SCHOOL OF
CHEMICAL ENGINEERING
College of Engineering, Architecture and Technology

CHE SEMINAR SERIES

Physics-Informed Bayesian Optimization: A Sequential Learning Framework for Accelerating Scientific Design and Discovery

JOEL PAULSON, PH.D.

NORTH CLASSROOM BUILDING 203
NOVEMBER 12, 10:30 - 11:45AM

Bayesian optimization (BO) is a powerful tool for optimizing non-convex black-box functions that are expensive and/or time-consuming to evaluate and subject to random noise in their observations. Many important real-world science and engineering problems belong to this class such as optimizing over high-fidelity computer simulations, tuning hyperparameters in machine learning algorithms, and efficient material and drug discovery. Traditionally, BO has been deployed as a purely black-box optimizer. However, this black-box approach can lead to significant performance losses, especially in high-dimensional, intricately constrained design spaces, such as those that appear in materials and molecular optimization. In most real-world applications, however, only a portion of the model is unknown, suggesting that we might (substantially) improve performance by "peeking inside the black box." In this talk, I will present an overview of advanced "physics-informed" Bayesian optimization (PIBO) methods recently developed by the Paulson Lab that selectively exploit problem structure to achieve state-of-the-art performance. Specifically, I will focus on a PIBO approach called MolDAIS, designed for molecular property optimization under small budgets. MolDAIS is built upon a conjecture that the properties of interest depend on a small subset of key molecular descriptors that can be actively learned from data using a particular type of sparsity-inducing probabilistic surrogate model. I will illustrate the effectiveness of MolDAIS on several molecule design benchmark problems as well as a real-world application to discovery of high-performance, low-cost organic electrode materials. By working closely with experimental collaborators, we used a variant of MolDAIS to find candidate materials with specific energy and cycling stability that match or surpass current state-of-the-art organic electrodes in aqueous zinc-ion batteries, while being synthesizable at a fraction of the cost.

Joel Paulson is the H.C. Slip "Slider" Assistant Professor of Chemical and Biomolecular Engineering at The Ohio State University (OSU) where he is also a core faculty member of the Sustainability Institute (SI) and an affiliate of the Translational Data Analytics Institute (TDAI). He joined OSU in 2019 after completing his Ph.D. at the Massachusetts Institute of Technology (MIT) in Chemical Engineering and a subsequent postdoctoral appointment at the University of California, Berkeley in systems and control theory. He has received several awards including the NSF CAREER Award, the AIChE 35 Under 35 Award, the Best Application Paper Prize from the 2020 IFAC World Congress, and the OSU Lumley Research Award. His research interests are mainly in the areas of data-driven optimization, physics-informed machine learning, and model predictive control. Methods developed by the Paulson group are being applied to a variety of next-generation biochemical systems including continuous pharmaceutical manufacturing, chemical looping combustion, sustainable battery systems, and non-equilibrium plasma jets.