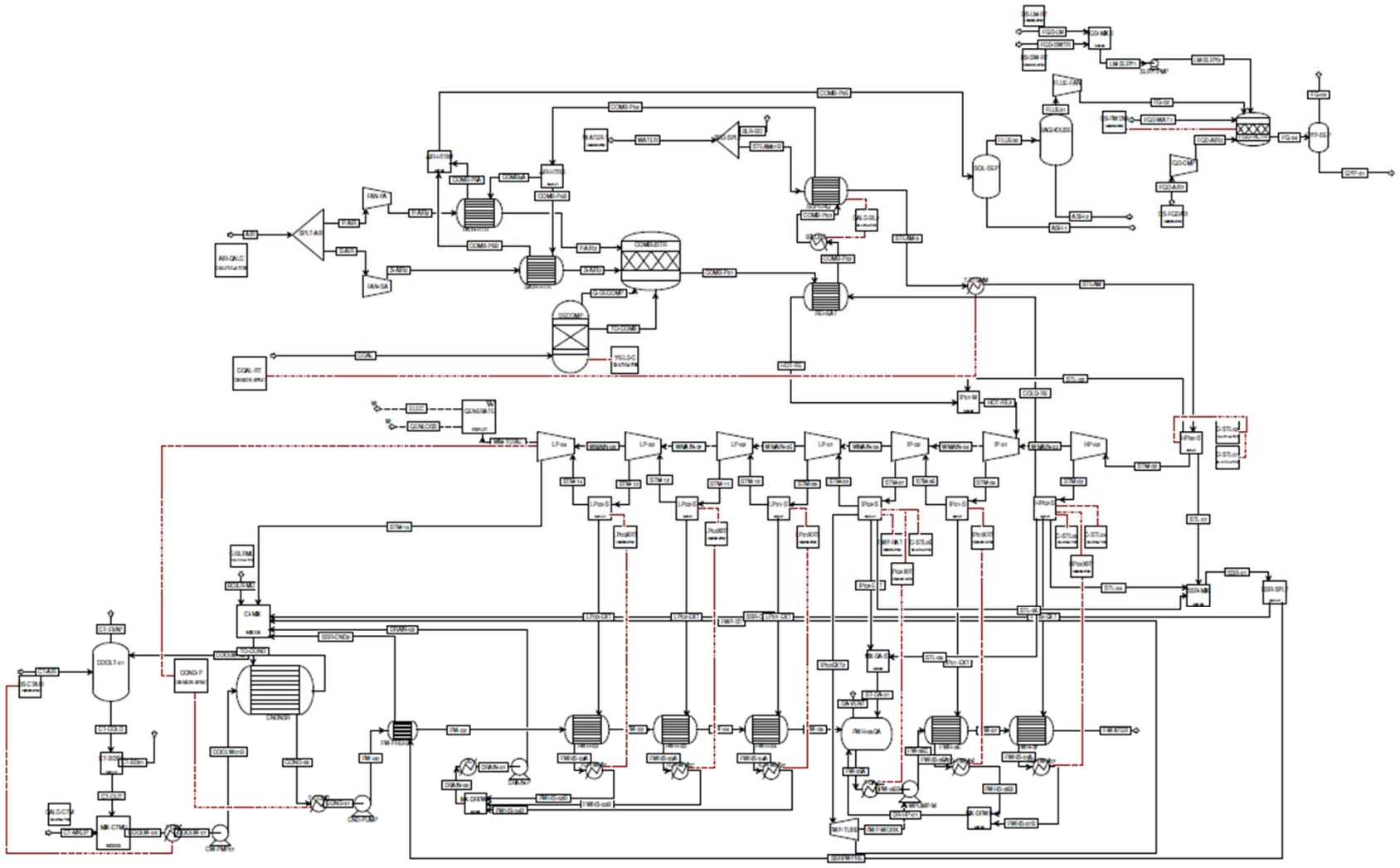
REDUCED-ORDER MODELING GAINS

- **For the benchmark study and SACROC application, surrogate models developed based on the proposed technique were found to be accurate.**

Case	Maximum relative error	CPU time to run surrogates in MATLAB	CPU time to run numerical simulator	Speedup
TOUGH2 Benchmark	6%	30 s	15 mins	10 x
SACROC Oilfield Case	7%	45 s	24 hrs	100 x

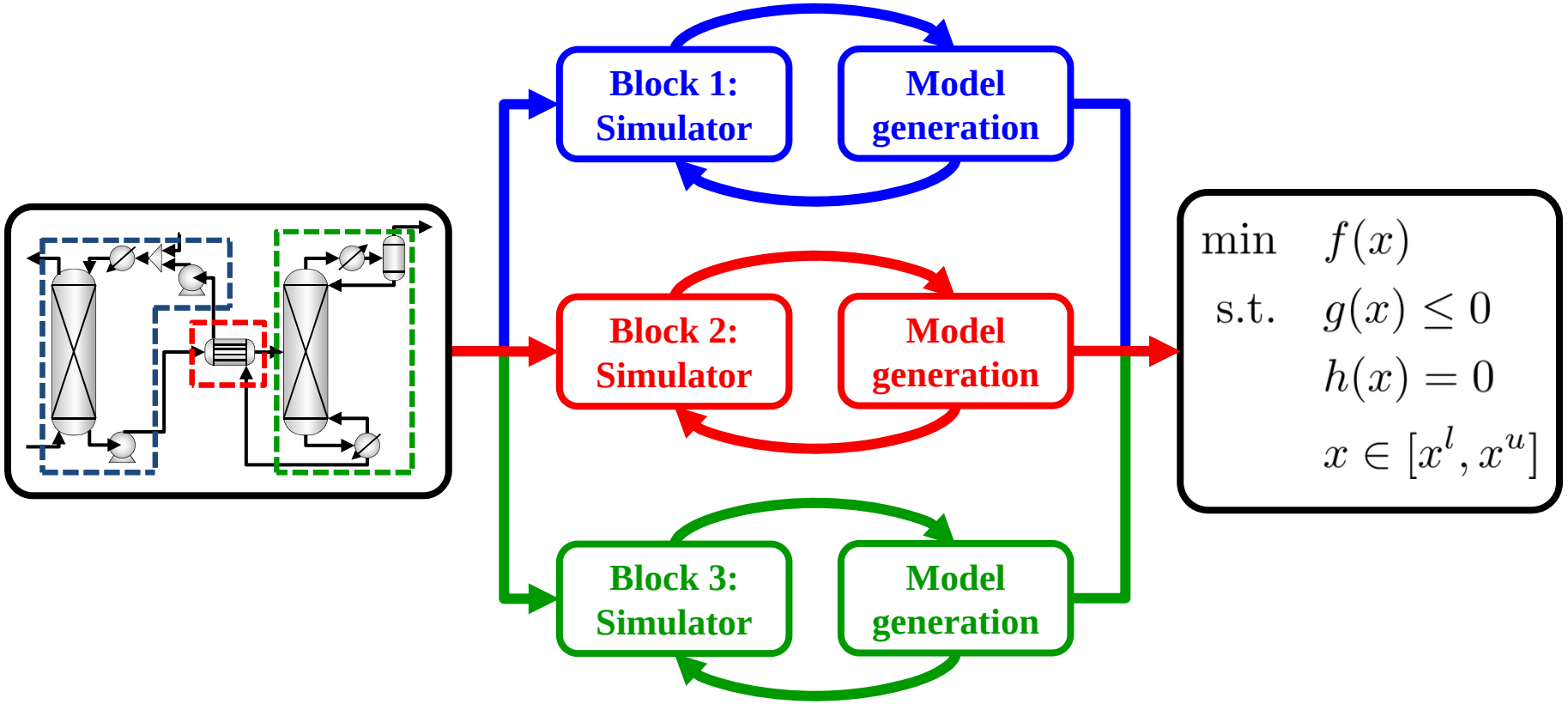
See Zhang and Sahinidis (IECR, 2013)

SIMULATION OPTIMIZATION



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

PROCESS DISAGGREGATION



Process Simulation

Disaggregate process into process blocks

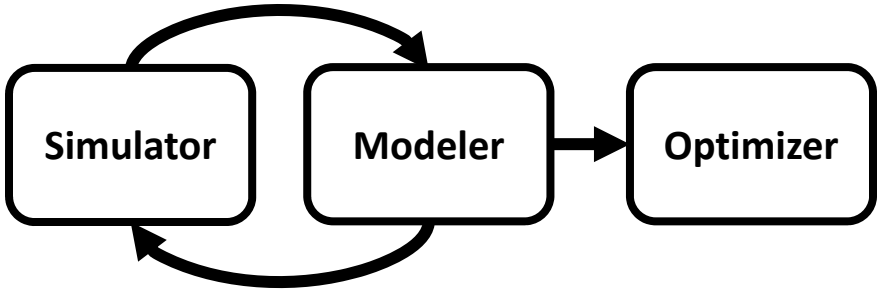
Surrogate Models

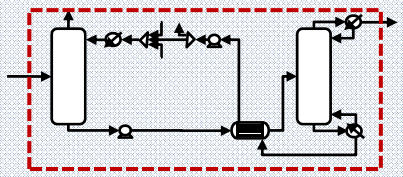
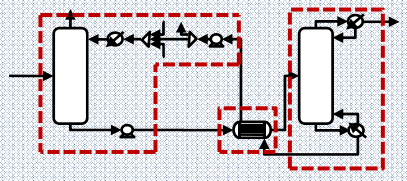
Build simple and accurate models with a functional form tailored for an optimization framework

Optimization Model

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

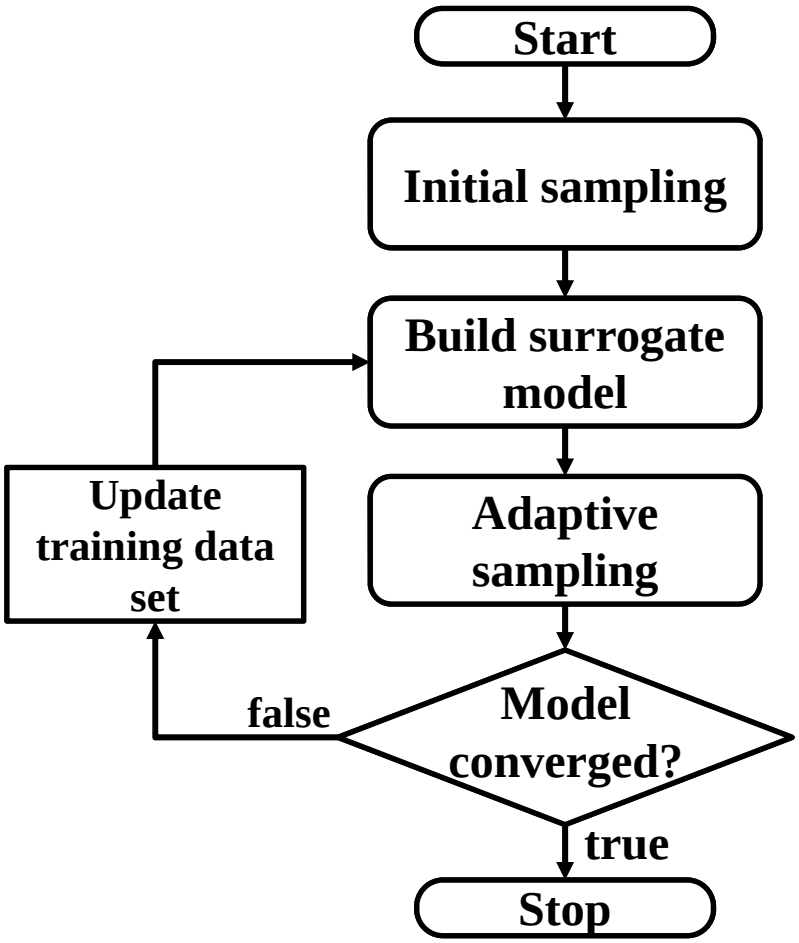
RECENT WORK IN CHEMICAL ENG

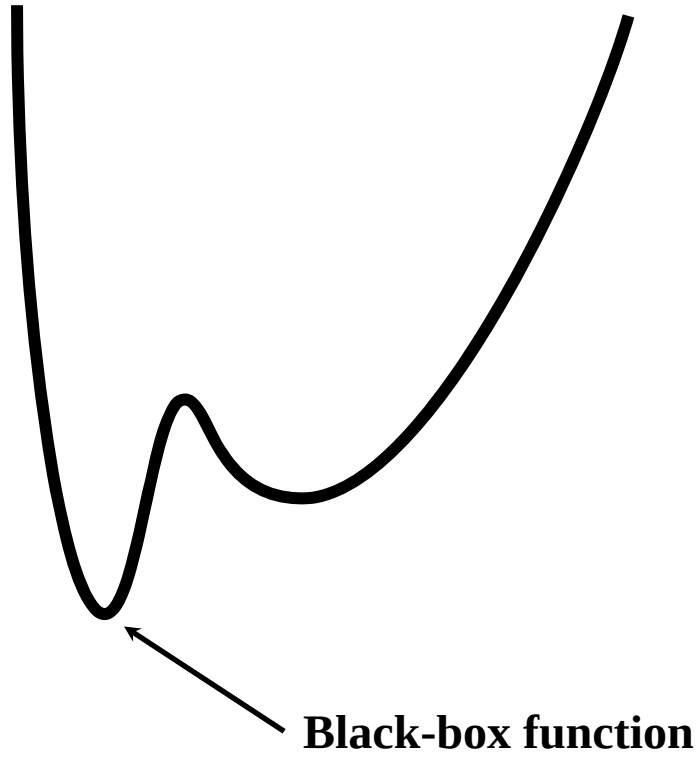


	Kriging	Neural nets	Polynomial-based
Full process 	▪ Palmer and Realff, 2002 ▪ Huang et al., 2006 ▪ Davis and Ierapetritou, 2012	▪ Michalopoulos et al., 2001	▪ Palmer and Realff, 2002
Disaggregated 	▪ Caballero and Grossmann, 2008	▪ Henao and Maravelias, 2011	

ALAMO

Automated Learning of Algebraic Models for Optimization





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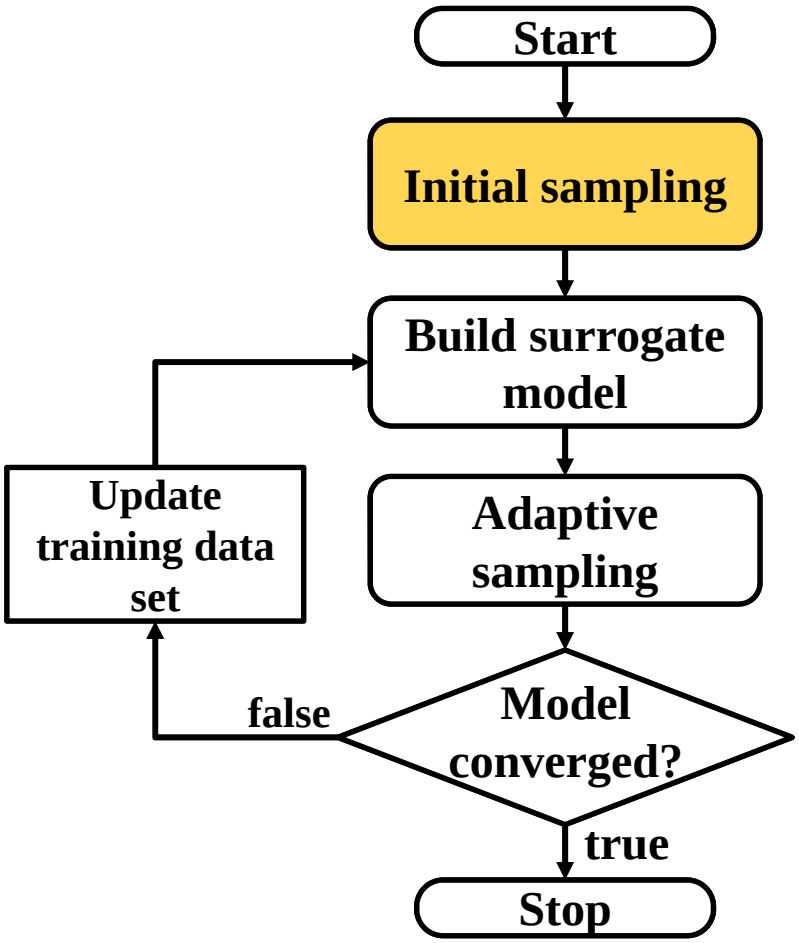

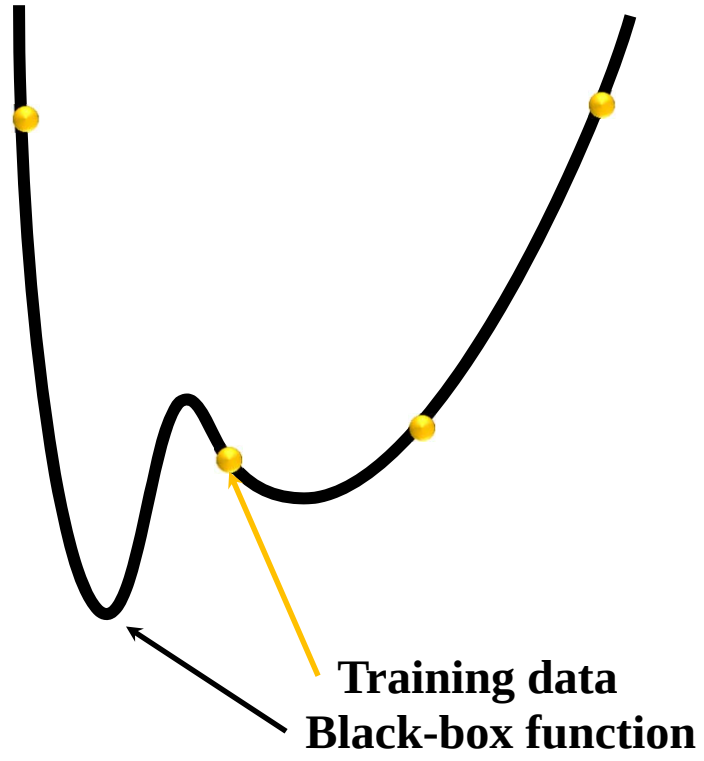

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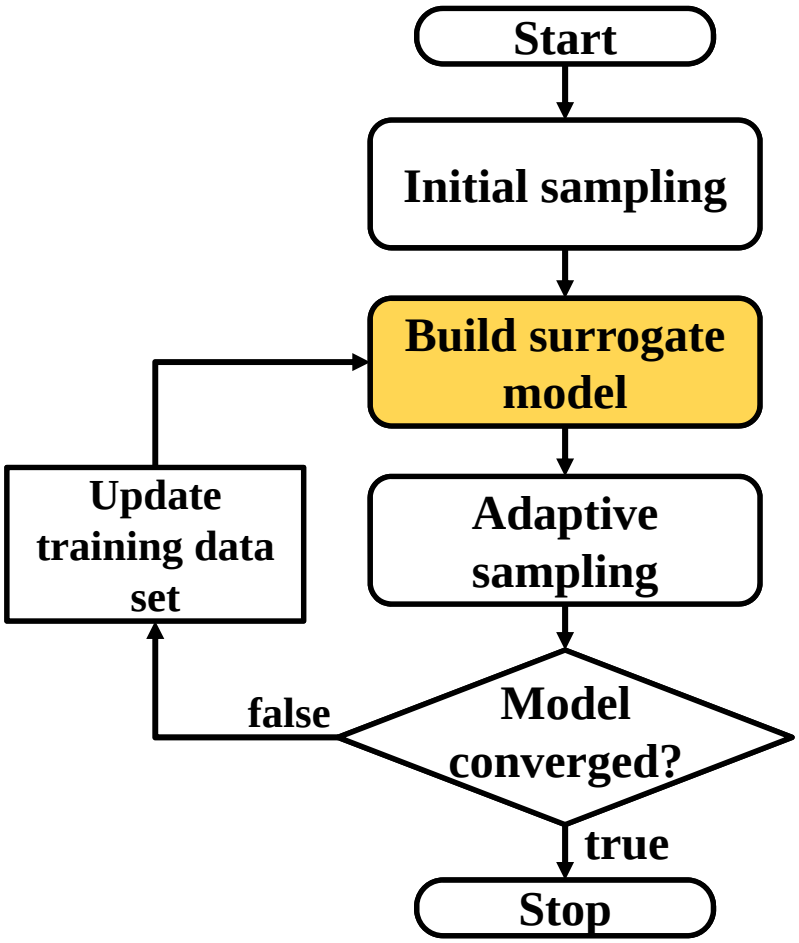

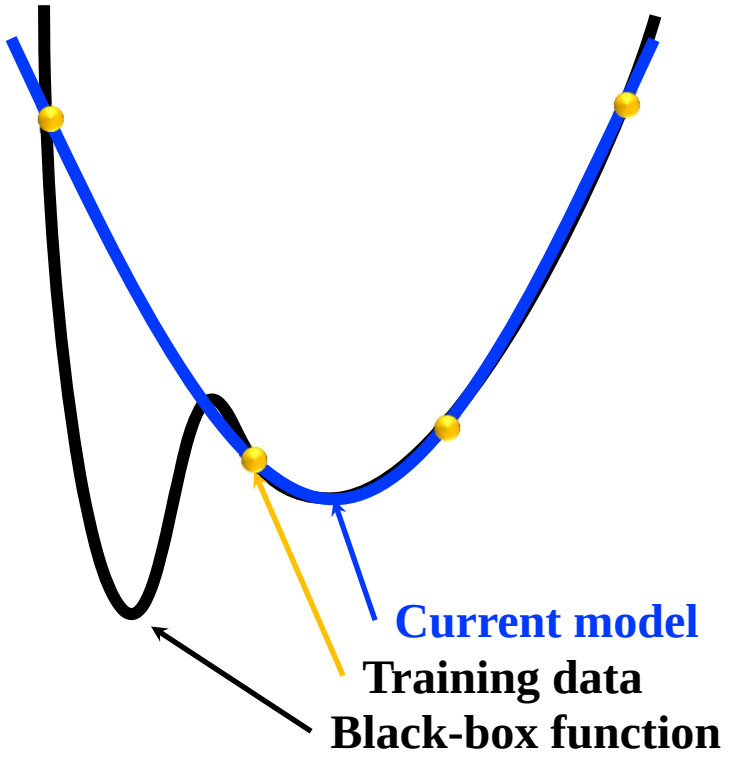

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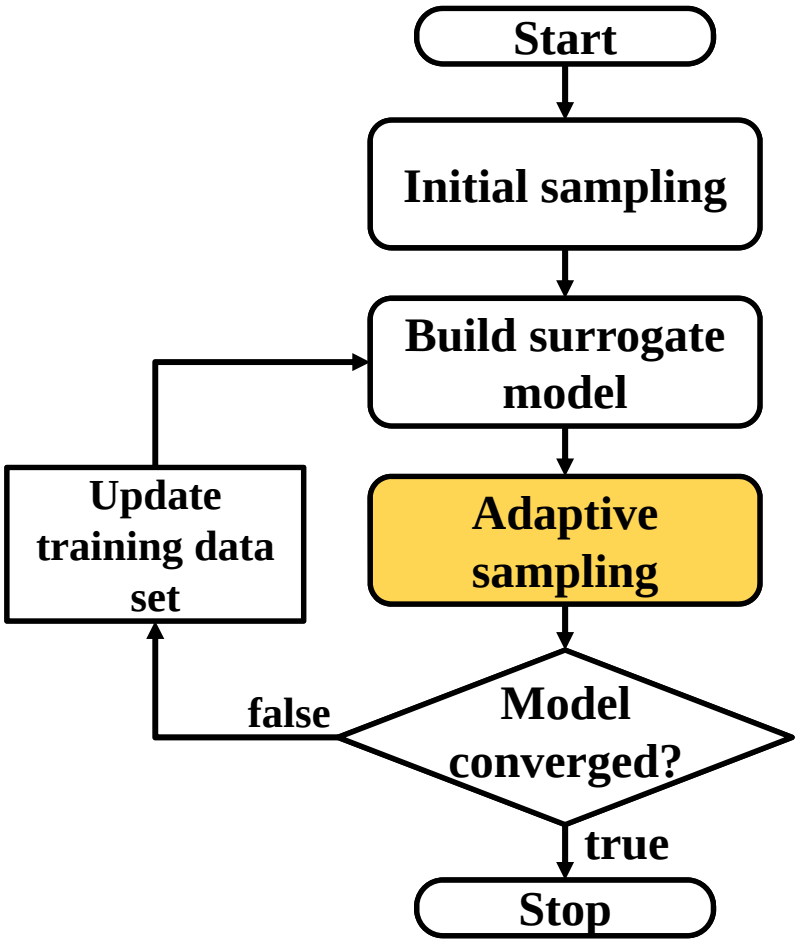

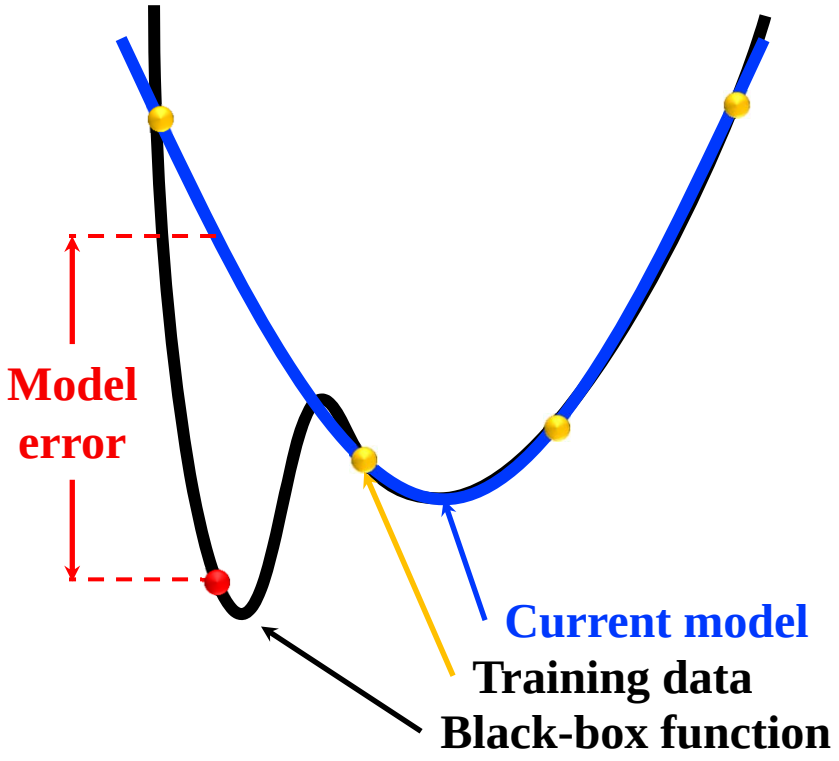

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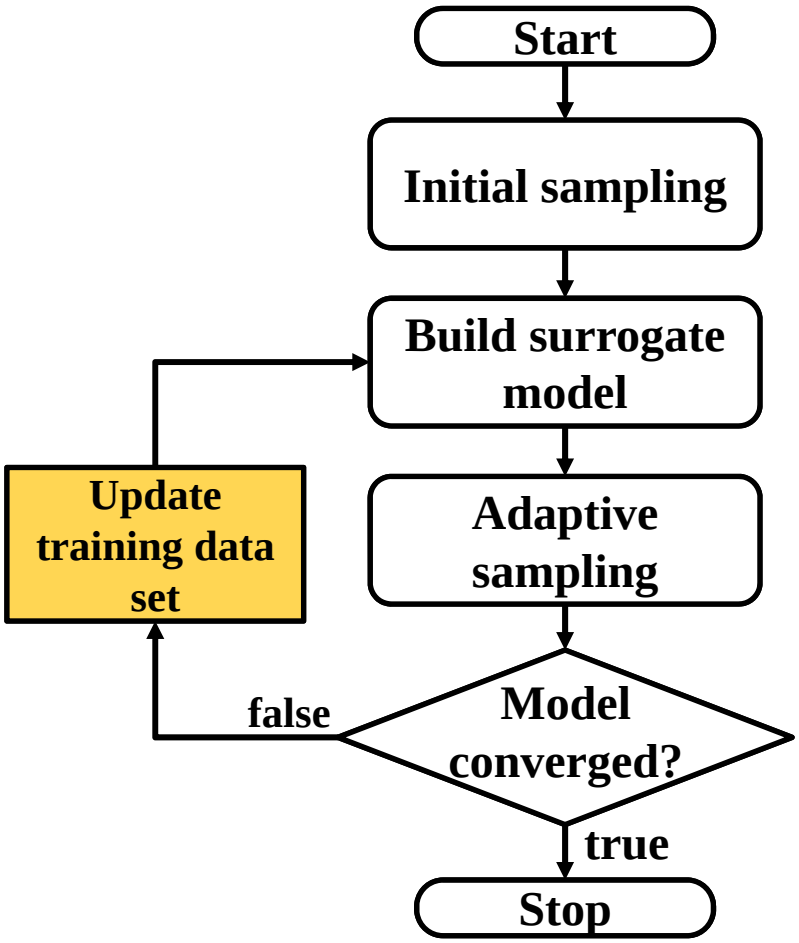

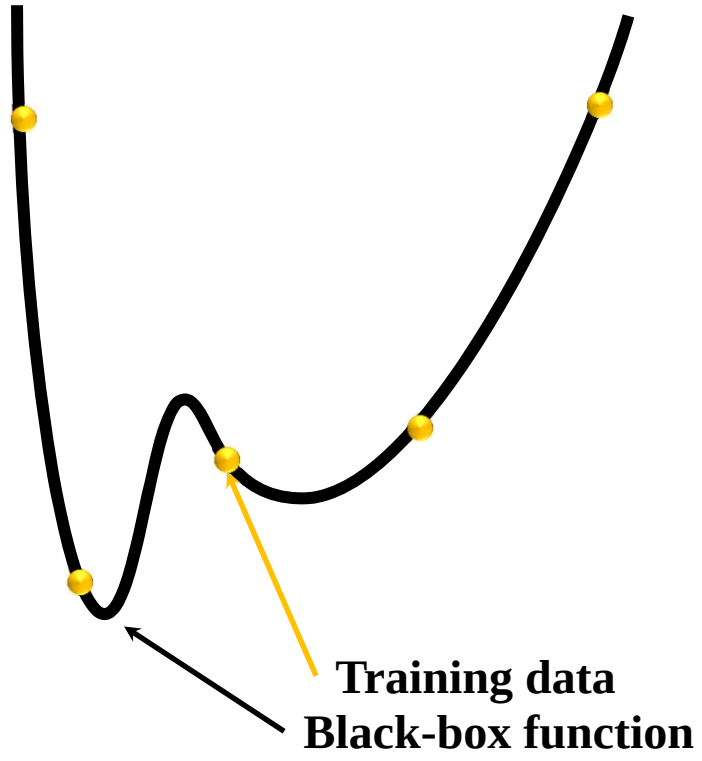

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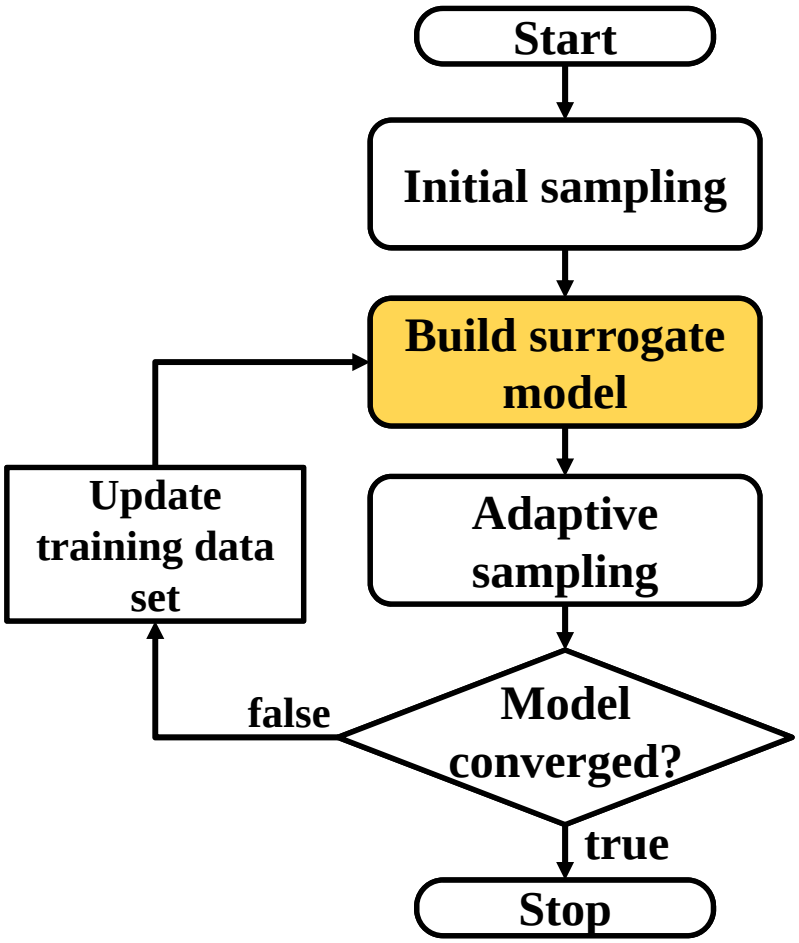

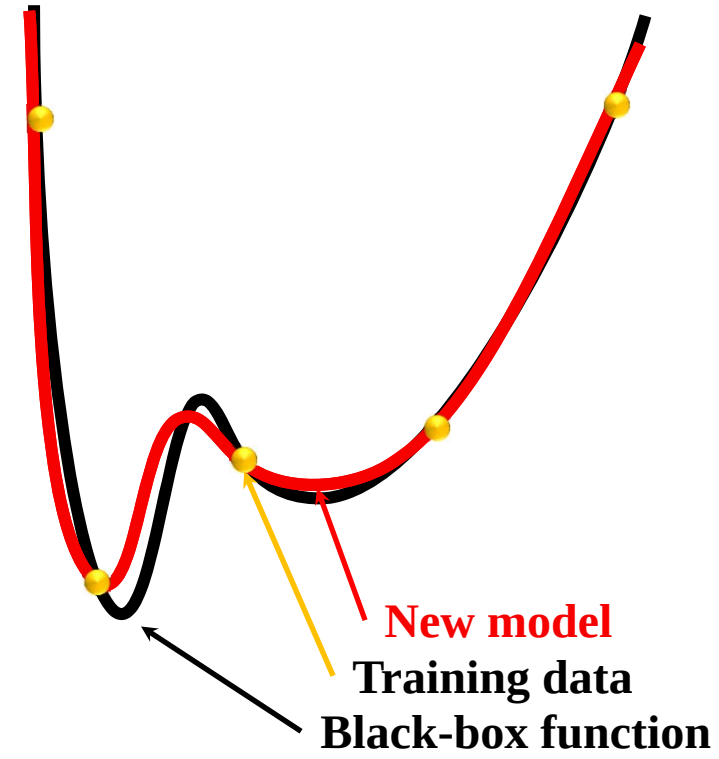

MODEL IDENTIFICATION

- **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 forms	$\exp\left(\frac{x_d}{\gamma}\right)^{\alpha}, \log\left(\frac{x_d}{\gamma}\right)^{\alpha}$
IV.	Expected bases	From experience, simple inspection, physical phenomena, etc.

BEST SUBSET SELECTION

Step 1: Define a large set of potential basis functions

$$\hat{z}(x) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1 x_2 + \beta_4 \frac{x_1}{x_2} + \beta_5 \frac{x_2}{x_1} + \beta_6 e^{x_1} + \beta_7 e^{x_2} + \dots$$

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Step 2: Model reduction

$$\hat{z}(x) = \beta_0 + \beta_2 x_2 + \beta_5 \frac{x_2}{x_1} + \beta_7 e^{x_2}$$

BEST SUBSET SELECTION

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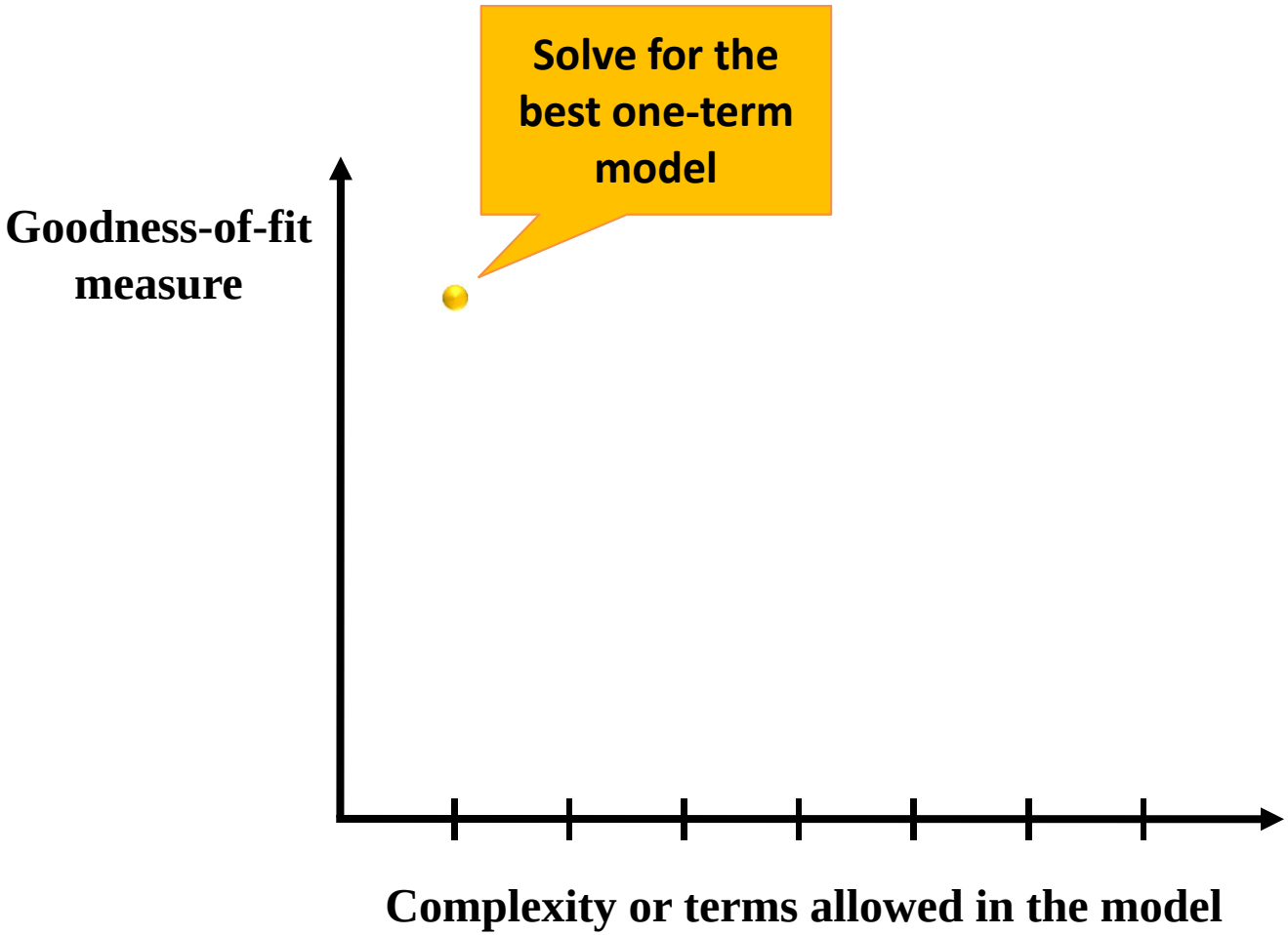
Step 2: Model reduction

$$\hat{z}(x) = \beta_0 + \beta_2 x_2 + \beta_5 \frac{x_2}{x_1} + \beta_7 e^{x_2}$$

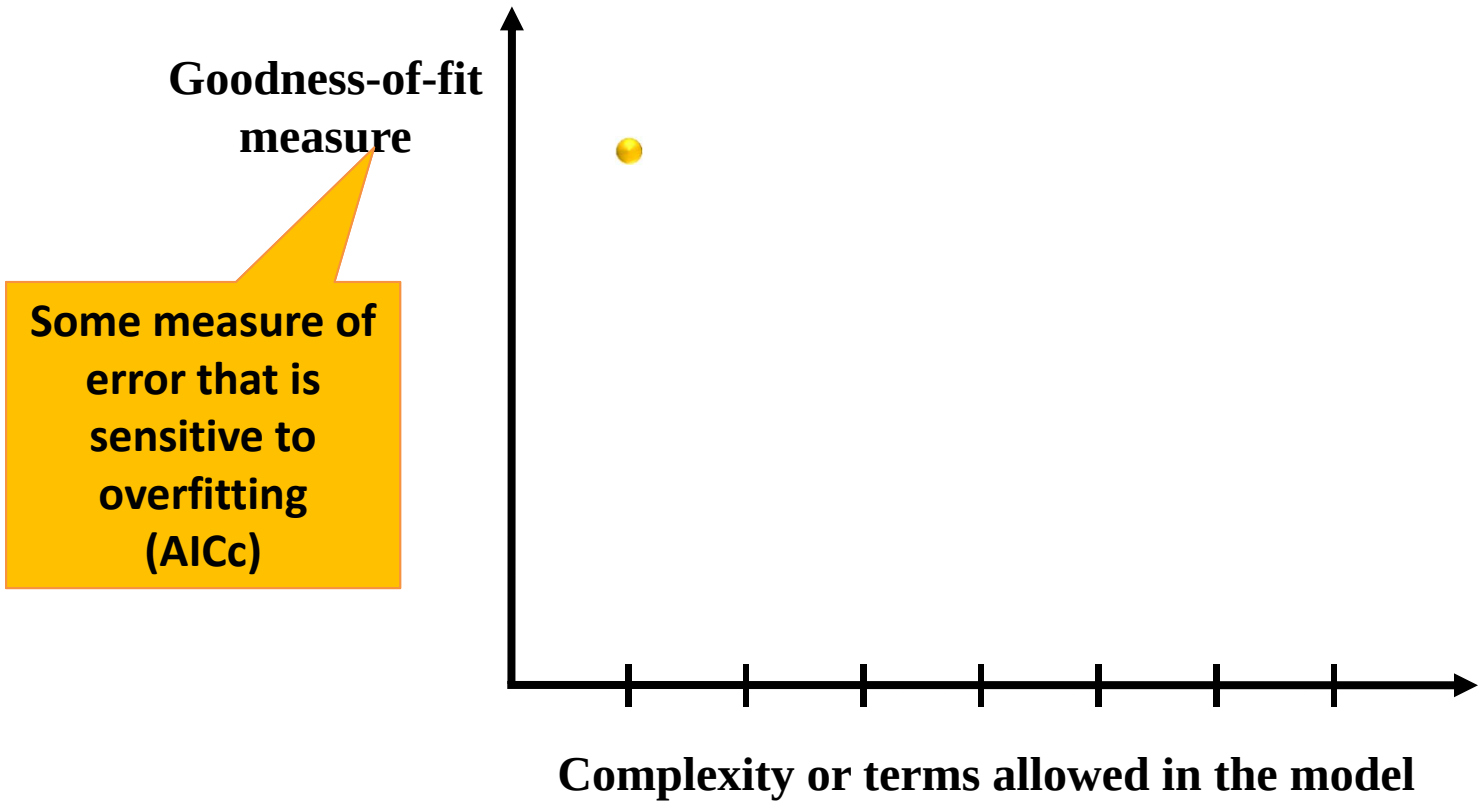
To identify a simple functional form we need to solve two problems:

1. **Model Sizing**
2. **Basis function selection**

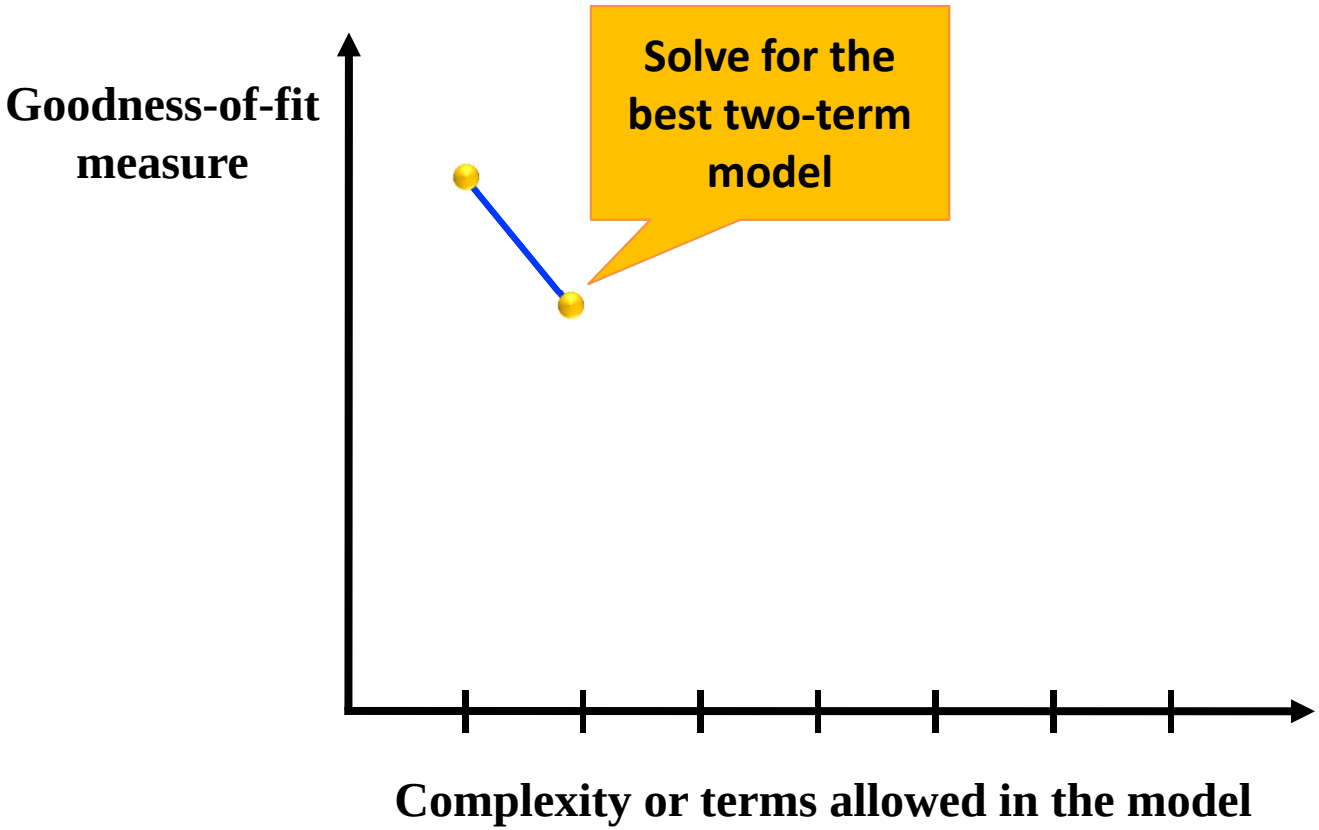
MODEL SIZING



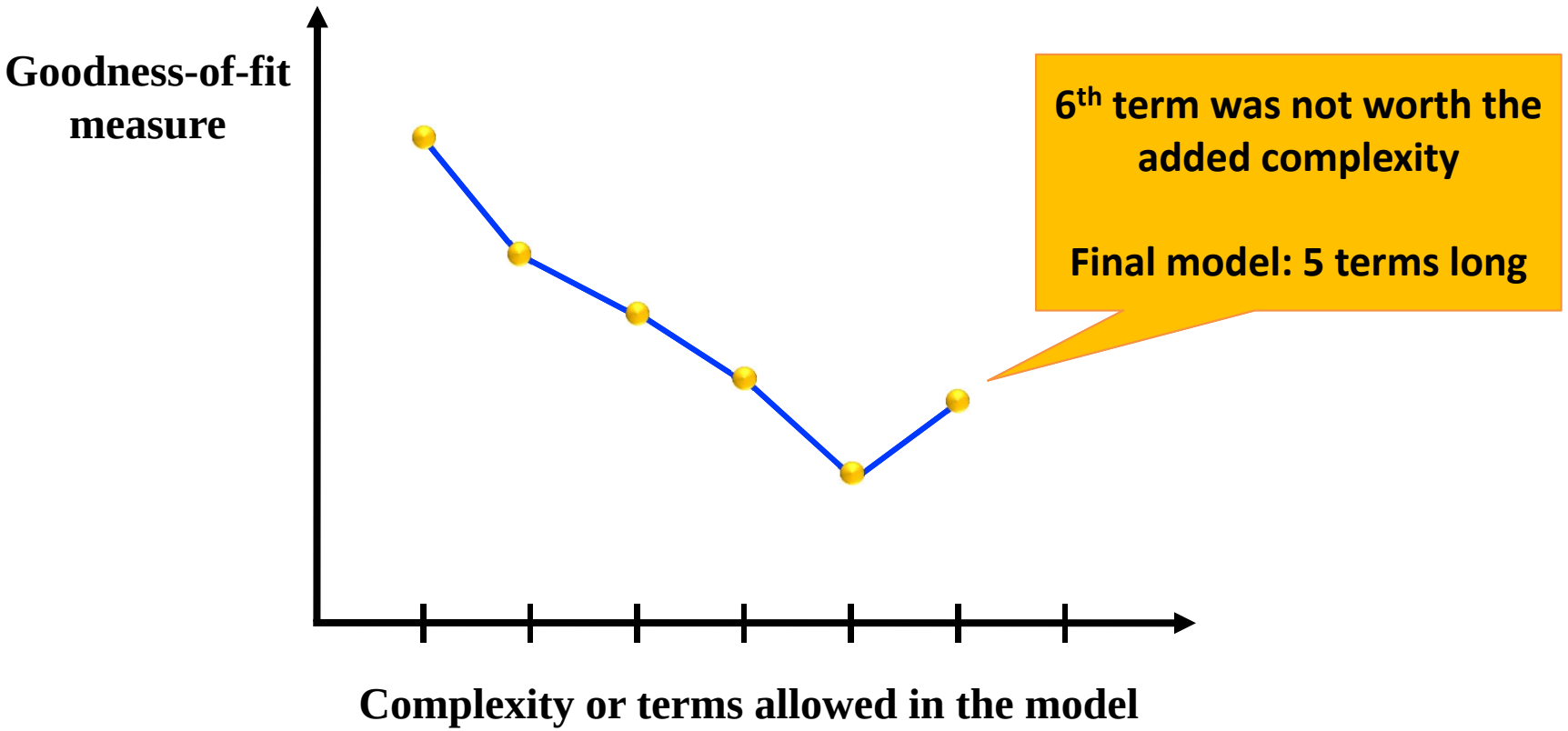
MODEL SIZING



MODEL SIZING

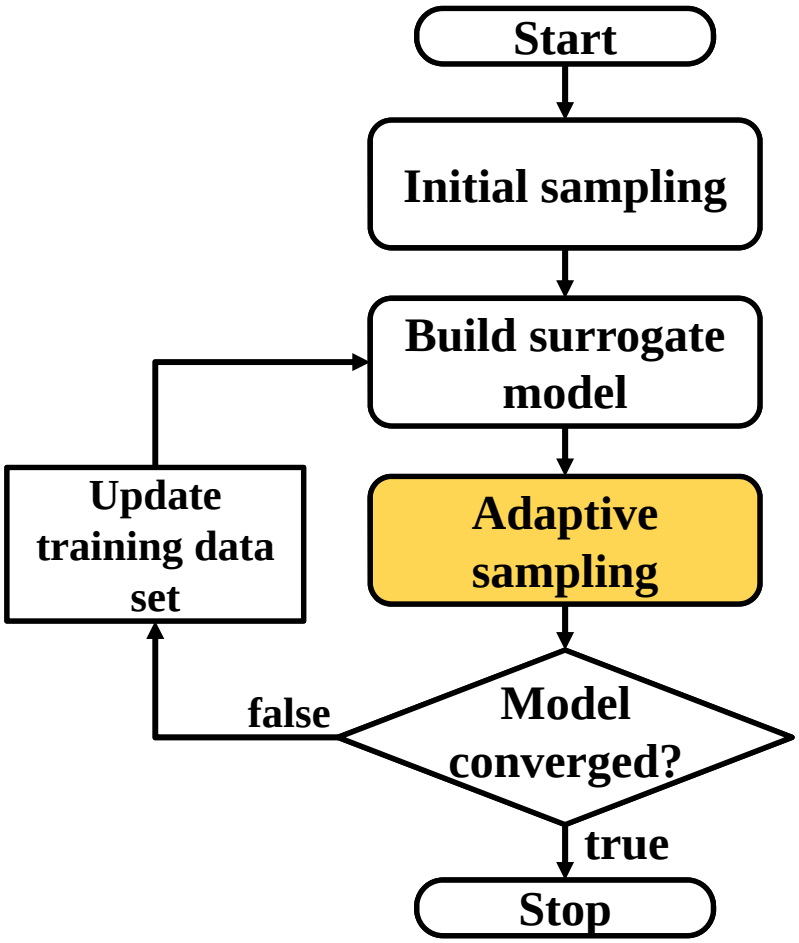


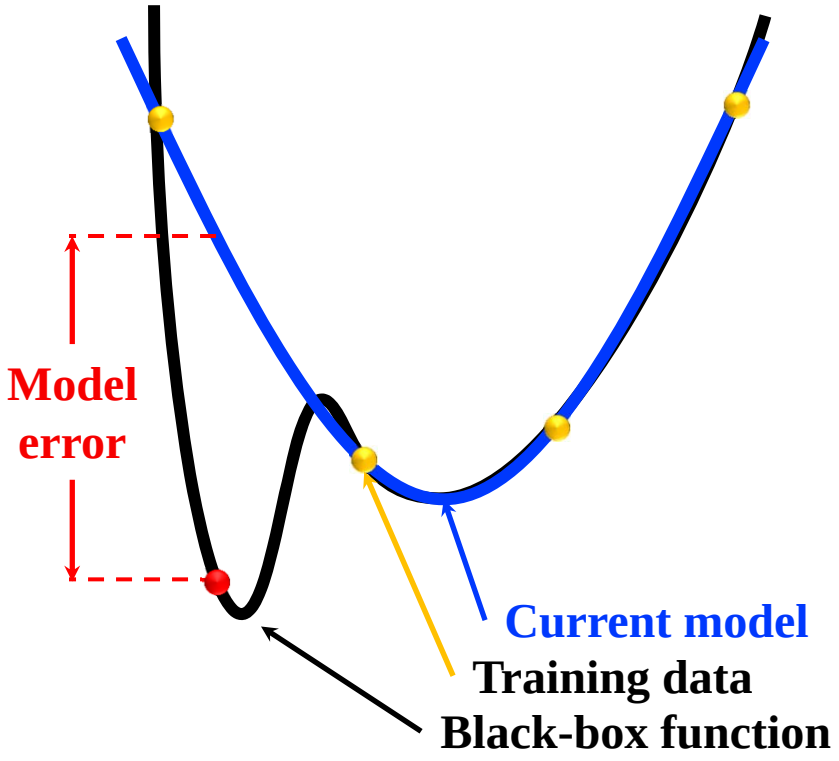
MODEL SIZING



ALAMO

Automated Learning of Algebraic Models for Optimization

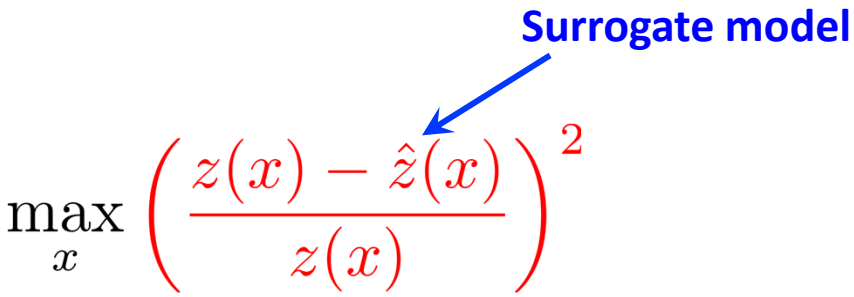




ERROR MAXIMIZATION SAMPLING

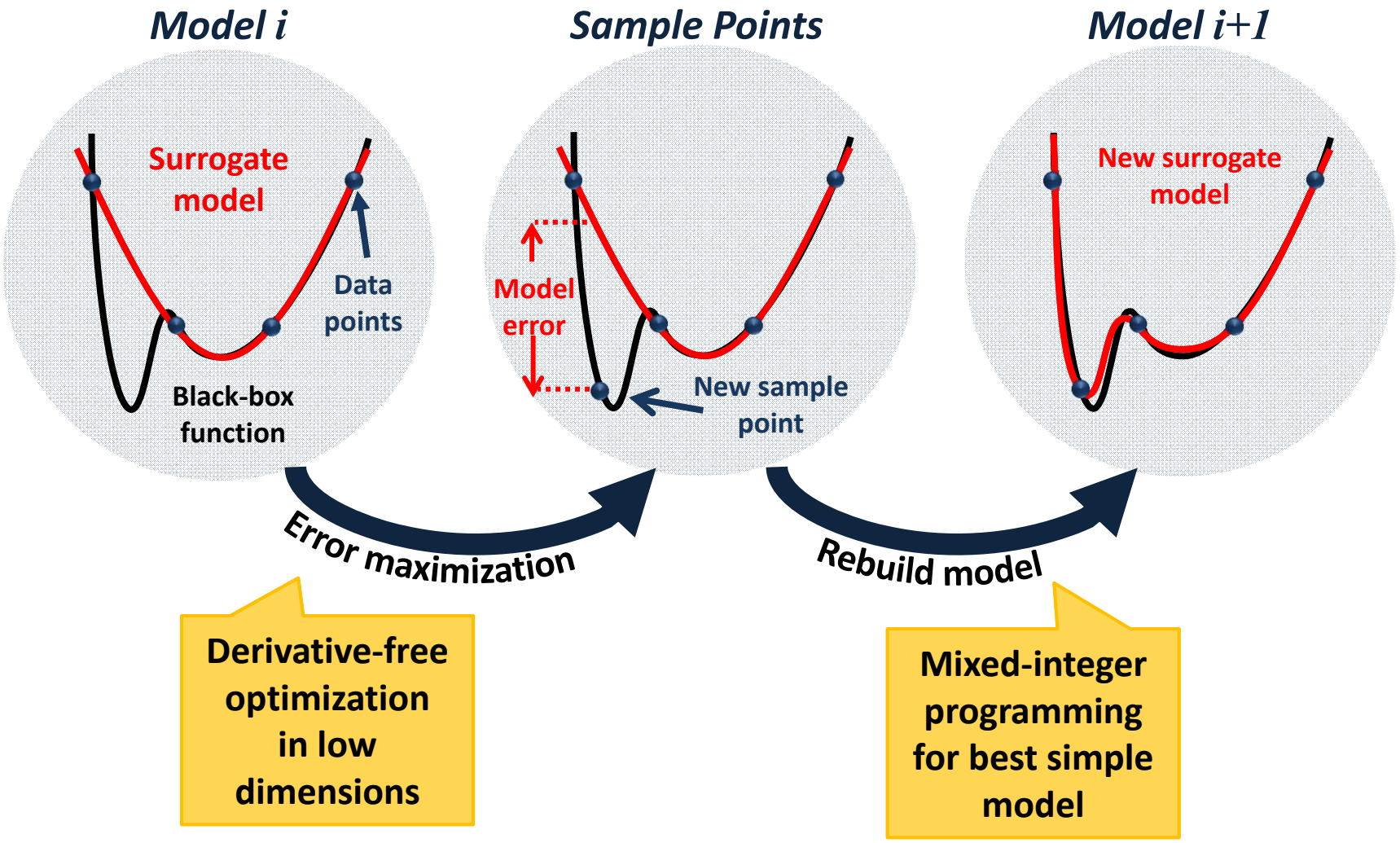
- **New goal: Search the problem space for areas of model inconsistency or model mismatch**

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



  - **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]

SYNOPSIS



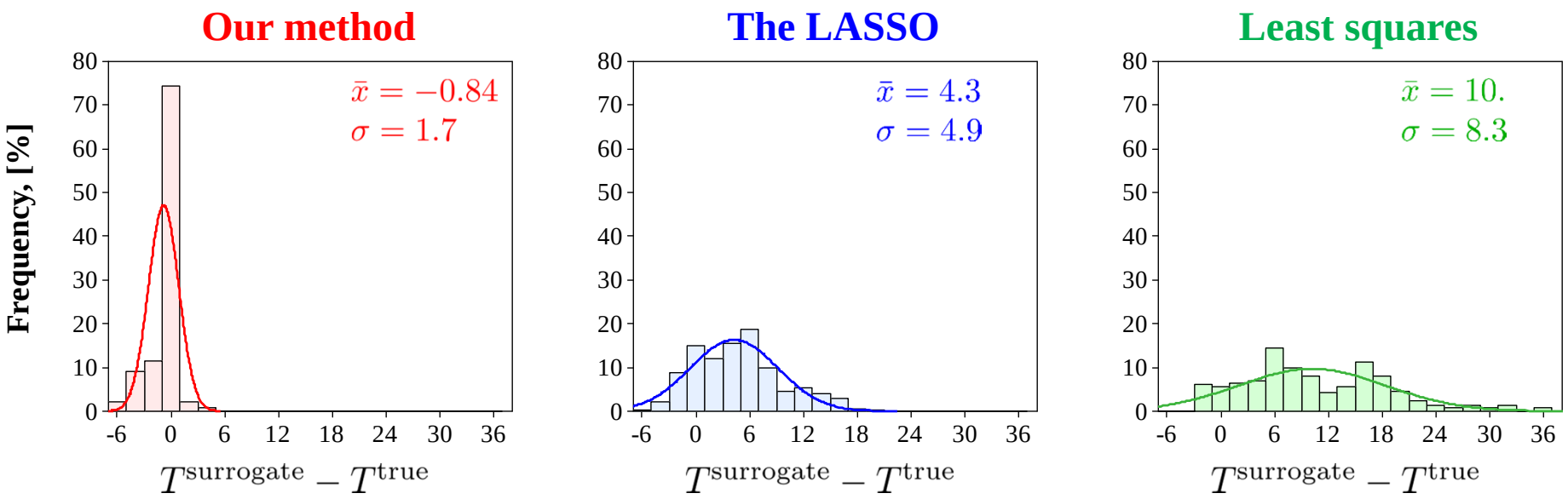
See paper 589b (Th 8:50 am)

COMPUTATIONAL TESTING

- **Paper 589b: Test the accuracy, efficiency, and model simplicity**
- **Modeling methods compared**
  - **MIP – Proposed methodology**
  - **LASSO – The lasso regularization**
  - **OLR – Ordinary least-squares regression**
- **Sampling methods compared**
  - **EMS – Proposed error maximization technique**
  - **SLH – Single Latin hypercube (no feedback)**

MODEL SIZING RESULTS

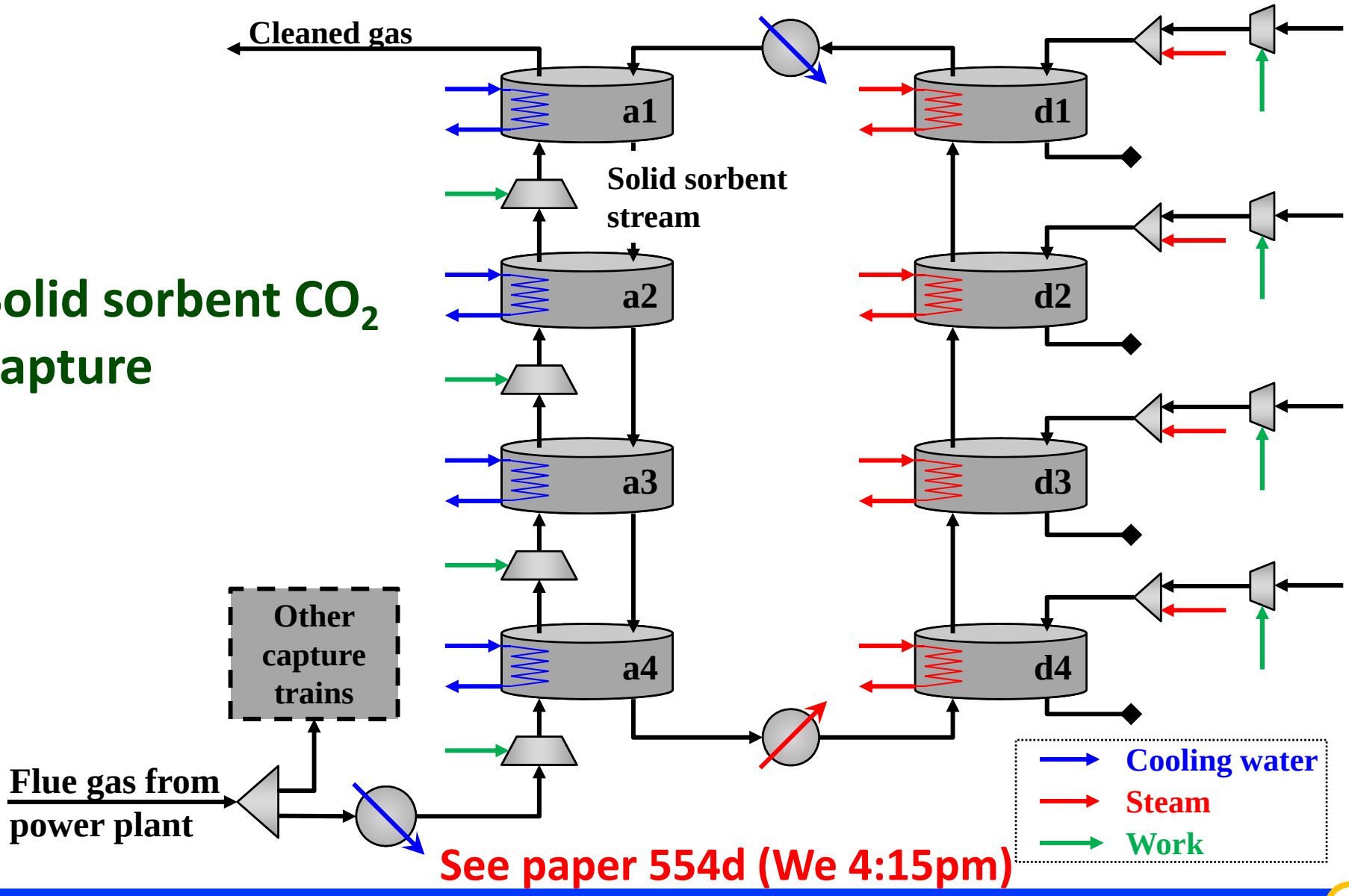
[Number of terms in the surrogate model] – [Number of terms in the true function]



45 problems with 2-10 available bases, 5 repeats

SUPERSTRUCTURE OPTIMIZATION

Solid sorbent CO_2 capture



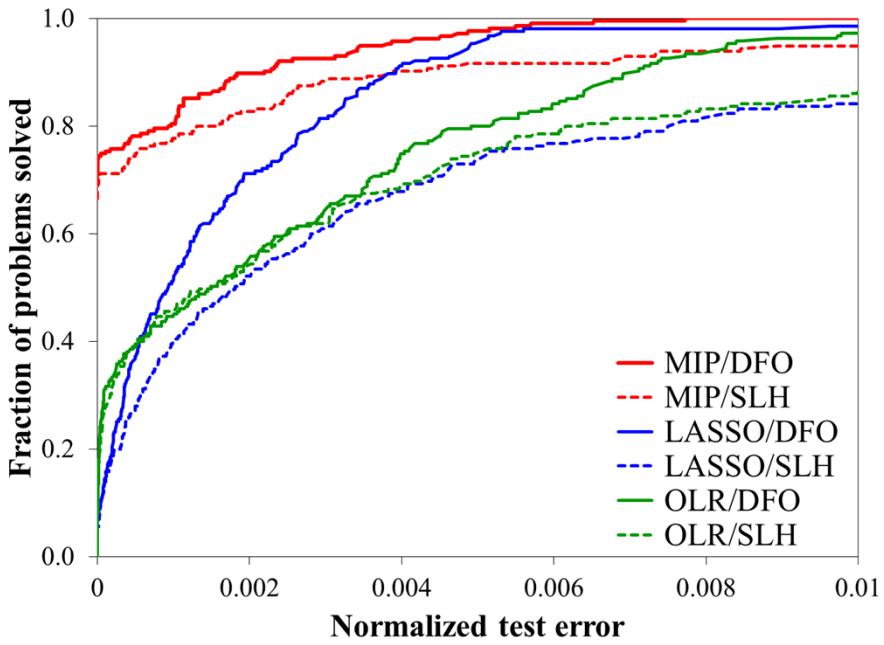
See paper 554d (We 4:15pm)

CONCLUSIONS

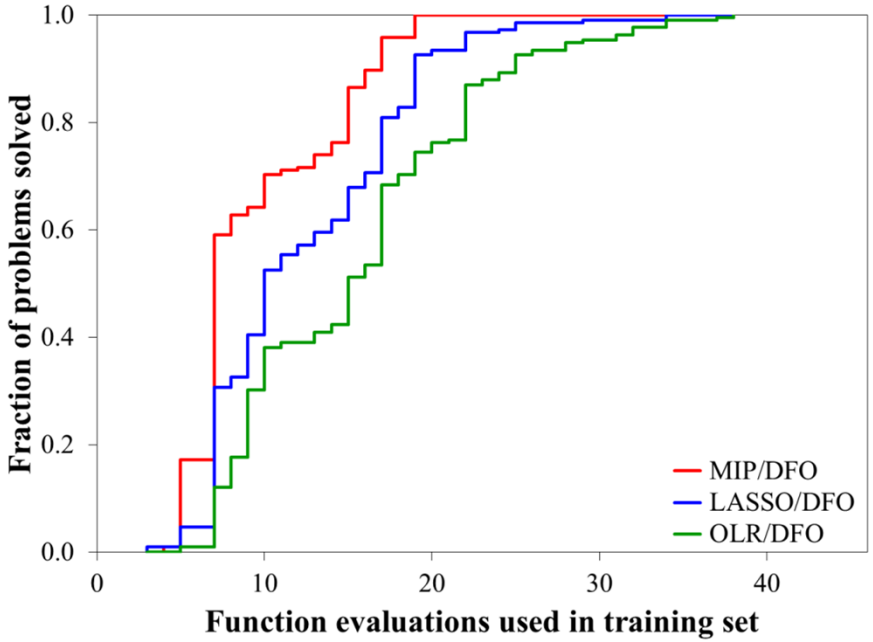
- **Best subset methods provide models that are**
  - ✓ **Accurate representations of black-box models**
- **ALAMO provides algebraic models that are**
  - ✓ **Generated from a minimal number of function evaluations**
  - ✓ **Tractable in an optimization framework (low-complexity models)**
- **Surrogate models can then be incorporated within an optimization or risk assessment framework**
- **Learning algorithms are domain independent**
- **ALAMO site: archimedes.cheme.cmu.edu/?q=alamo**

RESULTS

Model accuracy



Modeling efficiency



Modeling methods

- Our method
- LASSO
- Least squares

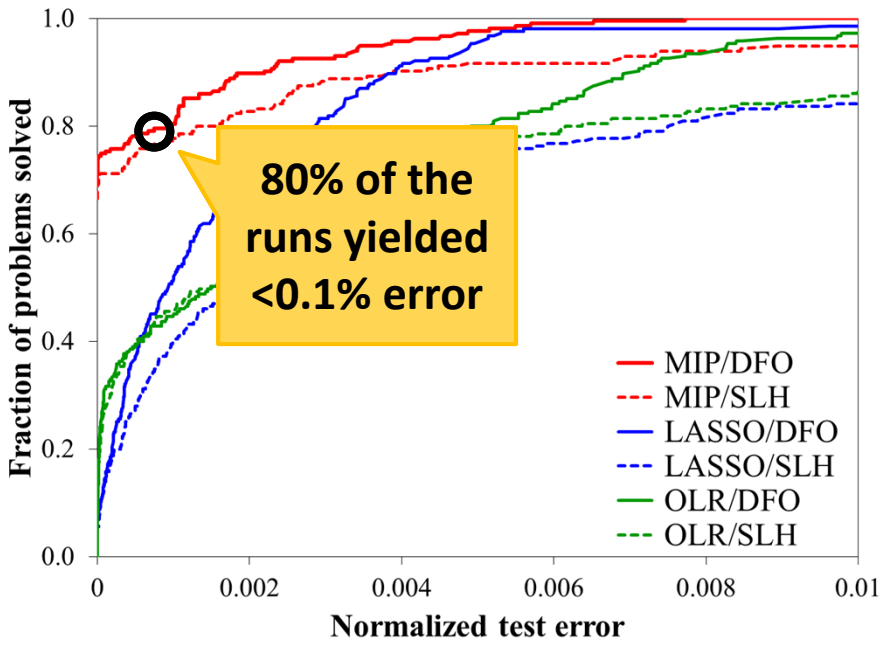
Sampling methods

- Error maximization
- Single Latin hypercube

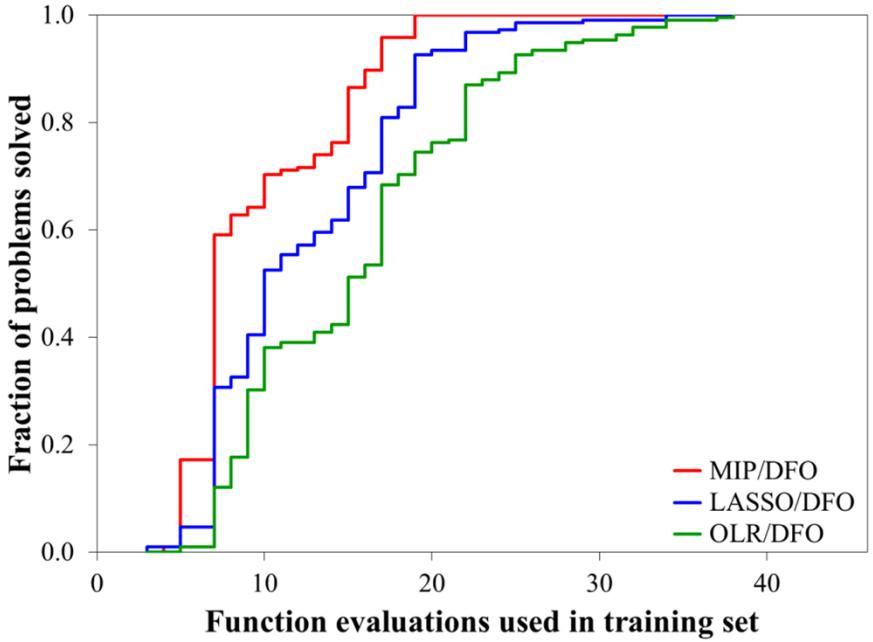
45 test problems, repeated 5 times, tested against 1000 independent data points

RESULTS

Model accuracy



Modeling efficiency



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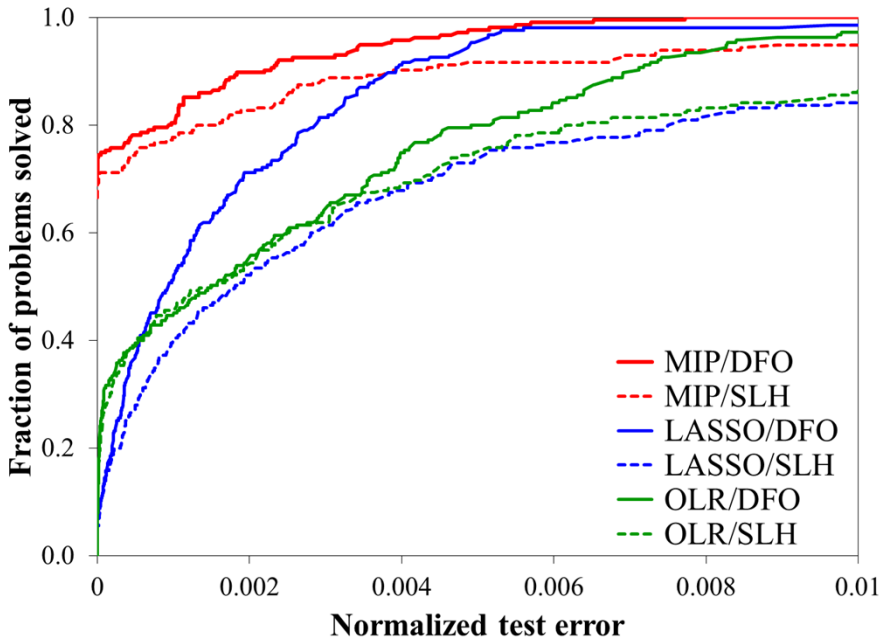

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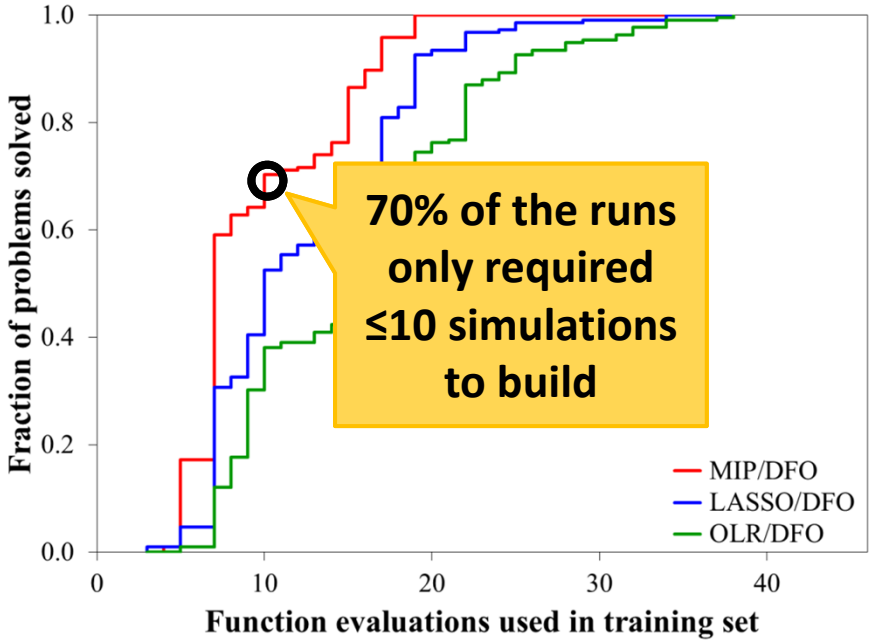

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