香港中文大學統計學系
Department of Statistics
THE CHINESE UNIVERSITY OF HONG KONG

SEMINAR

DEPARTMENT OF STATISTICS
THE CHINESE UNIVERSITY OF HONG KONG

Recent advances in Bayesian optimization for the physical and engineering sciences

INVITED SPEAKER

Dr. Simon Mak
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TIME

January 21st, 2025 (Tue) · 2:30 pm - 3:30 pm

VENUE

LSB LT1 (1/F) · Lady Shaw Building LT1 · CUHK

ABSTRACT

With advances in scientific computing, computer simulations are increasingly used for investigating complex physical phenomena. For many such applications, scientific decision-making involves optimizing the simulator output, which can be costly given the expensive nature of simulation runs. While Bayesian optimization (BO) offers a promising solution, there are key challenges that limit the use of existing BO methods in the physical sciences. The first is the presence of noise parameters, which are controllable in the simulator but uncontrollable in reality. For this, we propose a new Targeted Variance Reduction (TVR) method, for optimizing a black-box simulator given random uncertainty on noise parameters. Using a carefully specified Gaussian process surrogate, the TVR admits a closed-form acquisition function via normalizing flows, thus allowing for efficient sequential sampling. We explore the effectiveness of TVR in numerical experiments and an application for automobile brake design under operational uncertainties. The second challenge is the need for diverse optimization solutions, which provide users with a basket of "good" solutions for decision-making. For this, we propose a new Diverse Expected Improvement (DEI) method, which extends the popular Expected Improvement method to encourage diversity between near-optimal solutions. The DEI similarly yields a closed-form acquisition function, which reveals a novel exploration-exploitation-diversity trade-off for diverse black-box optimization. We explore the effectiveness of the DEI in two applications, the first on rover trajectory optimization and the second for optimizing diverse microbiome communities for biotic heterogeneity.