Exact hull reformulation for Quadratically Constrained Generalized Disjunctive Programs

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Background

Generalized Disjunctive Program (GDP) [1-4]

$$
\begin{aligned}
\min_{\mathbf{x},\mathbf{Y}} \quad & f(\mathbf{x}) \\
\text{s.t.} \quad & \mathbf{g}(\mathbf{x}) \le 0, \\
& \bigvee_{i\in D_k} \begin{bmatrix} Y_{ik} \\ h_{ik}(\mathbf{x}) \le 0 \end{bmatrix}, \quad \forall k \in K, \\
& \underline{\vee}_{i\in D_k} Y_{ik}, \quad \forall k \in K, \\
& \Omega(\mathbf{Y}) = \text{True}, \\
& \mathbf{x}^l \le \mathbf{x} \le \mathbf{x}^u, \\
& \mathbf{x} \in \mathbb{R}^n, \\
& Y_{ik} \in \{\text{False}, \text{True}\}, \quad \forall k \in K,\ i \in D_k.
\end{aligned}
$$

Hull reformulation of GDP

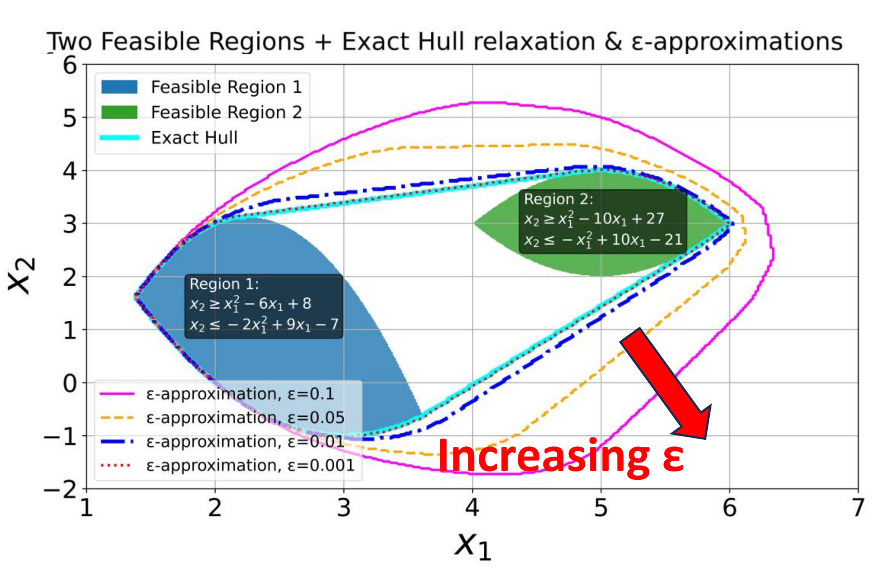
$$
\begin{aligned}
\min_{\mathbf{x},\mathbf{y}} \quad & f(\mathbf{x}) \\
\text{s.t.} \quad & \mathbf{g}(\mathbf{x}) \le 0, \\
& \sum_{i\in D_k} y_{ik} = 1 \quad \forall k \in K, \\
& \mathbf{E}\mathbf{y} \ge \mathbf{e}, \\
& \mathbf{x} = \sum_{i\in D_k} \mathbf{v}_{ik}, \quad k \in K \\
& \left(\text{cl}\,\widetilde{h}_{ik}\right)(\mathbf{v}_{ik}, y_{ik}) \le 0, \quad k \in K,\ i \in D_k \\
& \mathbf{v}_{ik} \in \mathbb{R}^n, \quad k \in K,\ i \in D_k \\
& \mathbf{x}^l \le \mathbf{x} \le \mathbf{x}^u, \\
& \mathbf{x} \in \mathbb{R}^n, \\
& y_{ik} \in \{0,1\} \quad \forall k \in K,\ i \in D_k.
\end{aligned}
$$

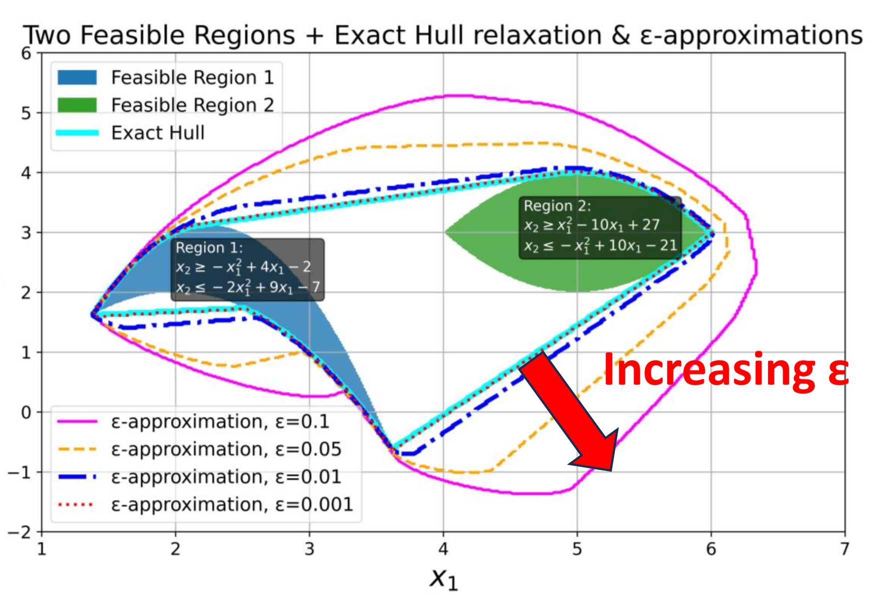
To calculate numerically the closure of a perspective function, an ε-approximation method (where ε is a small number, i.e. 10^{-4}) proposed by Furman, Sawaya, and Grossmann [5] is typically employed:

$$
\left(\text{cl}\,\widetilde{h}\right)(\mathbf{v}, y) \approx ((1-\varepsilon)y + \varepsilon)\, h\left(\frac{\mathbf{v}}{(1-\varepsilon)y+\varepsilon}\right) - \varepsilon\, h(0)(1-y),
$$

For the quadratic function $h(\mathbf{v}) = \mathbf{v}^\top Q\mathbf{v} + \mathbf{c}^\top\mathbf{v} + d$, where $Q \in \mathbb{R}^{n\times n}$, $\mathbf{c} \in \mathbb{R}^n$, and $d \in \mathbb{R}$, after simplification, an ε-approximation results in a general non-linear function:

$$
\left(\text{cl}\ \widetilde{h}\right)(\mathbf{v}, y) \approx \frac{\mathbf{v}^\top Q\mathbf{v}}{(1-\varepsilon)y+\varepsilon} + \mathbf{c}^\top\mathbf{v} + dy
$$





Exact Hull Reformulation of Quadratic GDP

Disjunctions of quadratically constrained GDP can be expressed as follows:

$$
\bigvee_{i\in D_k} \begin{bmatrix} Y_{ik} \\ \mathbf{x}^\top Q_{jik}\mathbf{x} + \mathbf{c}_{jik}^\top\mathbf{x} + d_{jik} \le 0,\ j \in J_{ik} \end{bmatrix}, \quad k \in K
$$

We propose the following reformulations:

Conic Exact Hull Reformulation (CEHR) for convex constraints:

$$
\begin{aligned}
& \mathbf{x} = \sum_{i\in D_k} \mathbf{v}_{ik}, \\
& \mathbf{x}^\ell y_{ik} \le \mathbf{v}_{ik} \le \mathbf{x}^u y_{ik}, \\
& \mathbf{v}_{ik}^\top Q_{jik}\mathbf{v}_{ik} \le t_{jik} y_{ik}, \\
& t_{jik} + \mathbf{c}_{jik}^\top\mathbf{v}_{ik} + d_{jik} y_{ik} \le 0, \\
& \mathbf{v}_{ik} \in \mathbb{R}^n, \quad t_{jik} \in \mathbb{R}_+.
\end{aligned}
$$

General Exact Hull Reformulation (GEHR) for nonconvex constraints:

$$
\begin{aligned}
& \mathbf{x} = \sum_{i\in D_k} \mathbf{v}_{ik}, \\
& \mathbf{v}_{ik}^\top Q_{jik}\mathbf{v}_{ik} + \mathbf{c}_{jik}^\top\mathbf{v}_{ik} y_{ik} + d_{jik} y_{ik}^2 \le 0, \\
& \mathbf{x}^\ell y_{ik} \le \mathbf{v}_{ik} \le \mathbf{x}^u y_{ik}, \\
& \mathbf{v}_{ik} \in \mathbb{R}^n.
\end{aligned}
$$

where $k \in K$ indexes disjunctions, $i \in D_k$ indexes disjuncts in disjunction k, and $j \in J_{ik}$ indexes quadratic constraints in disjunct i. Here, $\mathbf{v}_{ik}$ is the disaggregated variable, y_{ik} is the disjunct indicator, and Q_{jik}, $\mathbf{c}_{jik}$, and d_{jik} are the quadratic, linear, and constant coefficients.

Computational experiments

Computational experiments were conducted on various convex and non-convex quadratic GDPs, such as random convex and non-convex quadratic GDPs, convex k-means clustering, a non-convex CSTR network benchmark, and constrained layout instances.

Solver outcomes across reformulation strategies for **convex random** quadratic GDPs

Strategy	Optimal	Timeout	Infeasible	Objective mismatch	Total
Solver: `Gurobi`					
BigM	240	0	0	0	240
Hull ε-approx. ($\varepsilon = 10^{-4}$)	2	0	200	38	240
GEHR	240	0	0	0	240
CEHR	240	0	0	0	240
Binary Mult.	167	73	0	0	240
Solver: `BARON`					
BigM	233	7	0	0	240
Hull ε-approx. ($\varepsilon = 10^{-4}$)	5	233	0	2	240
GEHR	29	183	0	28	240
CEHR	20	190	0	30	240
Binary Mult.	180	60	0	0	240
Solver: `SCIP`					
BigM	240	0	0	0	240
Hull ε-approx. ($\varepsilon = 10^{-4}$)	47	182	0	11	240
GEHR	104	136	0	0	240
CEHR	240	0	0	0	240
Binary Mult.	94	146	0	0	240
Solver: `SCIP` **(convex flag)**					
BigM	240	0	0	0	240
Hull ε-approx. ($\varepsilon = 10^{-4}$)	238	0	0	2	240
GEHR	4	0	217	19	240
CEHR	240	0	0	0	240
Binary Mult.	0	0	219	21	240

Solver outcomes across reformulation strategies for non-**convex random** quadratic GDPs

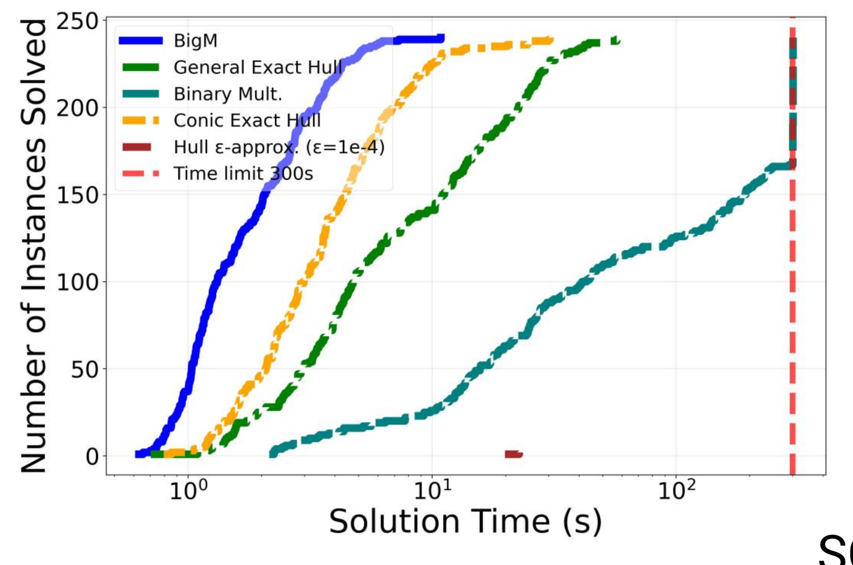
Strategy	Optimal	Timeout	Infeasible	Objective mismatch	Total
Solver: `Gurobi`					
BigM	91	9	0	0	100
Hull ε-approx. ($\varepsilon = 10^{-4}$)	2	86	0	12	100
GEHR	59	41	0	0	100
Binary Mult.	83	17	0	0	100
Solver: `BARON`					
BigM	95	4	0	1	100
Hull ε-approx. ($\varepsilon = 10^{-4}$)	0	99	1	0	100
GEHR	7	86	0	7	100
Binary Mult.	88	12	0	0	100
Solver: `SCIP`					
BigM	91	9	0	0	100
Hull ε-approx. ($\varepsilon = 10^{-4}$)	11	89	0	0	100
GEHR	41	59	0	0	100
Binary Mult.	39	61	0	0	100

Computational experiments

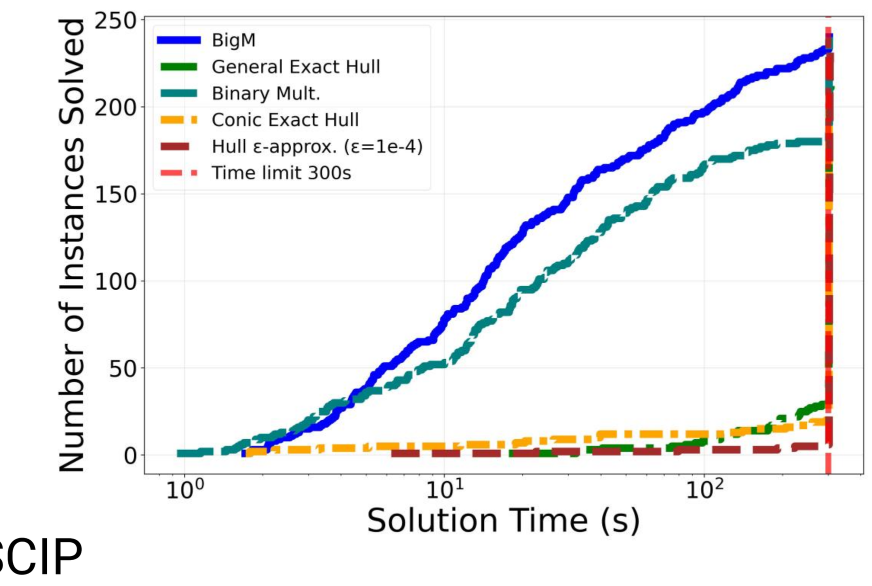
240 **Convex random instances** ($Q \succeq 0$) **:**

$3 \le |K| \le 10, \quad 10 \le |D_k| \le 15, \quad |J_{ik}| = 10, \quad 3 \le n \le 7$

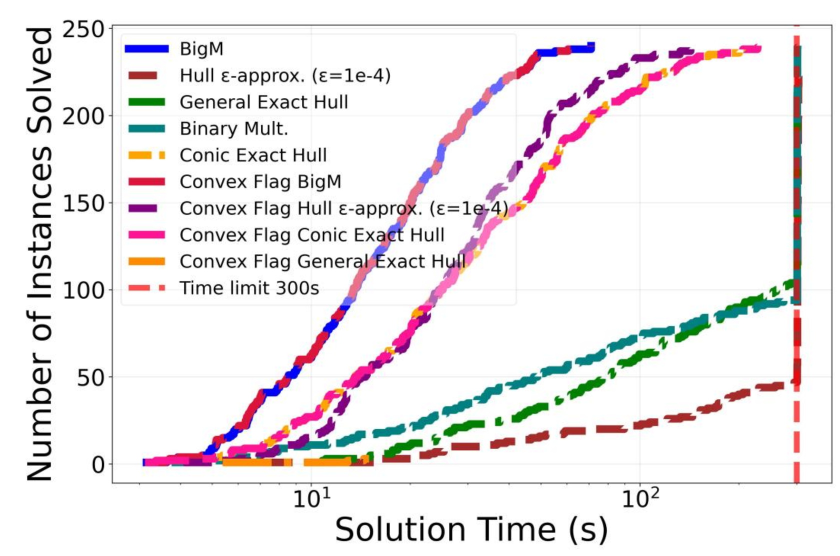
Gurobi



Baron



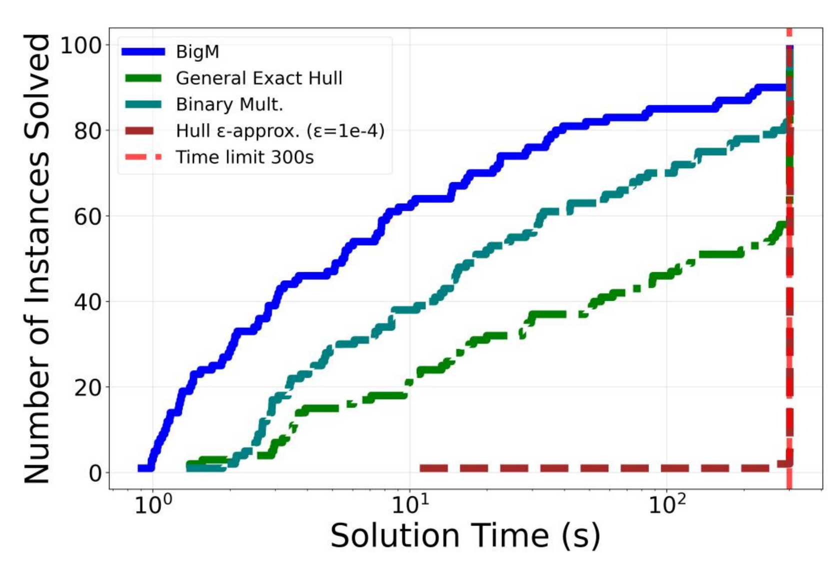
SCIP



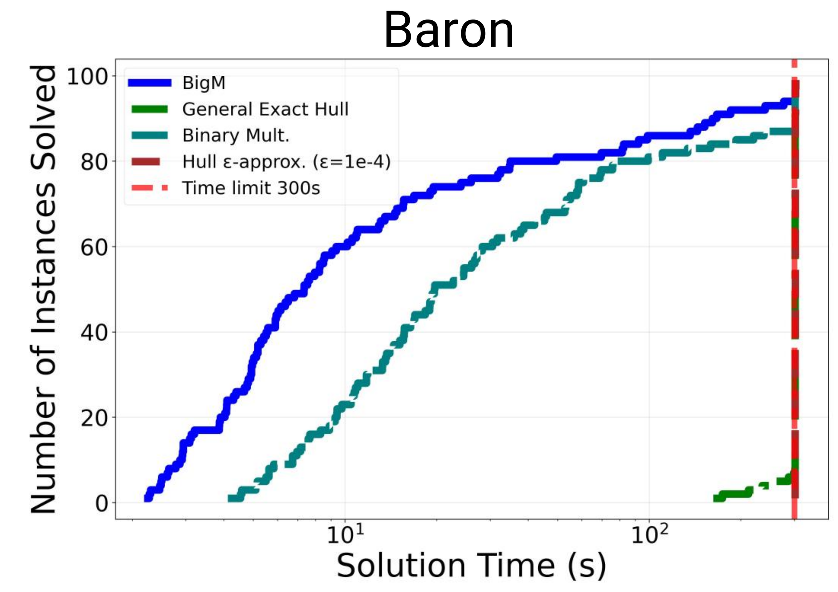
100 **Non-convex random instances:**

$3 \le |K| \le 10, \quad 10 \le |D_k| \le 15, \quad |J_{ik}| = 10, \quad 3 \le n \le 9$

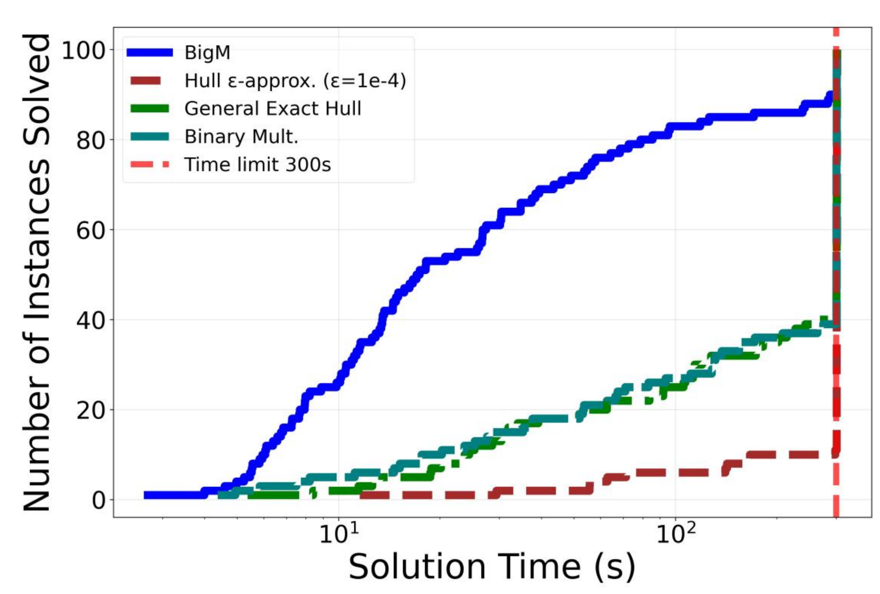
Gurobi



Baron



SCIP



Conclusion

- **Exact Hull Reformulation:** The proposed exact hull reformulation offers practical benefits by preserving the original quadratic problem structure and eliminating approximations in GDPs
- **Improved Solver Performance:** Numerical experiments show that state-of-the-art Mixed-Integer Nonlinear Programming (MINLP) solvers solve the proposed reformulations faster and more reliably than ε-approximation-based approaches.
- **Value of Customization:** Results highlight the importance of developing tailored, exact reformulations, especially when constraints exhibit simpler structural forms.

References

[1] I. E. Grossmann and S. Lee, "Generalized Convex Disjunctive Programming: Nonlinear Convex Hull Relaxation," *Comput. Optim. Appl.*, vol. 26, no. 1, pp. 83–100, Oct. 2003, doi: 10.1023/A:1025154322278.

[2] I. E. Grossmann and J. P. Ruiz, "Generalized Disjunctive Programming: A Framework for Formulation and Alternative Algorithms for MINLP Optimization," in *Mixed Integer Nonlinear Programming*, vol. 154, J. Lee and S. Leyffer, Eds., in The IMA Volumes in Mathematics and its Applications, vol. 154. , New York, NY: Springer New York, 2012, pp. 93–115. doi: 10.1007/978-1-4614-1927-3_4.

[3] P. Bonami, A. Lodi, A. Tramontani, and S. Wiese, "On mathematical programming with indicator constraints," *Math. Program.*, vol. 151, no. 1, pp. 191–223, Jun. 2015, doi: 10.1007/s10107-015-0891-4.

[4] D. E. Bernal Neira and I. E. Grossmann, "Convex Mixed-Integer Nonlinear Programs Derived from Generalized Disjunctive Programming using Cones," Feb. 19, 2024, *arXiv*: arXiv:2109.09657. doi: 10.48550/arXiv.2109.09657.

[5] K. C. Furman, N. W. Sawaya, and I. E. Grossmann, "A computationally useful algebraic representation of nonlinear disjunctive convex sets using the perspective function," *Comput. Optim. Appl.*, vol. 76, no. 2, pp. 589–614, Jun. 2020, doi: 10.1007/s10589-020-00176-0.

[6] O. Günlük and J. Linderoth, "Perspective Reformulation and Applications," in *Mixed Integer Nonlinear Programming*, vol. 154, J. Lee and S. Leyffer, Eds., in The IMA Volumes in Mathematics and its Applications, vol. 154. , New York, NY: Springer New York, 2012, pp. 61–89. doi: 10.1007/978-1-4614-1927-3_3.

[7] M. S. Aktürk, A. Atamtürk, and S. Gürel, "A strong conic quadratic reformulation for machine-job assignment with controllable processing times," *Oper. Res. Lett.*, vol. 37, no. 3, pp. 187–191, May 2009, doi: 10.1016/j.orl.2008.12.009.

[8] D. A. Liñán, D. E. Bernal, L. A. Ricardez-Sandoval, and J. M. Gómez, "Optimal design of superstructures for placing units and streams with multiple and ordered available locations. Part I: A new mathematical framework," *Comput. Chem. Eng.*, vol. 137, p. 106794, Jun. 2020, doi: 10.1016/j.compchemeng.2020.106794.

[9]D. Ovalle *et al.*, "Logic-Based Discrete-Steepest Descent: A solution method for process synthesis Generalized Disjunctive Programs," *Comput. Chem. Eng.*, vol. 195, p. 108993, Apr. 2025, doi: 10.1016/j.compchemeng.2024.108993.

[10] M. L. Bynum *et al.*, *Pyomo — Optimization Modeling in Python, Version 6.9.2*, vol. 67. in Springer Optimization and Its Applications, vol. 67. Cham: Springer International Publishing, 2021. doi: 10.1007/978-3-030-68928-5.

[11] GAMS Development Corporation. General Algebraic Modeling System (GAMS), Version 49.1.0. Available: https://www.gams.com/download/

[12] *Gurobi Optimization, LLC.* Version 12.0. Available: https://www.gurobi.com/

[13] *The Optimization Firm. BARON*. Available: https://minlp.com/baron-solver

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All experiments were run on a single thread of an AMD EPYC 7643 48-Core Processor (96 logical cores) with 256 MB of L3 cache in a server running Red Hat Enterprise Linux 9.5 (Plow). The server is equipped with 1 TB of RAM and 15 GB of Swap Space. Versions of software used: Pyomo - Version 6.9.2, GAMS - Version 49.1.0, Gurobi - Version 12.0