Optimizing Simulations and Black-boxes using a Surrogated-based Approach

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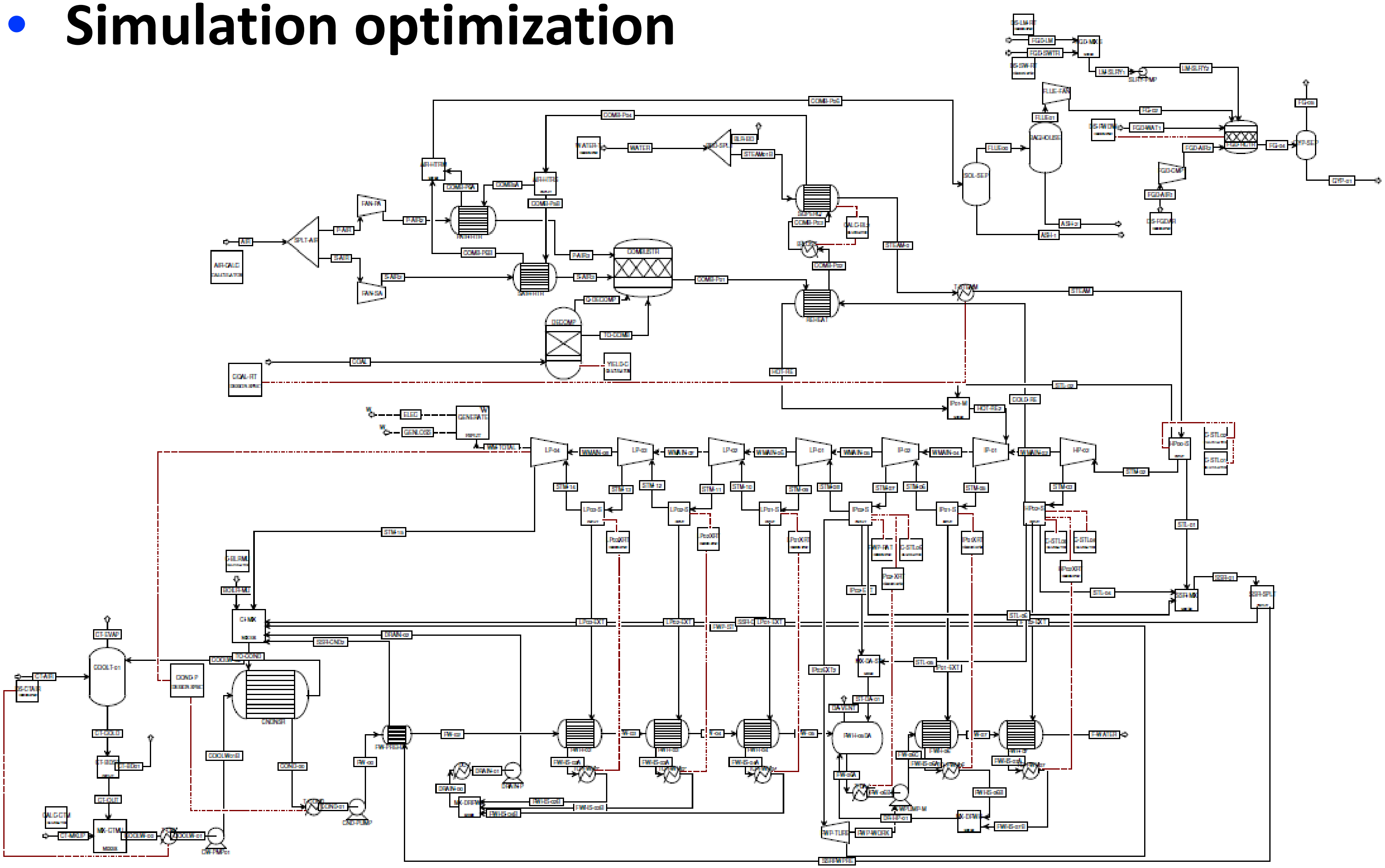
MOTIVATION

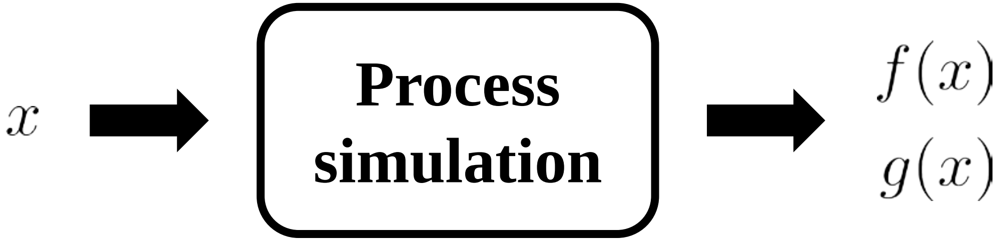
- **Simulation optimization**



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

PROBLEM STATEMENT

$$\begin{aligned} \min \quad & f(x) \\ \text{s.t.} \quad & g(x) \leq 0 \\ & h(x) = 0 \\ & x \in [x^l, x^u] \end{aligned}$$



x

Process simulation

$f(x)$

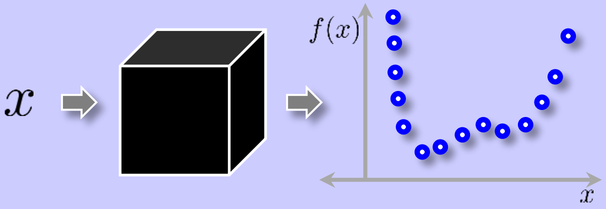
$g(x)$

Optimize simulations or black-box processes

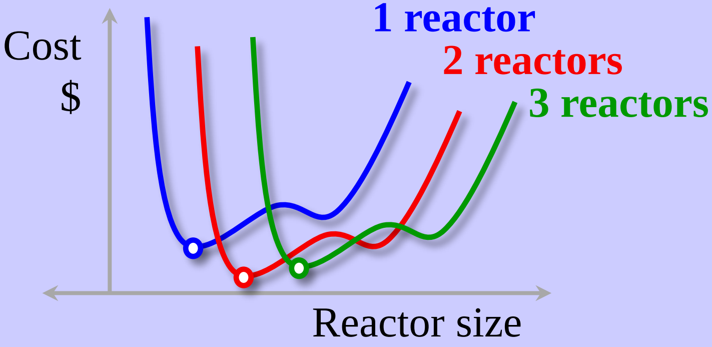
CHALLENGES

OPTIMIZER

No algebraic model



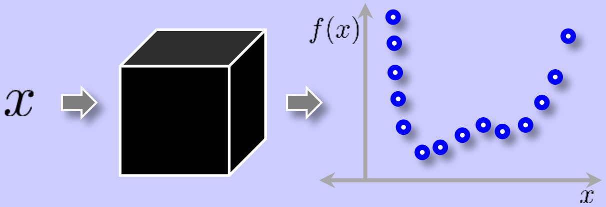
Complex process alternatives



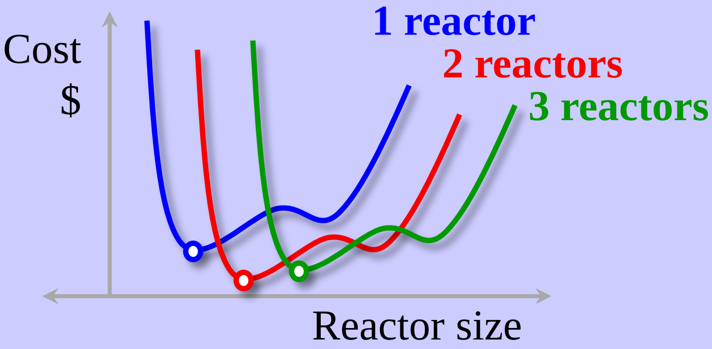
CHALLENGES

OPTIMIZER

No algebraic model

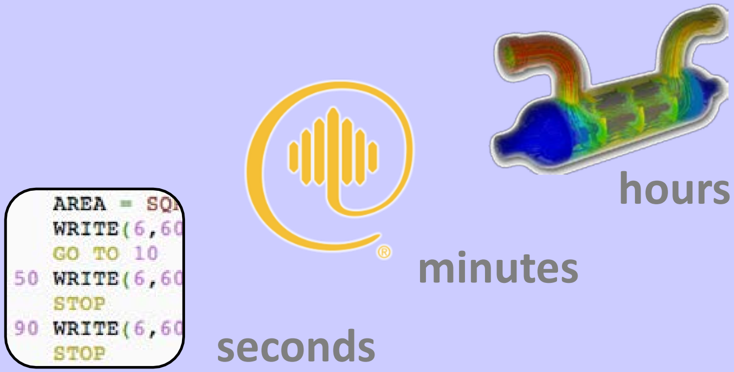


Complex process alternatives



SIMULATOR

Costly simulations



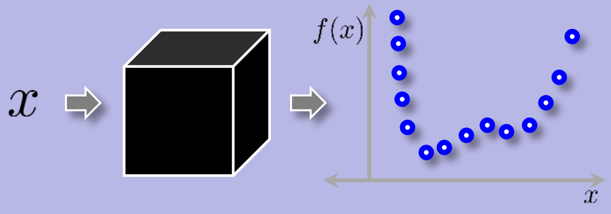
```
   AREA = SQ
   WRITE(6,60
   GO TO 10
50 WRITE(6,60
   STOP
90 WRITE(6,60
   STOP
```

Scarcity of fully robust simulations

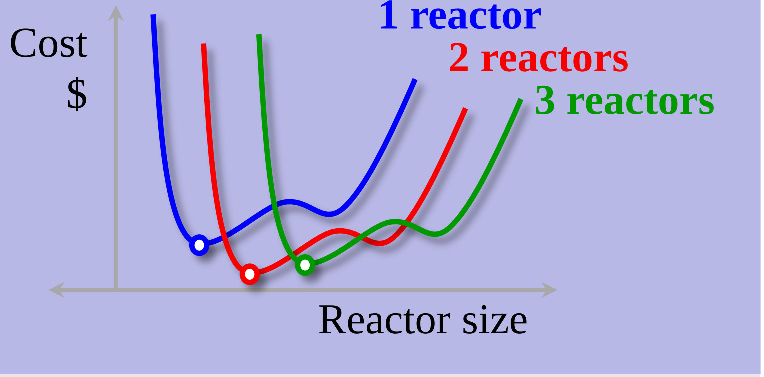
CHALLENGES

OPTIMIZER

No algebraic model

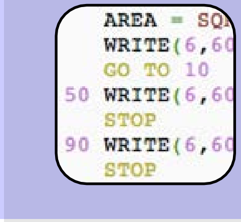


Complex process alternatives



SIMULATOR

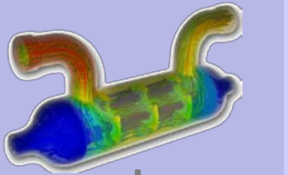
Costly simulations



```
   AREA = SQ
   WRITE(6,60
   GO TO 10
50 WRITE(6,60
   STOP
90 WRITE(6,60
   STOP
```

seconds

minutes



hours

Scarcity of fully robust simulations

✗ Gradient-based methods

✗ Derivative-free methods

OVERVIEW

1. **Surrogate-based optimization of process simulations**

2. **Surrogate model generation method**

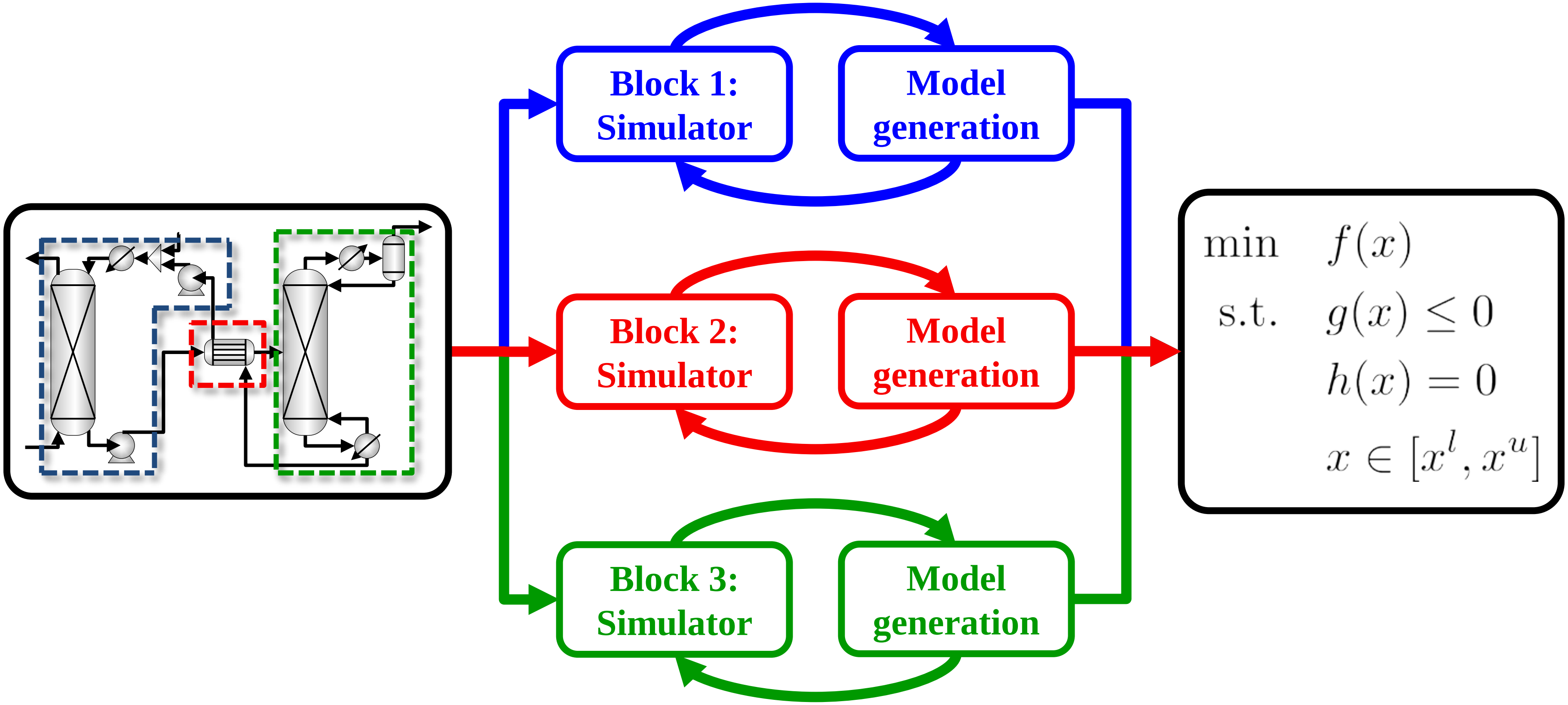
3. **Computational experiments**

4. **Case studies**

OVERVIEW

1. **Surrogate-based optimization of process simulations**
2. Surrogate model generation method
3. Computational experiments
4. Case studies

SOLUTION STRATEGY



Block 1: Simulator

Model generation

Block 2: Simulator

Model generation

Block 3: Simulator

Model generation

$$
\begin{aligned}
\min \quad & f(x) \\
\text{s.t.} \quad & g(x) \le 0 \\
& h(x) = 0 \\
& x \in [x^l, x^u]
\end{aligned}
$$

Process Simulation

Disaggregate process into process blocks

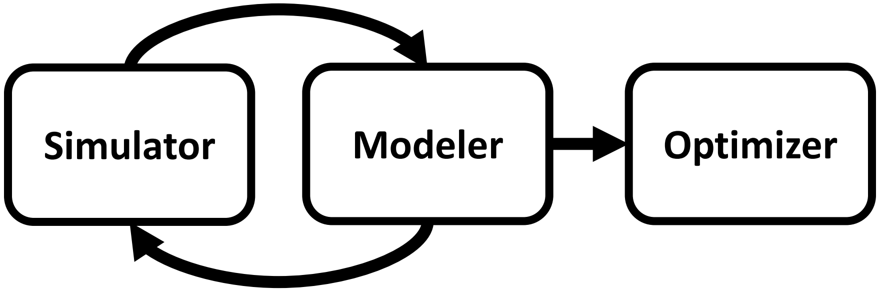
Surrogate Models

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

Optimization Model

Add algebraic constraints *h(x)*=0: design specs, heat/mass balances, and logic constraints

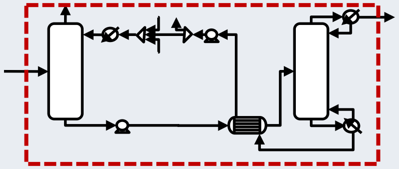
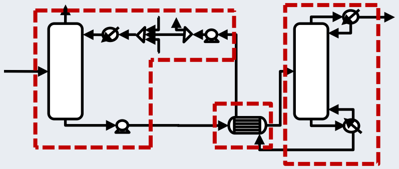
RECENT WORK IN CHEMICAL ENG



Simulator

Modeler

Optimizer

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

OVERVIEW

1. Surrogate-based optimization of process simulations

2. Surrogate model generation method
   - Efficiently generate simple and accurate algebraic models

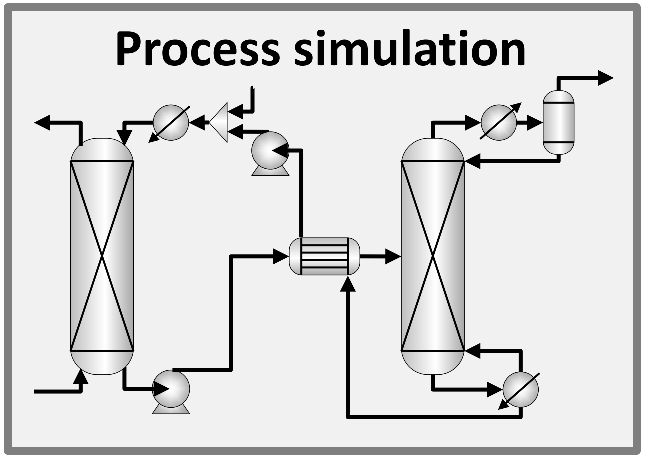
3. Computational experiments

4. Case studies

LEARNING PROBLEM STATEMENT

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

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



Process simulation

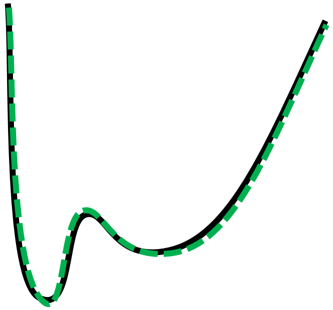
$$\begin{pmatrix} z_1 \\ z_2 \\ \vdots \\ z_k \\ \vdots \\ z_K \end{pmatrix} \qquad z \in \mathbb{R}^K \qquad z = f(x)$$

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

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

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*



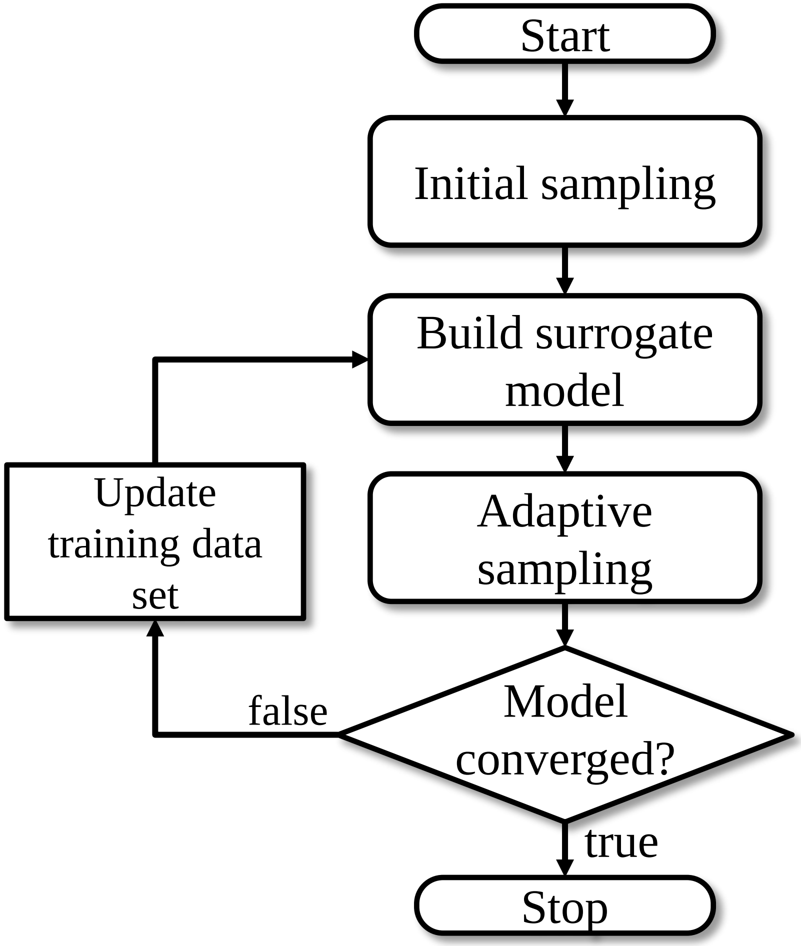
$$\hat{f}(x) = \sum_{i=1}^{n} \gamma_i \exp\left(\frac{\|x\|}{\sigma^2}\right) + \beta_0 + \beta_1 x + \ldots$$

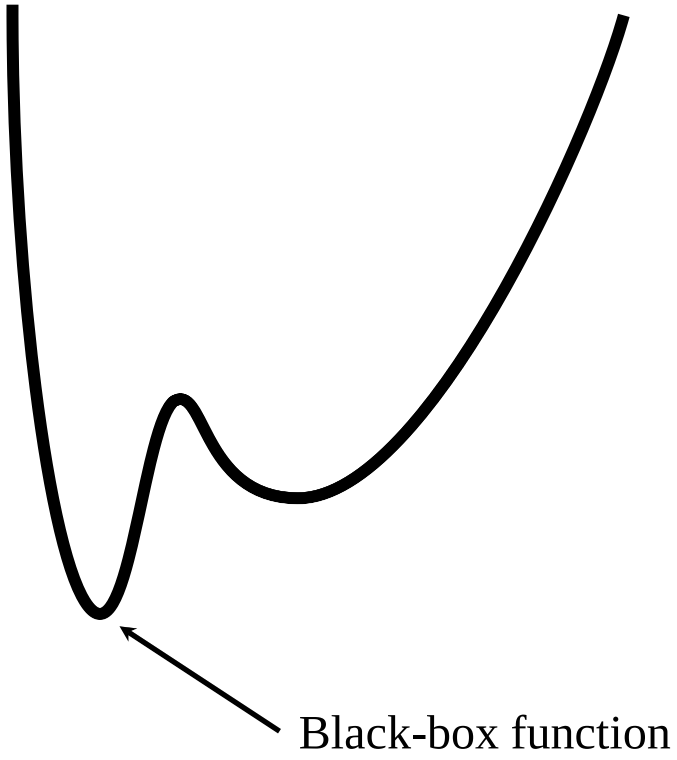
$$\hat{f}(x) = \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \beta_4 e^x$$

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

ALAMO

Automated Learning of Algebraic Models for Optimization





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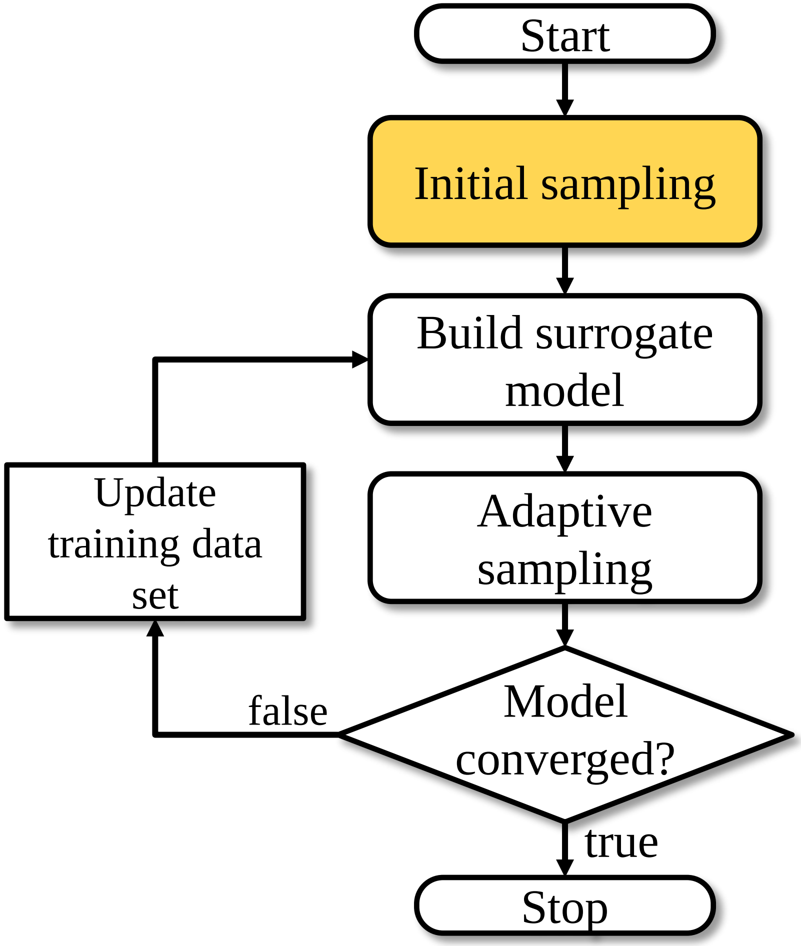
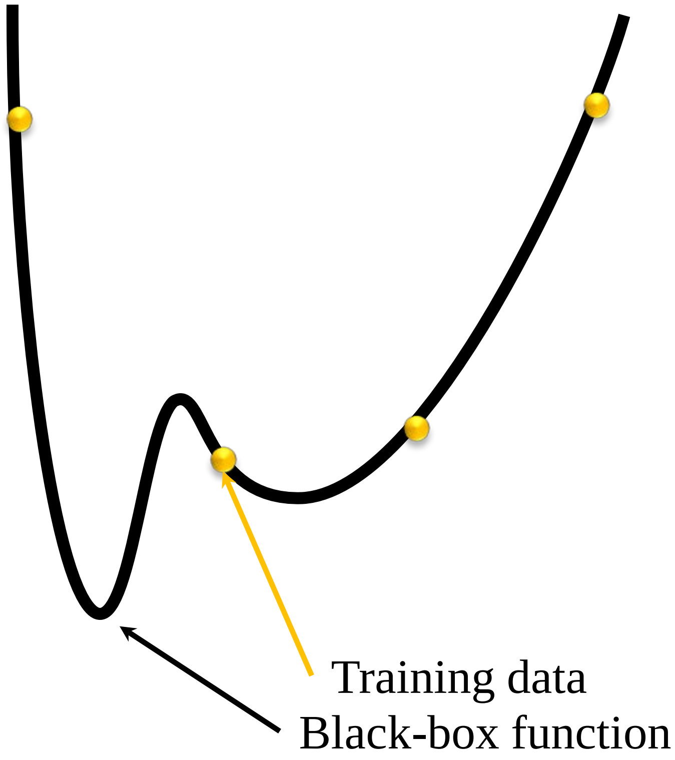
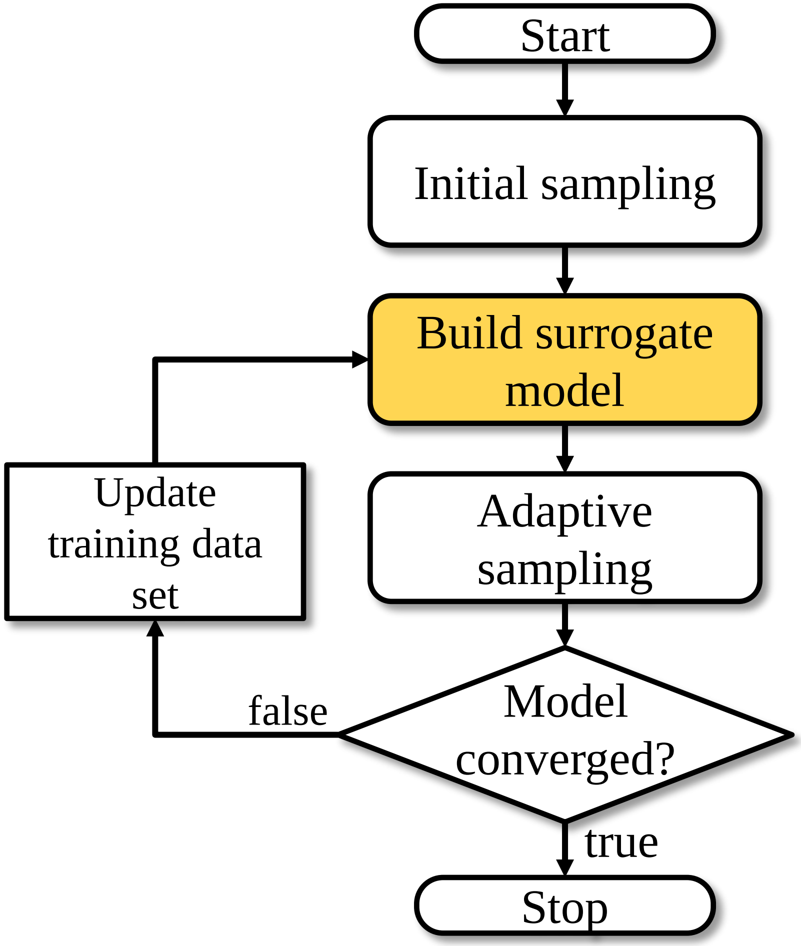




ALAMO

Automated Learning of Algebraic Models for Optimization


Start

Initial sampling

Build surrogate model

Adaptive sampling

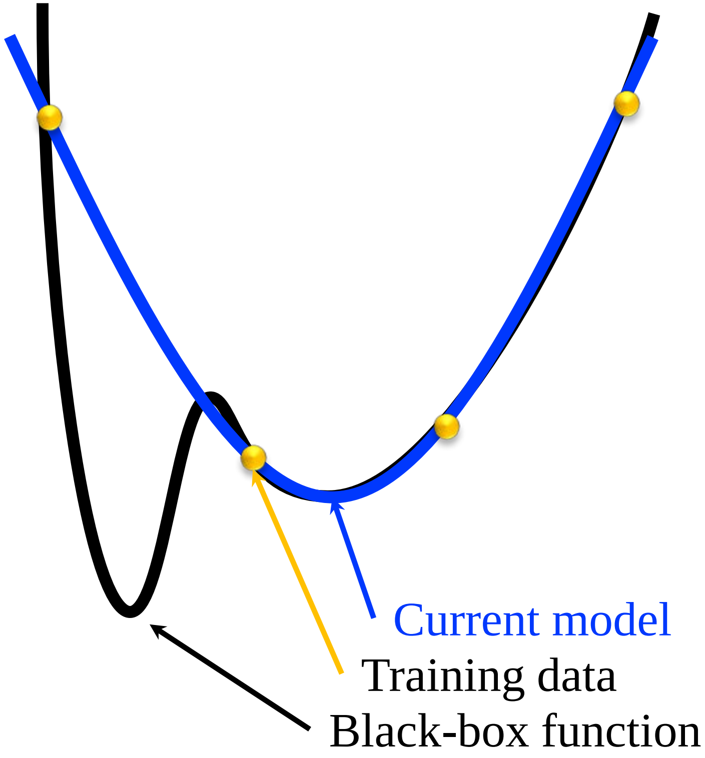
Model converged?

true

Stop

false

Update training data set



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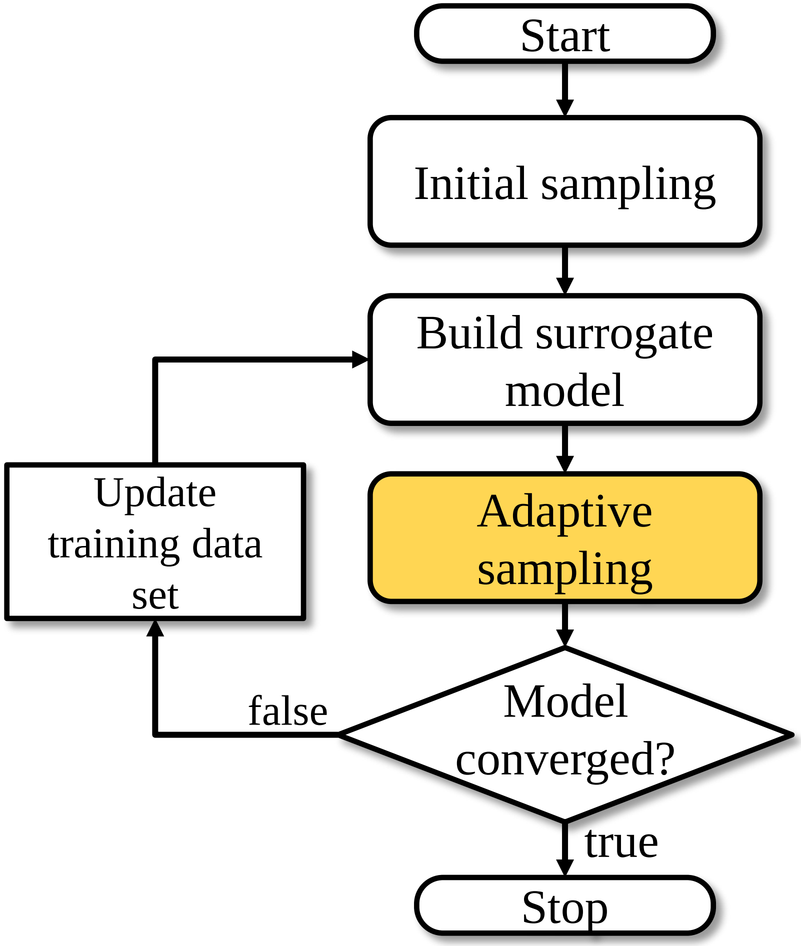

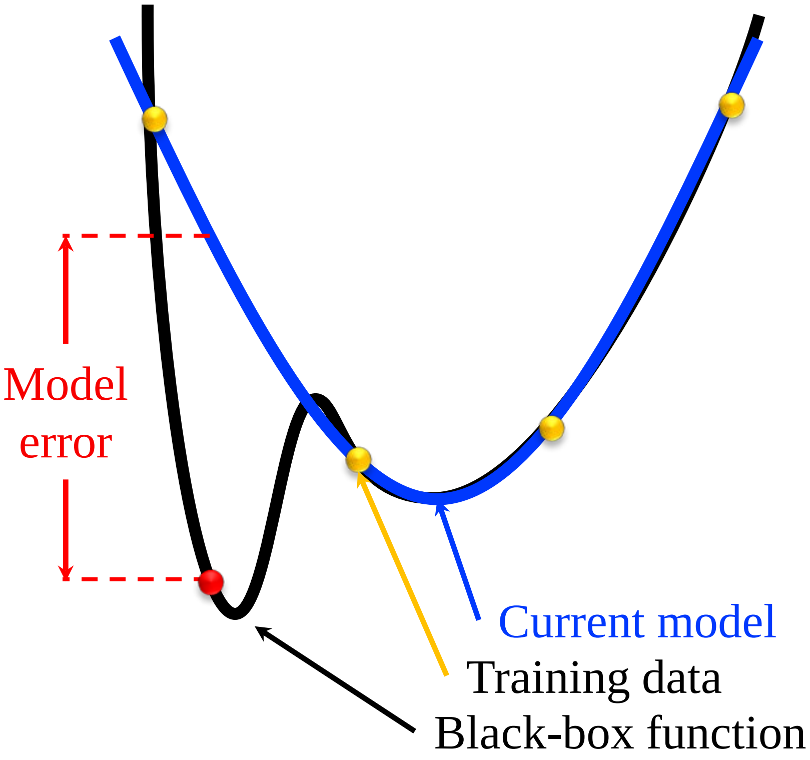

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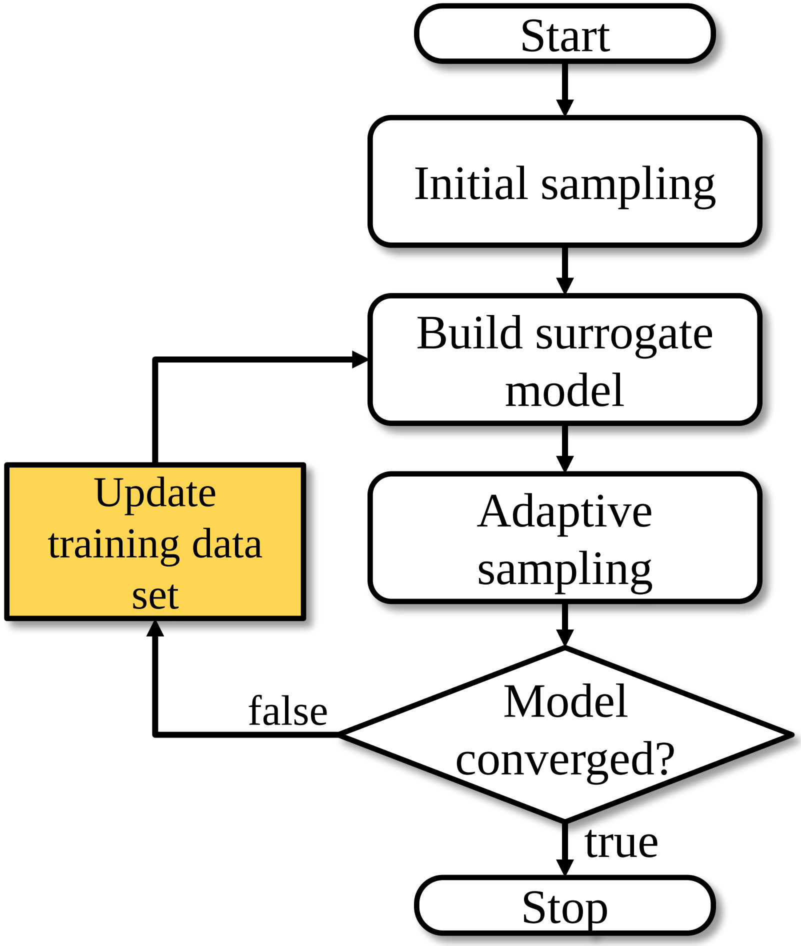

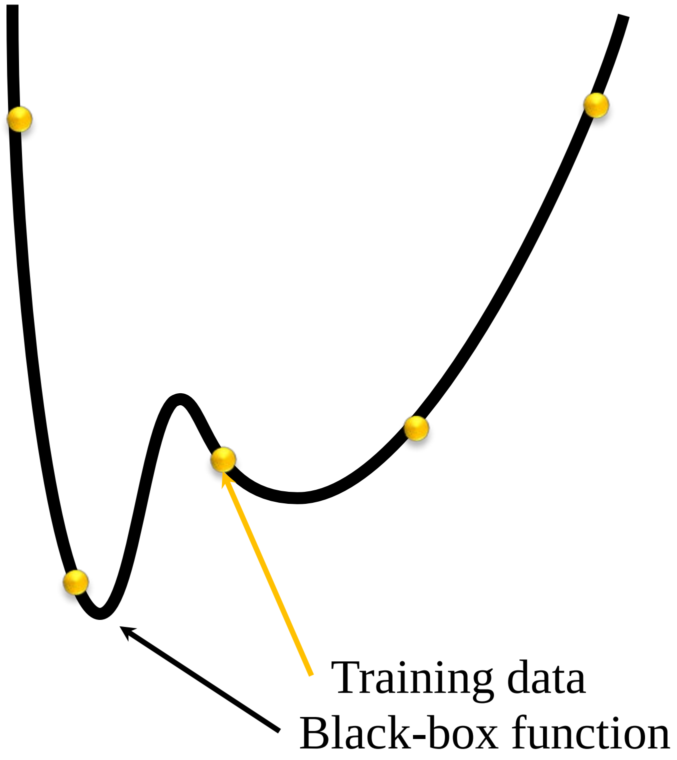

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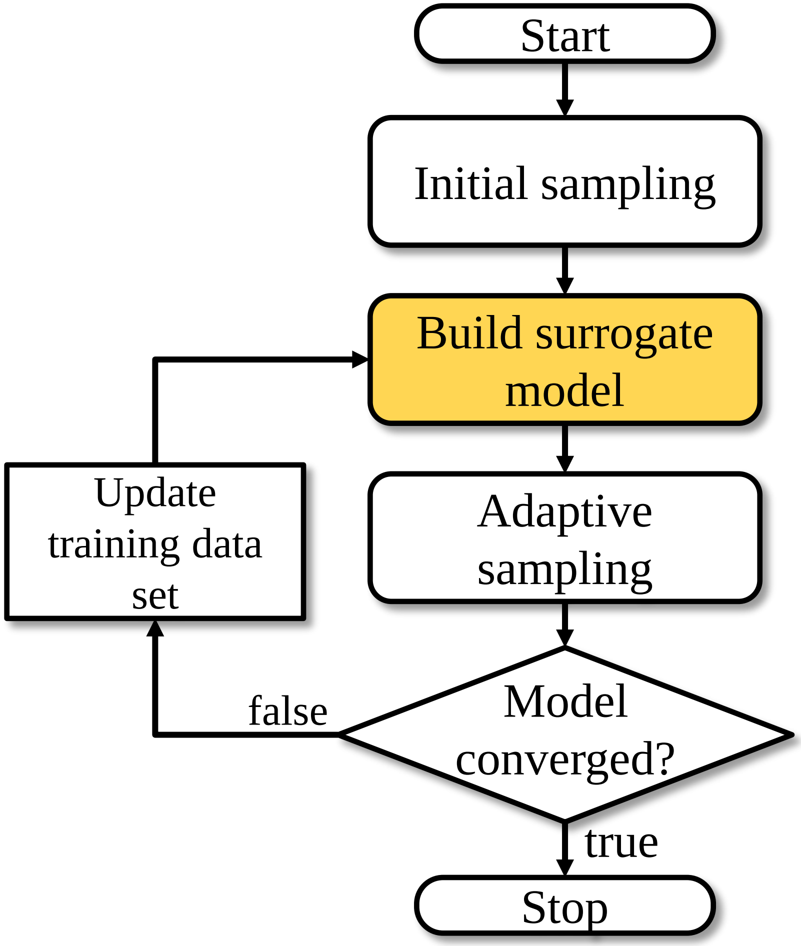
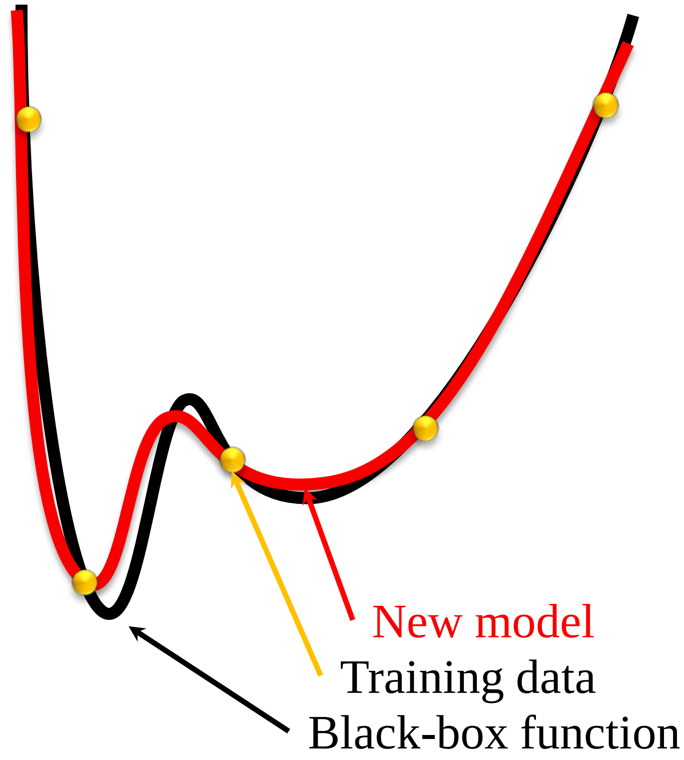
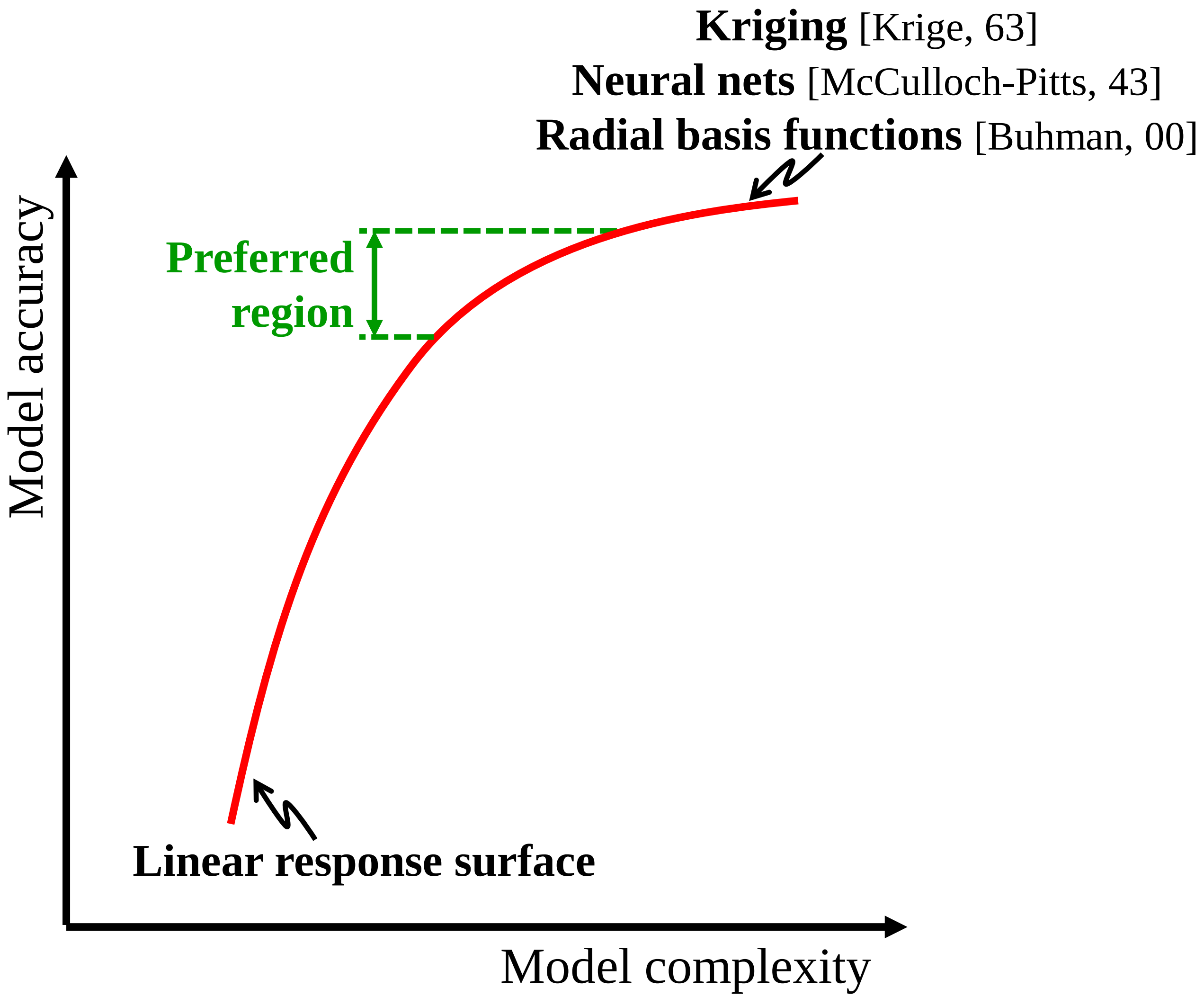




MODEL COMPLEXITY TRADEOFF

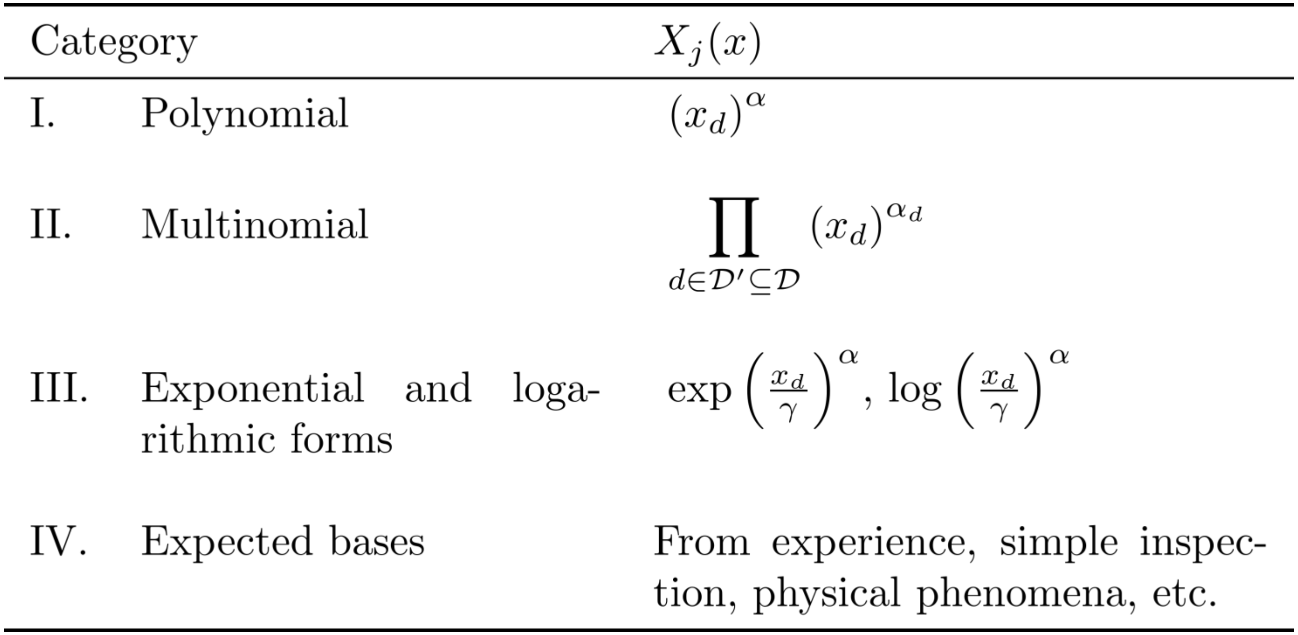


MODEL IDENTIFICATION

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

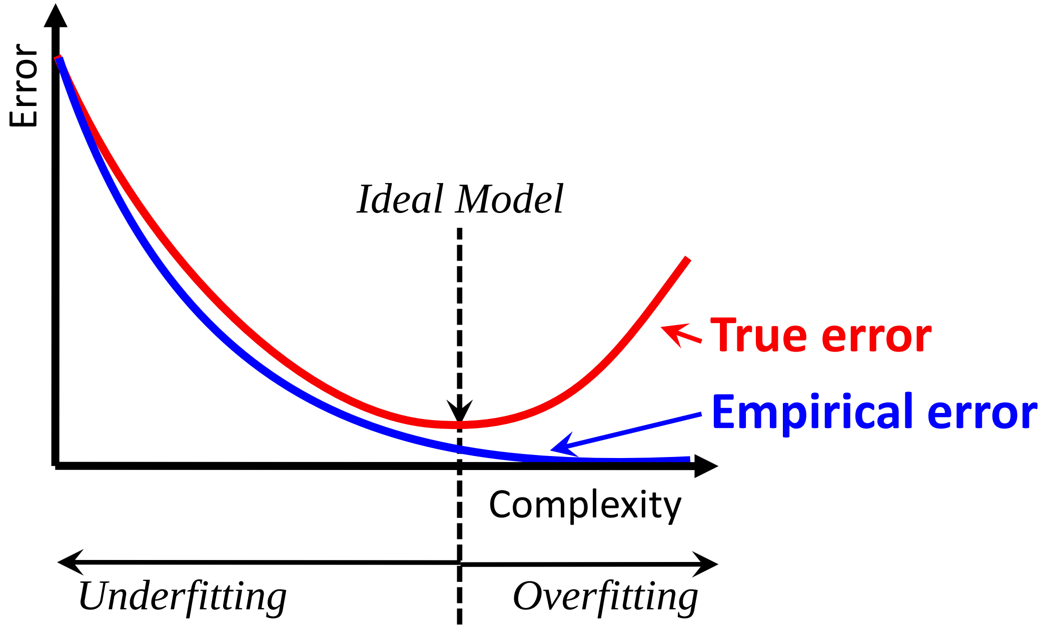
$$z = f(x)$$

- **Functional form:**
  - **General functional form is unknown: Our method will identify models with combinations of simple basis functions**

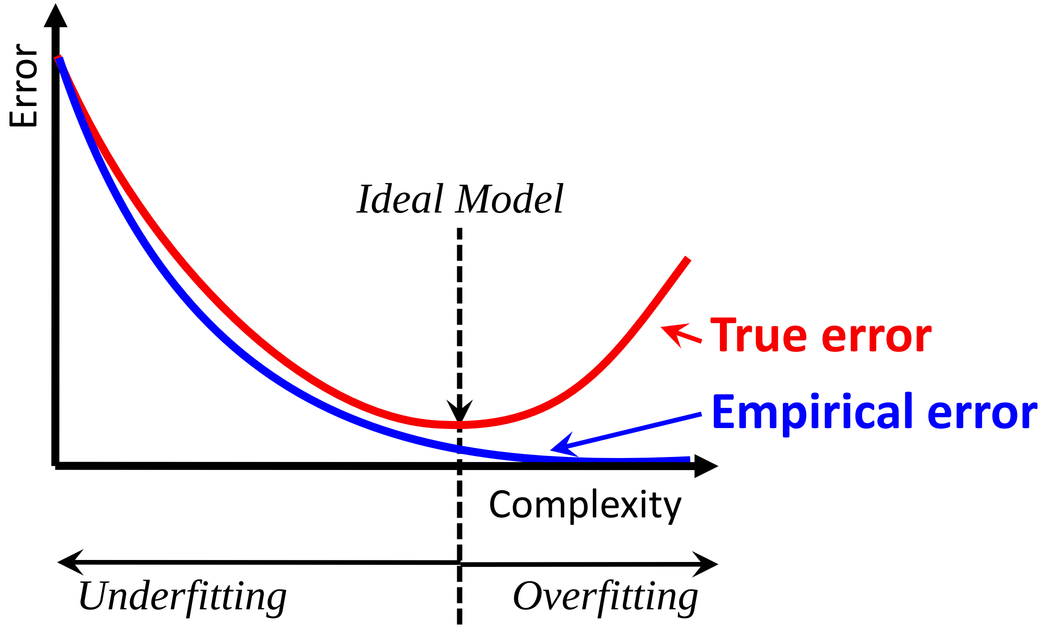


Category		$X_j(x)$
I.	Polynomial	$(x_d)^\alpha$
II.	Multinomial	$\prod_{d \in \mathcal{D}' \subseteq \mathcal{D}} (x_d)^{\alpha_d}$
III.	Exponential and logarithmic forms	$\exp\left(\frac{x_d}{\gamma}\right)^\alpha$, $\log\left(\frac{x_d}{\gamma}\right)^\alpha$
IV.	Expected bases	From experience, simple inspection, physical phenomena, etc.

OVERFITTING AND TRUE ERROR



OVERFITTING AND TRUE ERROR



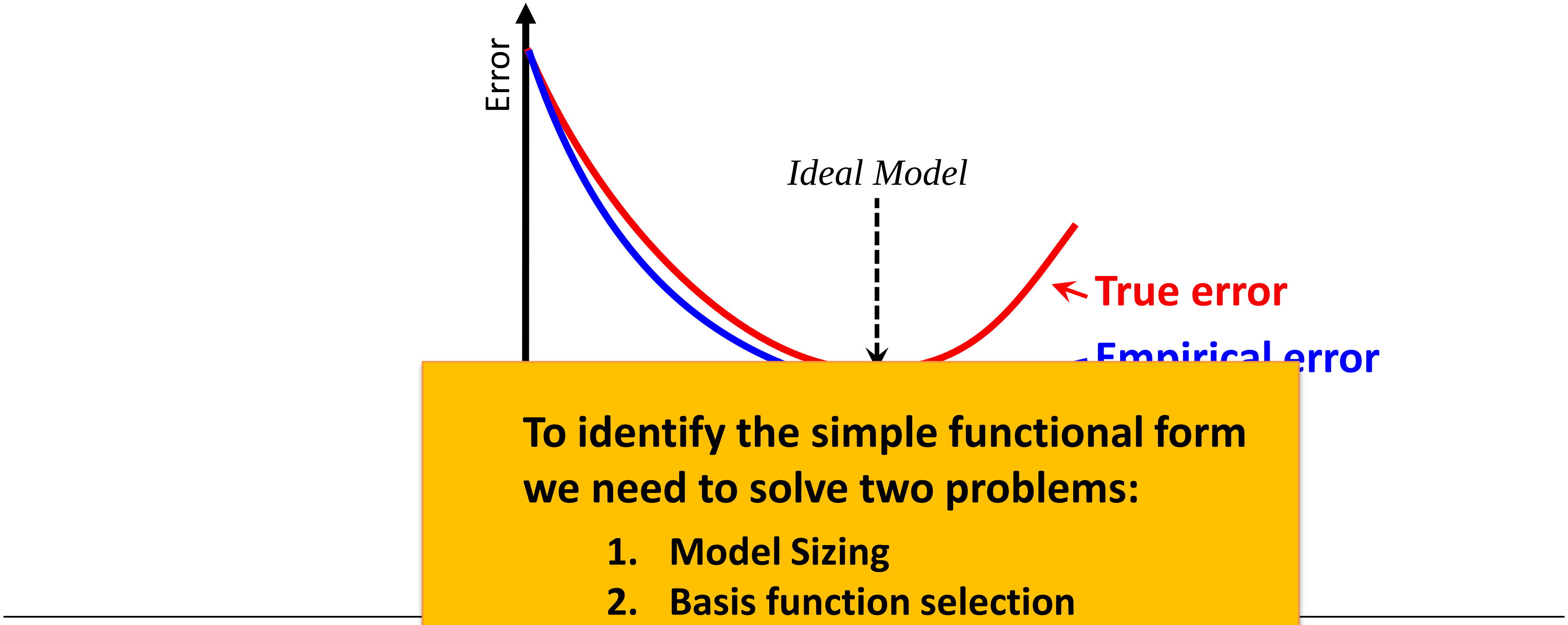
Step 1: Define a large set of potential basis functions

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

Step 2: Model reduction

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

OVERFITTING AND TRUE ERROR



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

1. Model Sizing
2. Basis function selection

Step 1: Define a large set of r   **is functions**

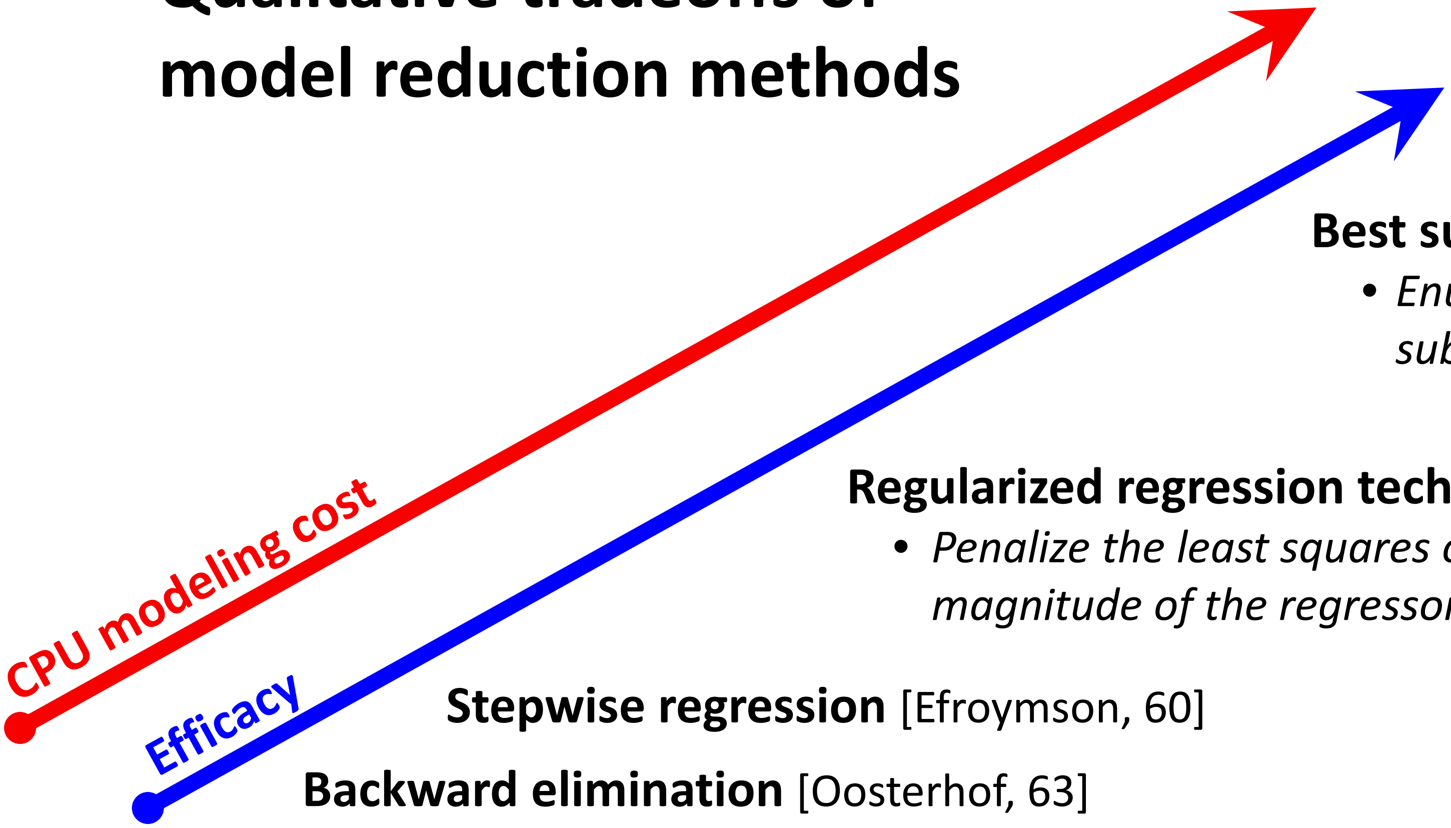
$$\hat{z}(x_1) = \beta_0 + \beta_1 x_1 \quad x_2 + \beta_3 x_1 x_2 + \beta_4 \frac{x_1}{x_2} + \beta_5 \frac{x_2}{x_1} + \beta_6 e^{x_1} + \beta_7 e^{x_2} + \dots$$

Step 2: Model reduction

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

MODEL REDUCTION TECHNIQUES

- **Qualitative tradeoffs of model reduction methods**



Best subset methods

- *Enumerate all possible subsets*

Regularized regression techniques

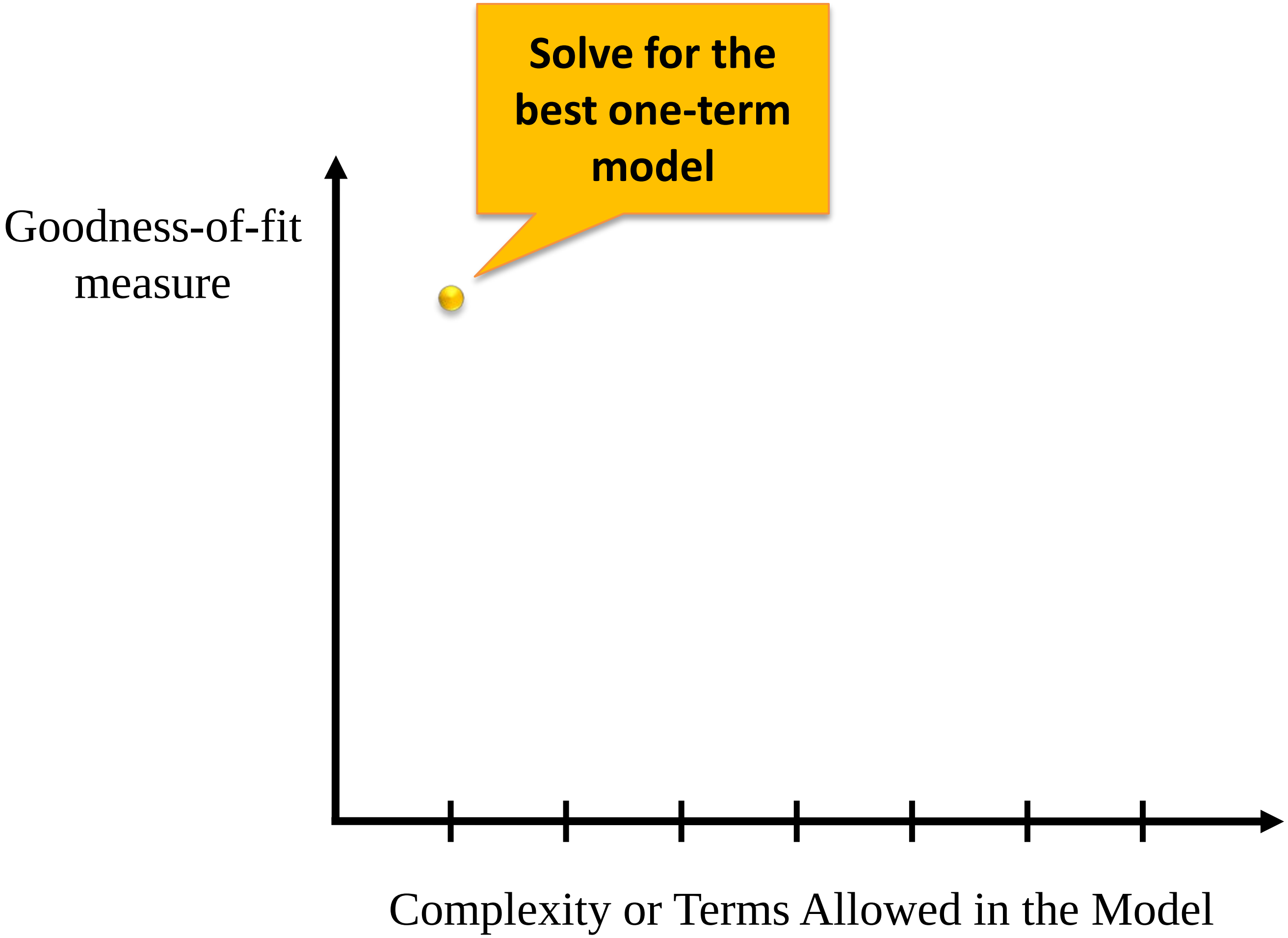
- *Penalize the least squares objective using the magnitude of the regressors*

Stepwise regression [Efroymson, 60]

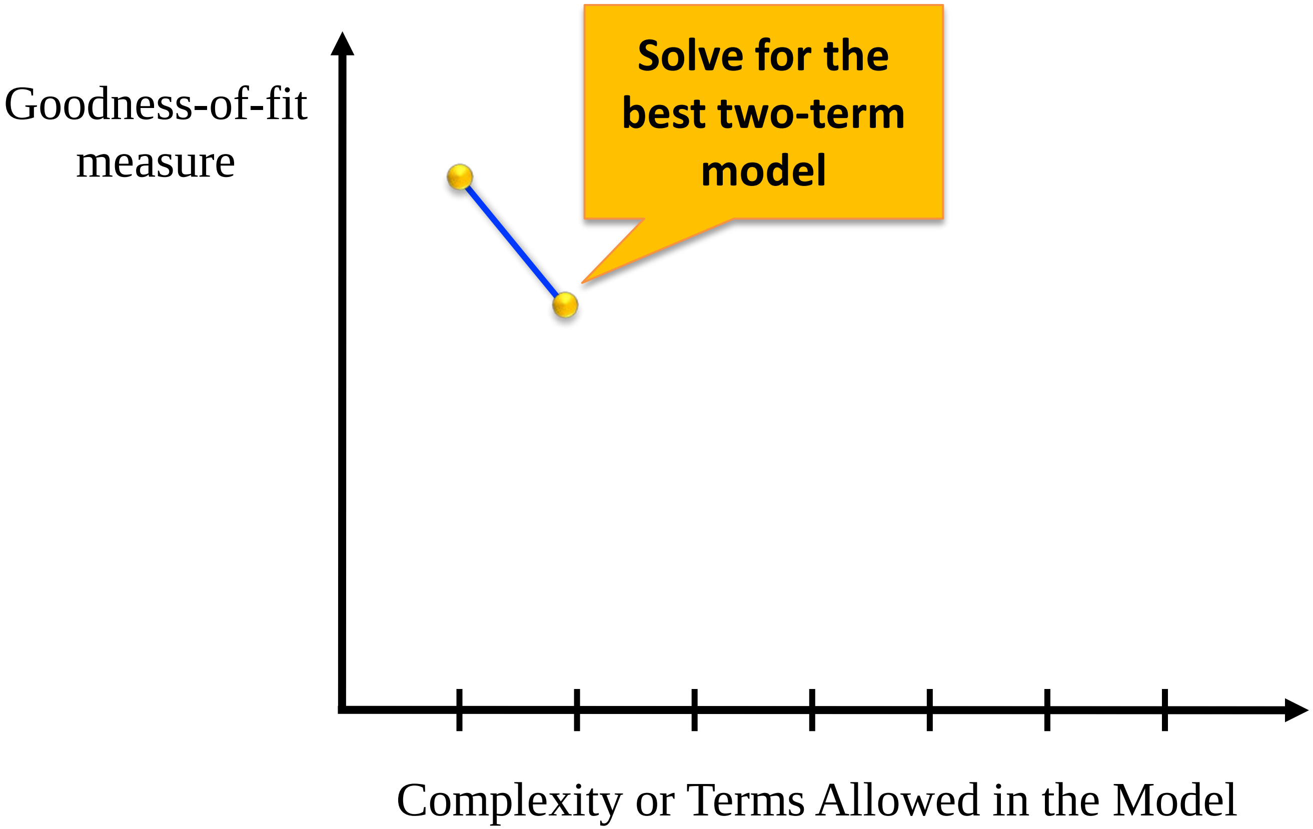
Backward elimination [Oosterhof, 63]

Forward selection [Hamaker, 62]

MODEL SIZING

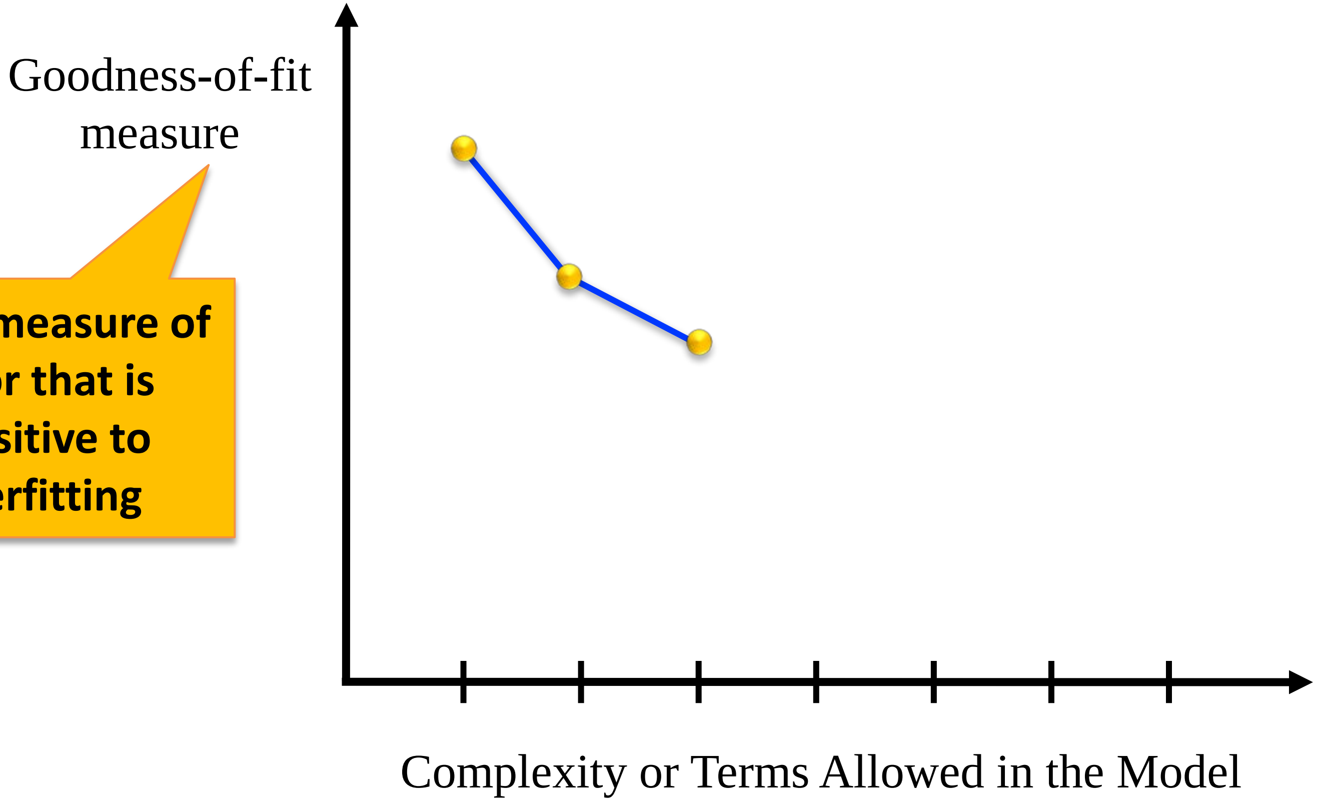


MODEL SIZING



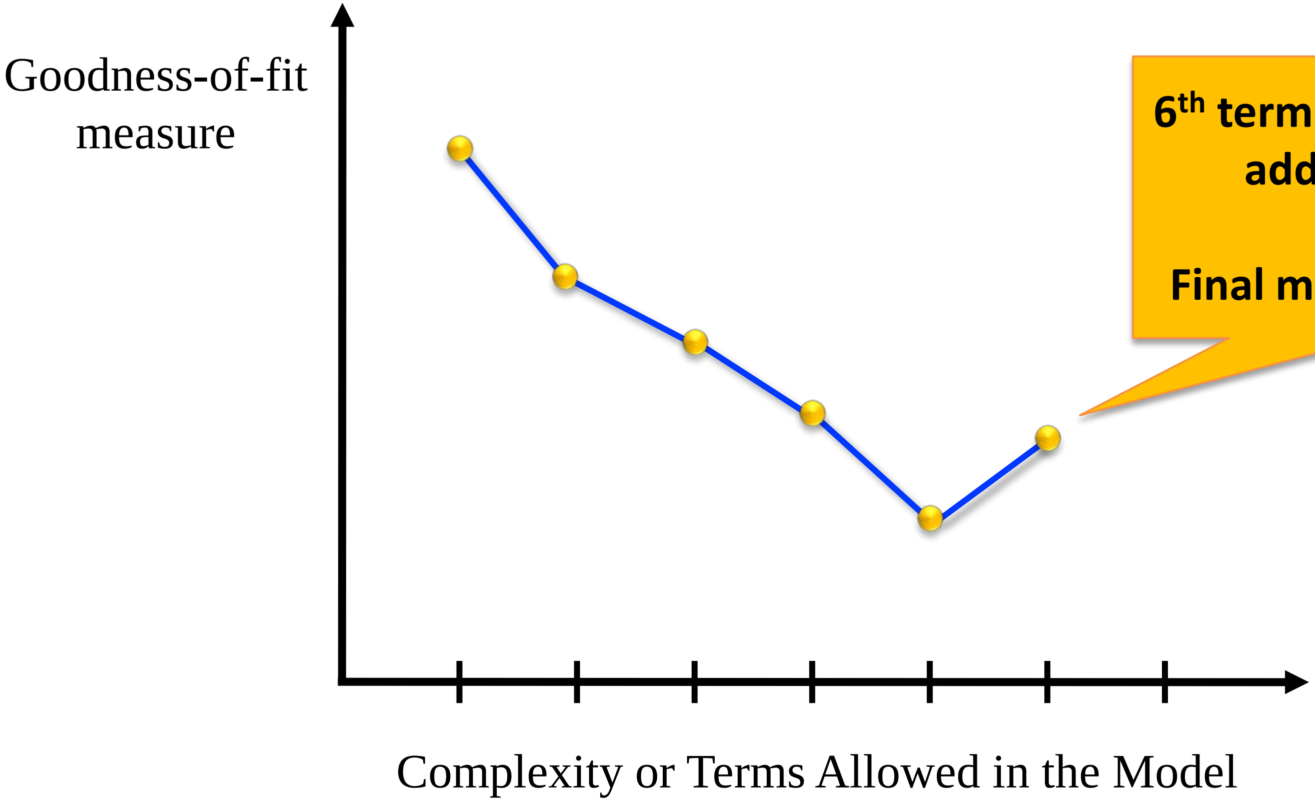
Solve for the best two-term model

MODEL SIZING



Some measure of error that is sensitive to overfitting

MODEL SIZING



6th term was not worth the added complexity

Final model: 5 terms long

BASIS FUNCTION SELECTION

$$
\begin{aligned}
\min \quad & SE = \sum_{i=1}^{N} \left| z_i - \sum_{j \in \mathcal{B}} \beta_j X_{ij} \right| \\
\text{s.t.} \quad & \sum_{j \in \mathcal{B}} y_j = T \\
& -U(1 - y_j) \le \sum_{i=1}^{N} X_{ij} \left(z^i - \sum_{j \in \mathcal{B}} \beta_j X_{ij} \right) \le U(1 - y_j) && j \in \mathcal{B} \\
& \beta^l y_j \le \beta_j \le \beta^u y_j && j \in \mathcal{B} \\
& y_j = \{0, 1\} && j \in \mathcal{B}
\end{aligned}
$$

BASIS FUNCTION SELECTION

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

Find the model with the least error

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

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

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

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

BASIS FUNCTION SELECTION

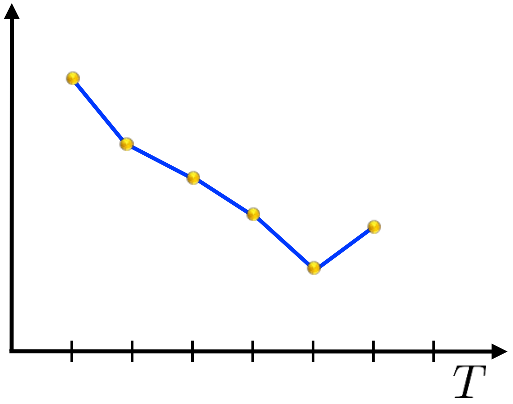
$$\min \quad SE = \sum_{i=1}^{N} \left| z_i - \sum_{j \in \mathcal{B}} \beta_j X_{ij} \right|$$

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

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

$$\beta^l y_j \leq \beta_j \leq \beta^u y_j$$

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



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

BASIS FUNCTION SELECTION

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

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

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

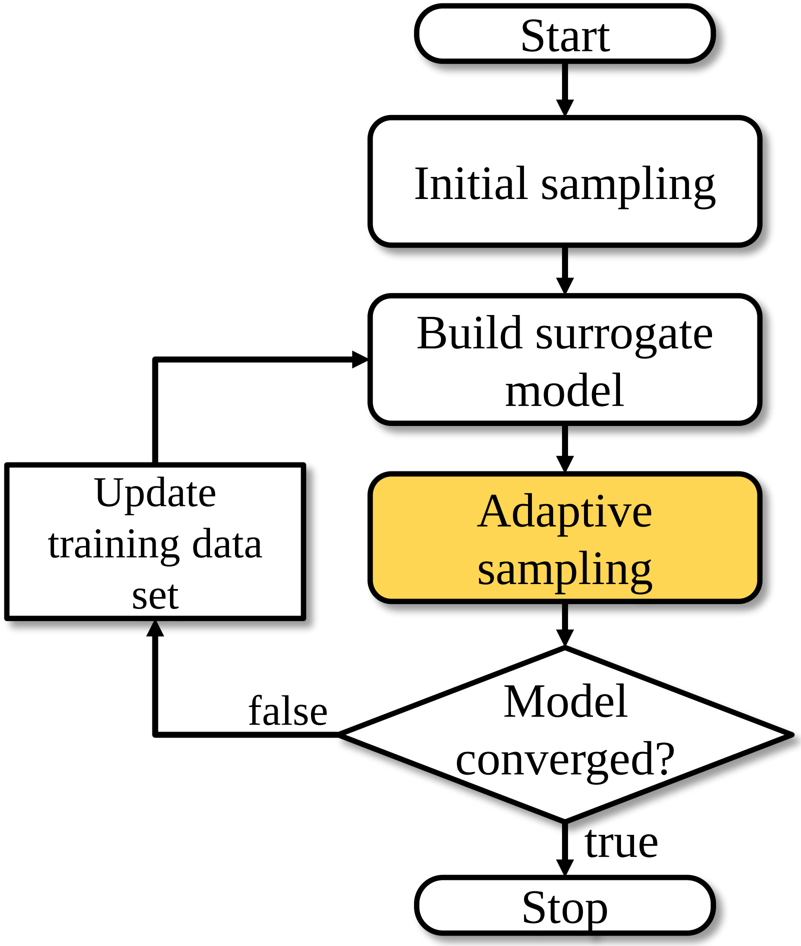
$$\beta^l y_j \le \beta_j \le \beta^u y_j \qquad j\in\mathcal{B}$$

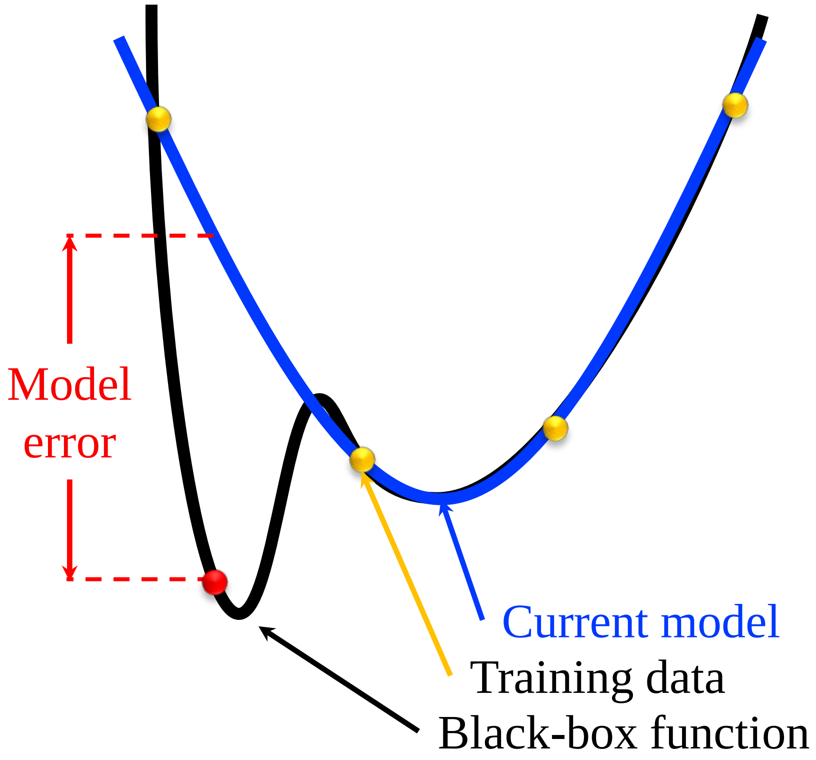
$$y_j = \{0,1\} \qquad j\in\mathcal{B}$$

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

ALAMO

Automated Learning of Algebraic Models for Optimization

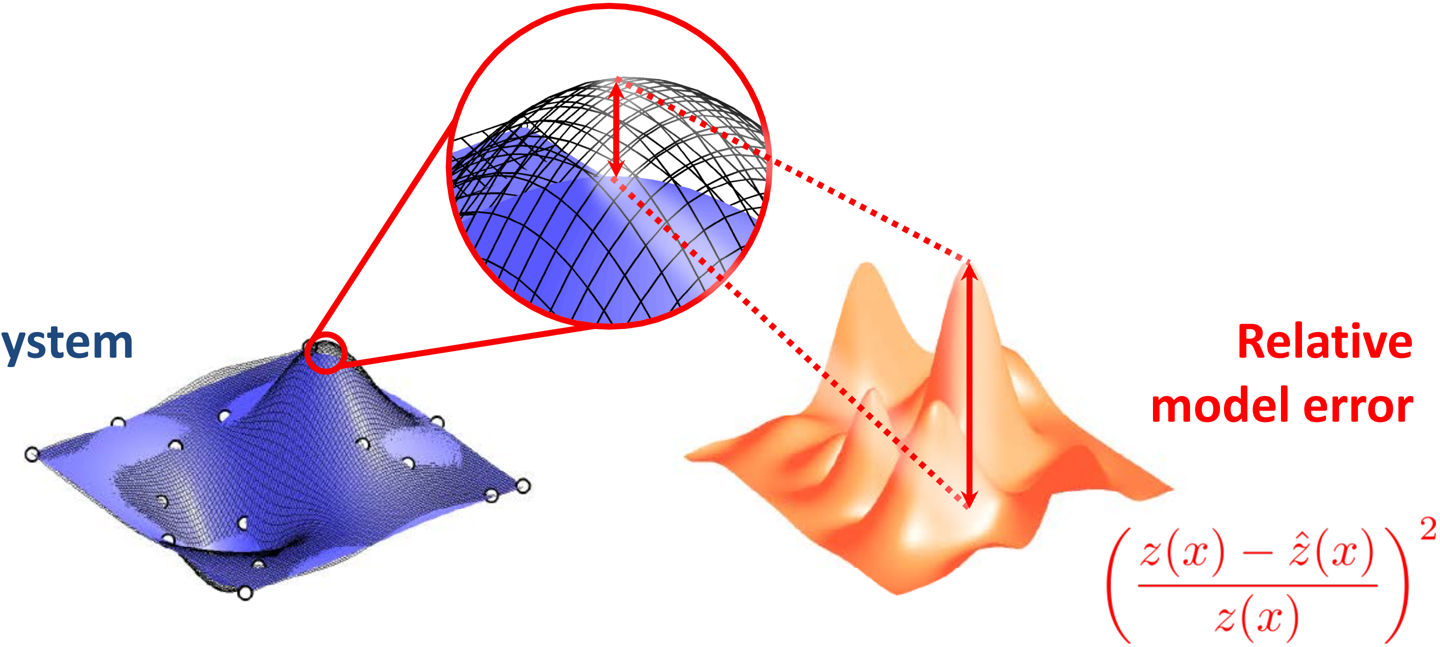




ADAPTIVE SAMPLING

- **Goal: Choose new locations to sample that can best be used to improve the model**

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



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

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

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

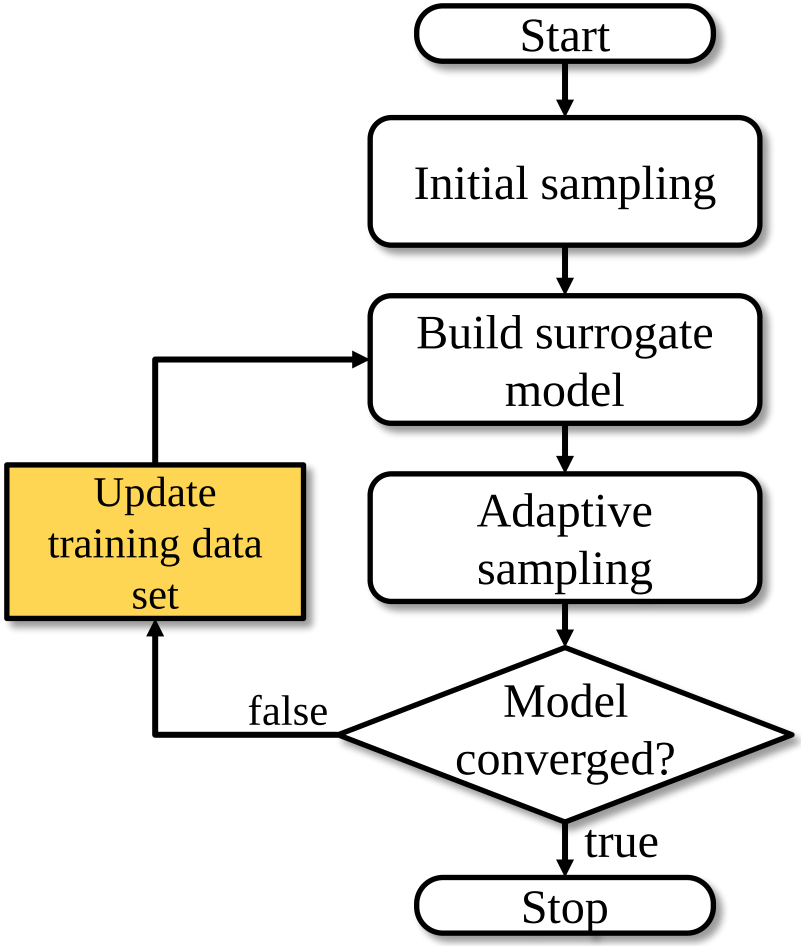
  - **Optimized using a black-box or derivative-free solver (SNOBFIT)** [Huyer and Neumaier, 08]

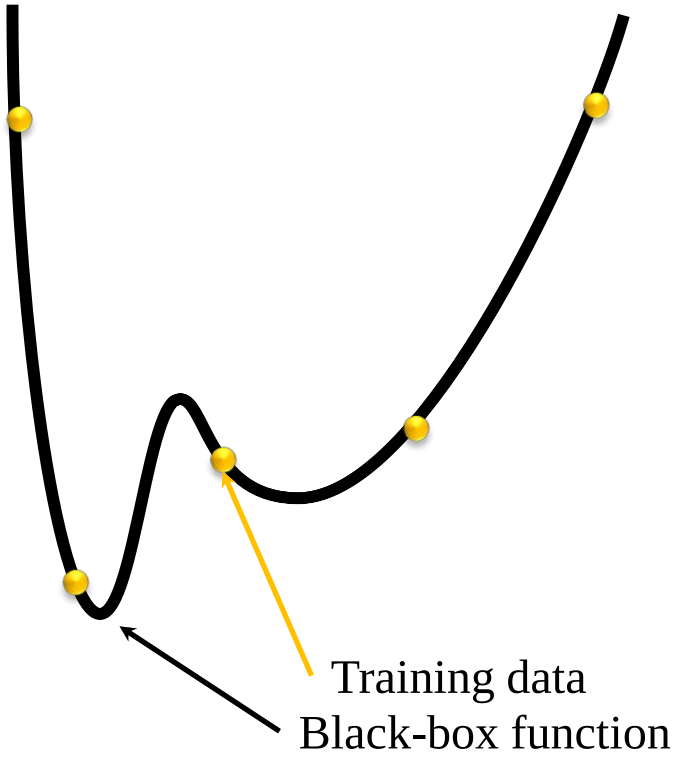
ERROR MAXIMIZATION SAMPLING

- **Information gained using error maximization sampling:**
  - **New data point locations that will be used to better train the next iteration's surrogate model**
  - **Conservative estimate of the true model error**
    - ***Defines a stopping criterion***
    - ***Estimates the final model error***

ALAMO

Automated Learning of Algebraic Models for Optimization





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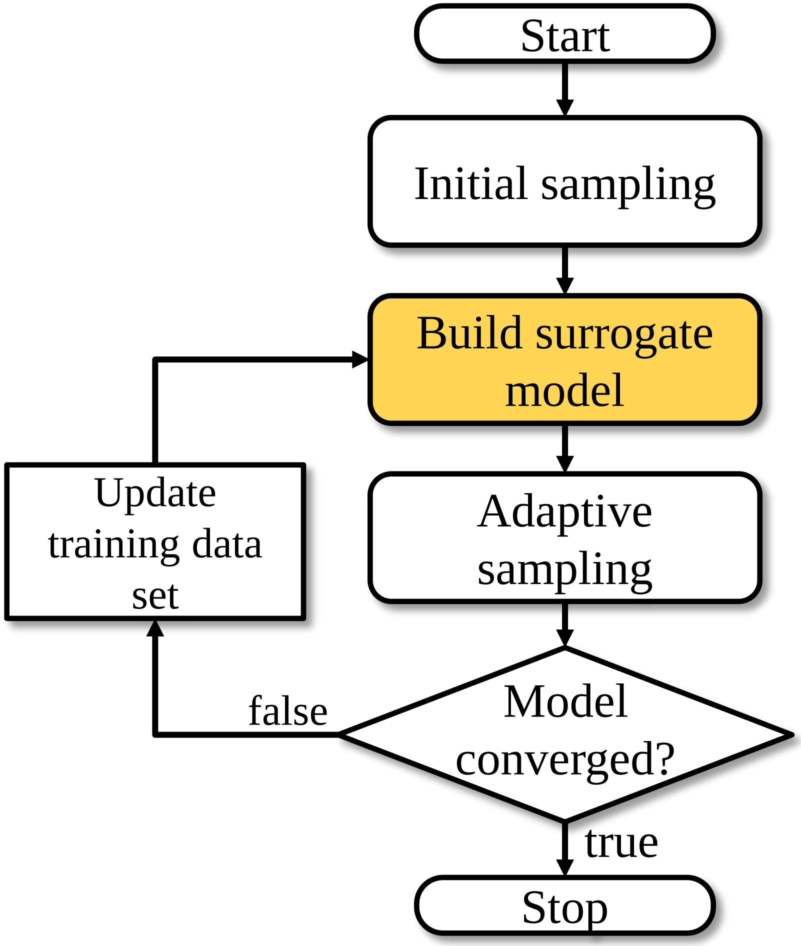
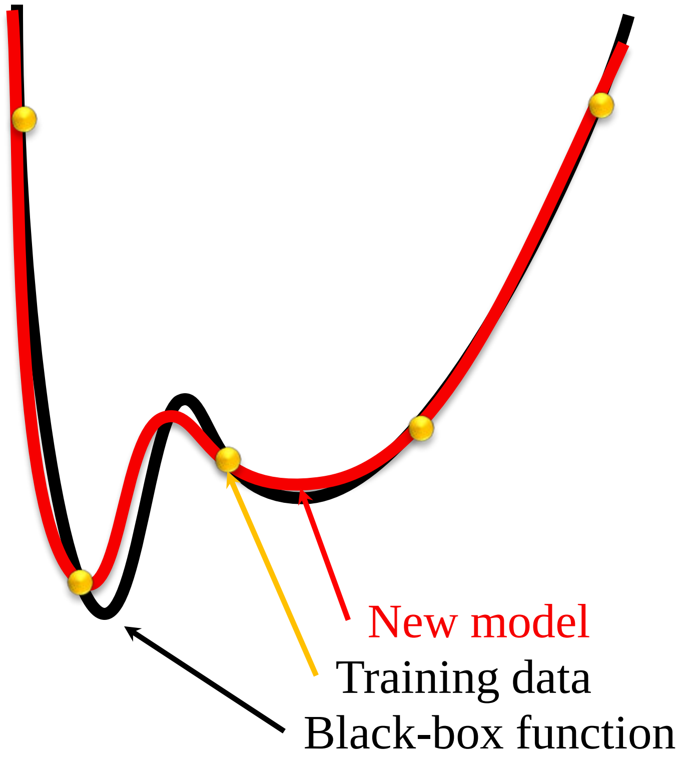




OVERVIEW

1. Surrogate-based optimization of process simulations

2. Surrogate model generation method

3. **Computational experiments**
   - **Validating modeling accuracy, efficiency, and parsimony**

4. Case studies

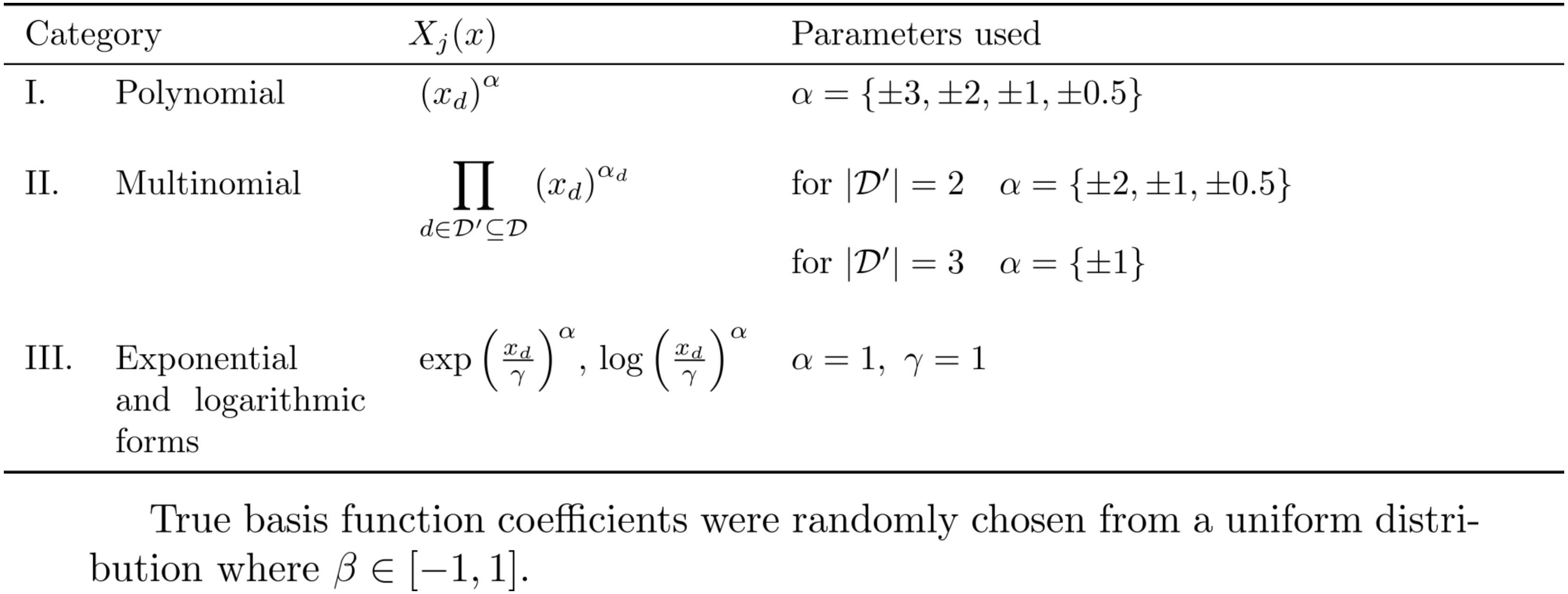
COMPUTATIONAL TESTING

- Goal - 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)
- Two test sets
  - Test set A – Generated from bases available to ALAMO
  - Test set B – Generated from functions with forms not available to ALAMO *(More real world test set)*

DESCRIPTION – TEST SET A

- **Two and three input black-box functions randomly chosen basis functions available to the algorithms with varying complexity from 2 to 10 terms**

- **Basis functions allowed:**



Category		$X_j(x)$	Parameters used
I.	Polynomial	$(x_d)^\alpha$	$\alpha = \{\pm 3, \pm 2, \pm 1, \pm 0.5\}$

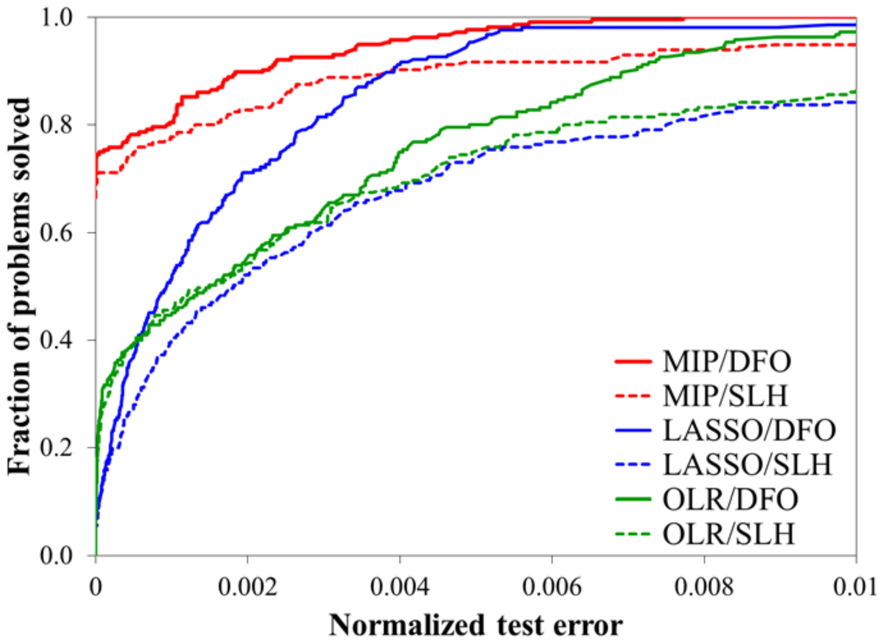
II.	Multinomial	$\prod_{d \in \mathcal{D}' \subseteq \mathcal{D}} (x_d)^{\alpha_d}$	for $\lvert\mathcal{D}'\rvert = 2 \quad \alpha = \{\pm 2, \pm 1, \pm 0.5\}$
			for $\lvert\mathcal{D}'\rvert = 3 \quad \alpha = \{\pm 1\}$

III.	Exponential and logarithmic forms	$\exp\left(\frac{x_d}{\gamma}\right)^\alpha, \log\left(\frac{x_d}{\gamma}\right)^\alpha$	$\alpha = 1, \ \gamma = 1$

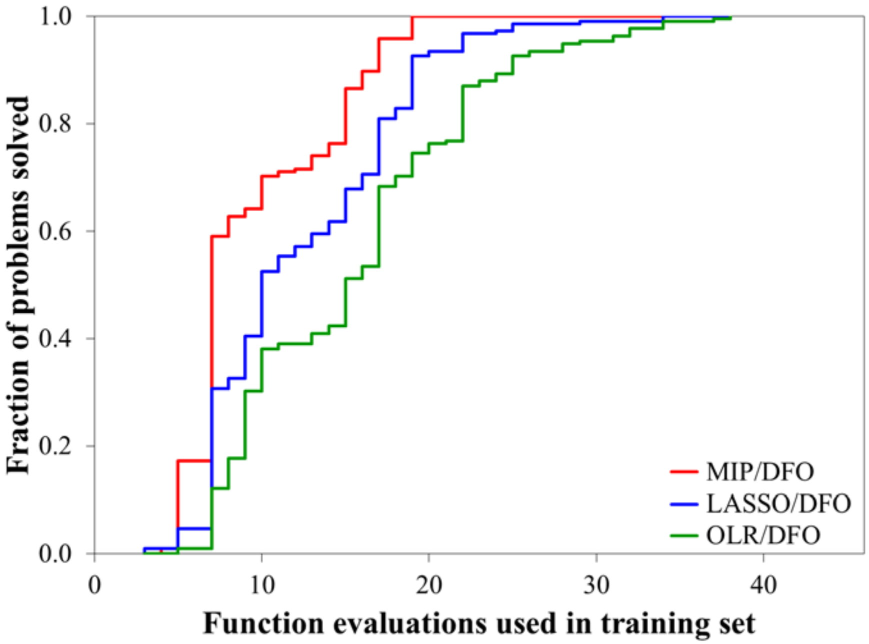
True basis function coefficients were randomly chosen from a uniform distribution where $\beta \in [-1, 1]$.

RESULTS – TEST SET A

Model accuracy



Modeling efficiency



Modeling methods

Our method

LASSO

Least squares

Sampling methods

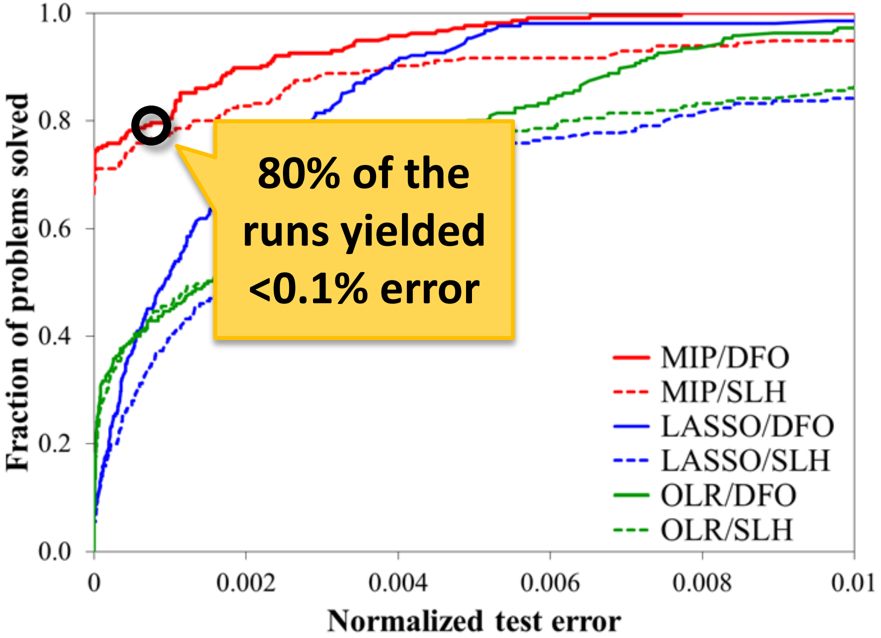
Error maximization

Single Latin hypercube

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

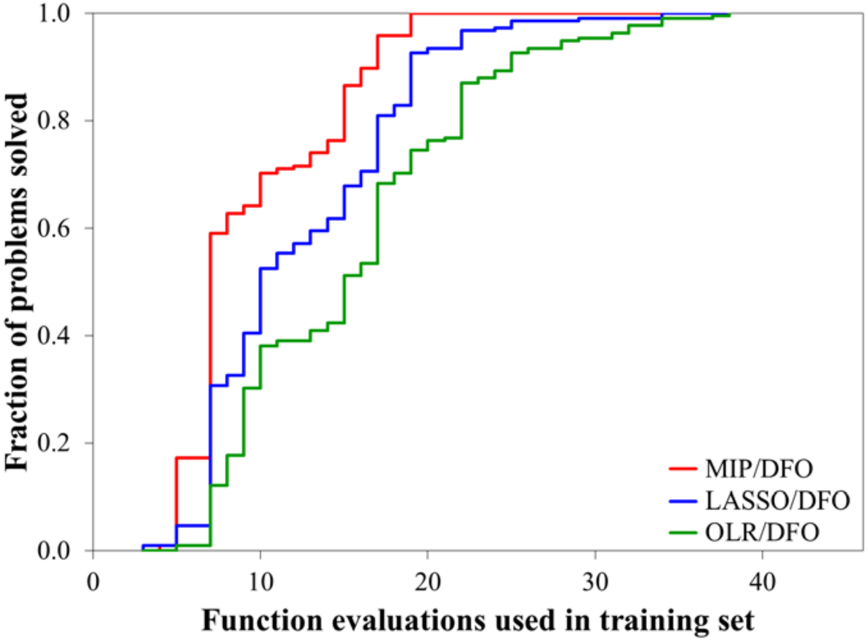
RESULTS – TEST SET A

Model accuracy



80% of the runs yielded <0.1% error

Modeling efficiency



Modeling methods

Our method	LASSO	Least squares

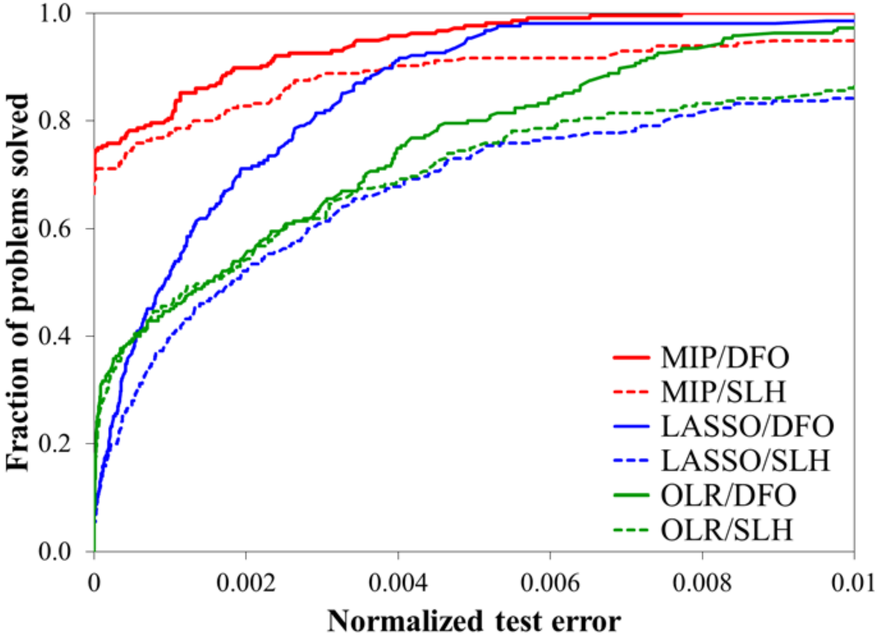
Sampling methods

Error maximization	Single Latin hypercube

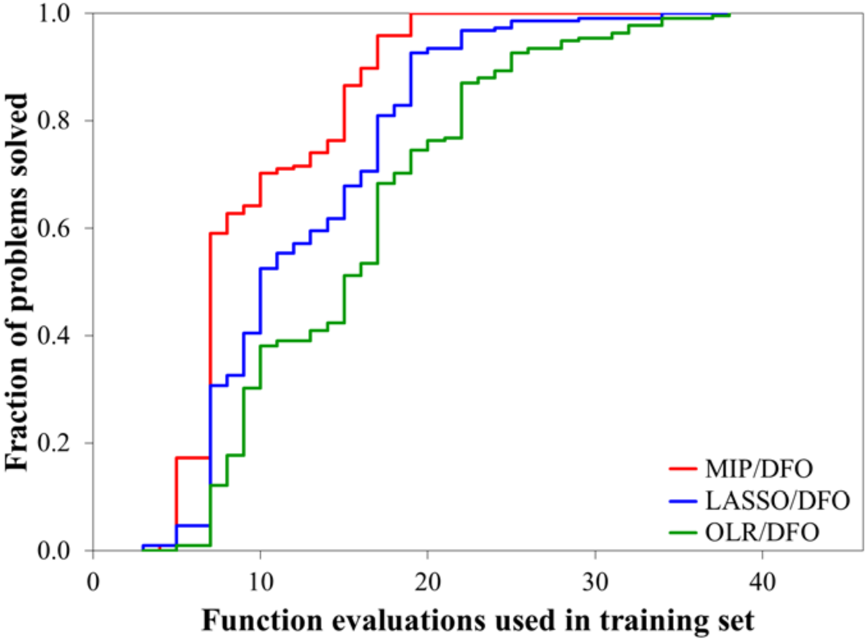
45 test problems, repeated 5 times, tested against 1000 independent data points

RESULTS – TEST SET A

Model accuracy



Modeling efficiency



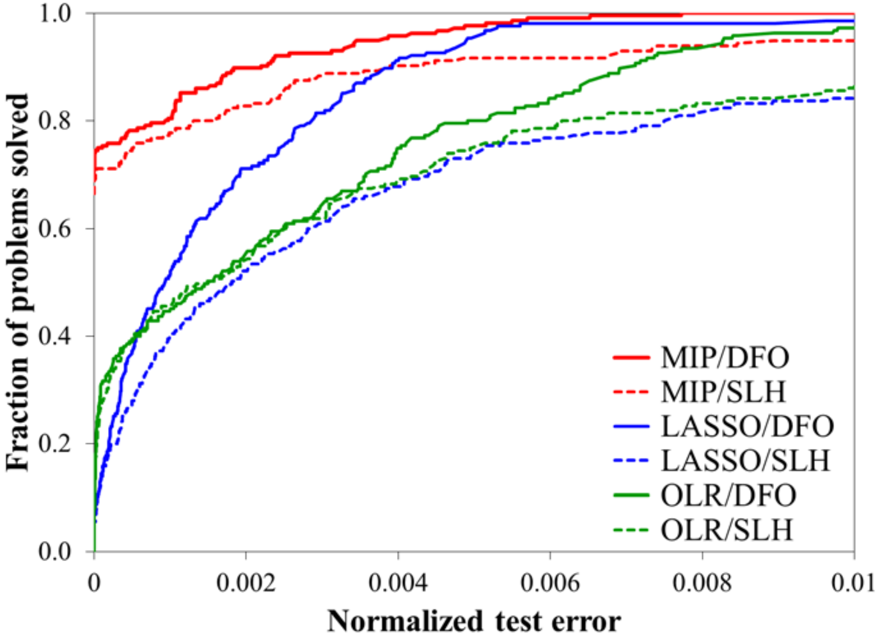
Modeling methods		
Our method	LASSO	Least squares

Sampling methods	
Error maximization	Single Latin hypercube

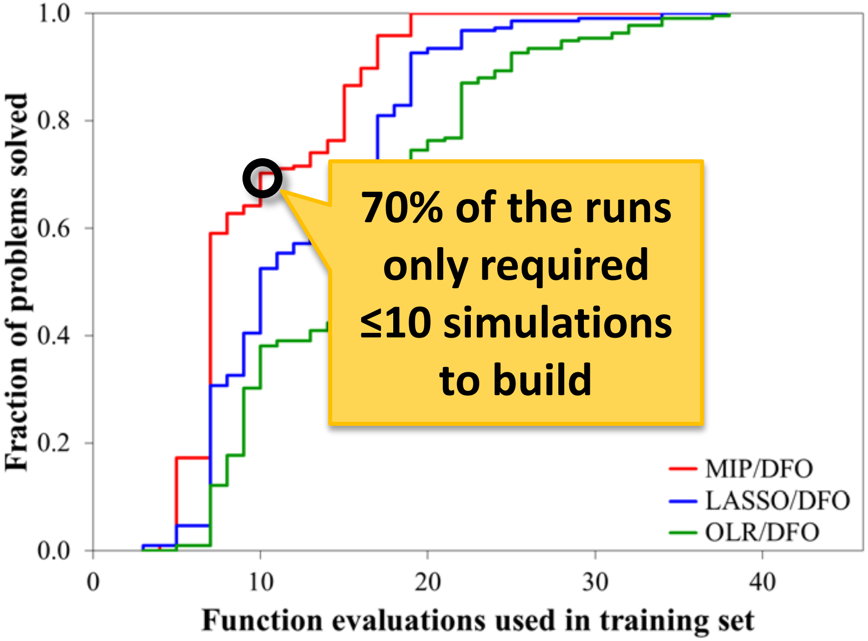
45 test problems, repeated 5 times, tested against 1000 independent data points

RESULTS – TEST SET A

Model accuracy



Modeling efficiency



70% of the runs only required ≤10 simulations to build

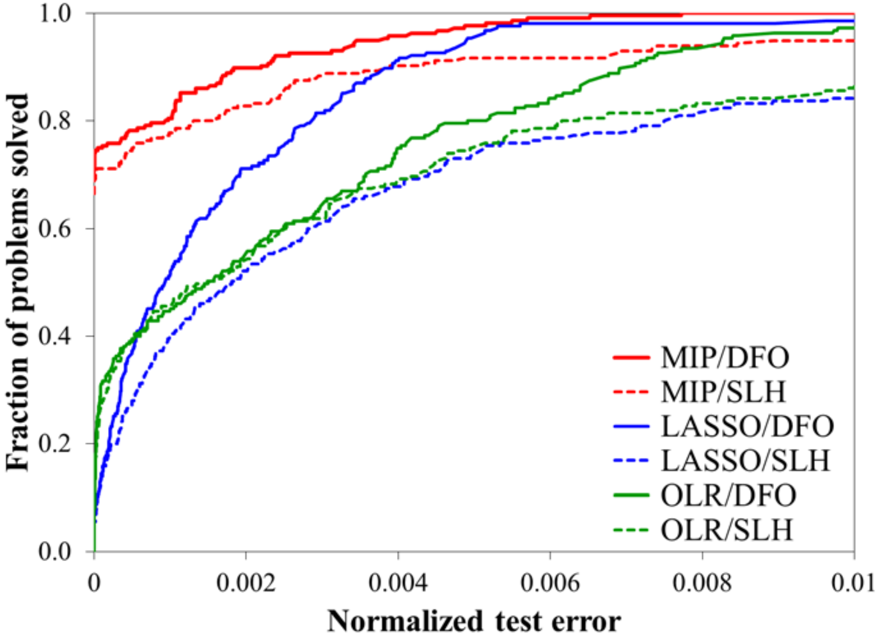
Modeling methods		
Our method	LASSO	Least squares

Sampling methods	
Error maximization	Single Latin hypercube

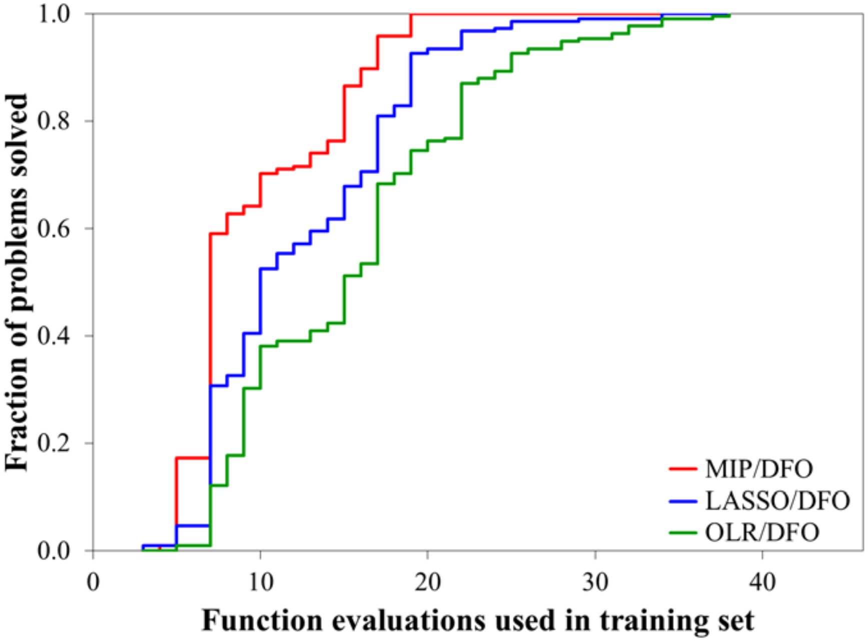
45 test problems, repeated 5 times, tested against 1000 independent data points

RESULTS – TEST SET A

Model accuracy



Modeling efficiency



Modeling methods

Our method | LASSO | Least squares

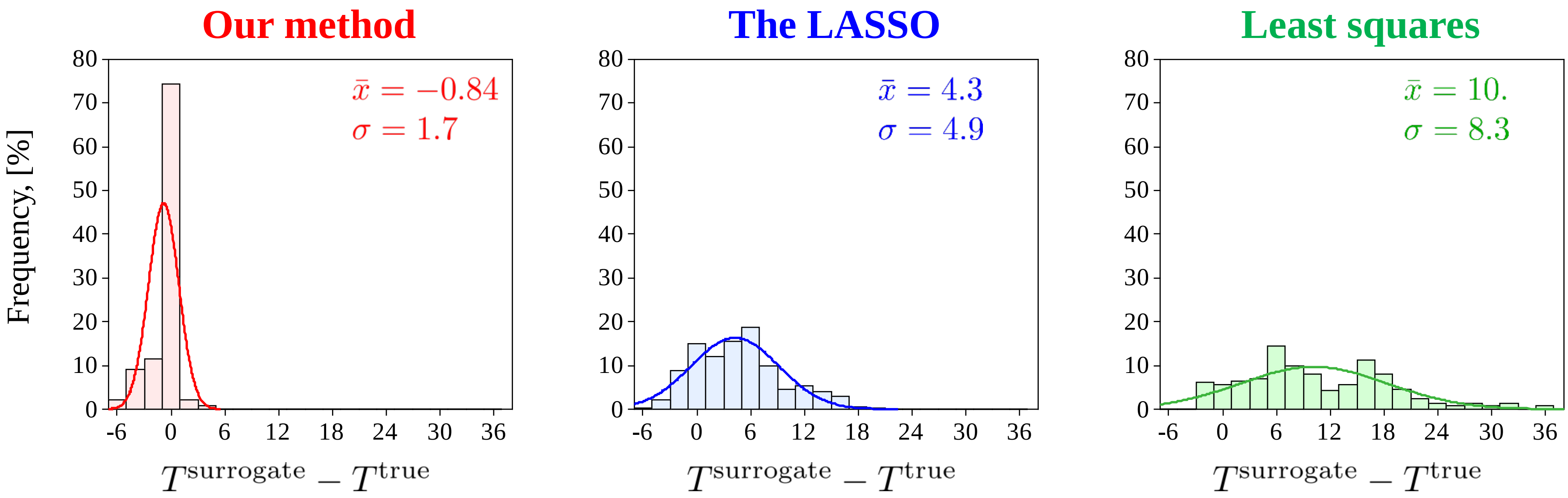
Sampling methods

Error maximization | Single Latin hypercube

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

MODEL SIZING RESULTS

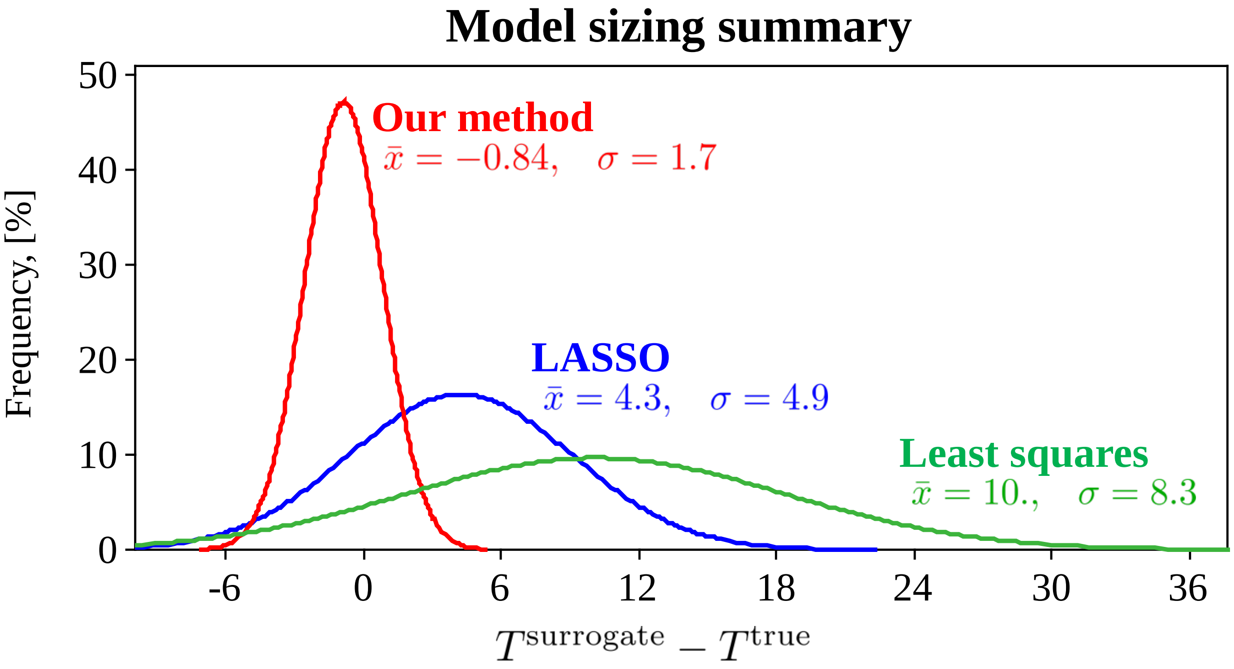
$$\left[\begin{array}{l}\text{No. of terms in the}\\ \text{surrogate model}\end{array}\right] - \left[\begin{array}{l}\text{No. of terms in}\\ \text{the true function}\end{array}\right]$$



45 problems with 2-10 available bases, 5 repeats

MODEL SIZING RESULTS

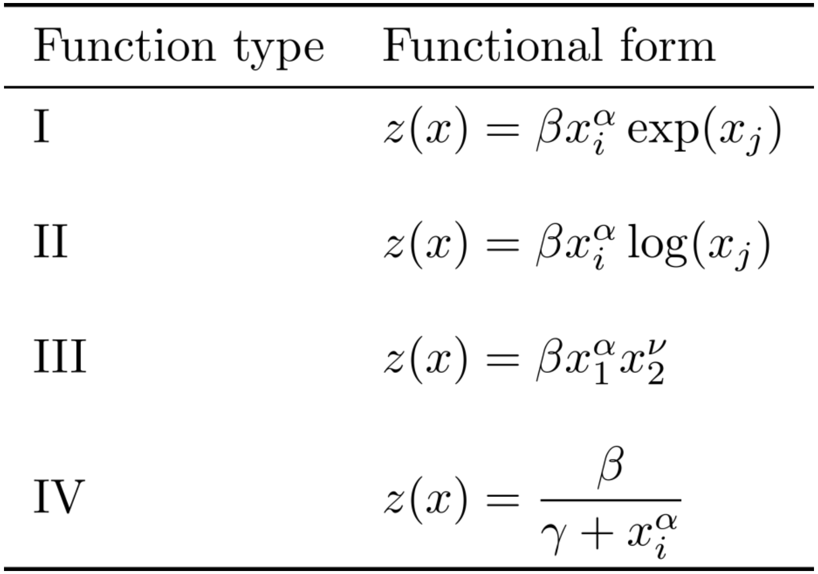
$$\begin{bmatrix}\text{No. of terms in the} \\ \text{surrogate model}\end{bmatrix} - \begin{bmatrix}\text{No. of terms in} \\ \text{the true function}\end{bmatrix}$$



45 problems with 2-10 available bases, 5 repeats

DESCRIPTION – TEST SET B

- **Two input black-box functions with basis functions unavailable to the algorithms with**

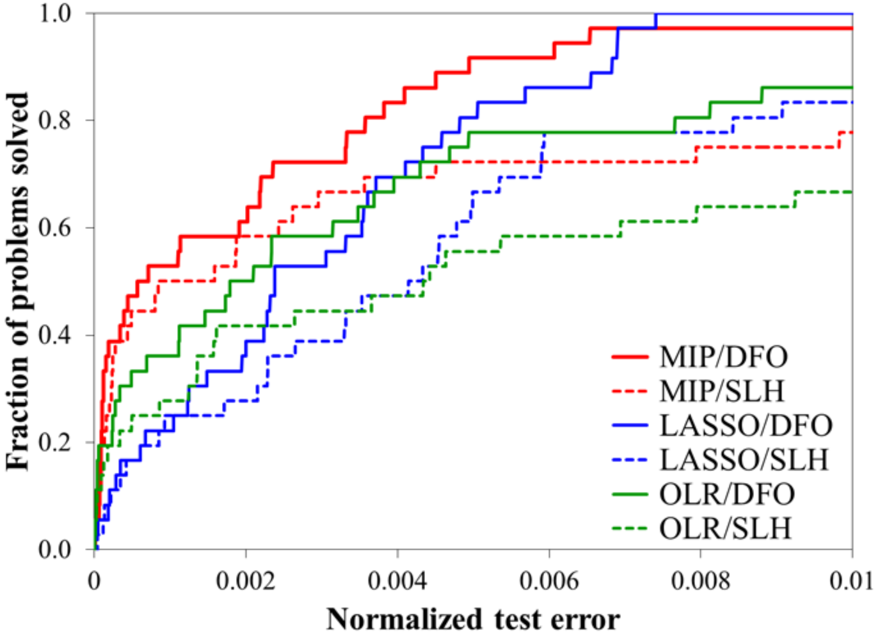


Function type	Functional form
I	$z(x) = \beta x_i^\alpha \exp(x_j)$
II	$z(x) = \beta x_i^\alpha \log(x_j)$
III	$z(x) = \beta x_1^\alpha x_2^\nu$
IV	$z(x) = \dfrac{\beta}{\gamma + x_i^\alpha}$

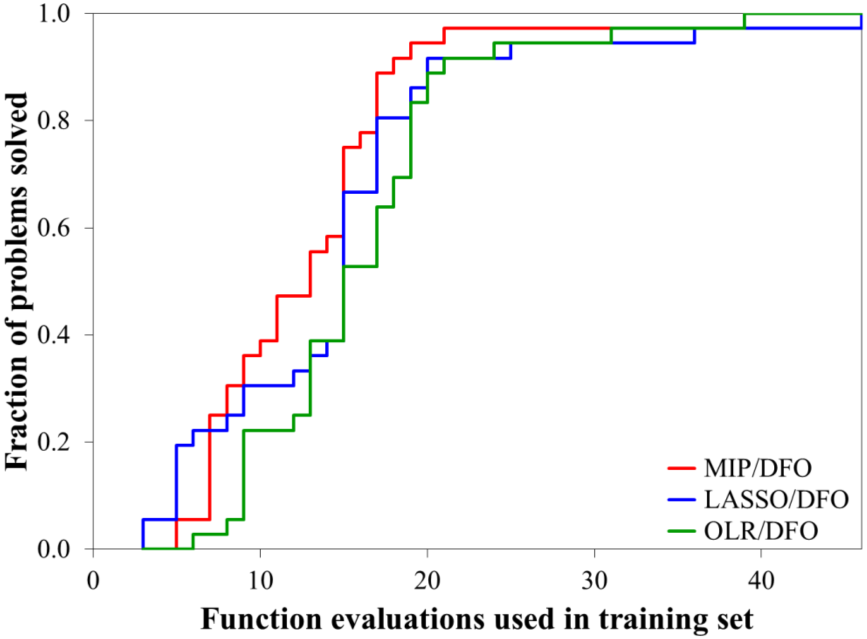
with true parameters chosen from a uniform distribution where $\beta \in [-1, 1]$, $\alpha, \nu \in [-3, 3]$, $\gamma \in [-5, 5]$, and $i, j \in \{1, 2\}$.

RESULTS – TEST SET B

Model accuracy



Modeling efficiency



Modeling methods

Our method

LASSO

Least squares

Sampling methods

Error maximization

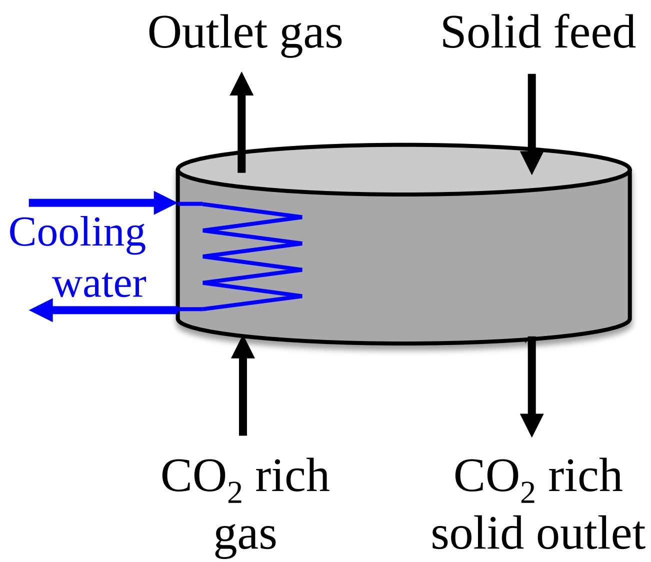
Single Latin hypercube

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

OVERVIEW

1. Surrogate-based optimization of process simulations
2. Surrogate model generation method
3. Computational experiments
4. **Case studies**
   - **Small example problem**
   - **Real world example**

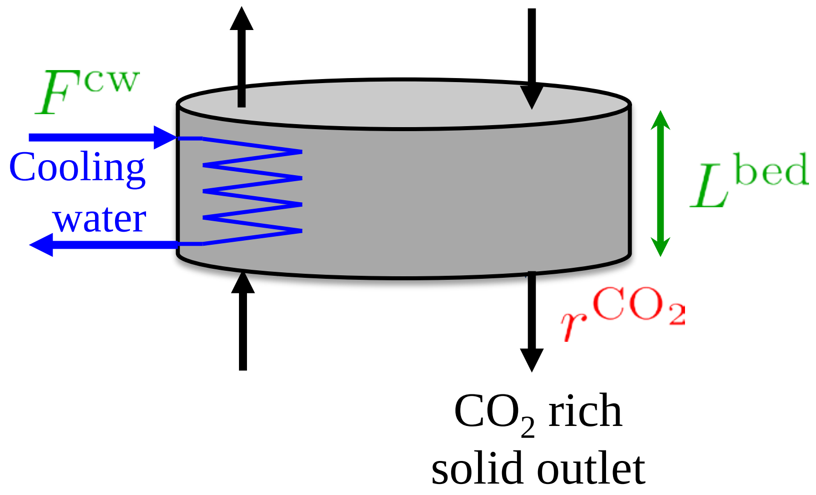
BUBBLING FLUIDIZED BED ADSORBER



Goal: Optimize a bubbling fluidized bed reactor by

- **Minimizing the increased cost of electricity**
- **Maximizing CO_2 removal**

BUBBLING FLUIDIZED BED ADSORBER



Generate model of % CO_2 removal:

$$r^{\mathrm{CO_2}}(L^{\mathrm{bed}}, F^{\mathrm{cw}}) = f_1(L^{\mathrm{bed}}, F^{\mathrm{cw}})$$

Over the Range:

$$\begin{aligned} 1\ \mathrm{m} &\leq L^{\mathrm{bed}} &&\leq 10\ \mathrm{m} \\ 1 \cdot 10^4\ \frac{\mathrm{kmol}}{\mathrm{h}} &\leq F^{\mathrm{cw}} &&\leq 20 \cdot 10^4\ \frac{\mathrm{kmol}}{\mathrm{h}} \end{aligned}$$

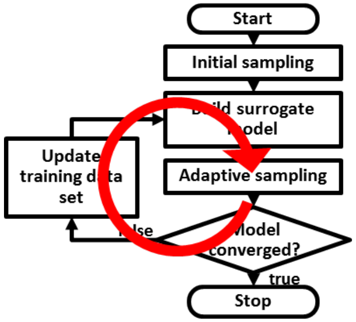
POTENTIAL MODEL

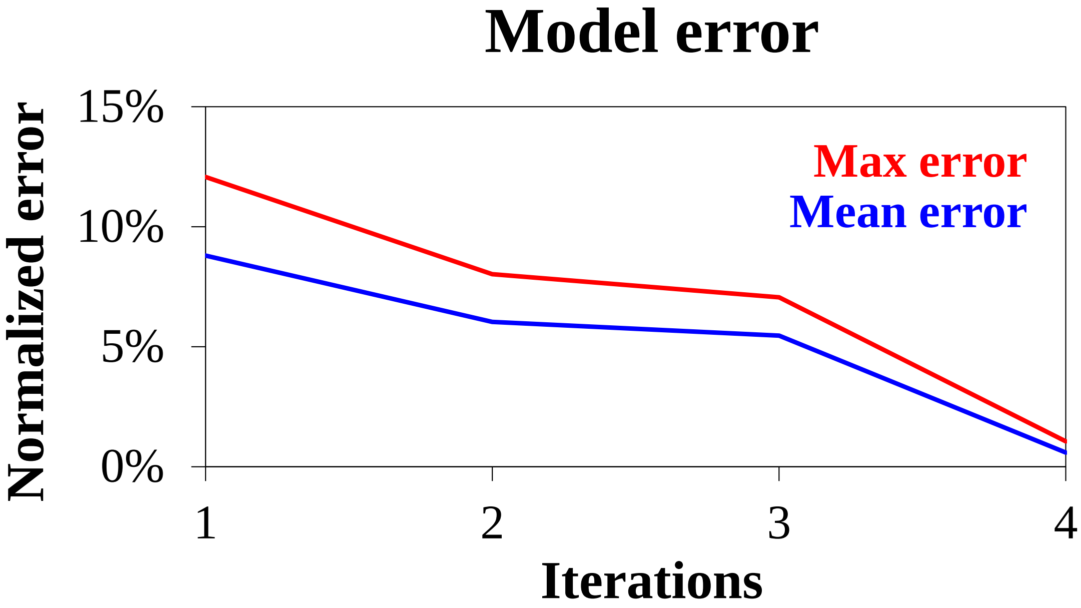
$$
\begin{aligned}
r^{\mathrm{CO_2}} = {} & \beta_0 + \beta_1 F + \beta_2 L + \beta_3 \mathrm{e}^F + \beta_4 \mathrm{e}^L + \beta_5 \ln(F) + \beta_6 \ln(L) + \beta_7 \frac{F}{L} + \beta_8 \frac{2\,F}{L^2} + \\
& \beta_9 F\,L^2 + \beta_{10} F^2\,L + \beta_{11} \frac{F}{\sqrt{L}} + \beta_{12} F\,\sqrt{L} + \beta_{13} \frac{L}{\sqrt{F}} + \beta_{14} \sqrt{F}\,L + \beta_{15} \frac{F}{L^{\frac{1}{3}}} + \beta_{16} F\,L^{\frac{1}{3}} + \\
& \beta_{17} \frac{L}{F^{\frac{1}{3}}} + \beta_{18} F^{\frac{1}{3}}\,L + \beta_{19} 2\,F\,\ln(F) + \beta_{20} F\,\ln(L) + \beta_{21} L\,\ln(F) + \beta_{22} L\,\ln(L) + \beta_{23} \frac{1}{F} + \\
& \beta_{24} \frac{1}{F^2} + \beta_{25} F^2 + \beta_{26} \frac{1}{F^3} + \beta_{27} \frac{1}{\sqrt{F}} + \beta_{28} \sqrt{F} + \beta_{29} F^3 + \beta_{30} \frac{1}{F^{\frac{1}{3}}} + \beta_{31} F^{\frac{1}{3}} + \beta_{32} \frac{1}{L} + \\
& \beta_{33} \frac{1}{L^2} + \beta_{34} L^2 + \beta_{35} \frac{1}{L^3} + \beta_{36} \frac{1}{\sqrt{L}} + \beta_{37} \sqrt{L} + \beta_{38} L^3 + \beta_{39} \frac{1}{L^{\frac{1}{3}}} + \beta_{40} L^{\frac{1}{3}} + \beta_{41} \frac{1}{F\,L} + \\
& \beta_{42} \frac{2\,L^2}{F} + \beta_{43} \frac{\sqrt{L}}{F} + \beta_{44} \frac{F^2}{L^2} + \beta_{45} F^2\,L^2 + \beta_{46} \frac{\sqrt{F}}{L} + \beta_{47} \frac{F^3}{L} + \beta_{48} \frac{1}{F^3\,L^3} + \beta_{49} \frac{1}{\sqrt{F}\,\sqrt{L}} + \\
& \beta_{50} \frac{\sqrt{F}}{\sqrt{L}} + \beta_{51} \sqrt{F}\,\sqrt{L} + \beta_{52} \frac{F^3}{L^3} + \beta_{53} F^3\,L^3 + \beta_{54} \frac{L^{\frac{1}{3}}}{F} + \beta_{55} \frac{F^{\frac{1}{3}}}{L} + \beta_{56} \frac{1}{F^{\frac{1}{3}}\,L^{\frac{1}{3}}} + \beta_{57} \frac{F^{\frac{1}{3}}}{L^{\frac{1}{3}}} + \\
& \beta_{58} F^{\frac{1}{3}}\,L^{\frac{1}{3}} + \beta_{59} F^{\frac{1}{3}}\,\ln(L) + \beta_{60} L^{\frac{1}{3}}\,\ln(F) + \beta_{61} L^{\frac{1}{3}}\,\ln(L) + \beta_{62} F\,L
\end{aligned}
$$

63 basis functions

Not tractable in an algebraic superstructure formulation!

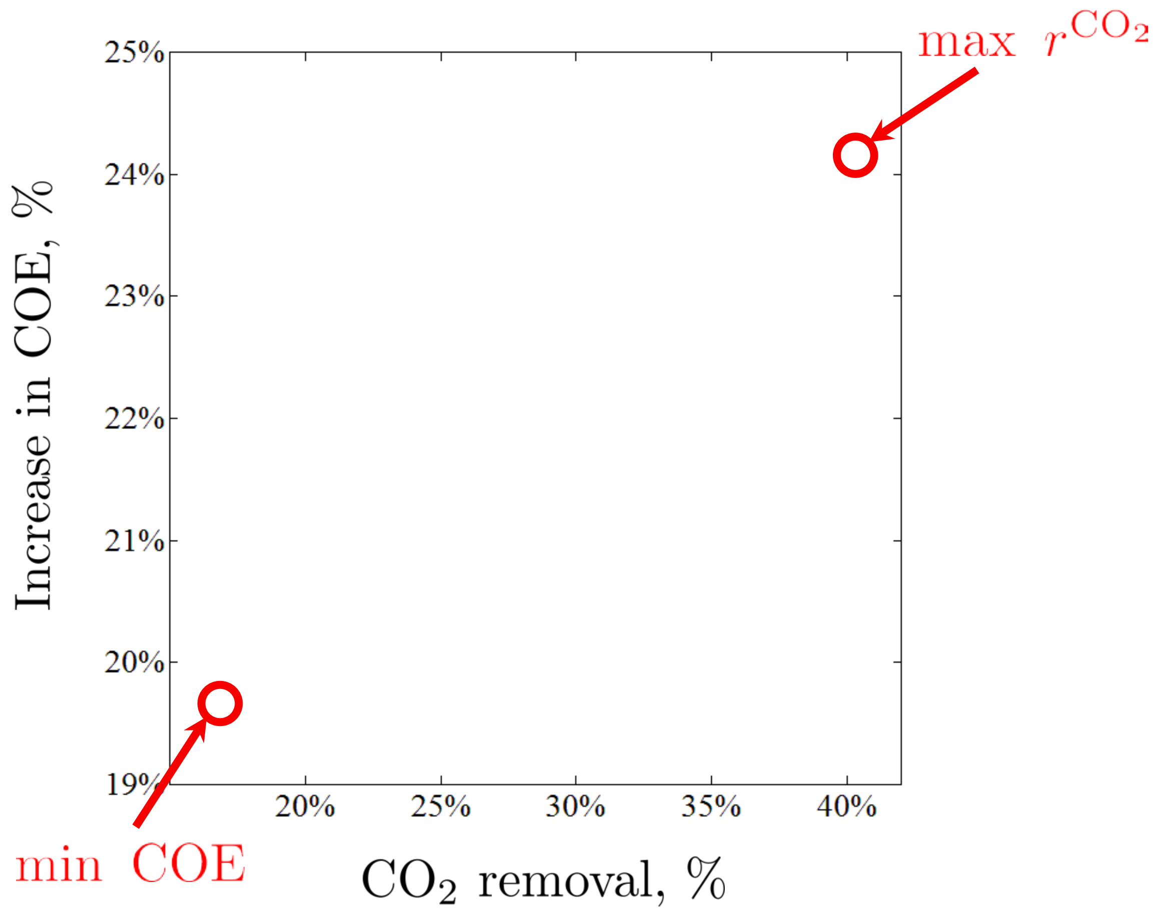
BUILDING THE MODEL



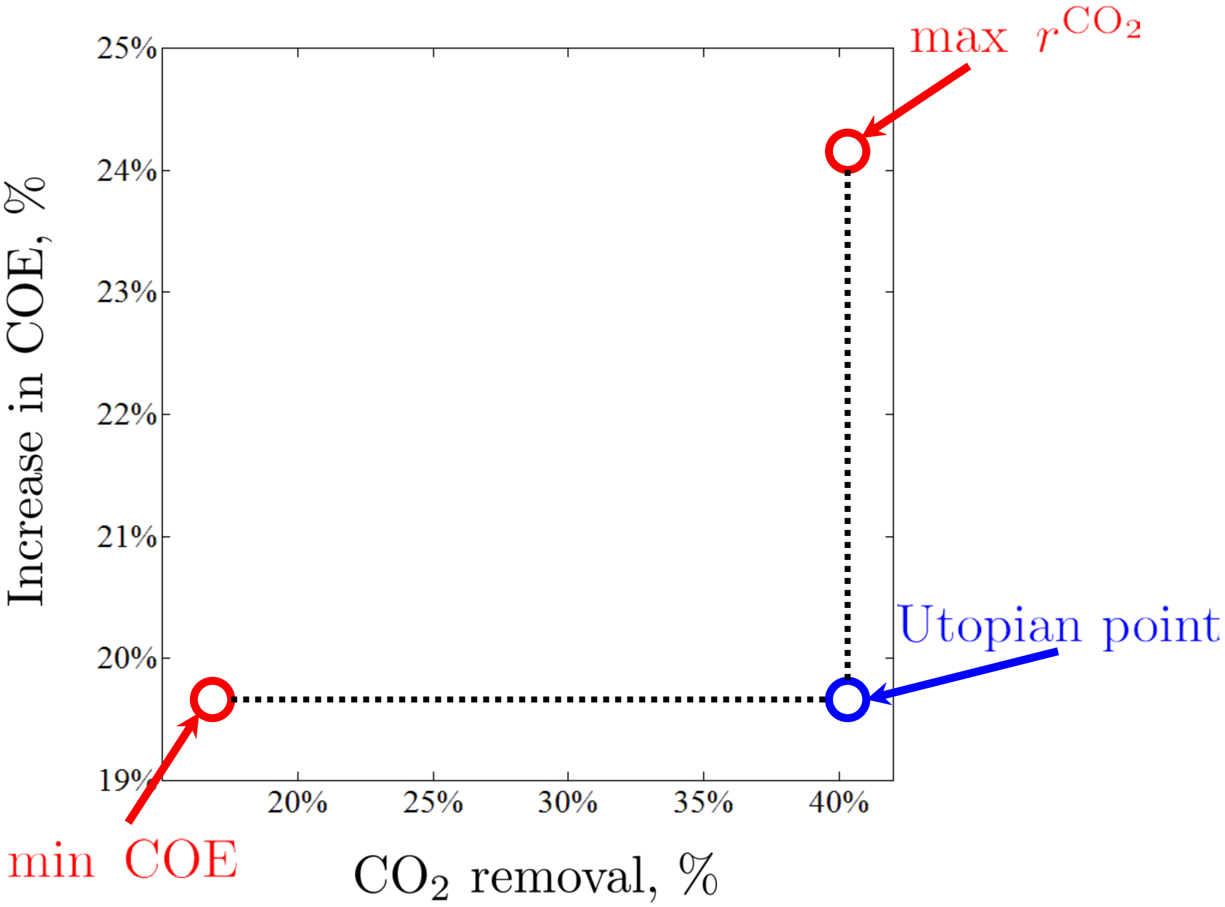


Iteration	Surrogate
1	$0.17\,\sqrt[3]{L}$
2	$0.22\,\sqrt{L} - 0.018\,L\,F - 0.015\frac{L}{\sqrt{F}}$
3	$0.18 + -0.02\,F^2 + 0.038\,L\,F + 0.061\log L - 0.003\,F\,L^2 - 5.1\cdot10^{-5}\,\frac{L^2}{F}$
4	$0.057\,F - \frac{0.033\,L}{\sqrt[3]{F}} + 0.29\,\sqrt{L} + \frac{\left(1.7\cdot10^{-4}\right)L^2}{F} - \frac{0.042\,\sqrt{F}}{L} - \frac{\left(1.6\cdot10^{-3}\right)\sqrt[3]{L}}{F} - 0.084\,\sqrt{F}\,\sqrt{L}$

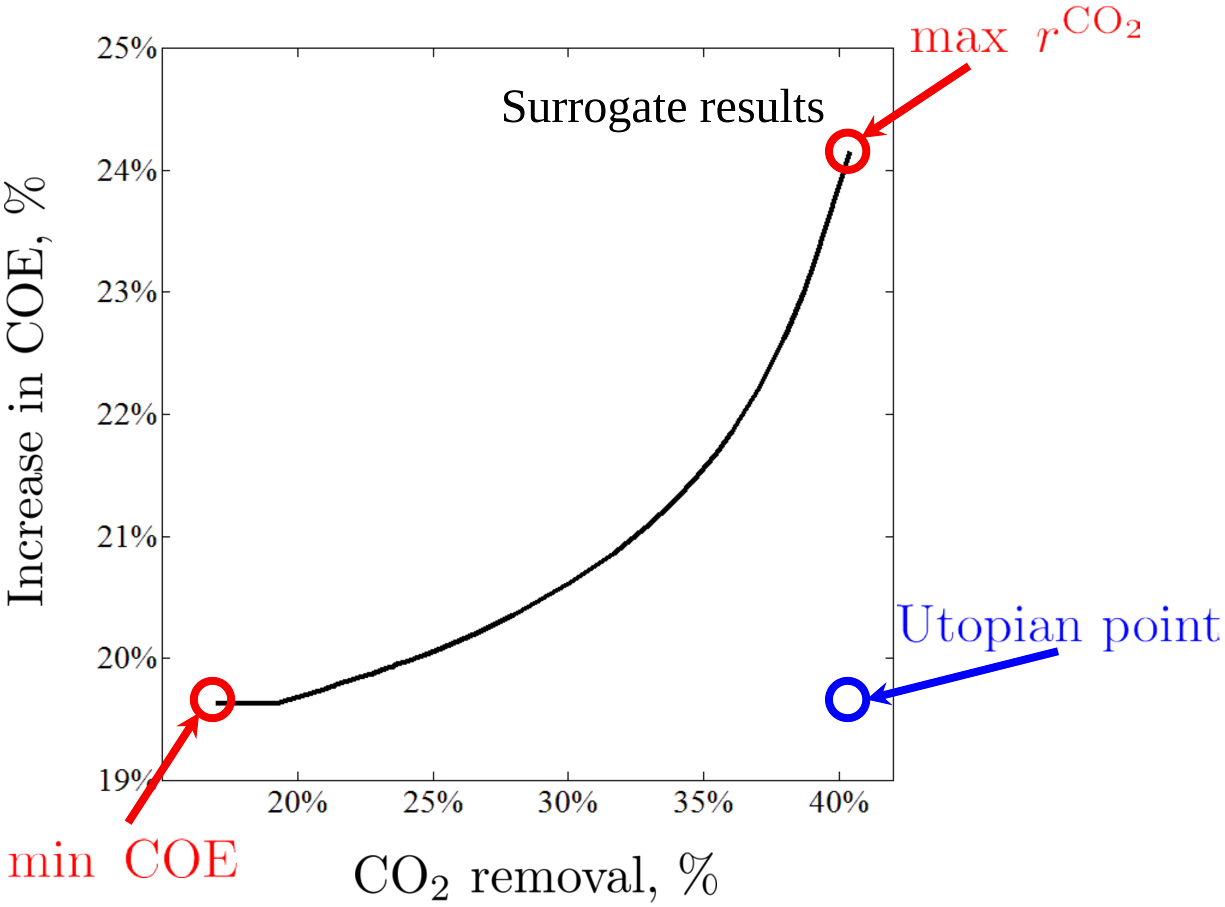
OPTIMAL PARETO CURVE



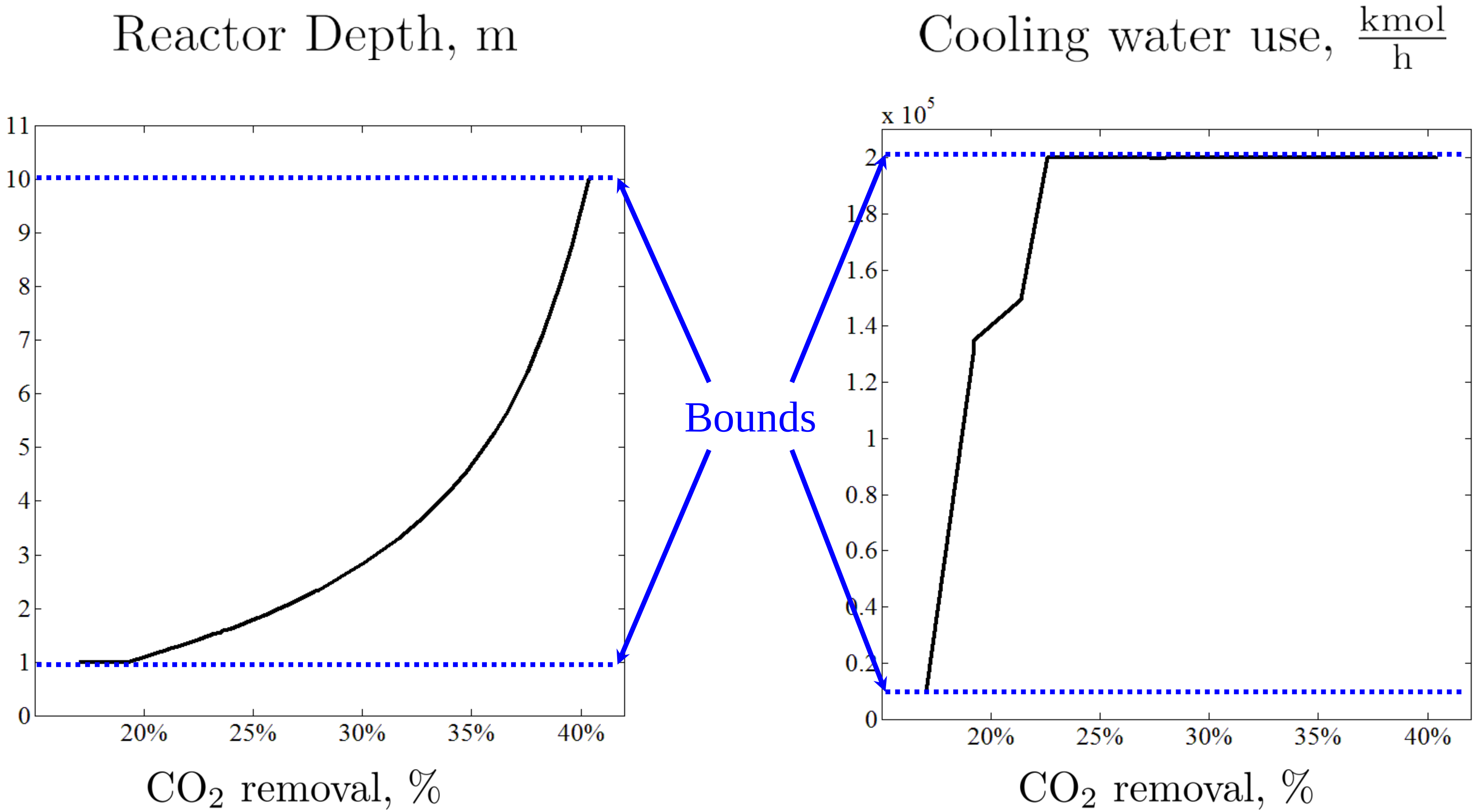
OPTIMAL PARETO CURVE



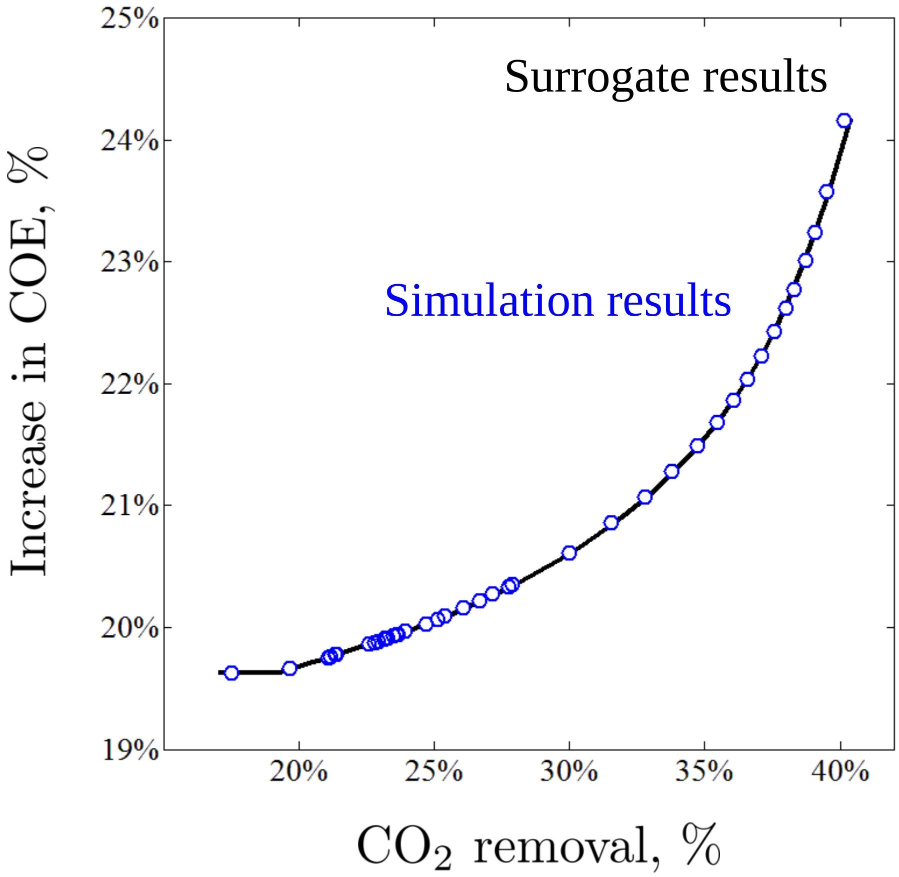
OPTIMAL PARETO CURVE



DESIGN VARIABLE RESULTS



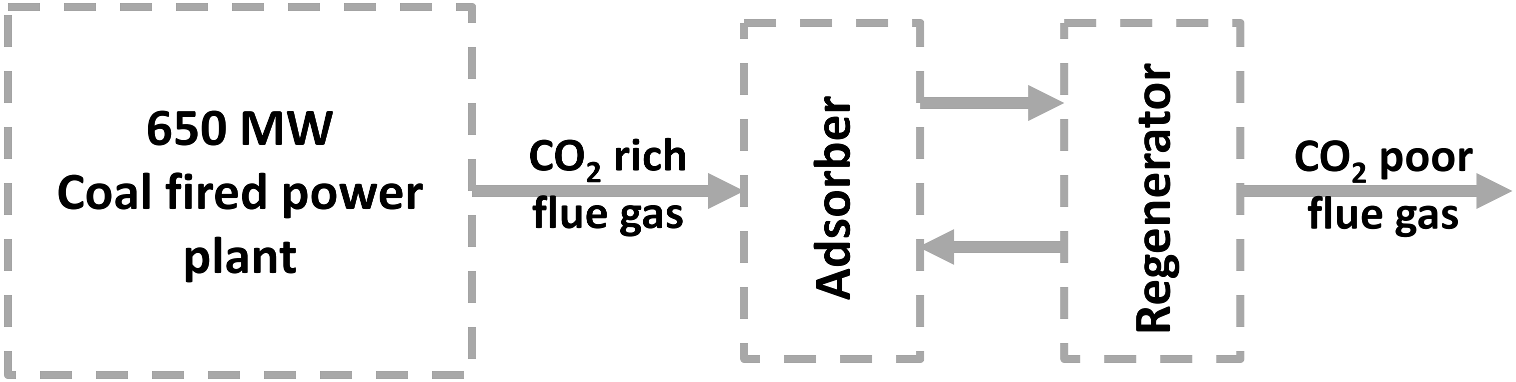
OPTIMAL PARETO CURVE



CARBON CAPTURE OPTIMIZATION

- **Problem statement:**

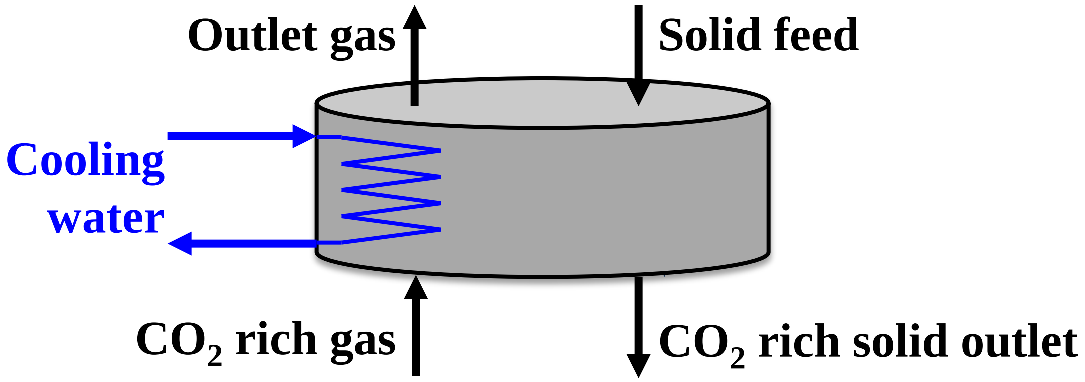
  Capture 90% of CO_2 from a 350MW power plant's post combustion flue gas with minimal increase in the cost of electricity



- **Design considerations:**
  - **Capture technology**
    - ***Bubbling fluidized bed, moving bed, fast fluidized bed, transport bed, etc.***
  - **Number of reactors**
  - **Reactor configuration and geometry**
  - **Operating conditions**

BUBBLING FLUIDIZED BED

Bubbling fluidized bed adsorber diagram

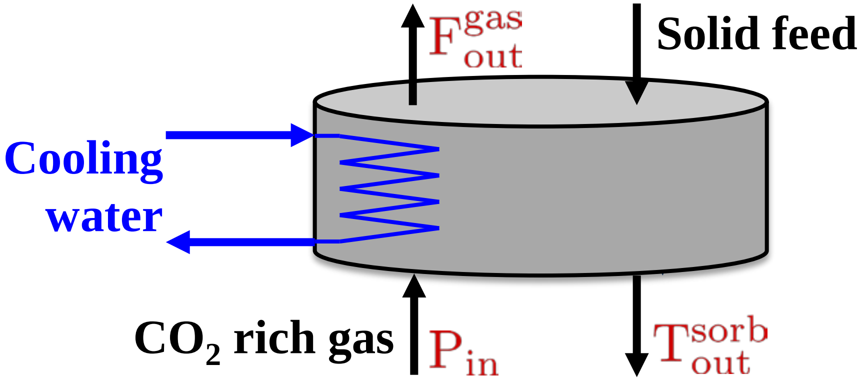


- **Model inputs (16 total)**
  - **Geometry (3)**
  - **Operating conditions (5)**
  - **Gas mole fractions (2)**
  - **Solid compositions (2)**
  - **Flow rates (4)**

- **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 and Technology Laboratory

EXAMPLE MODELS



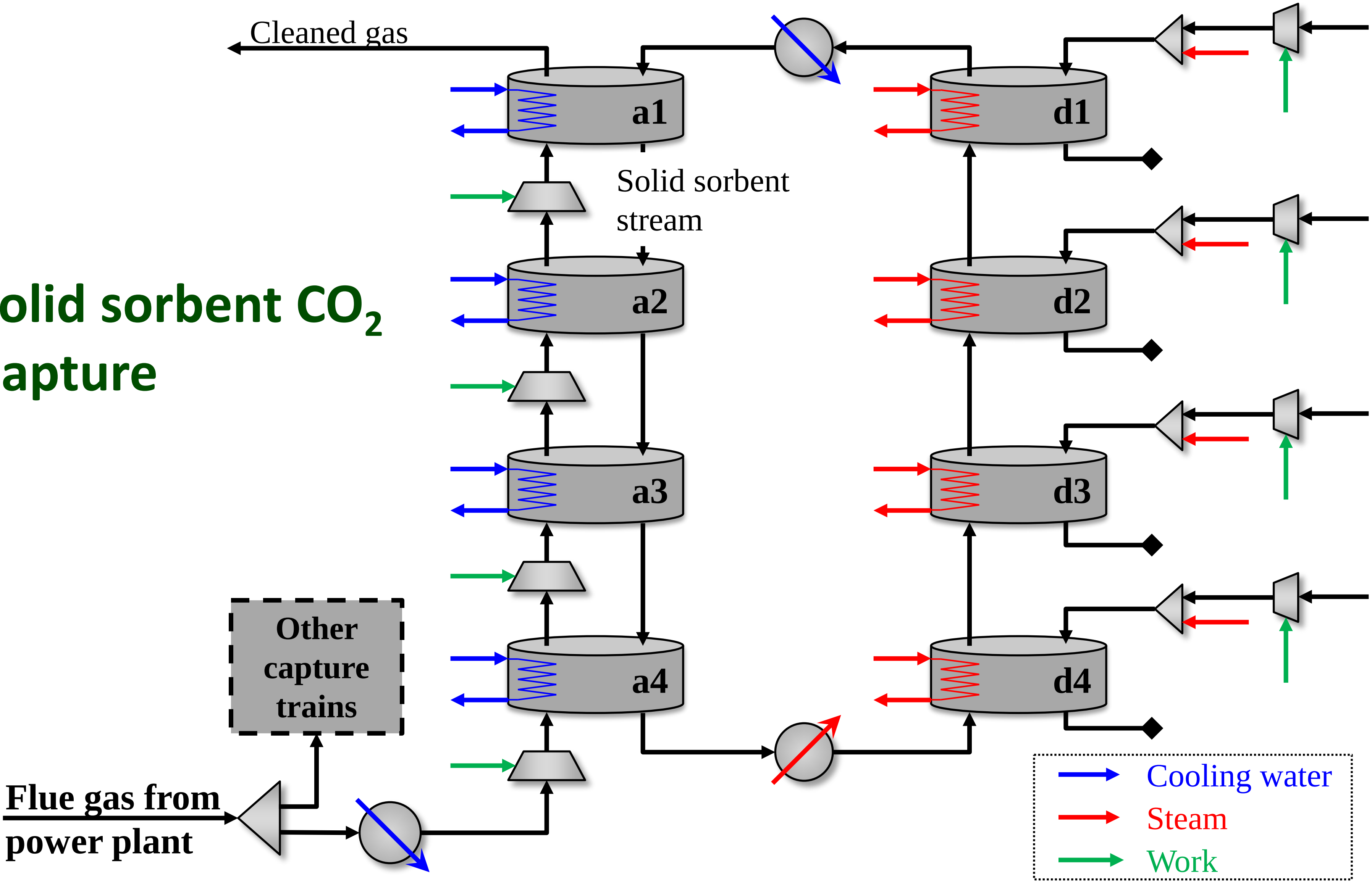
$$\mathrm{P_{in}} = 1.0\,\mathrm{P_{out}} + 0.0231\,L_b - 0.0187\,\ln(0.167\,L_b) - 0.00626\,\ln(0.667\,\mathrm{v_{gi}}) - \frac{51.1\,\mathrm{xHCO3^{ads}_{in}}}{\mathrm{F^{gas}_{in}}}$$

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

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

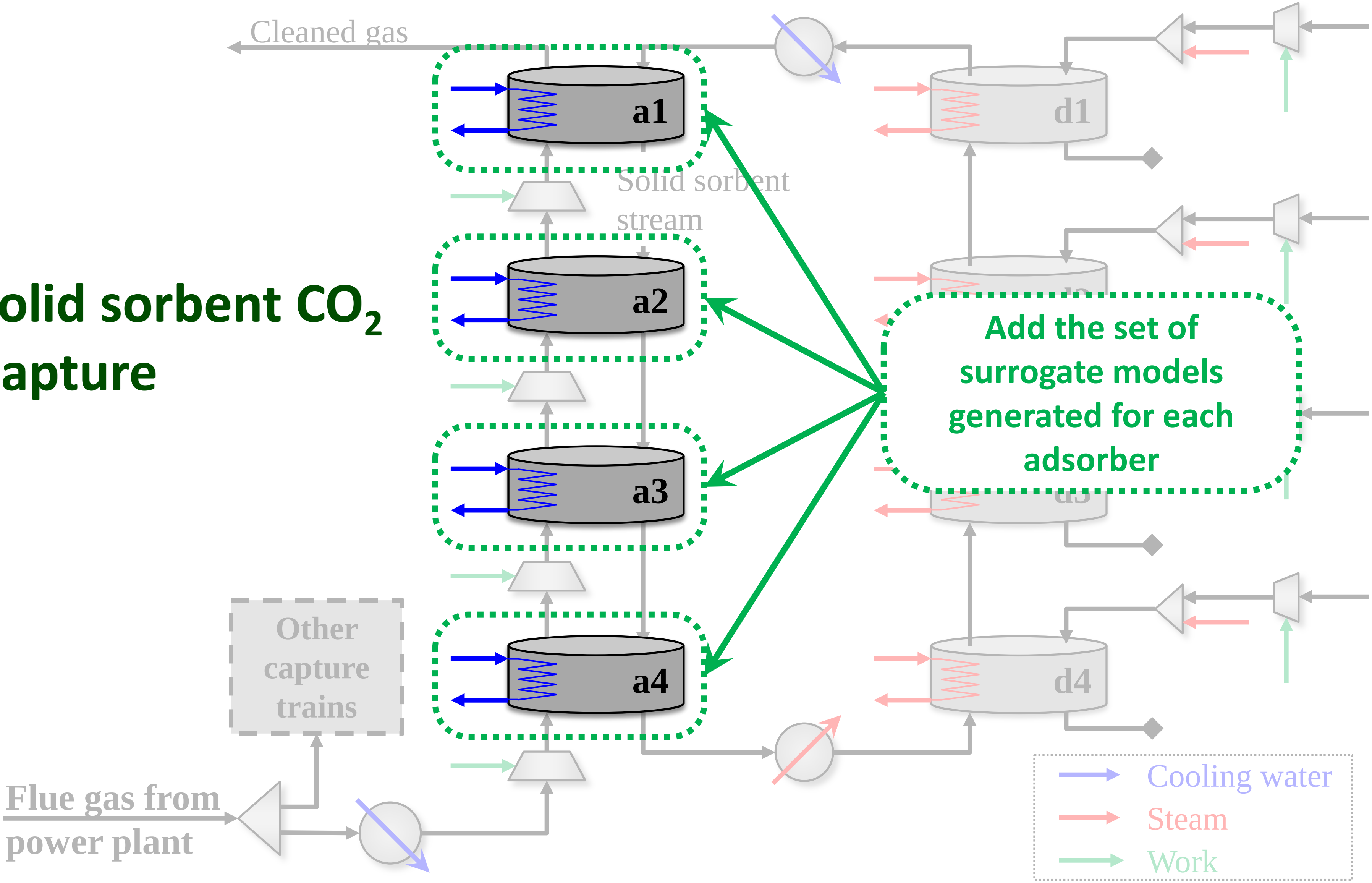
SUPERSTRUCTURE OPTIMIZATION

Solid sorbent CO_2 Capture



SUPERSTRUCTURE OPTIMIZATION

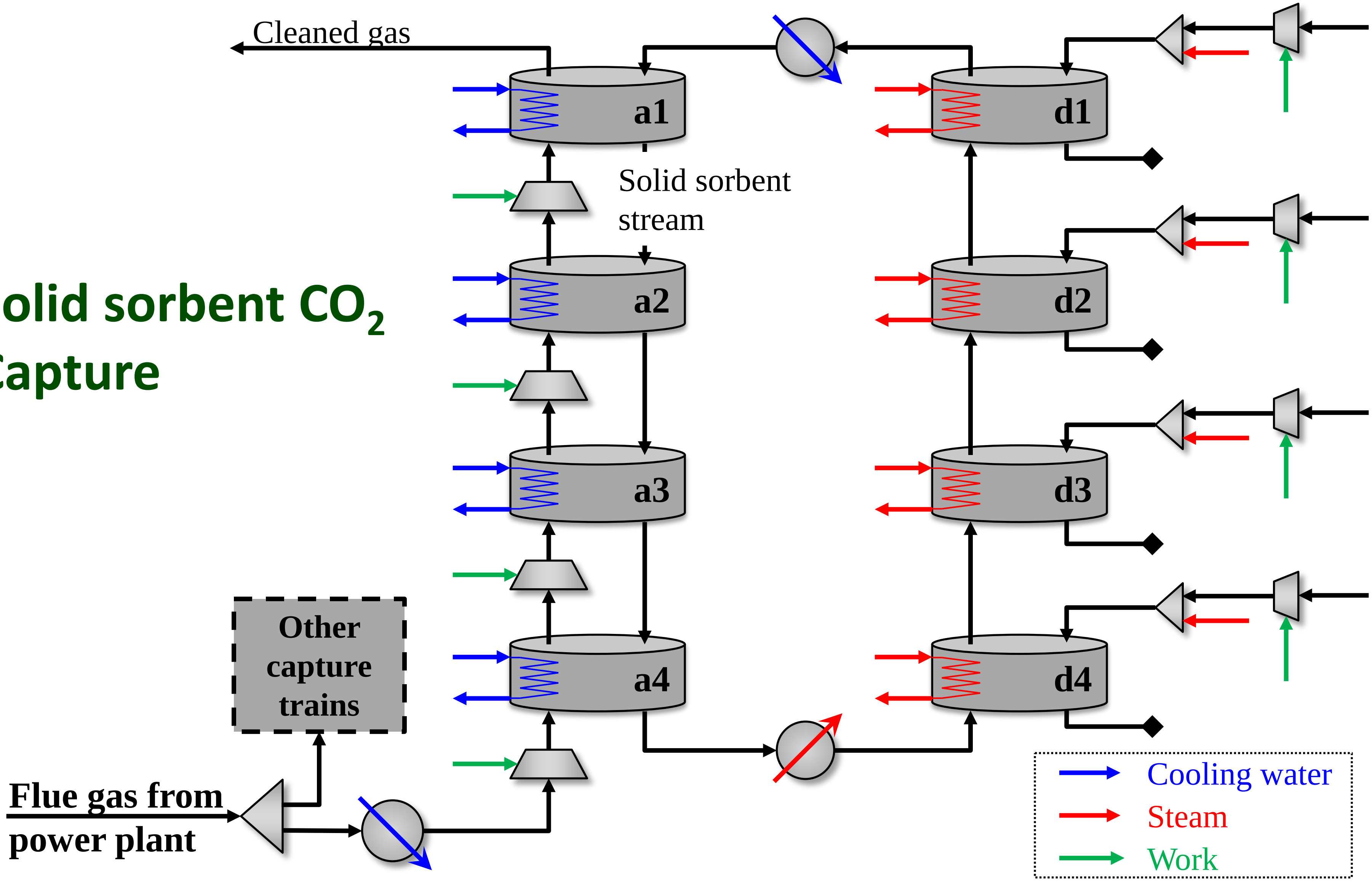
Solid sorbent CO_2 Capture



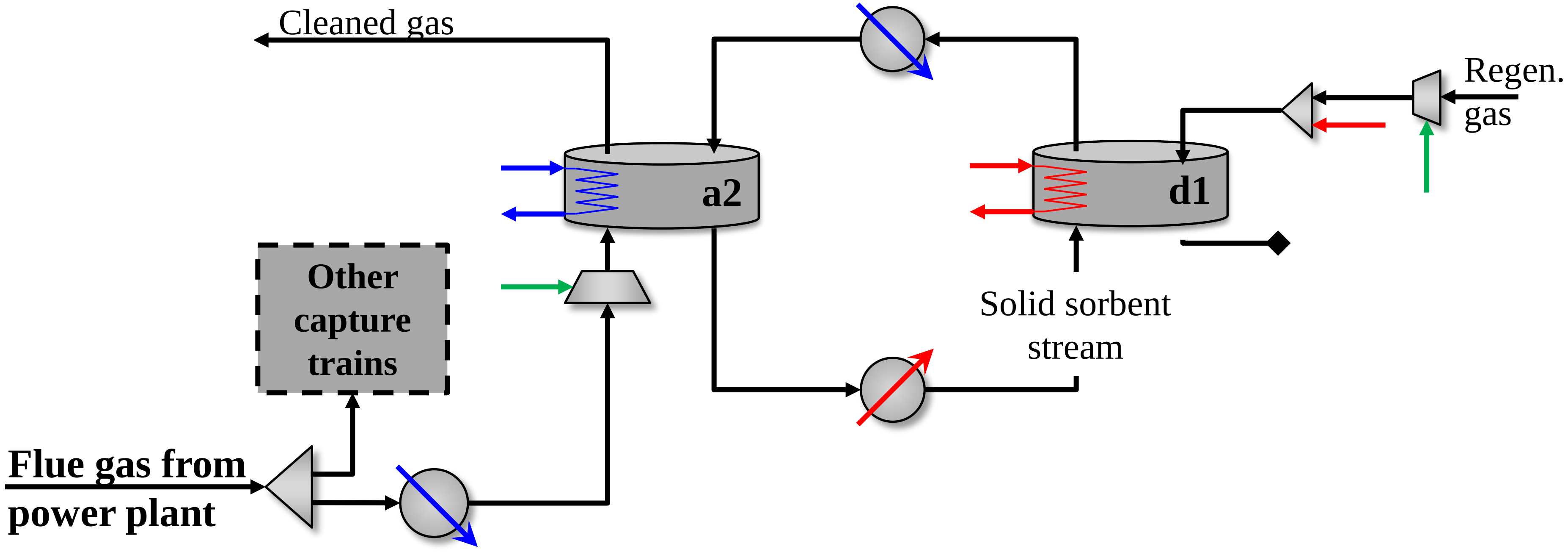
Add the set of surrogate models generated for each adsorber

SUPERSTRUCTURE OPTIMIZATION

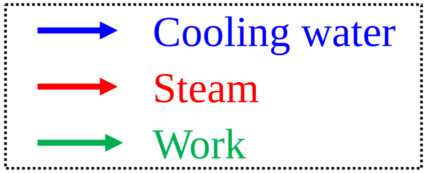
Solid sorbent CO_2 Capture



PRELIMINARY RESULTS



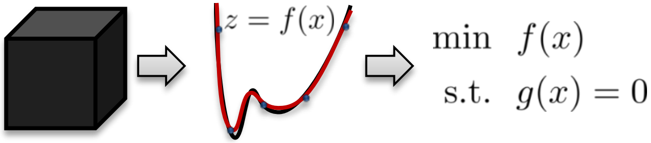
Variables	Value
COE ($/MWh)	92.3
CapEX ($)	1.05E+8
steamFlow (kg/s)	108
derate (MW)	114
utilInF (kgmol/s)	9.26



CONCLUSIONS

- **The algorithm we developed is able to model black-box functions for use in optimization such that the models are**
  - ✓ **Accurate**
  - ✓ **Tractable in an optimization framework (low-complexity models)**
  - ✓ **Generated from a minimal number of function evaluations**

- **Surrogate models can then be incorporated within a larger optimization framework**



$$\begin{aligned} \min \quad & f(x) \\ \text{s.t.} \quad & g(x) = 0 \end{aligned}$$

- **ALAMO site:** archimedes.cheme.cmu.edu/?q=alamo