

Data-Driven Optimization for Materials Discovery: Benchmarks and Case Studies

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and Zoom

Abstract

Self-driving laboratories can compress years of materials discovery into weeks. Instead of relying on trial-and-error, they use algorithms to learn from each experiment and decide what to try next. When experiments are expensive and budgets are limited, choosing the next experiment well can have a large impact on the quality of the material ultimately discovered.

I will present results from a recent benchmark of 46 data-driven optimization solvers on 502 problems, ranging from one to 300 dimensions and spanning a wide variety of mathematical behavior. Our new branch-and-model (BAM) algorithm achieves the highest overall success rate, outperforming several Bayesian optimizers as well as stochastic and deterministic derivative-free optimization solvers.

I will then show how branch-without-bound algorithms work in practice. In one example, an algorithm guided experiments on perovskite solar cells, jointly optimizing six processing parameters across three layers of the cell. I will also share results from optimizing digital twins and simulators developed by the self-driving-labs community.

Finally, I will discuss opportunities in batteries, semiconductors, catalysts, polymeric membranes, and biomolecules, and how deterministic methods such as BAM can help scientists discover better materials faster.

Biography

Nick Sahinidis is Gary C. Butler Family Chair Professor of Industrial & Systems Engineering and Chemical & Biomolecular Engineering at the Georgia Institute of Technology and a Hagler Fellow at Texas A&M. He previously held faculty positions at the University of Illinois at Urbana-Champaign (1991-2007) and at Carnegie Mellon University (2007-2020).

He is a pioneer in optimization and machine learning algorithms and the development of widely used optimization software. He is a member of the National Academy of Engineering and a fellow of INFORMS, AIChE and the Hagler Institute. His work has received major awards from INFORMS, the Mathematical Optimization Society, and AIChE. He is past Editor-in-Chief of Optimization and Engineering and current Editor-in-Chief of Mathematical Programming Computation.



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