Recent advances in ALAMO

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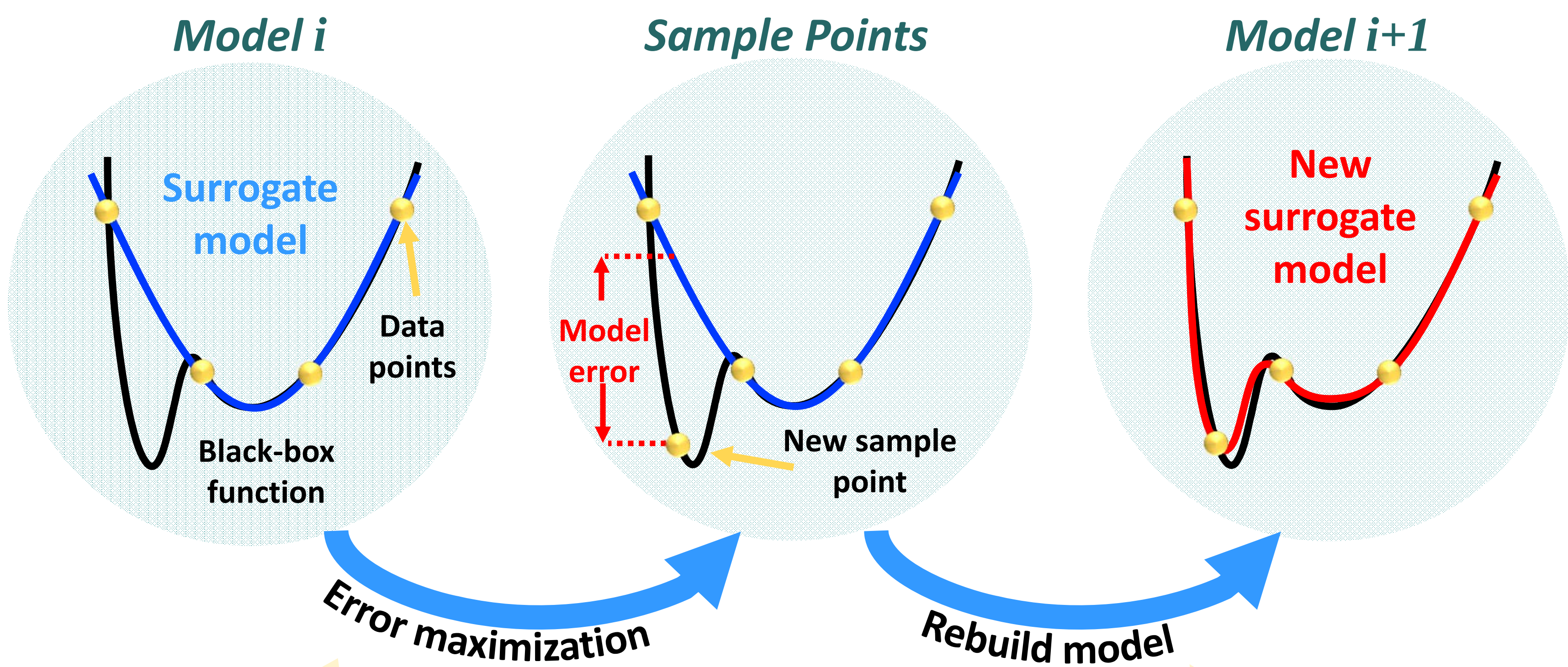
ALAMO METHODOLOGY



Derivative-free optimization
In low dimensions

Mixed-integer programming for best simple model

ALAMO SOFTWARE

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  - **4000 lines of Matlab code**
  - **Written in 2011-2013**
  - **Used GAMS to solve algebraic optimization subproblems**
  - **Demonstrated advantages vs. least squares and lasso**

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- **Current version**
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BASIC ALAMO FUNCTIONS

- **Curve fitting**
  - **Given a collection of points in an input-output space, find a function that relates inputs to outputs**
  - **ALAMO considers potential functions and automatically identifies a simple function that fits the data**

BASIC ALAMO FUNCTIONS

- **Curve fitting**
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  - **ALAMO considers potential functions and automatically identifies a simple function that fits the data**
- **Design of experiments**
  - **ALAMO can interface to a simulator (or experimental system) to guide collection of data with the aim to**
    - ***Build a model entirely from scratch***
    - ***Validate quality of model built based on a pre-existing data set***
    - ***Supplement existing experimental data***

EXAMPLE ALAMO INPUT FILE

Input-output data used to fit model

```
ninputs 1
noutputs 1
ndata 11

BEGIN_DATA
-5      25
-4      16
-3      9
-2      4
-1      1
0       0
1       1
2       4
3       9
4       16
5       25
END_DATA
```

ALAMO OUTPUT

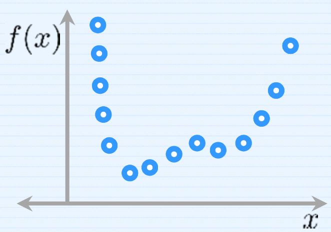
```
Step 1: Build model
Successive models for variable Z1
Z1 = 0.00
Z1 = 1.0 * X1**2.0

Calculating errors on observed data set
RMSE for observed data set:
Z1:            0.96E-05

Total execution time 0.72E-01 s
```

A DATA- AND THEORY-DRIVEN APPROACH

Empirical data



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System knowledge

output bounds

boundary conditions

derivative bounds

mass balances

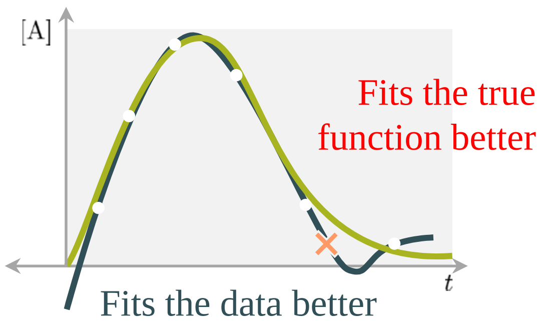
=

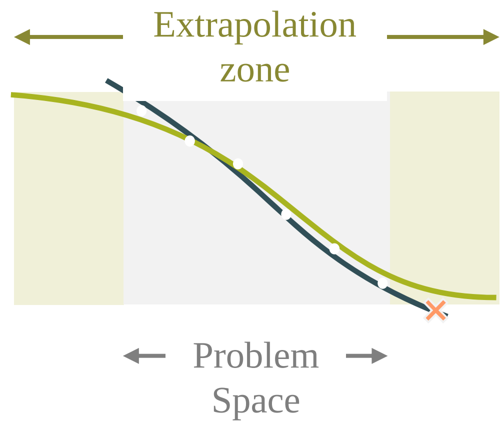
Richer models consistent with sampled data and theoretical insights

- **Apply system knowledge beyond sampled data to build regression models**
  - First principles derivation
  - Engineering insight
  - Output and derivative bounds
- **Insights that are generally available ‘free of charge’**

CONSTRAINED REGRESSION

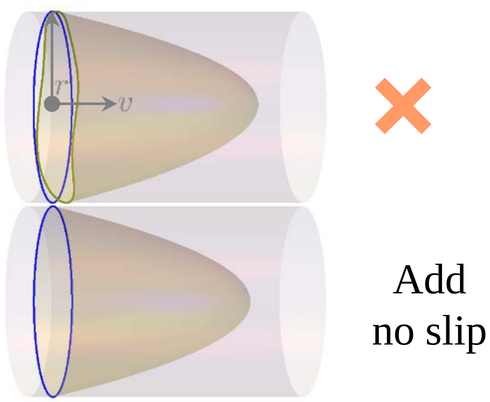
$0 \leq [\mathrm{A}]_t \leq [\mathrm{A}]^{\max}$





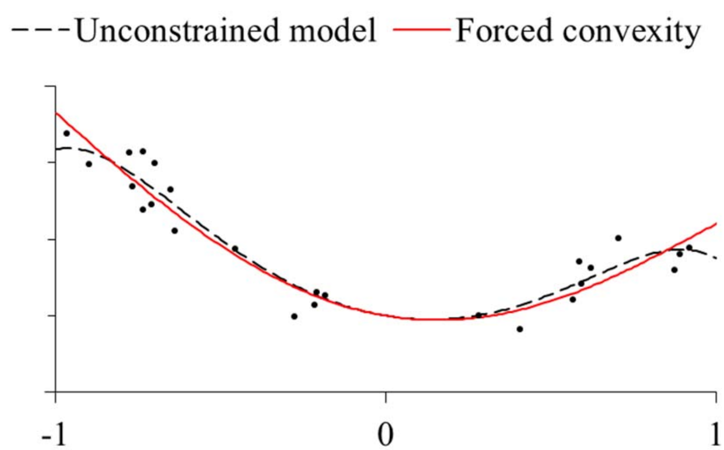
Safe Extrapolation

velocity profile model



$\hat{v}(R, \theta) = 0 \qquad \forall \theta$

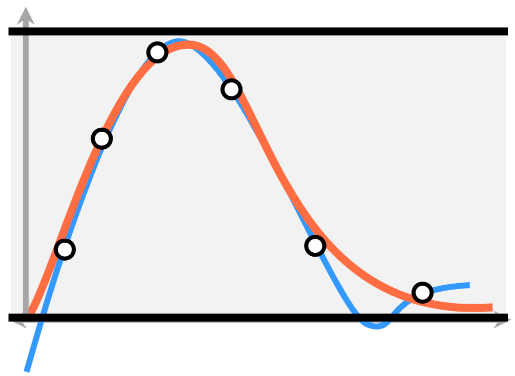
Boundary values



Convexity

IMPLEMENTATION

Enforced everywhere



$$\min_{\beta} \quad \sum_{i=1}^{N} \left(z_i - \left[\beta_0 + \beta_1\, x + \beta_2 x^2 + \ldots \right] \right)^2$$

$$\text{s.t.} \quad z^l \leq \beta_0 + \beta_1\, x + \beta_2 x^2 + \ldots \leq z^u \qquad \forall x$$

Ordinary least squares regression objective

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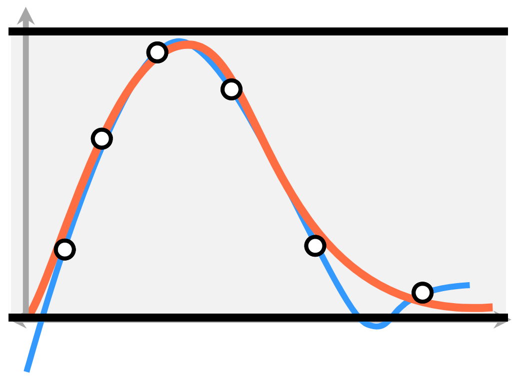

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Semi-infinite program

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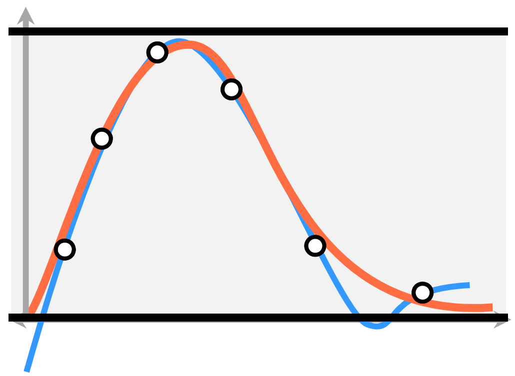

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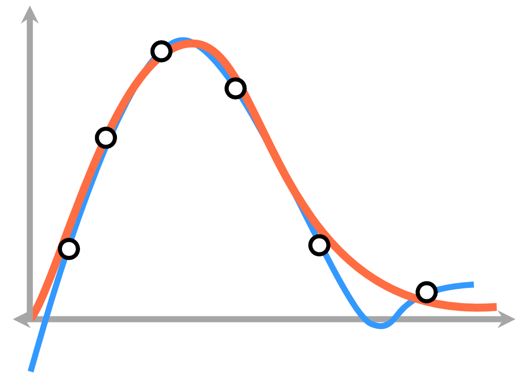
Semi-infinite program

Bounding set



$$\min_{\beta} \sum_{i=1}^{N} \left(z_i - [\beta_0 + \beta_1\, x + \beta_2 x^2 + \ldots]\right)^2$$

$$\text{s.t.} \quad z^l \leq \beta_0 + \beta_1\, x_j + \beta_2 x_j^2 + \ldots \leq z^u$$

$$\forall j \in \text{Bounding set}$$

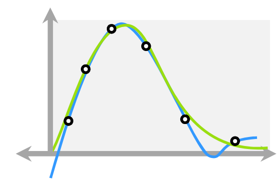
Simple linear constraints

CONCLUSIONS

- **Expanding the scope of MINLP algorithms**
  - Using low-complexity surrogate models to strike a balance between optimal decision-making and model fidelity

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

- **Enforcing theoretical insights to data-driven experimental science**
  - Iteratively use implicit regression constraints to ensure limits on models



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