Surrogate-based optimization of simulated energy systems

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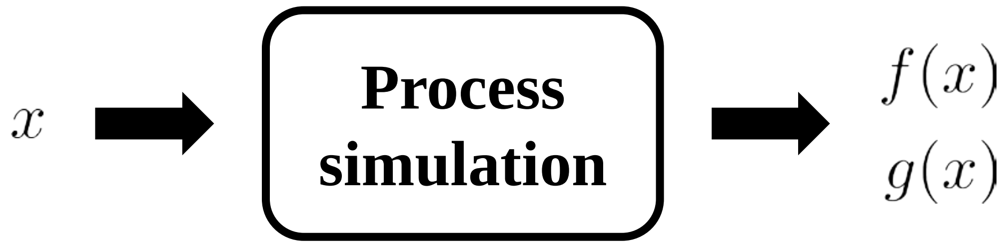
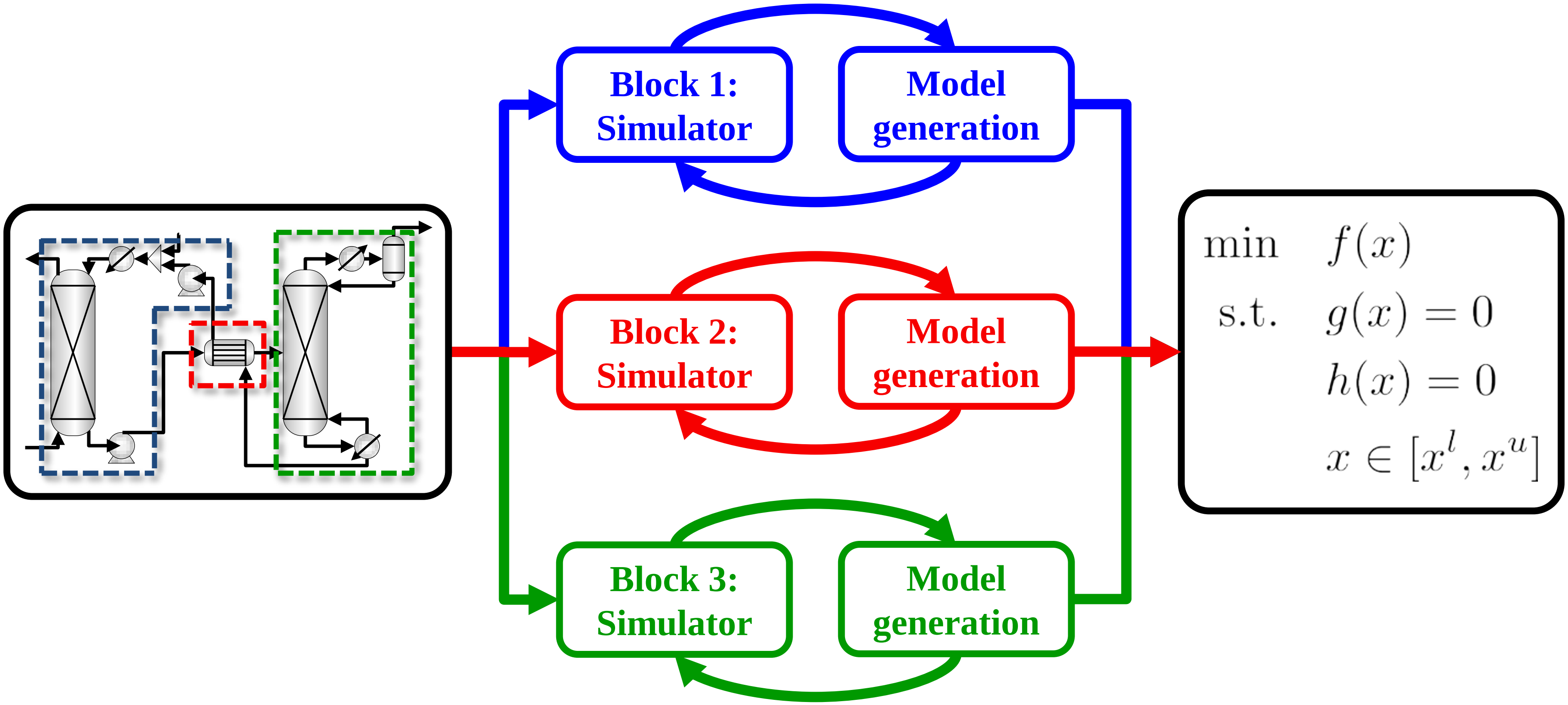
SIMULATION-BASED OPTIMIZATION

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



- **Challenges and solutions:**
  - **Lack of an algebraic model** → Build surrogate models
  - **Computationally costly simulations** → Selectively choose a minimal data set
  - **Often noisy function evaluations** → Use regression surrogate models
  - **Scarcity of fully robust simulations** → Disaggregate the process

PROCESS DISAGGREGATION



Process Simulation

Disaggregate process into process blocks

Surrogate Models

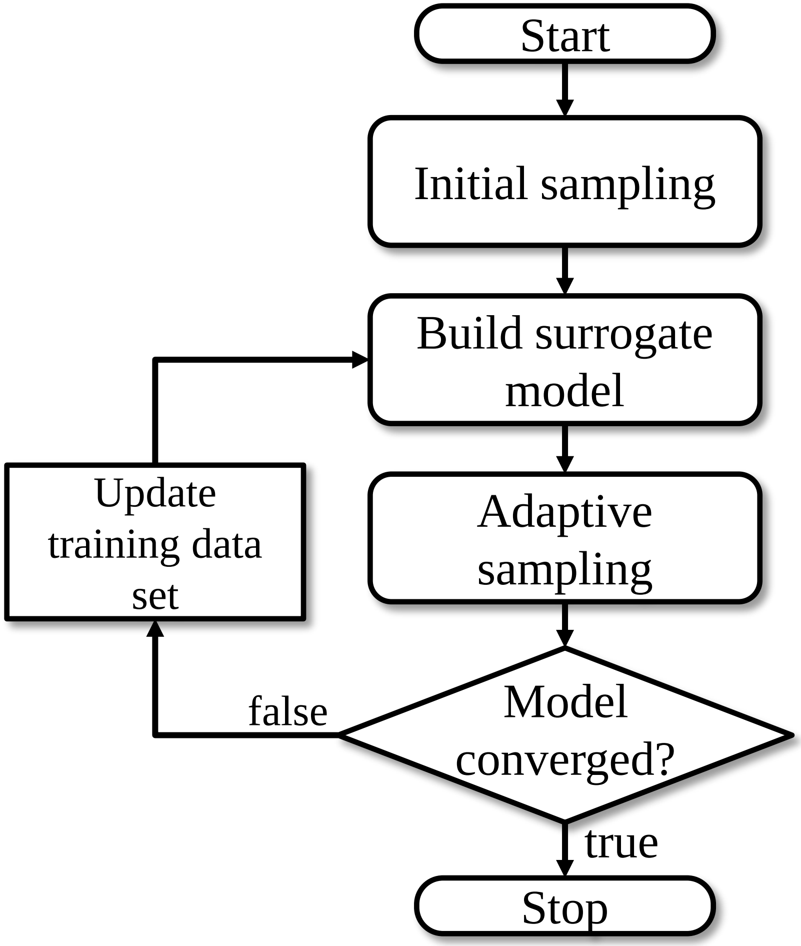
Build simple and accurate models with a functional form tailored for an optimization framework

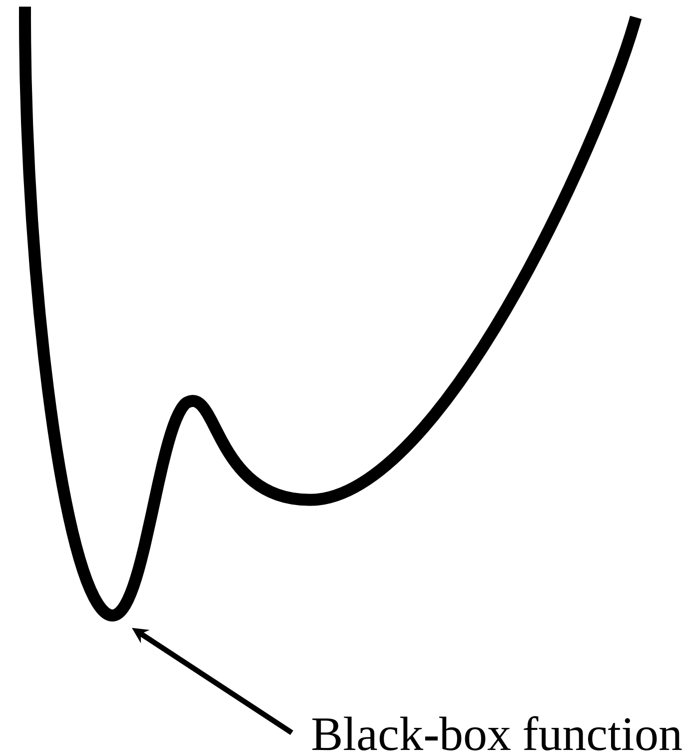
Optimization Model

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

ALAMO

Automated Learning of Algebraic Models for Optimization





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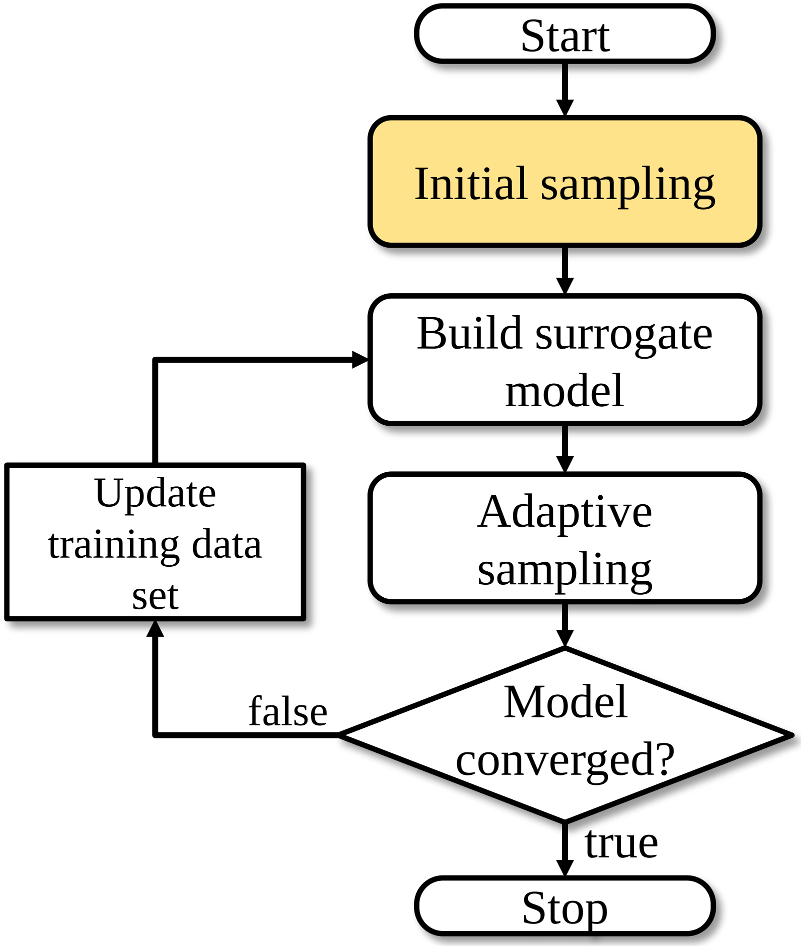

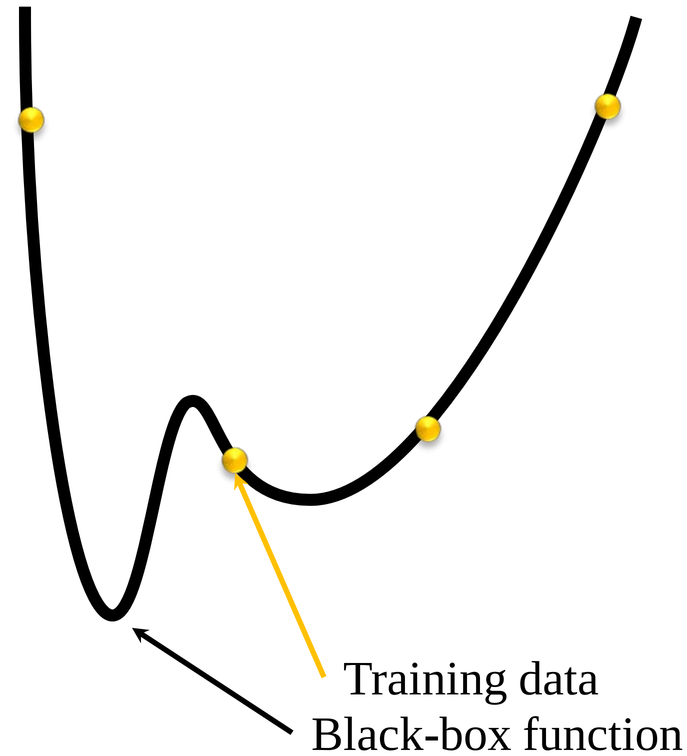

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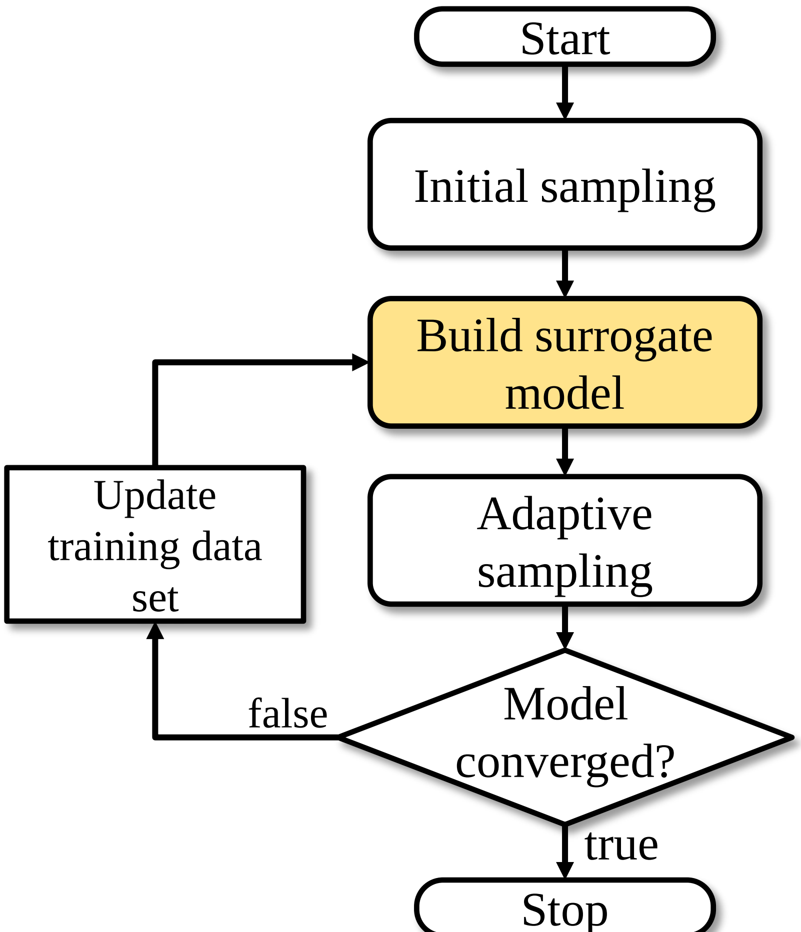

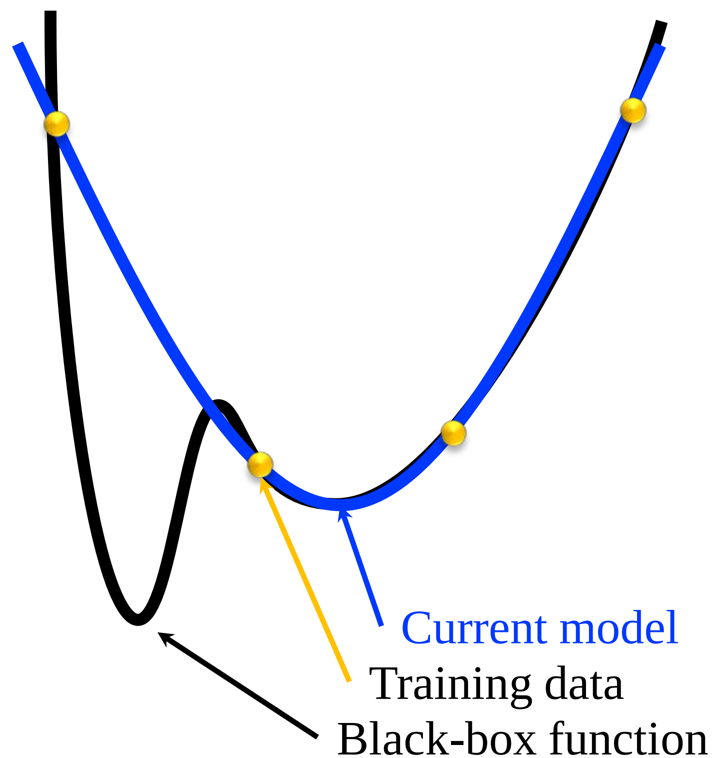

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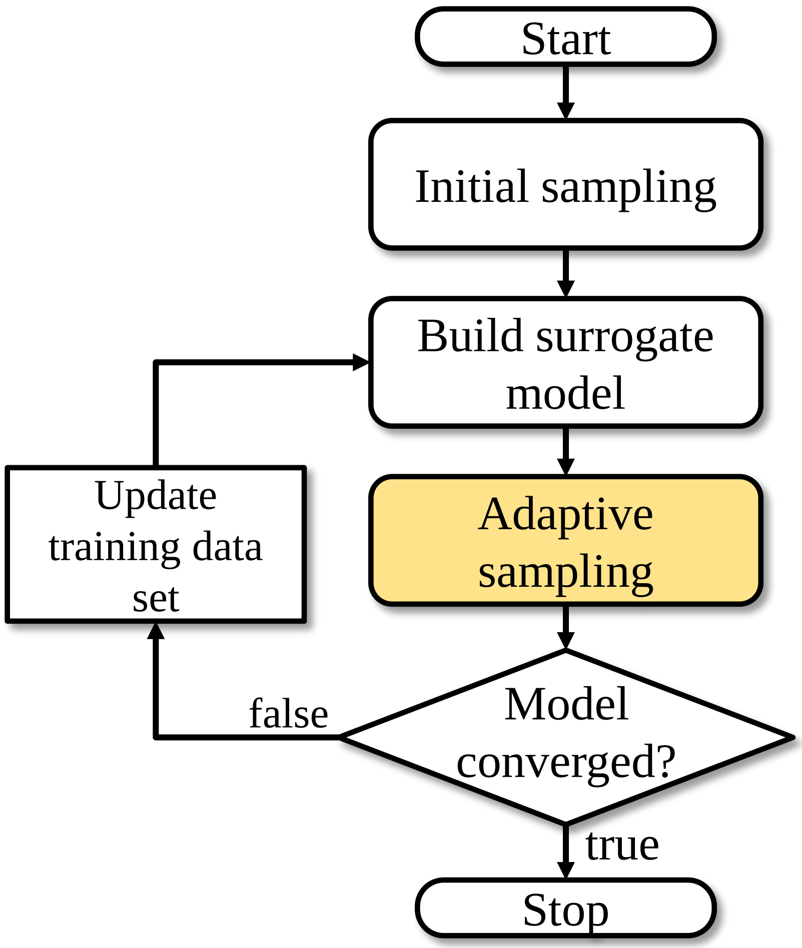
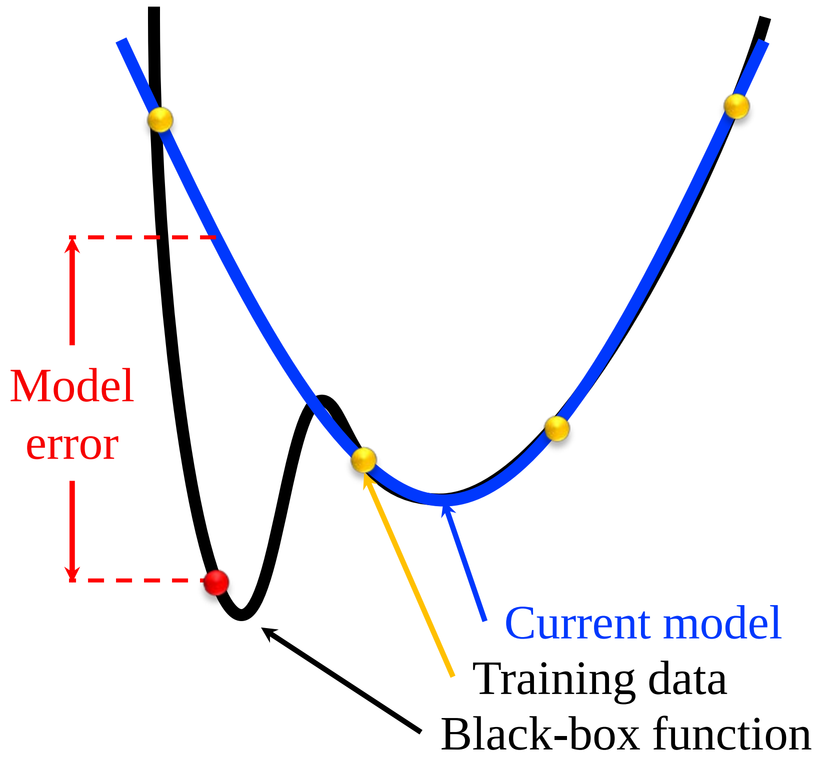
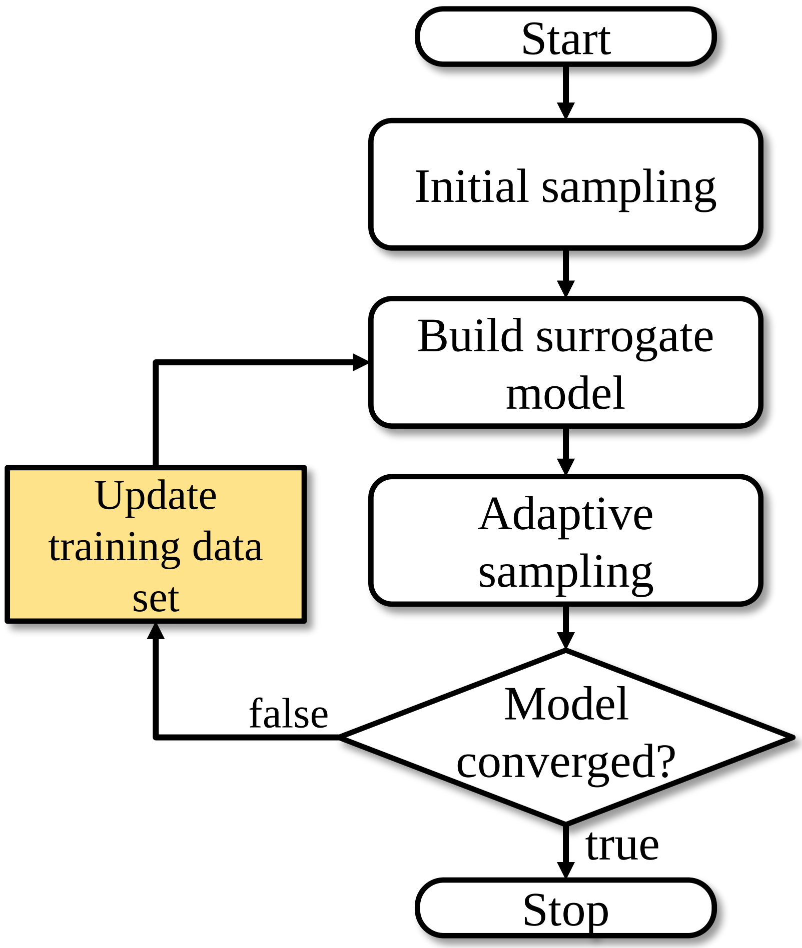
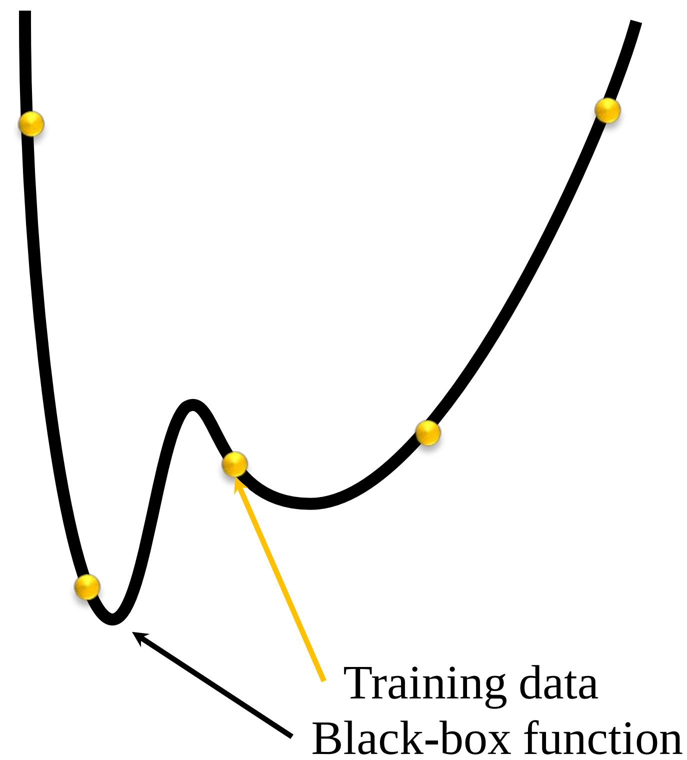




ALAMO

Automated **L**earning of **A**lgebraic **M**odels for **O**ptimization





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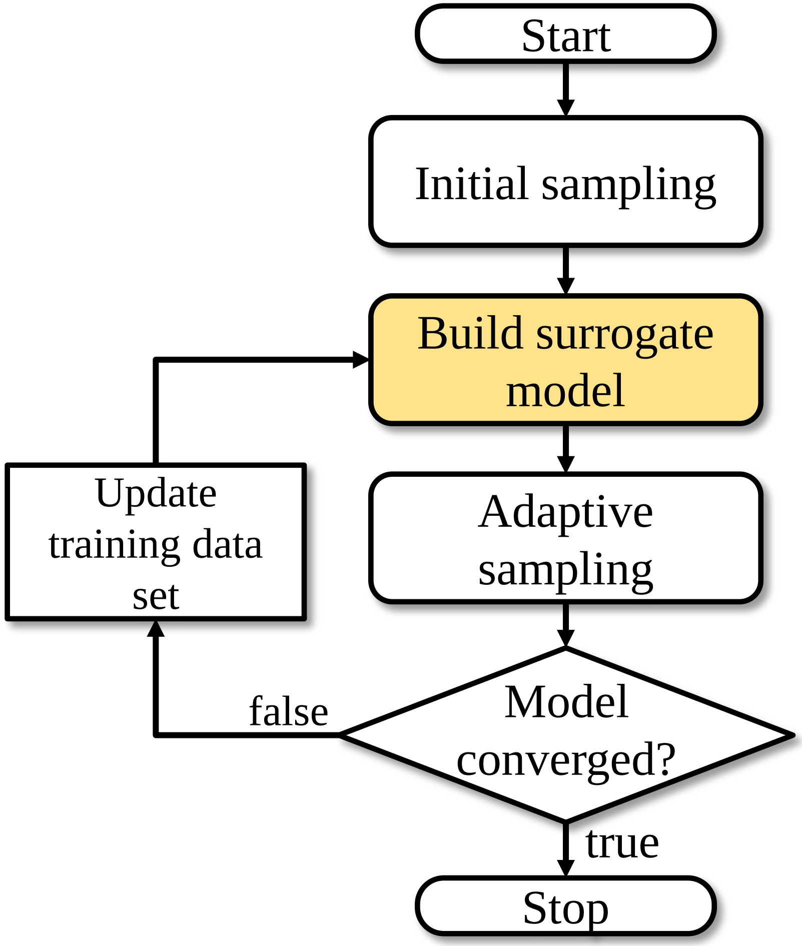
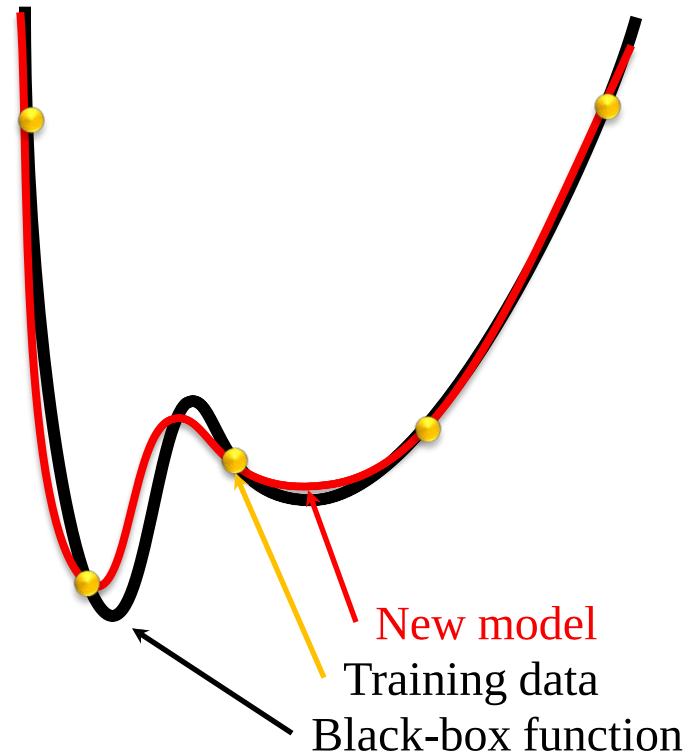
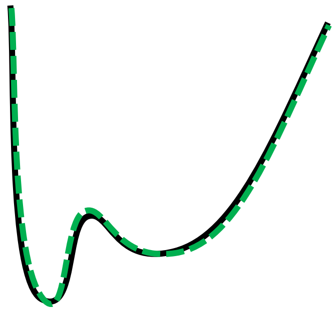




HOW TO BUILD THE SURROGATES

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

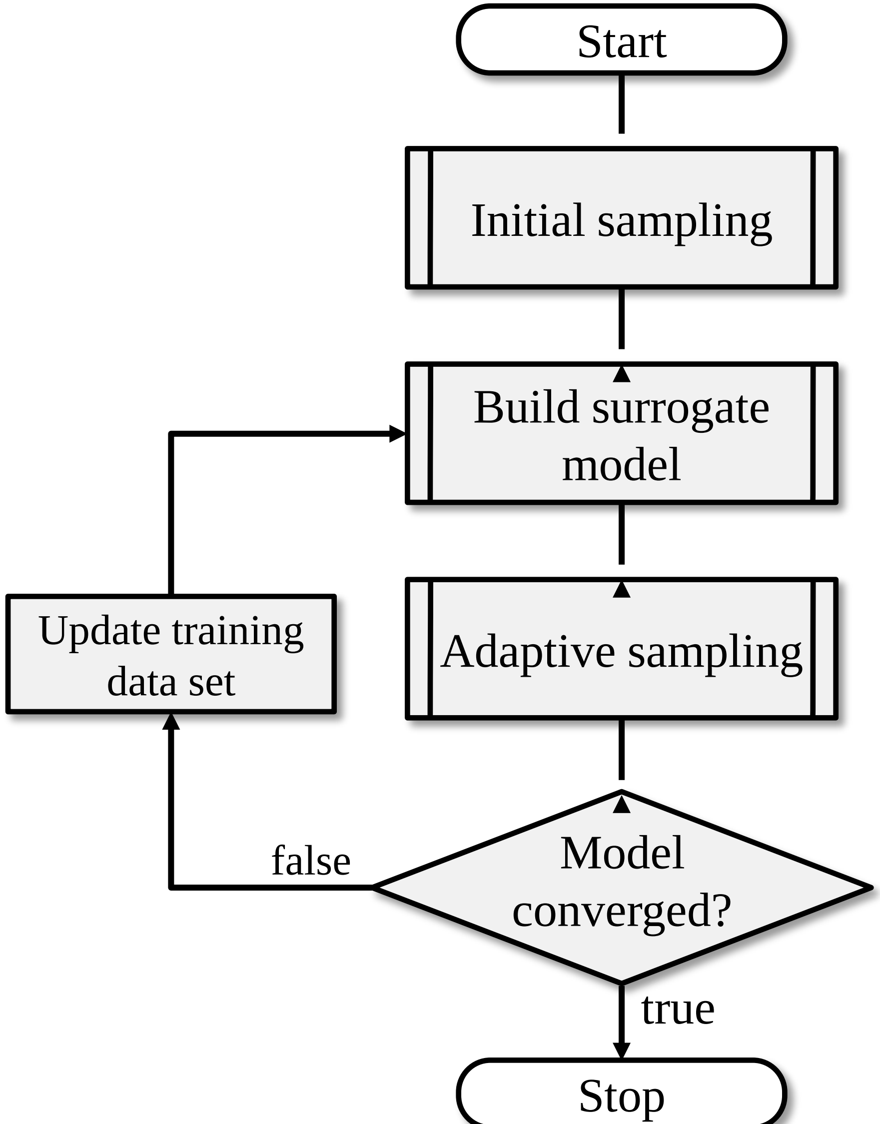


$$\hat{f}(x) = \sum_{i=1}^{n} \gamma_i exp\left(\frac{\|x\|}{\sigma^2}\right) + \beta_0 + \beta_1\, x + \ldots$$

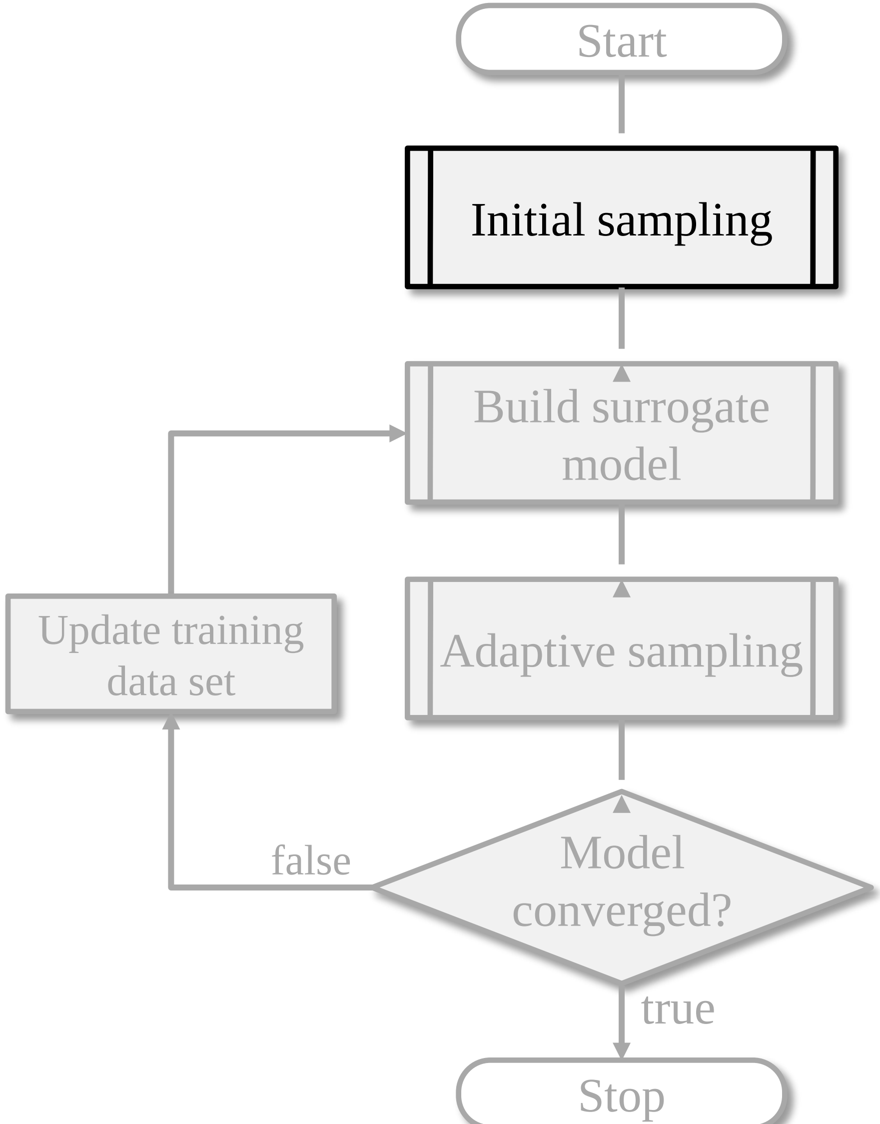
$$\hat{f}(x) = \beta_1\, x + \beta_2\, x^2 + \beta_3\, x^3 + \beta_4\, e^x$$

  - ✓ **Generated from a minimal data set**

ALGORITHMIC FLOWSHEET



ALGORITHMIC FLOWSHEET

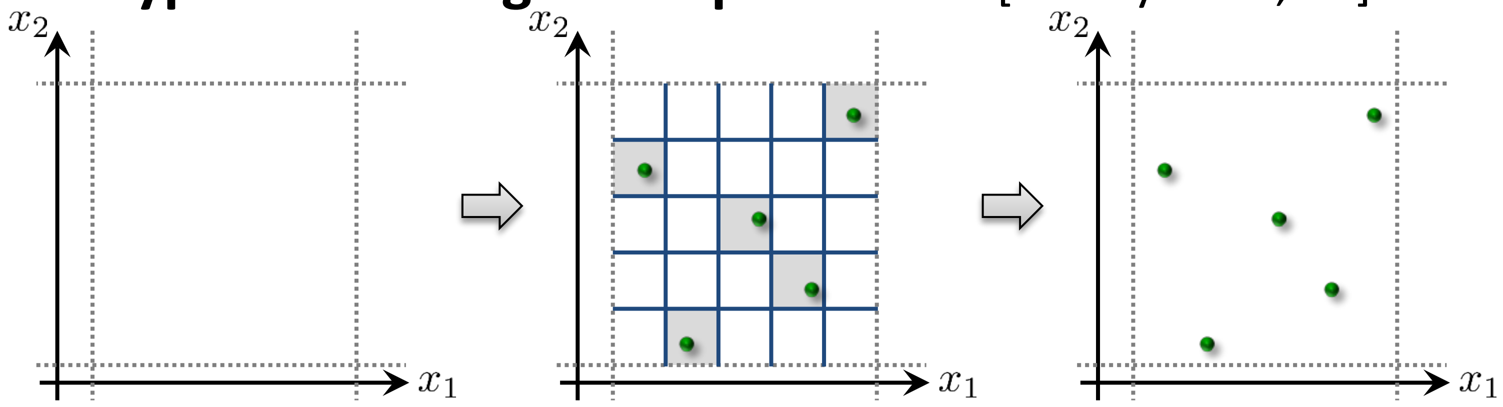


DESIGN OF EXPERIMENTS

- **Goal: To generate an initial set of input variables to evenly sample the problem space**

$$x = \begin{pmatrix} x^1 & x^2 & \cdots & x^i & \cdots & x^N \end{pmatrix} \qquad x^i = \begin{pmatrix} x_1^i \\ x_2^i \\ \vdots \\ x_d^i \\ \vdots \\ x_D^i \end{pmatrix}$$

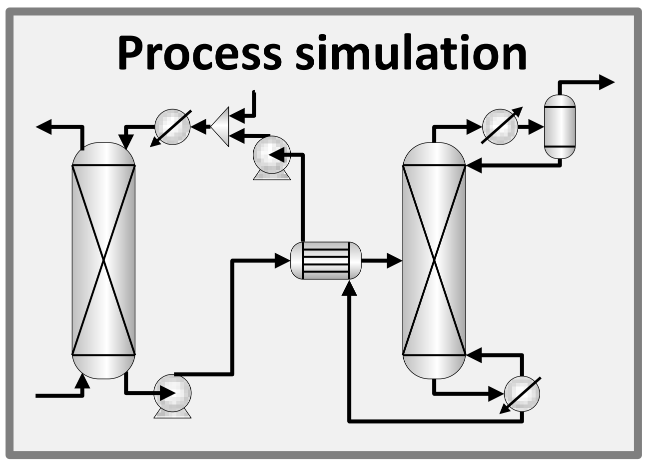
- **Latin hypercube design of experiments** [McKay et al., 79]



INITIAL SAMPLING

- **After running the design of experiments, we will evaluate the black-box function to determine each z^i**

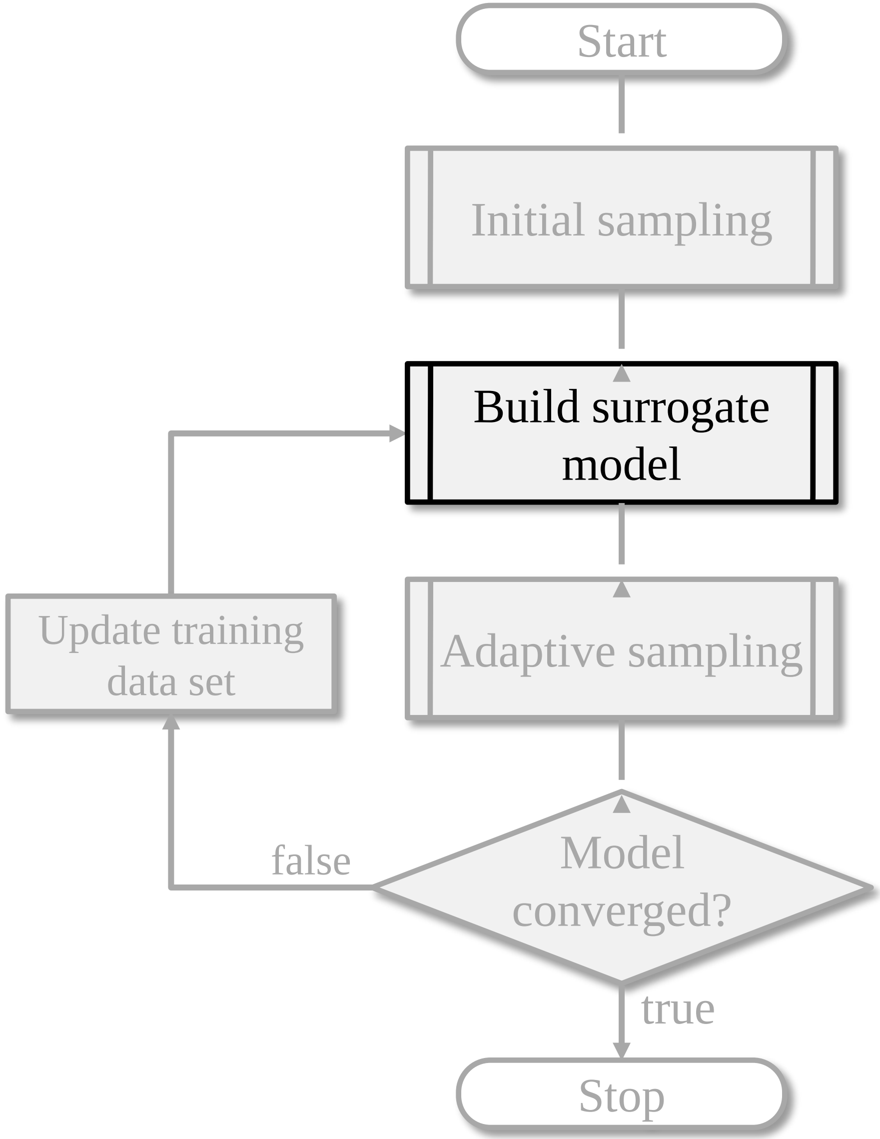
$$x = \begin{pmatrix} x^1 & x^2 & \cdots & x^i & \cdots & x^N \end{pmatrix}$$



$$z = \begin{pmatrix} z^1 & z^2 & \cdots & z^i & \cdots & z^N \end{pmatrix}$$

Initial training set

ALGORITHMIC FLOWSHEET



MODEL IDENTIFICATION

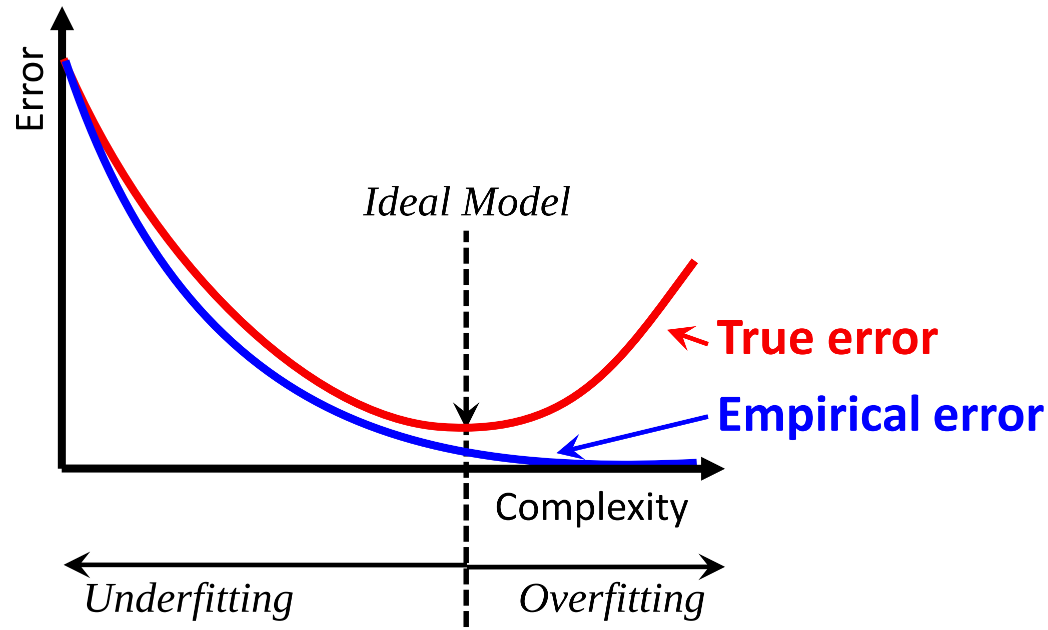
- **Goal: Identify the functional form and complexity of the surrogate models**

$$z = f(x)$$

- **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



Step 1: Define a large set of potential basis functions

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

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 METHOD

- **Generalized best subset problem:**

$$\min_{\mathcal{S},\beta} \quad \Phi(\mathcal{S}, \beta)$$
$$\text{s.t.} \quad \mathcal{S} \subseteq \mathcal{B}$$

where $\Phi(\mathcal{S}, \beta)$ is a goodness of fit measure for the subset of basis function, $\mathcal{S}$, and regression coefficients, β.

BEST SUBSET METHOD

- **Surrogate subset model:**

$$\hat{z}(x) = \sum_{j \in \mathcal{S}} \beta_j X_j(x)$$

- **Mixed-integer surrogate subset model:**

$$\hat{z}(x) = \sum_{j \in \mathcal{B}} (y_j \beta_j) X_j(x) \quad \text{such that} \quad \begin{array}{ll} y_j = 1 & j \in \mathcal{S} \\ y_j = 0 & j \notin \mathcal{S} \end{array}$$

- **Generalized best subset problem mixed-integer formulation:**

$$\begin{aligned} \min_{\beta, y} \quad & \Phi(\beta, y) \\ \text{s.t.} \quad & y_j = \{0, 1\} \end{aligned}$$

MIXED-INTEGER AICC

- **Corrected Akaike information criterion (AICc)** [Hurvich and Tsai, 93]

$$AICc(\mathcal{S}, \beta) = N \log\left(\frac{1}{N}\sum_{i=1}^{N}\left(z_i - \sum_{j\in\mathcal{S}}\beta_j X_{ij}\right)^2\right) + 2|\mathcal{S}| + \frac{2|\mathcal{S}|\left(|\mathcal{S}|+1\right)}{N-|\mathcal{S}|-1}$$

- **Substituting the mixed integer surrogate form into AICc:**

$$AICc(\beta, y_j) = N \log\left(\frac{1}{N}\sum_{i=1}^{N}\left(z_i - \sum_{j\in\mathcal{B}}\left(y_j\beta_j\right)X_{ij}\right)^2\right) + 2\sum_j y_j + \frac{2\sum_j y_j\left(\sum_j y_j + 1\right)}{N-\sum_j y_j - 1}$$

$$\textbf{OR} \text{ if } \sum_j y_j = T$$

$$AICc(\beta, y_j) = N \log\left(\frac{1}{N}\sum_{i=1}^{N}\left(z_i - \sum_{j\in\mathcal{B}}\left(y_j\beta_j\right)X_{ij}\right)^2\right) + 2T + \frac{2T\left(T+1\right)}{N-T-1}$$

MIXED-INTEGER PROBLEM

$$\min_{\beta,T,y} \quad AICc(\beta,T,y) = N\log\left(\frac{1}{N}\sum_{i=1}^{N}\left(z_i - \sum_{j\in\mathcal{B}}(y_j\beta_j)\,X_{ij}\right)^2\right) + 2T + \frac{2T\,(T+1)}{N-T-1}$$

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

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

MIXED-INTEGER PROBLEM

- **Further reformulation**
  - **Replace bilinear terms with big-M constraints**

$$y_j \beta_j \quad \longrightarrow \quad \beta_j^l y_j \leq \beta_j \leq \beta_j^u y_j$$

  - **Decouple objective into two problems**

a) model sizing

$$\text{General:} \qquad \min_{\beta,T,y} \Phi(\beta,T,y) = \min_T \left\{ \min_{\beta,y} \left[\Phi_{\beta,y}(\beta,y)|_T\right] + \Phi_T(T) \right\}$$

b) basis and coefficient selection

$$AICc(\beta,T): \qquad AICc_{\beta,y}(\beta,y)|_T = N \log\left(\frac{1}{N} \sum_{i=1}^{N} \left(z_i - \sum_{j \in \mathcal{B}} (y_j \beta_j) X_{ij} \right)^2 \right)$$

$$AICc_T(T) = 2T + \frac{2T(T+1)}{N-T-1}$$

  - **Inner minimization objective reformulation**

NESTED MIXED-INTEGER PROBLEM

$$\min_{T \in \{1,\ldots,T^u\}} \quad N \log\left(\frac{1}{N}\sum_{i=1}^{N}\left(z_i - \sum_{j\in\mathcal{B}}(y_j\beta_j)\,X_{ij}\right)^2\right) + 2T + \frac{2T\,(T+1)}{N-T-1}$$

$$\text{s.t.} \quad \min_{\beta,y} \quad \sum_{i=1}^{N}\left(z_i - \sum_{j\in\mathcal{B}}\beta_j X_{ij}\right)^2$$

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

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

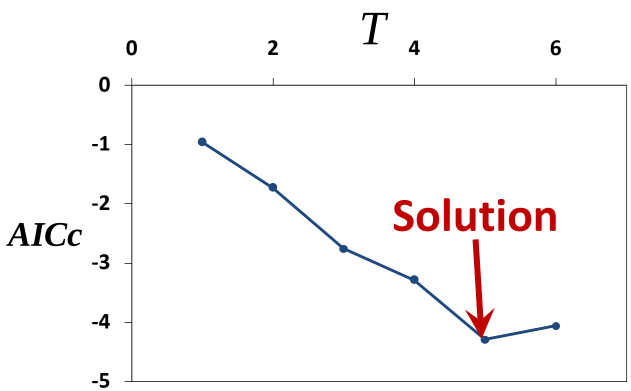
$$y_j = \{0,1\} \qquad j \in \mathcal{B}$$

a) **Model sizing**

b) **Basis and coefficient selection**

PROBLEM SIMPLIFICATIONS

- **Simplifications:**
  - **Outer problem**
    - ***The outer problem is parameterized by T and a local minima is found***



  - **Inner problem**
    - ***Stationarity condition used to solve for continuous variables***

$$\frac{d}{d\beta_j}\sum_{i=1}^{N}\left(z_i-\sum_{j\in\mathcal{S}}\beta_j X_{ij}\right)^2 \propto \sum_{i=1}^{N} X_{ij}\left(z_i-\sum_{j\in\mathcal{S}}\beta_j X_{ij}\right)=0, \quad j\in\mathcal{S}$$

    - ***Linear objective used to solved for integer variables***

$$\text{Objective:} \quad \sum_{i=1}^{N}\left|z_i-\sum_{j\in\mathcal{S}}\beta_j X_{ij}\right|$$

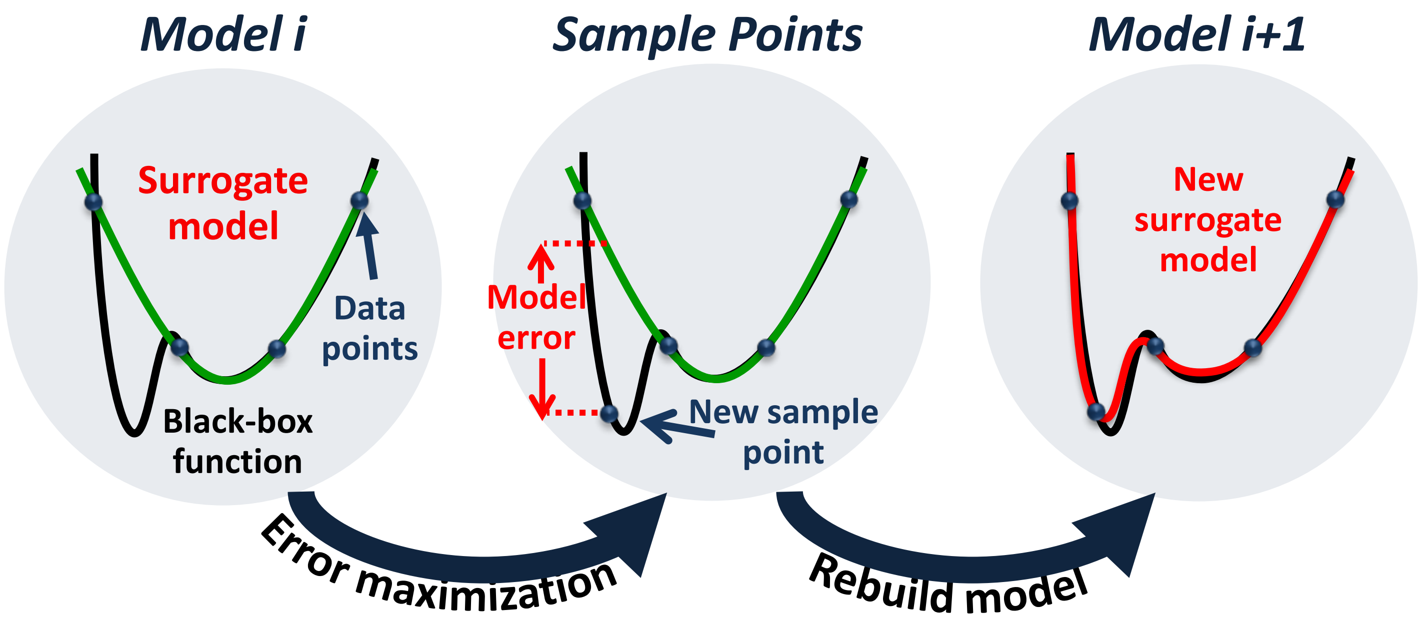
FINAL BEST SUBSET MODEL

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

- **This model is solved for increasing values of *T* until the *AICc* worsens**

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**



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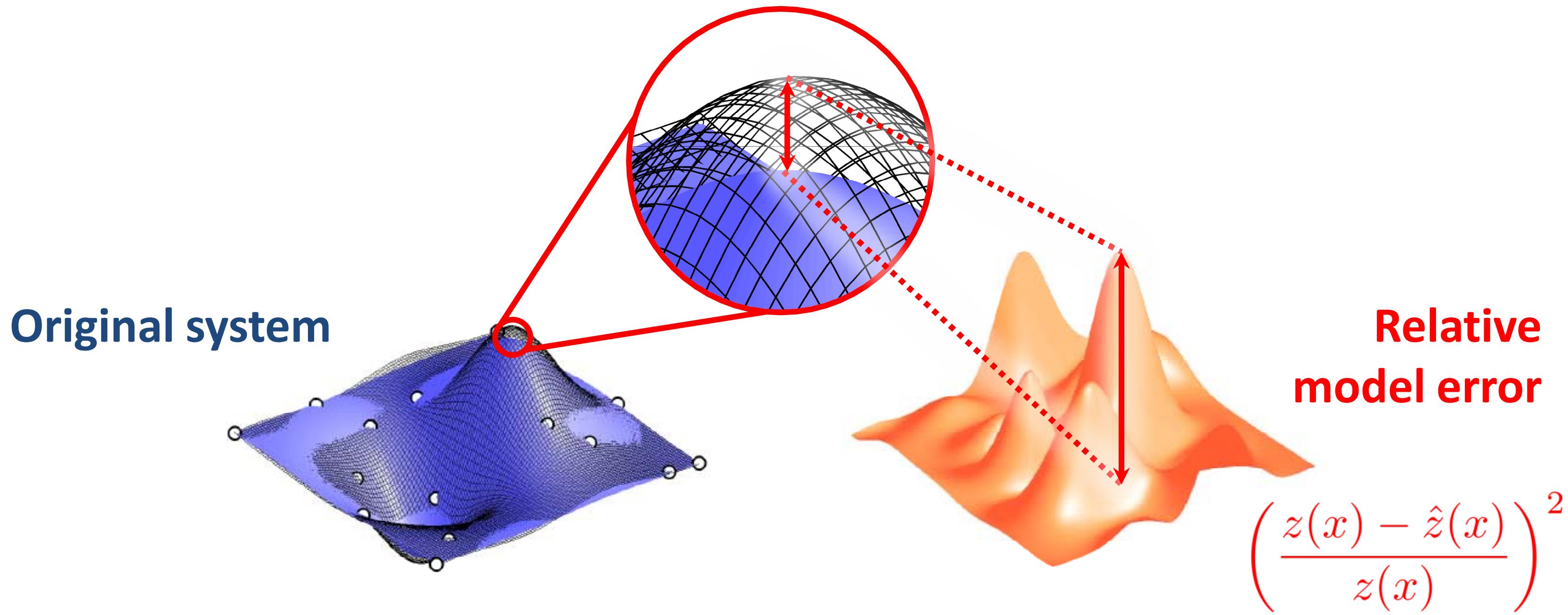

ADAPTIVE SAMPLING

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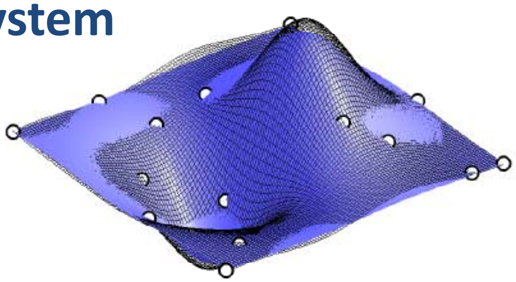
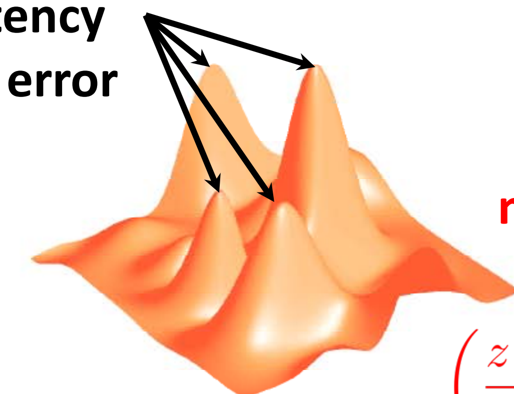
Original system



High model inconsistency or model error



Relative model error

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

ERROR MAXIMIZATION SAMPLING

- **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]

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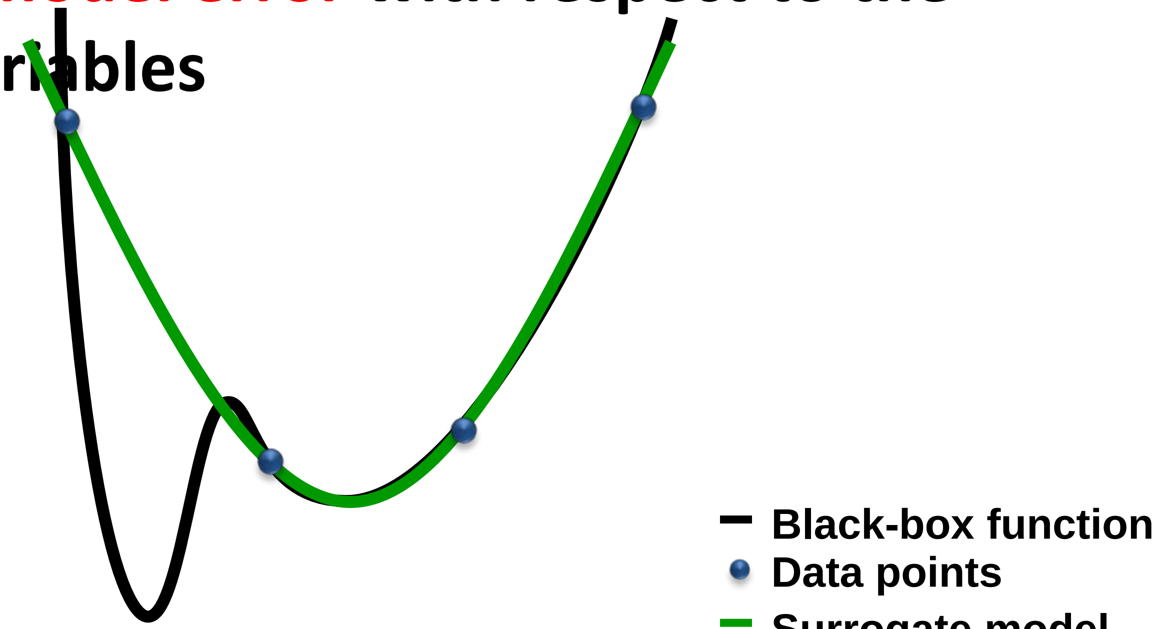
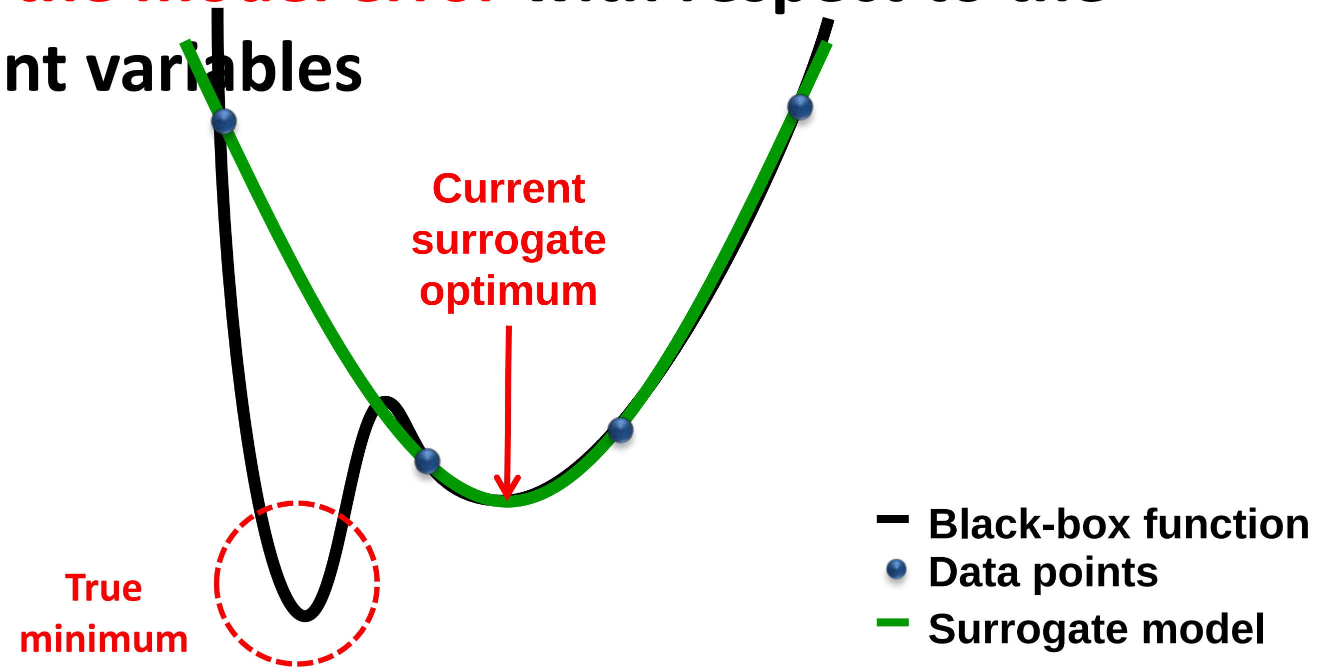


ADAPTIVE SAMPLING

- 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



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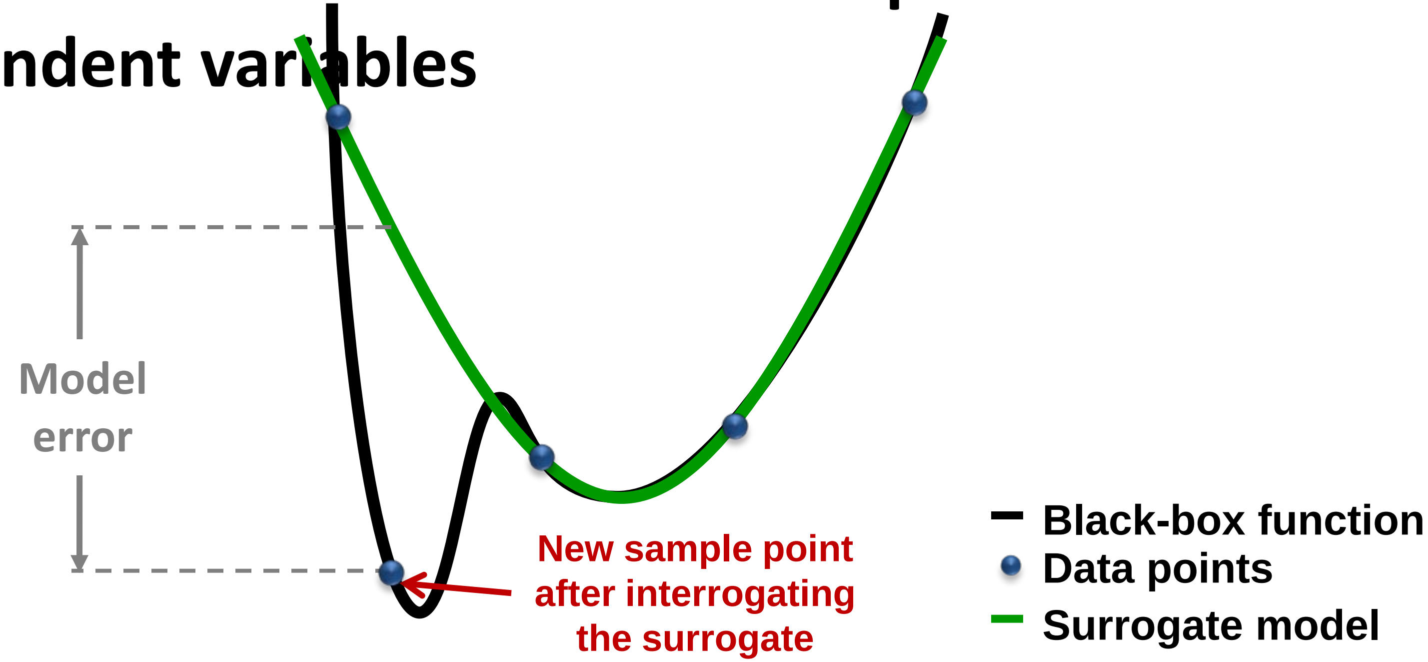

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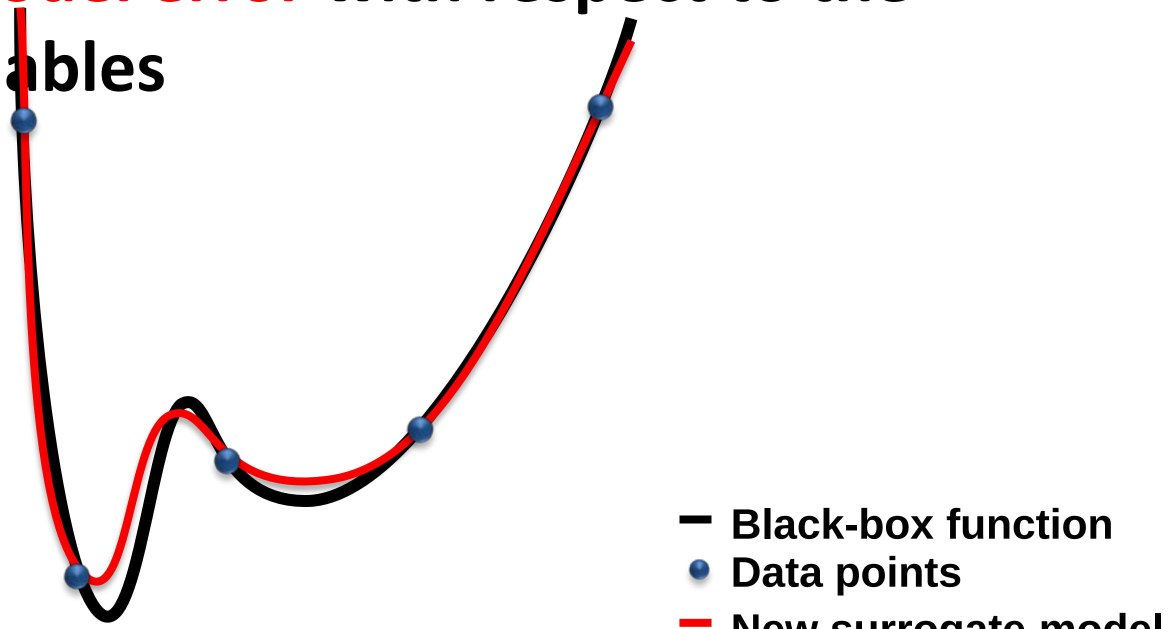


ERROR MAXIMIZATION SAMPLING

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

COMPUTATIONAL TESTING

- **Surrogate generation methods have been implemented into a package:**

ALAMO

(Automated Learning of Algebraic Models for Optimization)

- **Modeling methods compared**
  - **MIP – Proposed methodology**
  - **EBS – Exhaustive best subset method**
    - ***Note: due to high CPU times this was only tested on smaller problems***
  - **LASSO – The lasso regularization**
  - **OLR – Ordinary least-squares regression**

- **Sampling methods compared**
  - **DFO – Proposed error maximization technique**
  - **SLH – Single latin hypercube (no feedback)**

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**

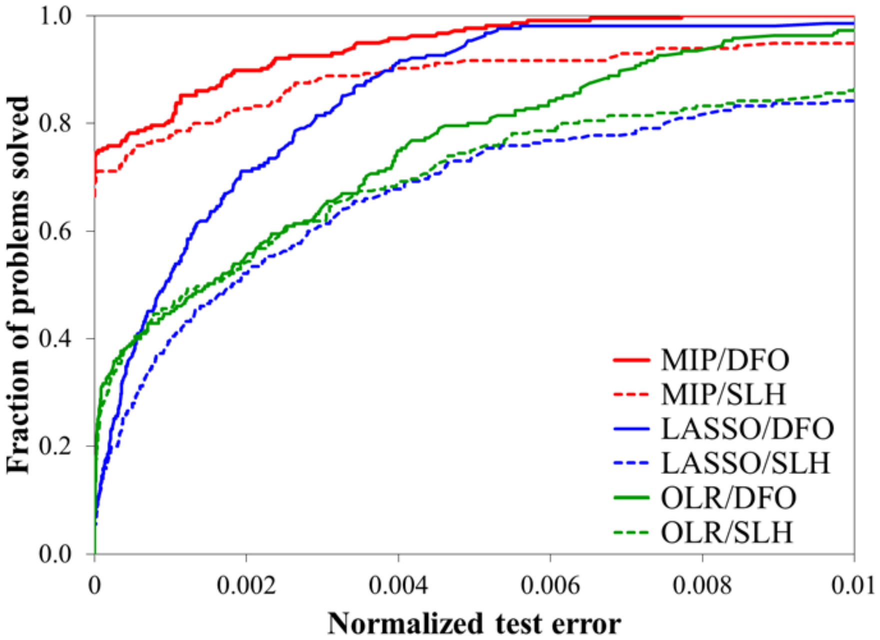
- **Basis functions allowed:**

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	$\exp\left(\frac{x_d}{\gamma}\right)^\alpha$, $\log\left(\frac{x_d}{\gamma}\right)^\alpha$	$\alpha = 1,\ \gamma = 1$

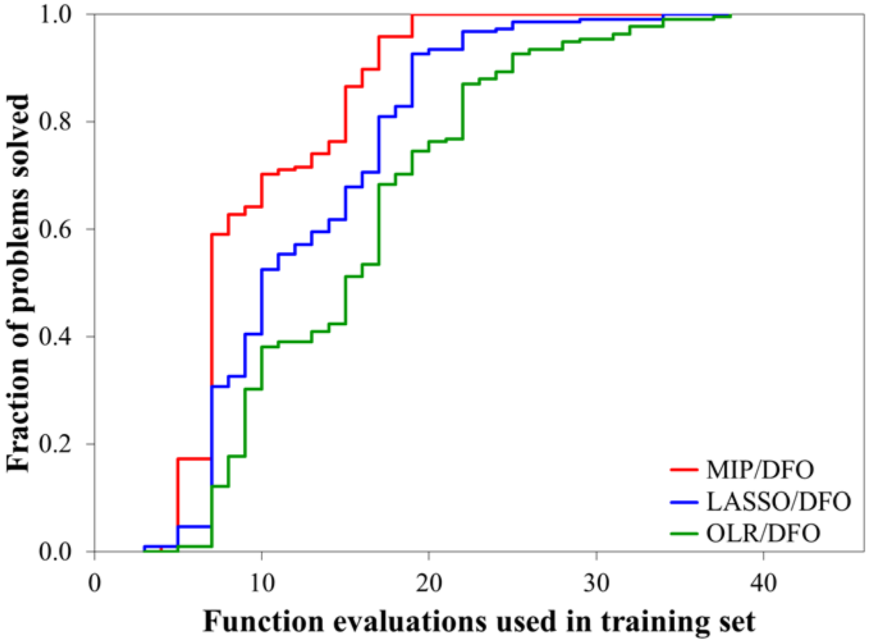
True basis function coefficients were randomly chosen from a uniform distribution where $\beta \in [-1, 1]$.

RESULTS – TEST SET A

Model accuracy



Function evaluations



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

MODEL COMPLEXITY – TEST SET A

No. inputs	No. true terms	MIP/ DFO	MIP/ SLH	EBS/ DFO	EBS/ SLH	LASSO/ DFO	LASSO/ SLH	OLR/ DFO	OLR/ SLH
2	2	2	[2, 2]	2	2	[6, 8]	[6, 11]	[12, 15]	[12, 15]
2	3	3	3	3	3	[5, 12]	[5, 10]	[12, 14]	[12, 14]
2	4	[3, 4]	[3, 4]	[3, 4]	[3, 4]	[8, 11]	[8, 10]	[11, 12]	[11, 12]
2	5	[2, 4]	[2, 4]	[2, 5]	[2, 5]	[3, 12]	[4, 11]	[10, 16]	[10, 16]
2	6	[5, 6]	[6, 6]	[5, 6]	[6, 6]	[7, 10]	[6, 7]	[11, 13]	[11, 13]
2	7	[4, 6]	[4, 6]	[4, 7]	[4, 7]	[7, 11]	[6, 12]	[8, 13]	[8, 13]
2	8	[4, 5]	[5, 6]	[4, 5]	[5, 6]	[6, 8]	[6, 9]	[10, 15]	[10, 15]
2	9	[4, 6]	[4, 6]	NA	NA	[6, 14]	[7, 12]	[10, 17]	[10, 17]
2	10	[4, 8]	[4, 8]	NA	NA	[5, 14]	[7, 14]	[10, 14]	[10, 14]
3	2	[2, 3]	[2, 3]	NA	NA	[6, 12]	[7, 13]	[27, 29]	[27, 29]
3	3	[3, 3]	[3, 3]	NA	NA	[8, 16]	[7, 15]	[19, 22]	[19, 22]
3	4	4	[3, 4]	NA	NA	[10, 13]	[9, 10]	[16, 21]	[16, 21]
3	5	5	5	NA	NA	[11, 17]	[9, 15]	[15, 23]	[15, 23]
3	6	[5, 6]	[6, 6]	NA	NA	[9, 18]	[10, 13]	[15, 26]	[15, 26]
3	7	7	[7, 8]	NA	NA	[10, 22]	[10, 22]	22	22

DESCRIPTION – TEST SET B

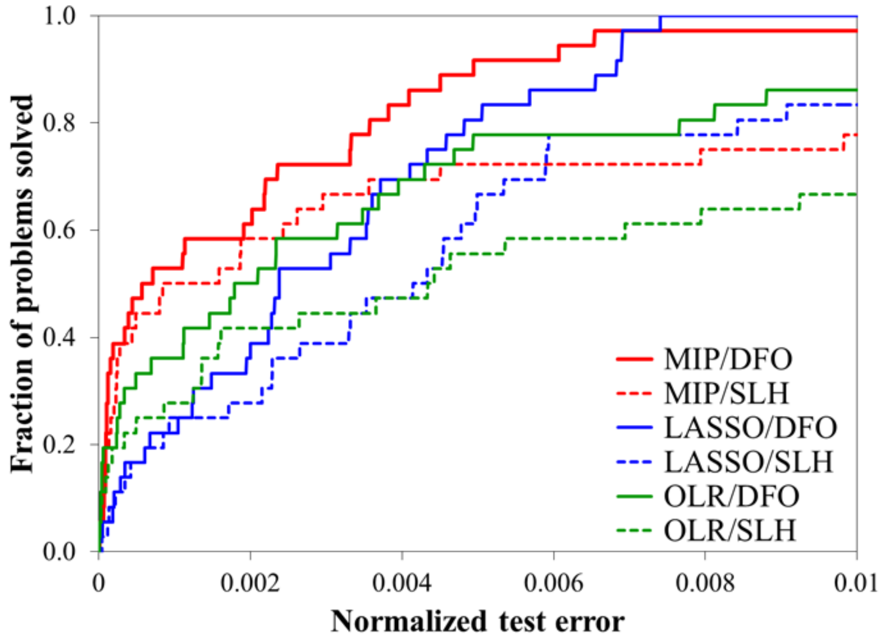
- **Two input black-box functions with basis functions unavailable to the algorithms with**

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	$z(x) = \dfrac{\beta}{\gamma + x_i^\alpha}$

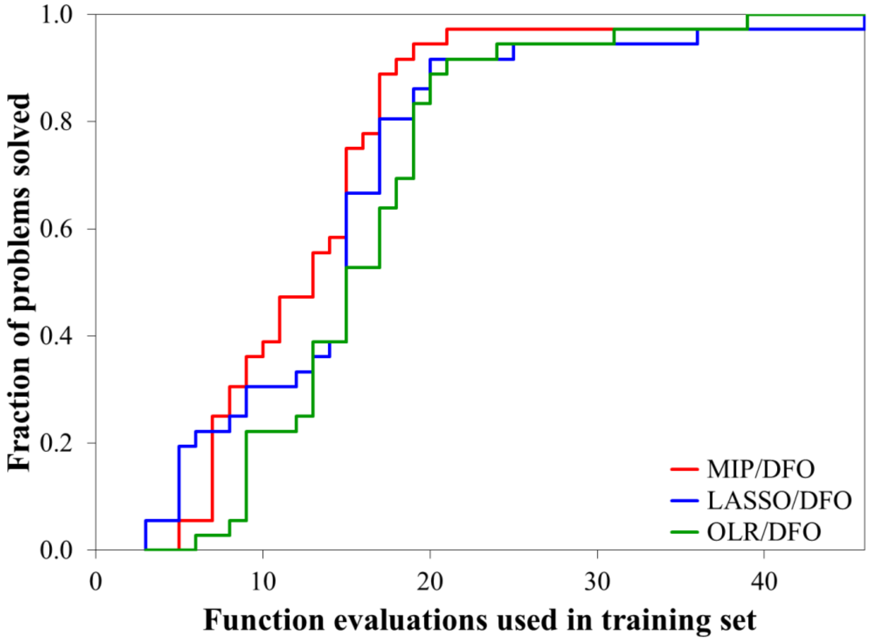
with true parameters chosen from a uniform distribution where $\beta \in [-1, 1]$, $\alpha, \nu \in [-3, 3]$, $\gamma \in [-5, 5]$, and $i, j \in \{1, 2\}$.

RESULTS – TEST SET B

Model accuracy



Function evaluations



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

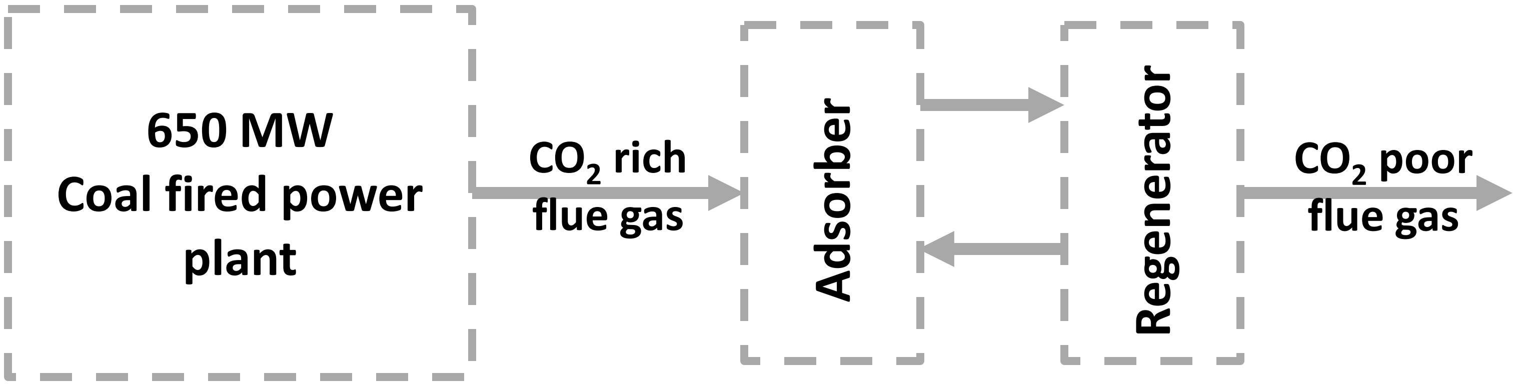
MODEL COMPLEXITY – TEST SET B

True function type	Function ID	MIP/ DFO	MIP/ SLH	LASSO/ DFO	LASSO/ SLH	OLR/ DFO	OLR/ SLH
I	a	5	5	[3, 5]	[4, 9]	[6, 17]	[6, 17]
I	b	[4, 10]	[4, 10]	[10, 14]	[5, 8]	[8, 17]	[8, 17]
I	c	[3, 10]	[6, 9]	[8, 9]	[4, 10]	[13, 17]	[13, 17]
II	a	[4, 6]	[4, 10]	[8, 15]	[7, 9]	[15, 19]	[15, 19]
II	b	[1, 7]	[1, 9]	[13, 16]	[11, 17]	[13, 30]	[13, 30]
II	c	[5, 12]	[5, 12]	[9, 13]	[9, 16]	[9, 19]	[9, 19]
III	a	[3, 4]	[1, 4]	[2, 5]	[2, 5]	[9, 20]	[9, 20]
III	b	4	[1, 4]	5	5	[9, 20]	[9, 20]
III	c	[3, 4]	[3, 4]	[5, 8]	[5, 9]	[18, 24]	[18, 24]
IV	a	[7, 8]	[4, 10]	[8, 17]	[11, 18]	[13, 19]	[13, 19]
IV	b	[8, 9]	[9, 10]	[8, 12]	[10, 14]	[9, 17]	[9, 17]
IV	c	[6, 9]	[9, 10]	[5, 13]	[4, 12]	[13, 15]	[13, 15]

CARBON CAPTURE OPTIMIZATION

- **Problem statement:**

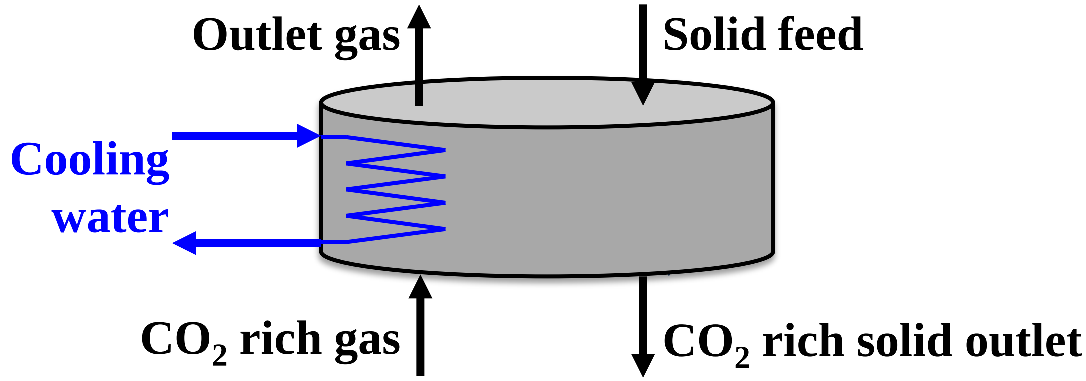
  Capture 90% of CO_2 from a 350MW power plant's post combustion flue gas with minimal increase in the cost of electricity



- **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



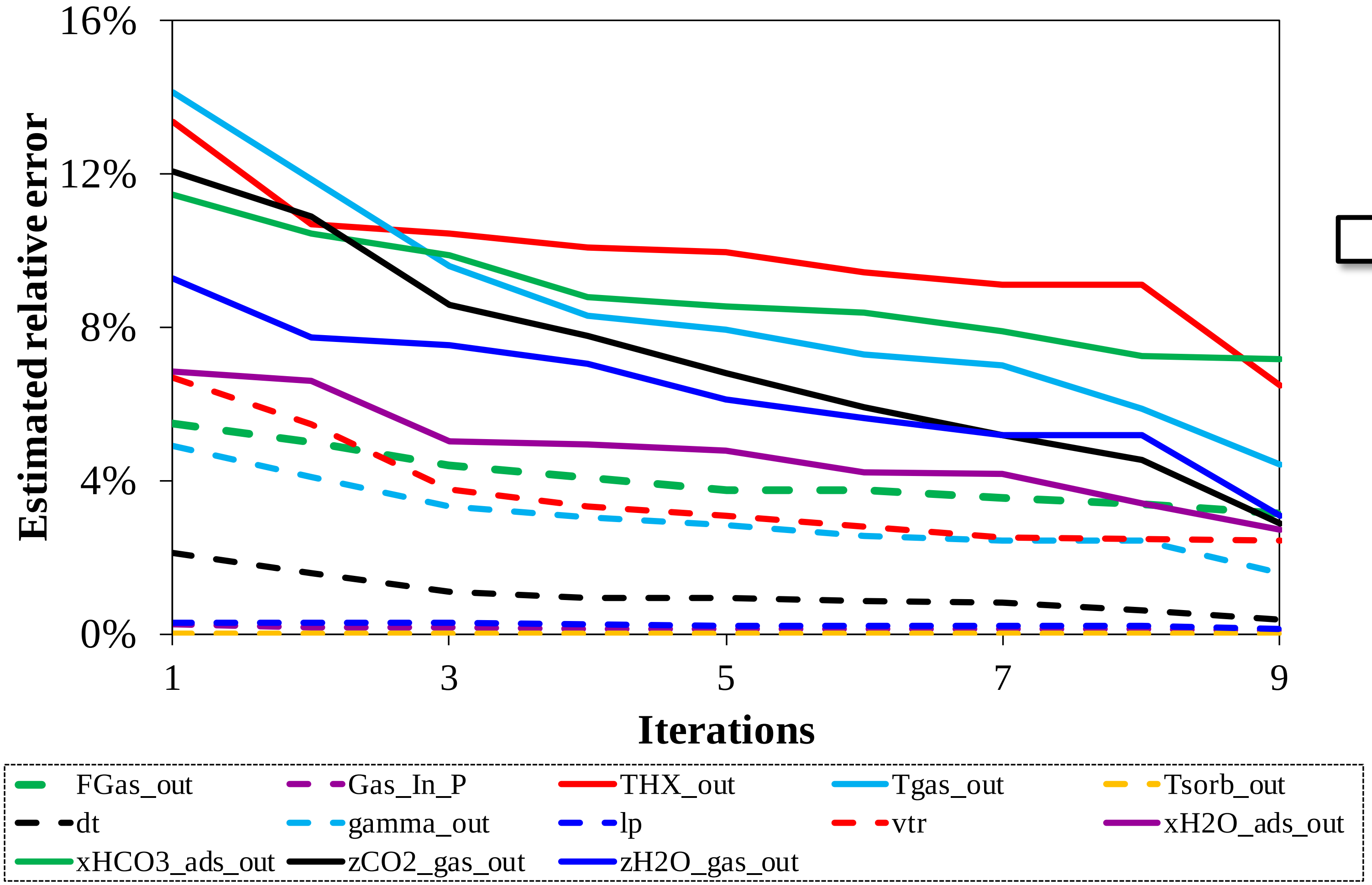
- **Model inputs (14 total)**
  - Geometry (3)
  - Operating conditions (4)
  - Gas mole fractions (2)
  - Solid compositions (2)
  - Flow rates (4)

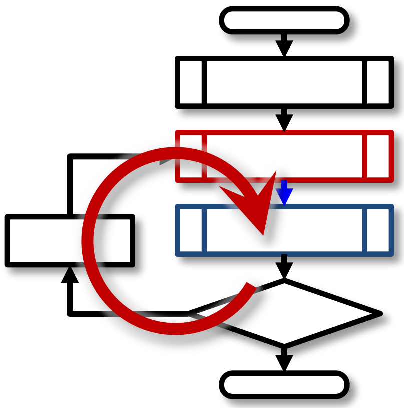
- **Model outputs (13 total)**
  - Geometry required (2)
  - Operating condition required (1)
  - Gas mole fractions (2)
  - Solid compositions (2)
  - Flow rates (2)
  - Outlet temperatures (3)
  - Design constraint (1)

Model created by Andrew Lee at the National Energy and Technology Laboratory

ADAPTIVE SAMPLING

Progression of mean error through the algorithm

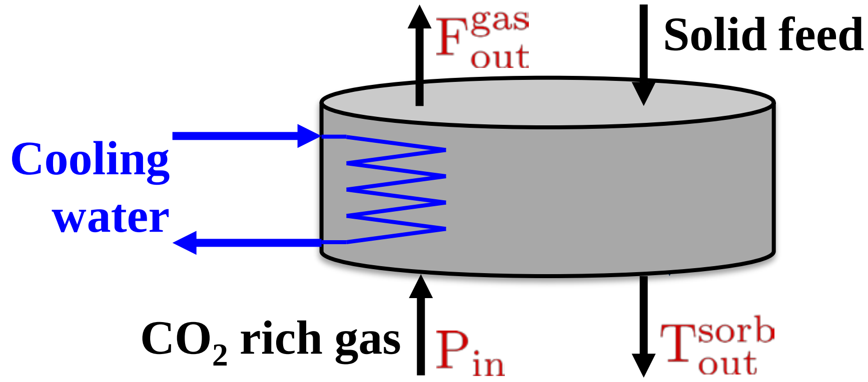




Initial data set: 137 pts

Final data set: 261

EXAMPLE MODELS



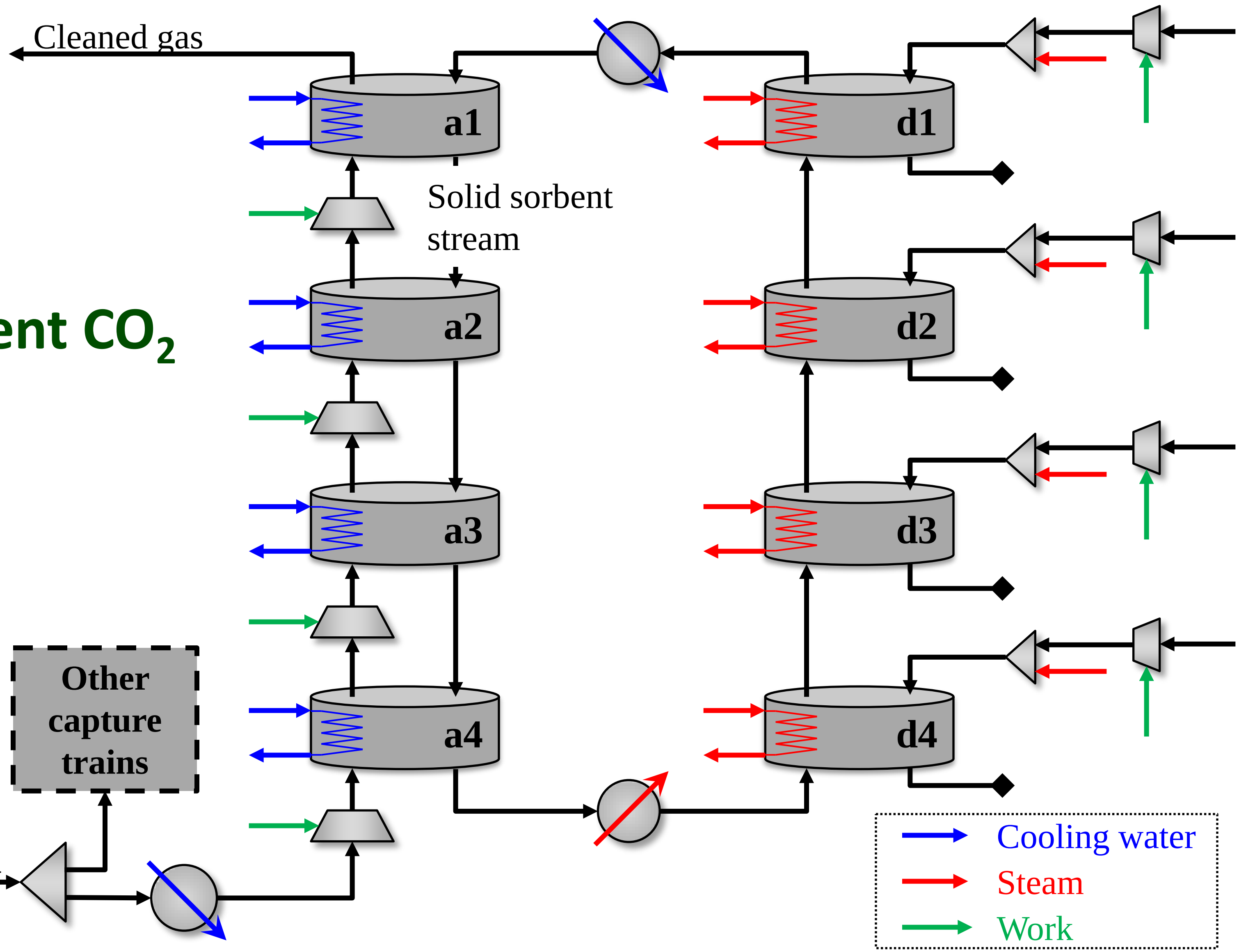
$$\mathrm{P_{in}} = 1.0\,\mathrm{P_{out}} + 0.0231\,L_b - 0.0187\,\ln(0.167\,L_b) - 0.00626\,\ln(0.667\,\mathrm{v_{gi}}) - \frac{51.1\,\mathrm{xHCO3^{ads}_{in}}}{\mathrm{F^{gas}_{in}}}$$

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

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

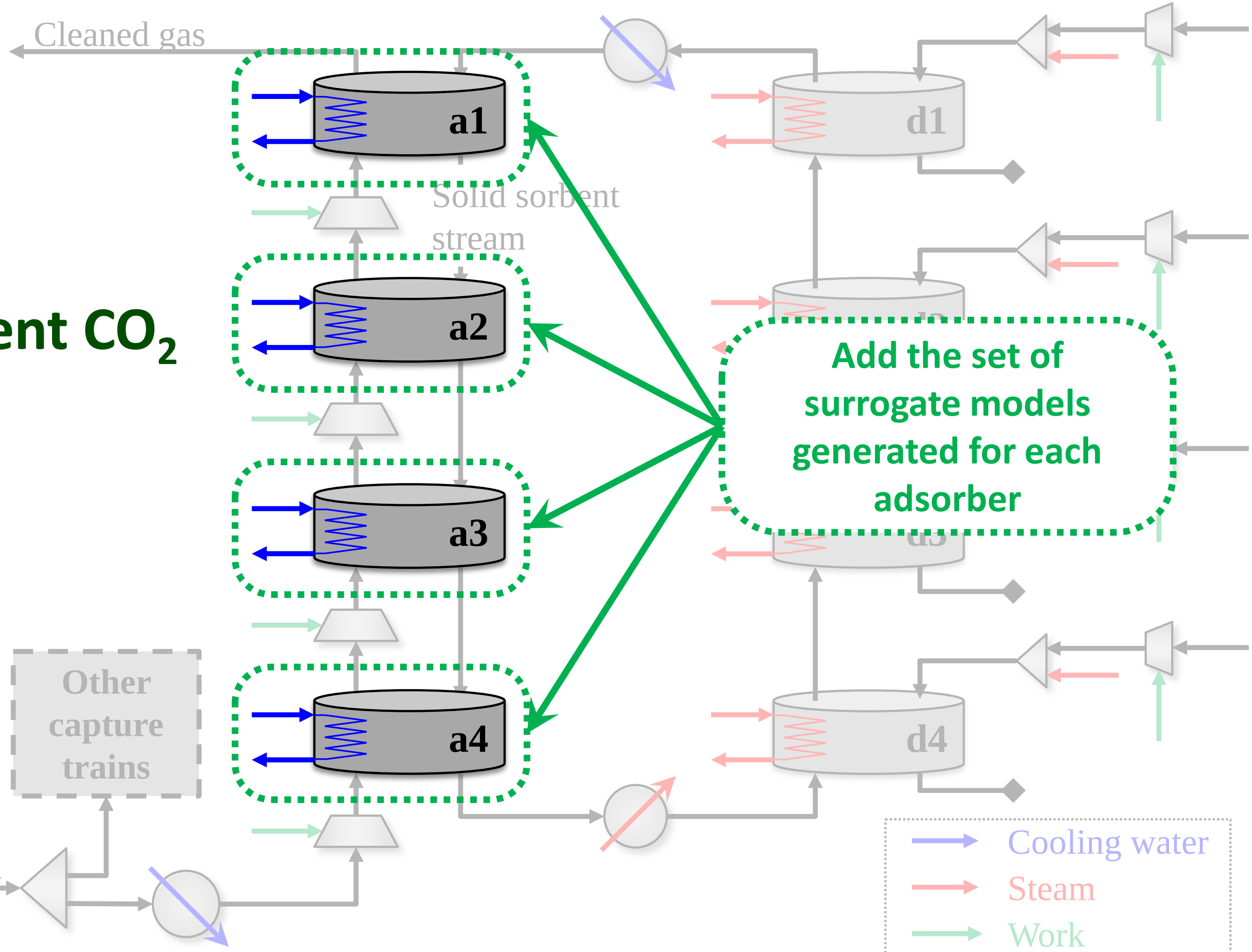
SUPERSTRUCTURE OPTIMIZATION

Solid sorbent CO_2 Capture

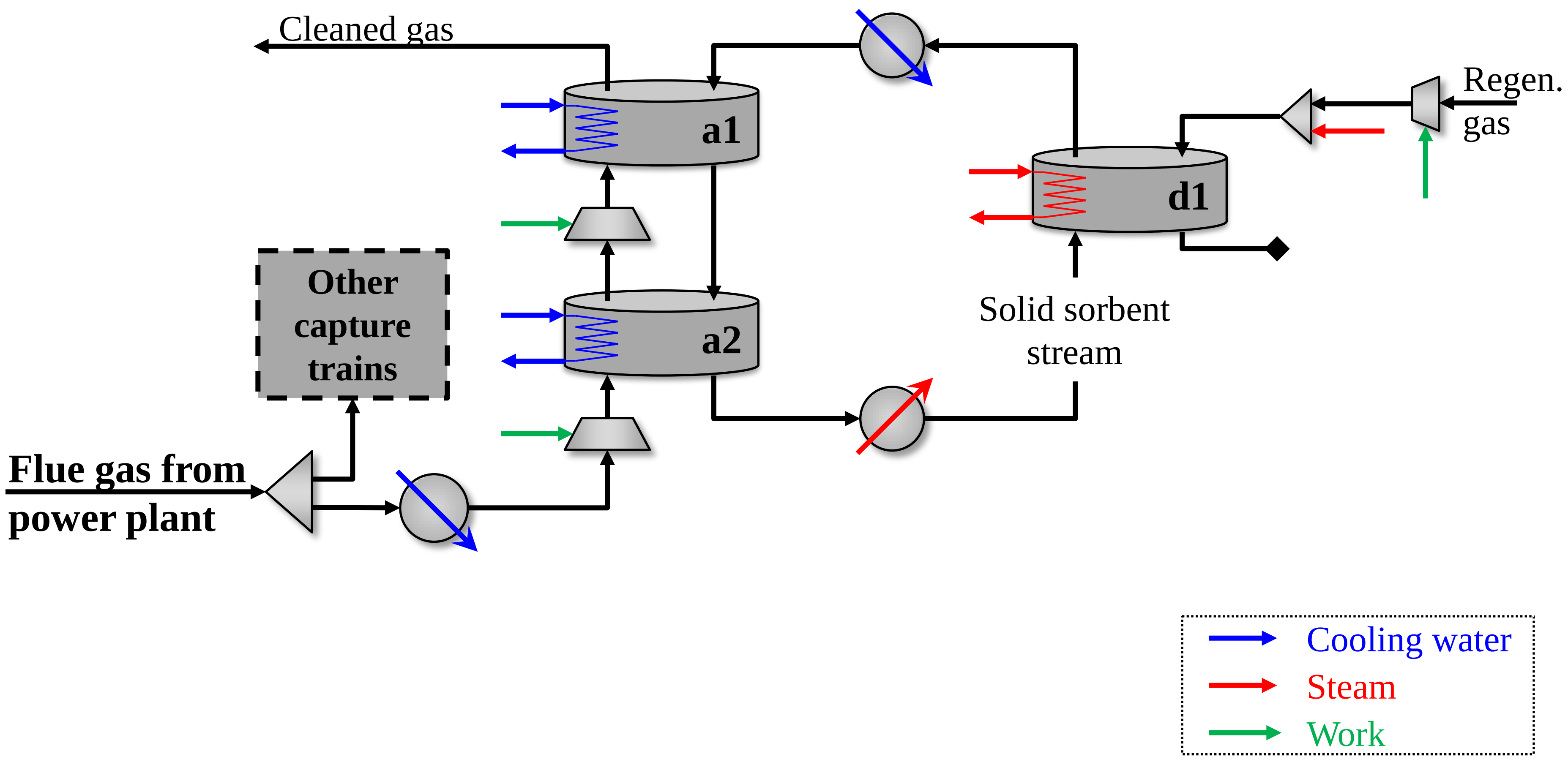


SUPERSTRUCTURE OPTIMIZATION

Solid sorbent CO_2 Capture



PRELIMINARY RESULTS



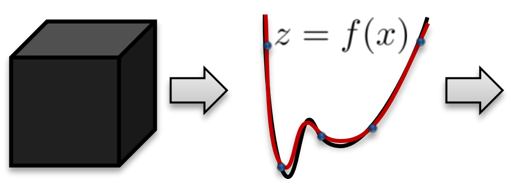
CONCLUSIONS

- **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 optimization framework flexible objective functions and additional constraints**

ALAMO

Automated **L**earning of **A**lgebraic **M**odels for **O**ptimization



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