Learning Process Models from Simulations

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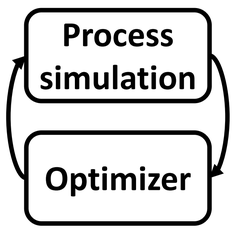
Overview

Objective

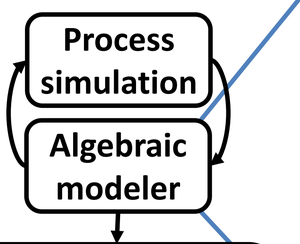
Optimize simulated processes

Direct



- ✗ No algebraic model
- ✗ Costly simulations
- ✗ Robust simulation complications

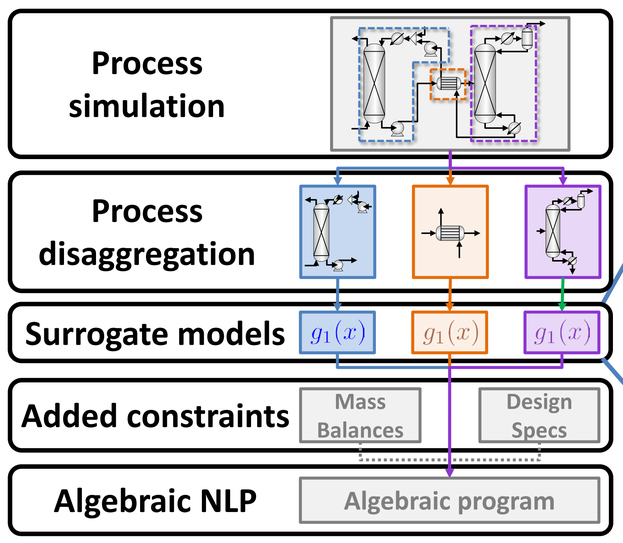
Indirect



Algebraic program

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

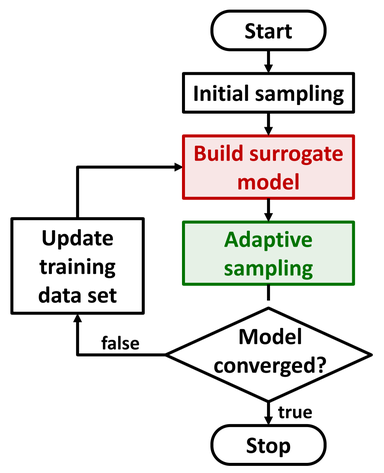
Approach



Surrogate Model Generation

ALAMO

Automated Learning of Algebraic Models for Optimization



- ✓ Accurate
- ✓ Tractable in algebraic optimization: Simple functional forms
- ✓ Generated from a minimal data set

Build surrogate model

Goal: Build a model $\hat{z}(x)$ for each output $z(x)$.

Inputs: $x \in [x^l, x^u]^D$ ⇒ **Process block** ⇒ **Outputs:** $z \in \mathbb{R}^K$

Q: How to determine the unknown functional form?

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

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

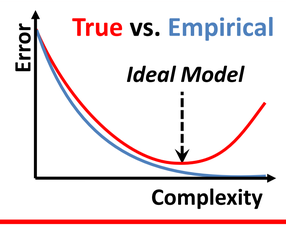
Step 2: Model reduction

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

Q: How to define the complexity of the model?

A: Estimate the true model error using Information Criterion

$$AICc = \underbrace{N \log\left(\frac{1}{N}\sum_{i=1}^{N}(z_i - \hat{z}(x_i))^2\right)}_{\text{Accuracy}} + \underbrace{2T + \frac{2T(T+1)}{N-T-1}}_{\text{Complexity}}$$



Adaptive Sampling

Q: Where should new points be sampled?

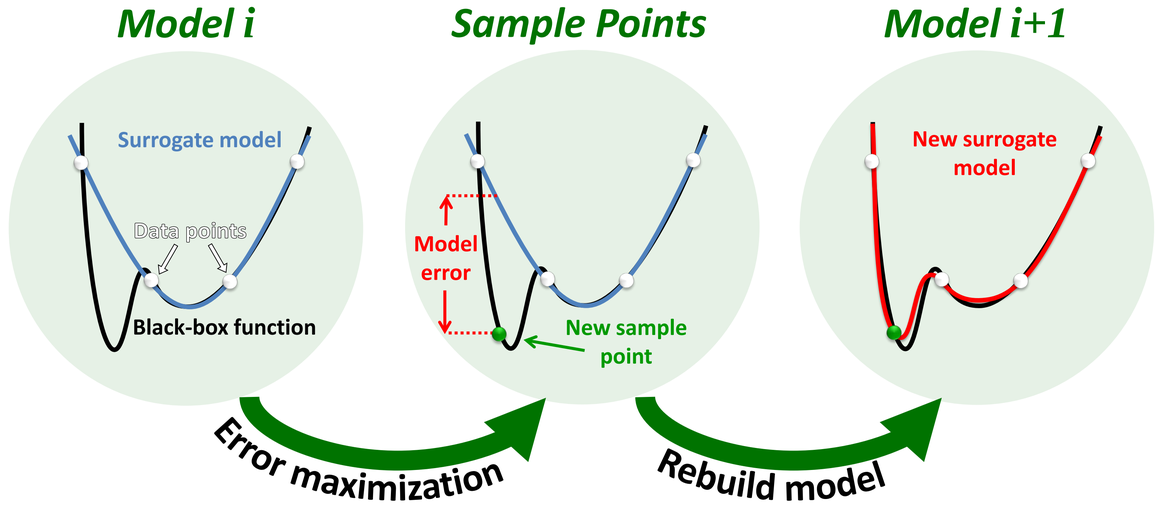
A: Error maximization

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

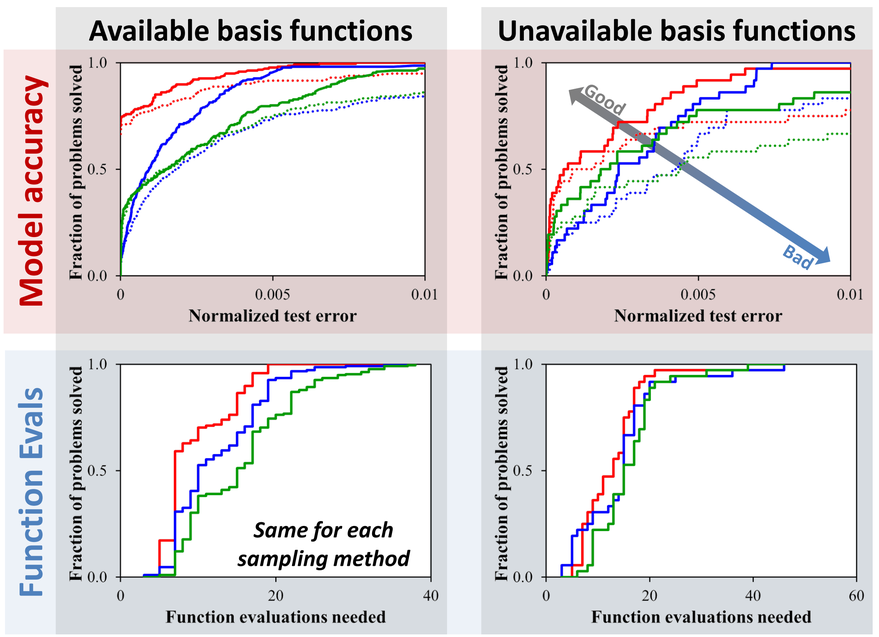
Surrogate model

Simulation/black-box

Search the problem space for areas of model inconsistency or model mismatch



Computational Experiments



Modeling methods

- Our method
- LASSO
- Least squares

Sampling methods

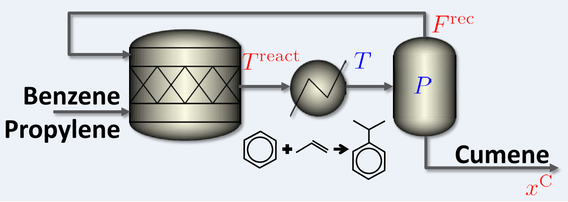
- Error maximization
- Single Latin hypercube

Test Case

Process simulation

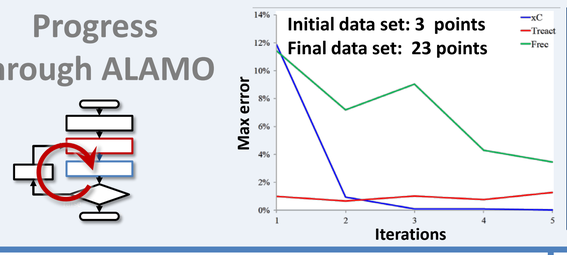
Cumene production

$$\begin{aligned} 100^\circ F &\le T \le 250^\circ F \\ 0.82 \text{ atm} &\le P \le 1.36 \text{ atm} \end{aligned}$$



Algebraic modeler

Progress through ALAMO



$$\begin{aligned} x^C(T,P) &= 0.002\,T - (5\cdot 10^{-6})\,(T)^2 + \frac{3.1}{P\,T} - \frac{12\sqrt{P}}{\sqrt{T}} + \frac{7\sqrt[3]{P}}{\sqrt[3]{T}} + \\ &\quad 0.4 + \dots \text{ small correction terms} \\ T^{react}(T,P) &= \frac{77}{\sqrt[3]{P}} + 780 \\ F^{rec}(T,P) &= (5\cdot 10^4)\,\sqrt{0.01\,T}\,\sqrt{1\,P} - 163\,T - \\ &\quad (6\cdot 10^4)\,(0.01\,T)^{\frac{1}{3}}\,(1\,P)^{\frac{1}{3}} + \frac{206\,T}{P} + \frac{9377}{\sqrt{0.01\,T}} - \\ &\quad \frac{2055}{P^3} + \dots \text{ small correction terms} \end{aligned}$$

Algebraic program

$\max \; x^C$

$T^{sp} = 250^\circ\text{F}$, $P = 0.82\text{atm}$

$x^C = 0.981$

$T^{react} = 828.1^\circ\text{F}$

$F^{rec} = 645.7 \frac{\text{lb}}{\text{hr}}$

$\le 5.2\%$error

Surrogate models can then be incorporated within a optimization framework with flexible objective functions and additional constraints

$\min \; \text{Utilities}$

$T^{sp} = 250^\circ\text{F}$, $P = 1.36\text{atm}$

$x^C = 0.964$

$T^{react} = 848.9^\circ\text{F}$

$\dot{m}^{cw} = 4.04 \cdot 10^4 \frac{\text{lb}}{\text{hr}}$

$F^{rec} = 373.16 \frac{\text{lb}}{\text{hr}}$

$A = 2,364\text{ft}^2$

$\le 3.0\%$error