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Sandia National Laboratories

Software and Advanced Solution Methods for Flexibility Analysis

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U.S. DEPARTMENT OF ENERGY

National Nuclear Security Administration

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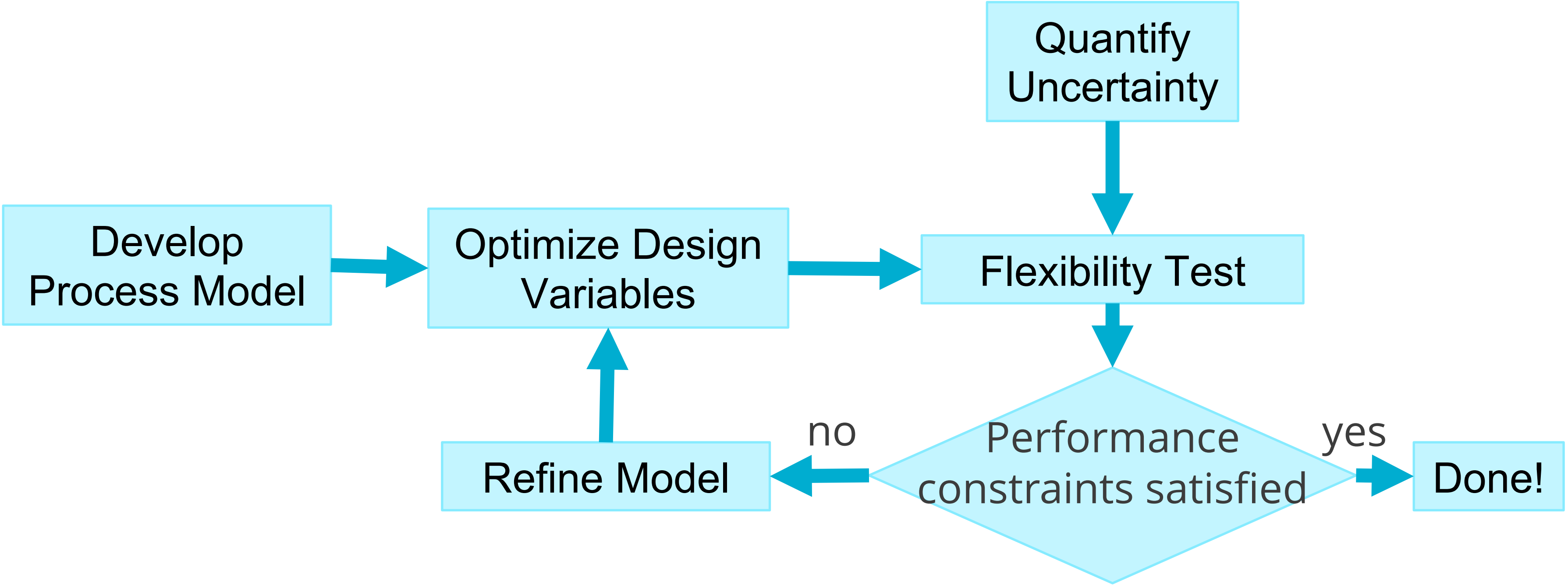
Why Flexibility Analysis?

Modern energy and process systems must satisfy performance criteria under a wide range of operating conditions, such as variable feed compositions and product demand.

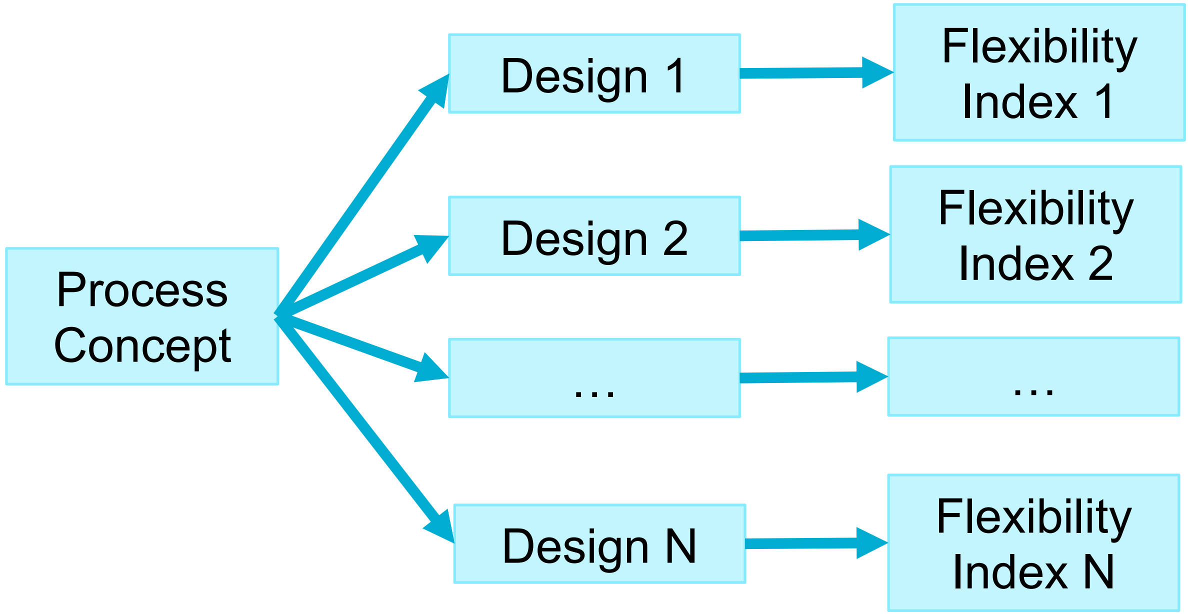
Flexibility Test: Design Refinement



Why Flexibility Analysis?

Modern energy and process systems must satisfy performance criteria under a wide range of operating conditions, such as variable feed compositions and product demand.

Flexibility Index:
Quantified comparison of designs



Flexibility Analysis provides a rigorous framework to quantify the flexible operation of a system given an uncertain parameter set.

The Flexibility Test

$$\phi(\underline{\theta}, \overline{\theta}) = \max_{\theta} \min_{z} u$$
$$\text{s.t.}$$
$$g_j(x, z, \theta) \leq u$$
$$h(x, z, \theta) = 0$$
$$\underline{\theta} \leq \theta \leq \overline{\theta}$$

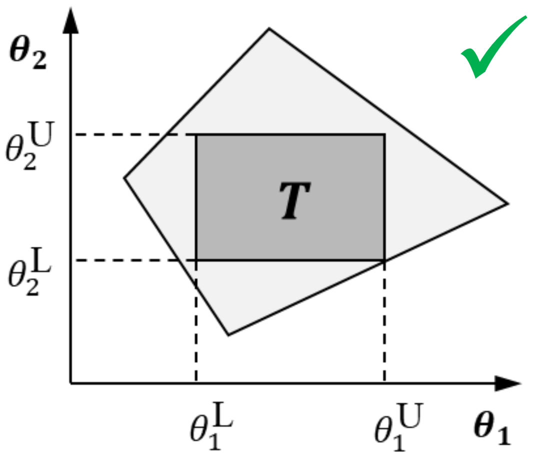
θ : Uncertain parameters

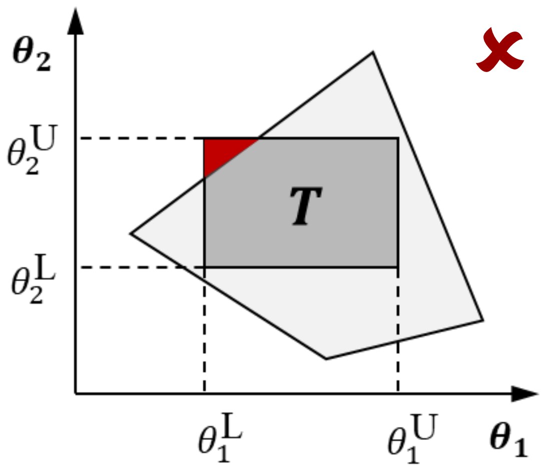
z : Controls

u : Maximum constraint violation

g_j : Performance constraints

h : Physics constraints (e.g., mass balance)





$u > 0$: Flexibility Test fails
$u \leq 0$: Flexibility Test passes

Halemane & Grossmann (1983)

The Flexibility Index

Find the largest uncertainty set around a nominal point such that the flexibility test passes.

$$\phi(\underline{\theta}, \overline{\theta}) = \max_{\theta} \min_{z} u$$

s.t.

$$g_j(x, z, \theta) \leq u$$

$$h(x, z, \theta) = 0$$

$$\underline{\theta} \leq \theta \leq \overline{\theta}$$

$$FI(\theta^N, \Delta\theta) = \max \delta$$

s.t.

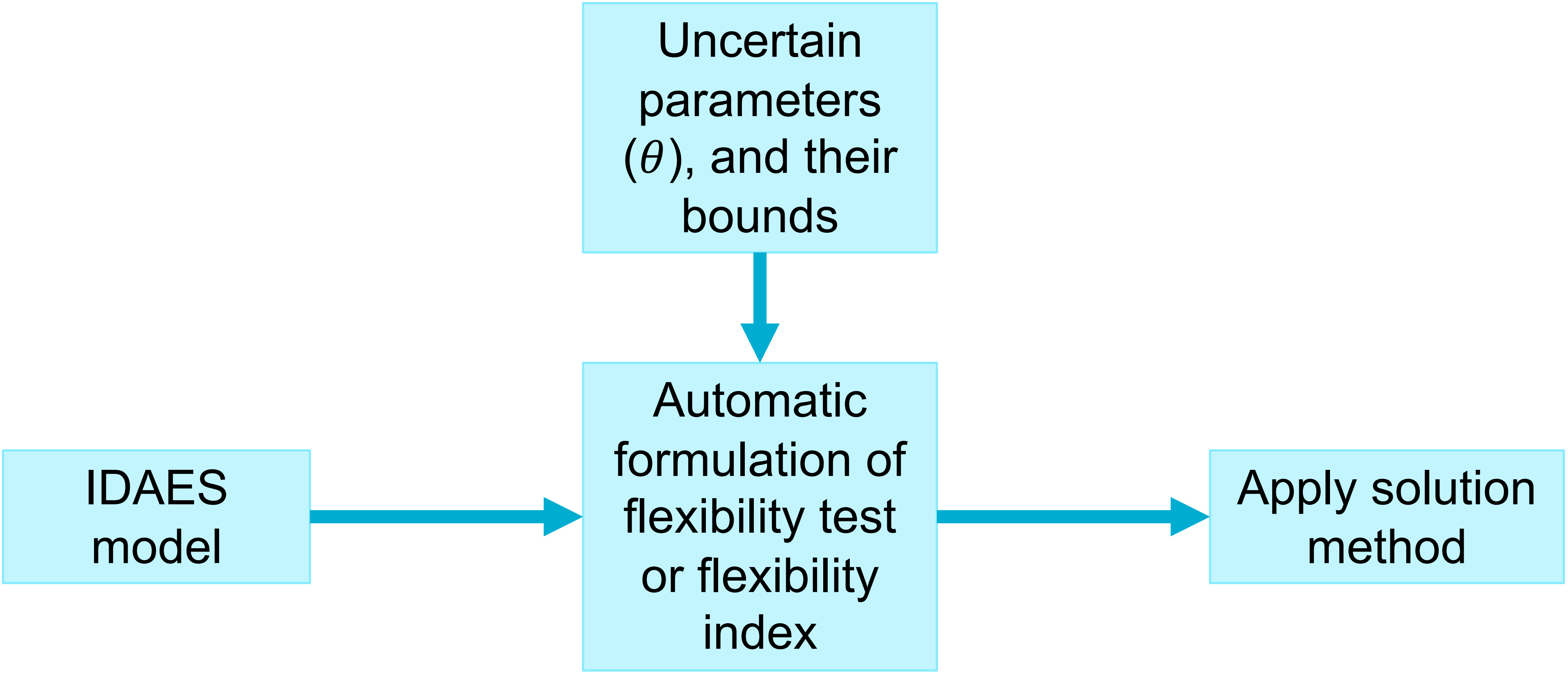
$$\phi(\underline{\theta}, \overline{\theta}) \leq 0$$

$$\underline{\theta} = \theta^N - \delta\Delta\theta$$

$$\overline{\theta} = \theta^N + \delta\Delta\theta$$

Swaney & Grossmann (1985)
Grossmann & Floudas (1987)

A Module for Flexibility Analysis with IDAES



A Module for Flexibility Analysis with IDAES

Method	*IDAES Implementation?	Advantages	Disadvantages
Vertex Enumeration	✓	• Requires NLPs • Supports external functions	• Heuristic for nonconvex problems • $2^{\# \, uncertain \, parameters}$
Sampling	✓	• Requires NLPs • Supports external functions	• $N^{\# \, uncertain \, parameters}$
Active Constraint	✓	• # of uncertain parameters	• Requires MINLP • Conservative for nonconvex problems
Linear Decision Rules	✓	• Much simpler MINLP	• Conservative
NN Decision Rules	✓	• Usually accurate, even for nonconvex problems	• Requires MINLP • Requires training a neural network
Global Optimization	Future Work	• Correct solution guaranteed	• Iterative solution of MINLPs

Machine Learning Approaches for Improved Solution of Nonconvex Problems

Challenge: Nonconvex bilevel problems are particularly challenging to solve, and nearly all IDAES problems are nonconvex.

Idea: Convert the bilevel problem (flexibility test) to a single-level problem by training a machine-learning (ML) based decision rule to approximate the optimal control action of the inner problem.

Machine Learning Approaches for Improved Solution of Nonconvex Problems

$$\max_{\theta \in \Theta} \quad \min_{z} u$$

s.t.

$$g_j(x, z, \theta) \leq u$$

$$h(x, z, \theta) = 0$$

$$\max_{\theta \in \Theta} \quad \overline{u}$$

s.t.

$$g_j(x, z, \theta) = u_j$$

$$h(x, z, \theta) = 0$$

$$\overline{u} = \sum u_j y_j$$

$$\sum y_j = 1$$

Select the most violated constraint

$$z = N(\theta)$$

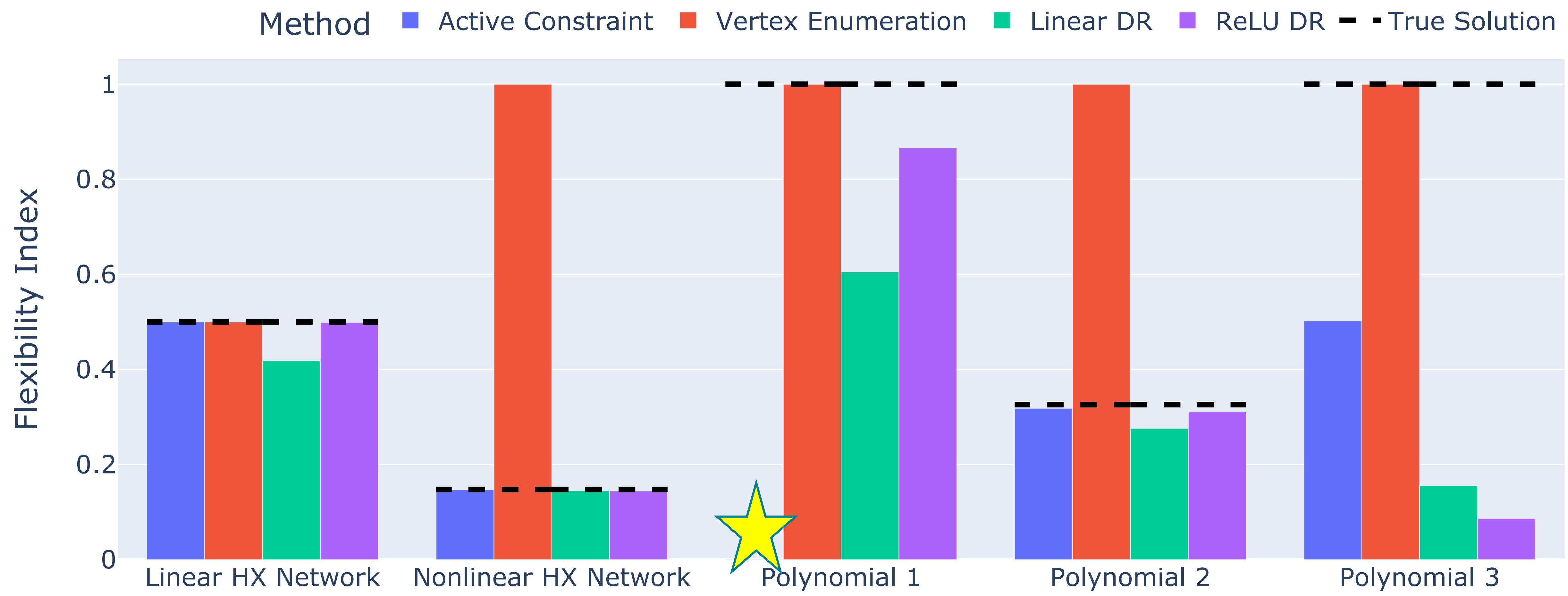
Machine Learning Decision Rule

Machine Learning Approaches for Improved Solution of Nonconvex Problems

Key Concepts:

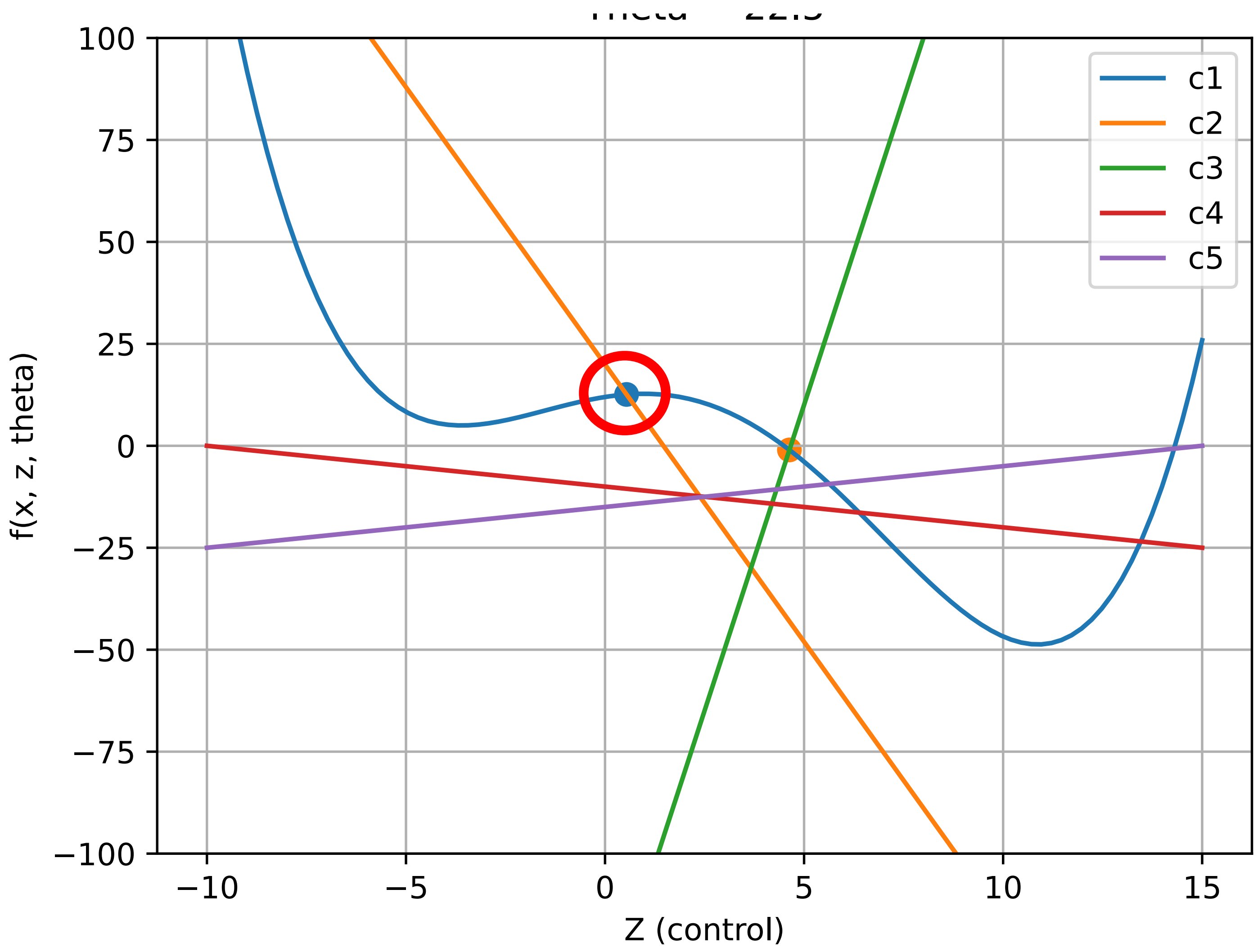
- The outputs of the ML surrogate must define all degrees of freedom of the inner problem.
- If the inner problem is always feasible, then this approach provides an upper bound on the maximum constraint violation.

Machine Learning Approaches for Improved Solution of Nonconvex Problems



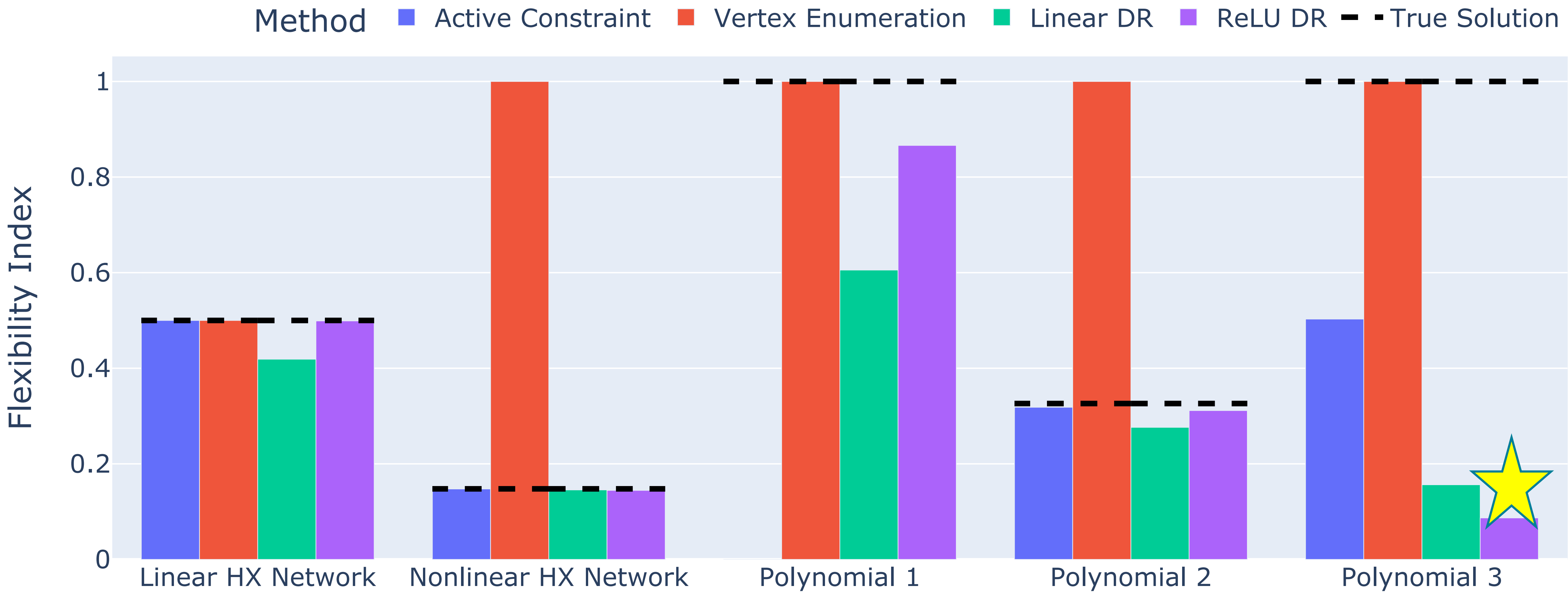
Keras: Chollet, et al. (2015) OMLT: Ceccon, et al. (2022) SCIP 7.0.2: Vigerske & Gleixner (2018) Pyomo 6.4: Bynum, et al. (2021) Gurobi 9.5.2

Machine Learning Approaches for Improved Solution of Nonconvex Problems

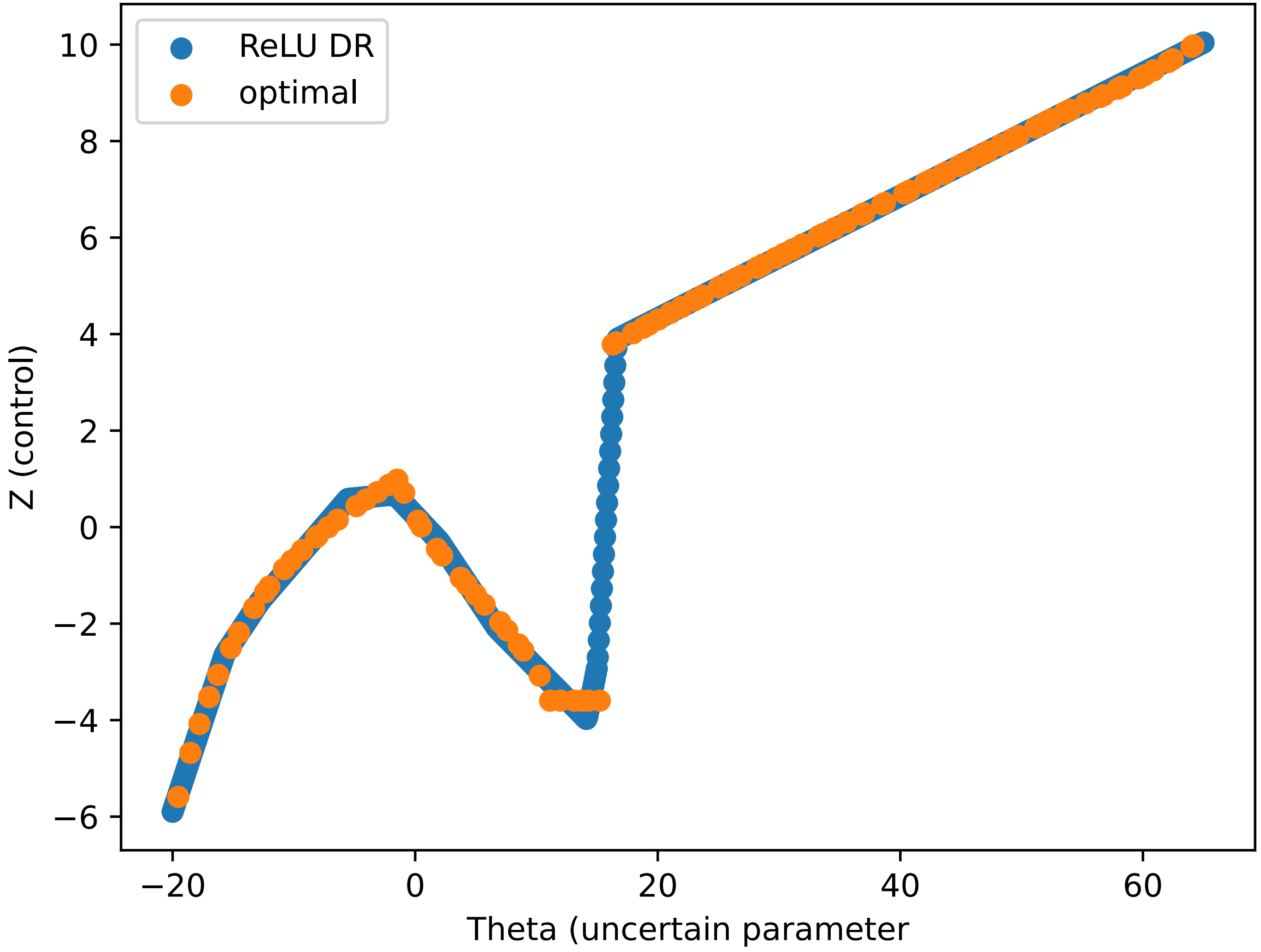


Polynomial 1 – Active Constraint: Local minima in the constraint violation causes the active constraint method to report the nominal point as infeasible.

Machine Learning Approaches for Improved Solution of Nonconvex Problems



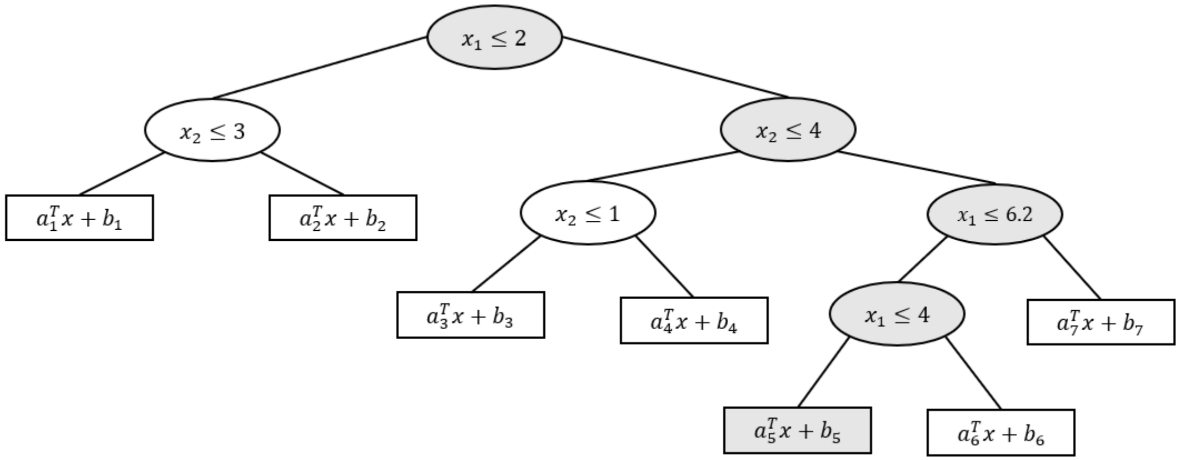
Machine Learning Approaches for Improved Solution of Nonconvex Problems

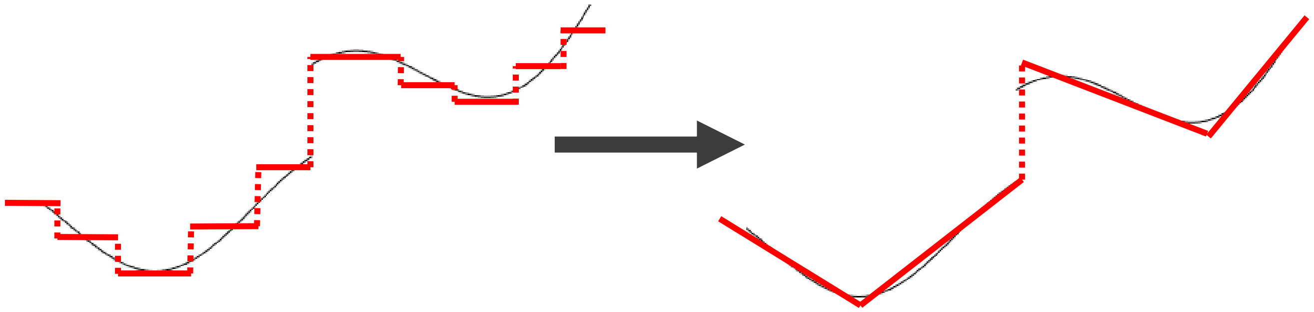


Polynomial 3 - ReLU DR: Discontinuity in the optimal control profile causes ReLU NN to underpredict the flexibility index.

Linear Model Decision Trees

Linear Model Decision Trees





Formulations

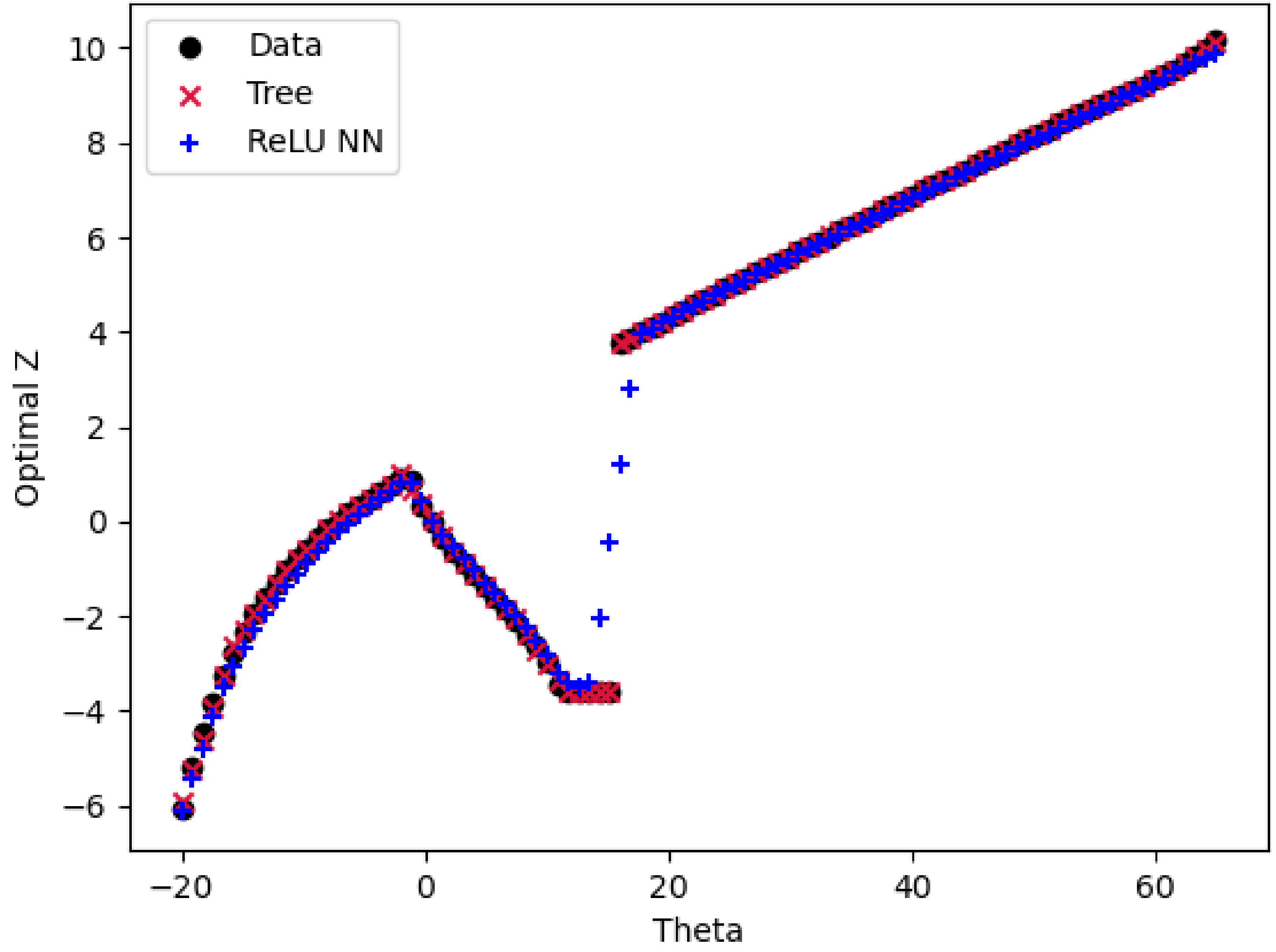
$$\bigvee \begin{bmatrix} Z_\ell \\ x_i \leq v_{i,\ell}^U \quad \forall\, i \in [n] \\ x_i \geq v_{i,\ell}^L \quad \forall\, i \in [n] \\ a_\ell^T x + b_\ell = d \end{bmatrix}$$

$$\begin{aligned}
\text{s.t.} \quad & d = \sum_{\ell \in L} (a_\ell^T x + b_\ell) z_\ell \\
& \sum_{\ell \in L} z_\ell = 1 \\
& \sum_{\ell \in \text{Left}_s} z_\ell \leq y_{i(s),j(s)} && \forall s \in S \\
& \sum_{\ell \in \text{Right}_s} z_\ell \leq 1 - y_{i(s),j(s)} && \forall s \in S \\
& y_{i,j} \leq y_{i,j+1} && \forall i \in [n], j \in [m_i - 1] \\
& x_i \geq v_{i,0} + \sum_{j=1}^{m_i} (v_{i,j} - v_{i,j-1})(1 - y_{i,j}) && \forall i \in [n] \\
& x_i \leq v_{i,m_i+1} + \sum_{j=1}^{m_i} (v_{i,j} - v_{i,j+1}) y_{i,j} && \forall i \in [n] \\
& x \in \mathbb{R}^n \\
& y_{i,j} \in \{0,1\} && \forall i \in [n], j \in [m_i] \\
& z_\ell \in \{0,1\} && \forall \ell \in L
\end{aligned}$$

⟷

$$\begin{aligned}
\text{s.t.} \quad & a_\ell^T x + b_\ell \leq d + M_\ell^U (1 - z_\ell) && \forall \ell \in L \\
& a_\ell^T x + b_\ell \geq d - M_\ell^L (1 - z_\ell) && \forall \ell \in L
\end{aligned}$$

Linear Model Decision Trees



Method	δ
True Solution	1
Vertex	1
ReLU NN	0.152
Linear Tree	0.890
Active Set	0.300

Remarks and Future Work

- IDAES is developing rigorous, general-purpose capabilities for quantified analysis of process system flexibility.
- The flexibility analysis module will be incorporated into the IDAES platform after documentation and unit tests have been developed.
- Machine-learning based decision rules provide a viable solution approach for nonconvex problems.
- The optimal control profile may be a discontinuous function of the uncertain parameters. Linear decision trees are likely to be an excellent solution.
- Because a decision rule can provide an upper bound on the maximum constraint violation, future work will investigate strategies to bound the true solution and iteratively refine the ML-based decision rule.

Acknowledgements

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