Optimization of Industrial Processes Using ALAMO

NETL-RUA
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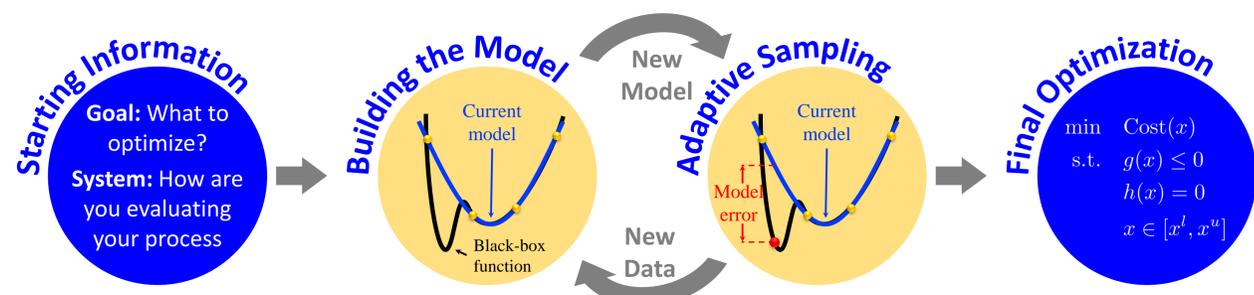Chemical Engineering

CAPD CENTER

Motivation and Challenges

When optimizing using black-boxes or simulations, a few challenges are seen:
(a) No algebraic models, (b) Costly simulations, and (c) Robust simulation complications

To over come this, ALAMO generates a set of simple algebraic surrogate models of detailed simulations or black-boxes to make, previously unusable, advanced optimization tools accessible for solving simulation-based process synthesis.

Technology/Capability Overview

Starting Information
Goal: What to optimize?
System: How are you evaluating your process

Building the Model
Current model
Black-box function

New Model
New Data

Adaptive Sampling
Current model
Model error

Final Optimization
$$\min \quad \text{Cost}(x)$$
$$\text{s.t.} \quad g(x) \leq 0$$
$$h(x) = 0$$
$$x \in [x^l, x^u]$$

How to identify a model?

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
$$\hat{z}(x) = \beta_0 + \beta_2 x_2 + \beta_5 e^{x_2}$$
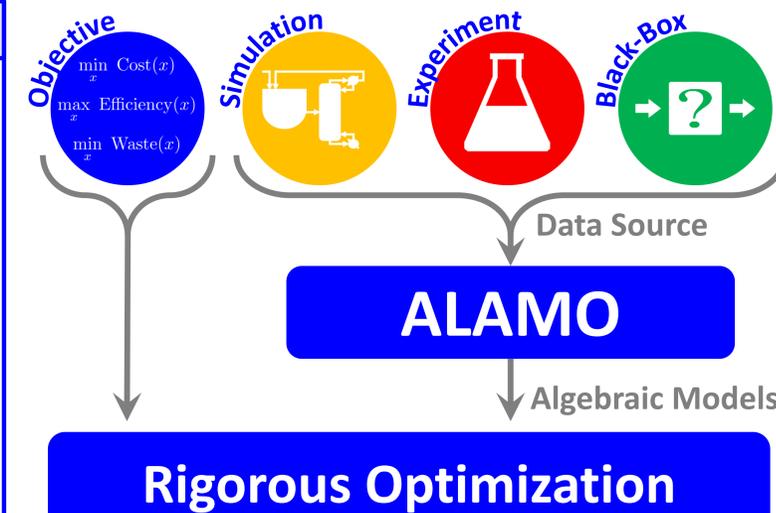
Where should new points be sampled?

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

Surrogate model
Simulation/black-box

Error maximization sampling: Search the problem space for areas of model inconsistency or **model mismatch**

Industry Significance

Improve processes using historical data, industrial simulations, and experimental set-ups. Here we show an example of using ALAMO to balance the optimal trade-off of cost and environmental impact

1. Optimize CO2 Capture

Outlet gas   Solid feed
F^{cw}
Cooling water L^{bed}
r^{CO_2}
CO_2 rich gas CO_2 rich solid outlet

Goal: Optimize a CO2 Capture Unit

2. Model Generation

Generate a low-complexity surrogate model of %CO₂ removal as a function of reactor bed depth and cooling water flow.

Now, set up the optimization...

3. Results: Pareto Analysis

Increase in cost, %
— Surrogate results
○ Simulation results
max r^{CO_2}
min cost
Utopian point
24%
22%
20%
20%   30%   40%
CO₂ removal, %

Benefits to Partner

Features

✓ **Optimize simulations**
✓ Increase profit by experimentations
✓ **Reduce process waste using historical and new data**
✓ Leverage simulations to reduce environmental impact
✓ **Use any black-box for complex optimization**

Objective
$$\min_x \text{Cost}(x)$$
$$\max_x \text{Efficiency}(x)$$
$$\min_x \text{Waste}(x)$$

Simulation   **Experiment**   **Black-Box**

Data Source

ALAMO

Algebraic Models

Rigorous Optimization

Opportunity

ALAMO works well on the test set of systems it has already been applied to, but what about others? Through testing on new systems, we aim towards two goals: (a) showcasing the ALAMO method with rich new problems and (b) locate areas of improvement throughout the software suite.

Development Status

This work has been compiled into a Matlab-based software suite that was published for pre-release at The Carbon Capture Simulation Initiative Industrial Advisory Board Program Review Meeting this October 10th-11th in San Francisco.

Contact
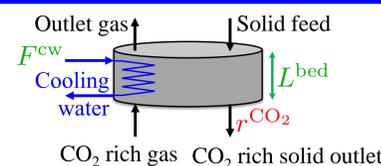
Alison Cozad
acozad@andrew.cmu.edu

Nick Sahinidis
sahinidis@cmu.edu

Department of Chemical Engineering, Carnegie Mellon University