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Leveraging Machine Learning for Multi-Level Optimization In Energy-Water Nexus Systems

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ABSTRACT

The energy-water nexus emerged in response to global challenges associated with energy and water resources. Along with their existing residential, commercial, and industrial commitments, the intrinsically complex system now faces additional pressure from the rampant rise in demands from data centers. To factor in the impacts of these new circumstances while accounting for the interdependent and interconnected nature of energy and water supply systems, the nexus holistically manages these resources and their corresponding decisions [1].

However, while these decisions are conventionally modeled from a centralized perspective through representative mathematical programs whose optimal decisions can then be optimized, a more realistic perspective models these decisions sequentially. Here, rather than all involved systems making their decision in a simultaneous fashion, decisions are made one after another in sequential order and characterized using multilevel programming. Bilevel programming, the most well-established multilevel problem, fundamentally consists of an upper-level optimization problem that has a lower-level optimization problem embedded within its constraints. Bilevel programming has been applied to challenges within the energy-water nexus through several traditional solution strategies such as reformulations into a single level, iterative procedures combined with decomposition, and more recently, a more nuanced approach that involves multi-parametric programming [2]. Through this approach, solutions of an optimization problem for all feasible values of uncertain parameters are determined without iteratively varying parameter values and resolving the problem. The feasible parameter space is demarcated into areas referred to as critical regions, each defined by a specific set of affine functions defining the optimal solution in terms of the uncertain parameter.

The key idea behind the application of this advanced optimization technique to multilevel programs is that decisions of the lower-level problem can be represented in terms of decisions of the upper-level problem or the uncertain parameters in this case [3]. While several works have demonstrated the applicability of this approach to nexus applications and beyond, a major limitation is the complexity that accompanies the scale of multi-parametric problems. The complexity of these problems shows combinatorial growth with the number of uncertain parameters and levels considered, thereby requiring faster approximations that can allow for practical implementations. In this work, seeking inspiration from multi-parametric programming, machine learning strategies will be employed to approximate the behavior of the optimal solution or the decisions of the lower-level problem in terms of the uncertain parameter or the upper-level variables in an energy-water nexus. The approximations determined will then be embedded with the upper-level problem to identify the optimal solution of the bilevel problem. With the increasing number of applications that utilize machine learning, even within nexus studies for the approximation of energy and water system behaviors, it is evident that machine learning strategies provide a unique and innovative

means for approximating the relationship between the upper-level and lower-level decision-makers [4].

REFERENCES

1. Di Martino M, Linke P, Pistikopoulos EN. Overcoming modeling and computational complexity challenges in food-energy-water nexus optimization. *Comput Chem Eng* 195:108902 (2025). https://doi.org/10.1016/j.compchemeng.2024.108902
2. Abraham EJ, Di Martino M, Kenefake D, Al-Mohannadi DM, Pistikopoulos EN. A multi-parametric approach for bi-level optimization within the energy-water nexus. *Comput Chem Eng* 202:109256 (2025). https://doi.org/10.1016/j.compchemeng.2025.109256
3. Avraamidou S, Pistikopoulos EN. Multi-level Mixed-Integer Optimization: Parametric Programming Approach. Walter de Gruyter GmbH & Co KG, 2022.
4. Bagloee SA, Asadi M, Sarvi M, Patriksson M. A hybrid machine-learning and optimization method to solve bi-level problems. *Expert Systems with Applications* 95:142–152 (2018). https://doi.org/10.1016/j.eswa.2017.11.039