中央研究院統計科學研究所

學 術 演 講

講 題： Recent advances in Bayesian optimization for the physical and engineering sciences

演 講 人： Prof. Simon Mak
Department of Statistical Science, Duke University, U.S.A.

時 間： 2025-02-12 (Wed.) 10:30-12:00

地 點： Auditorium, B1F, Institute of Statistical Science；The tea reception will be held at 10:10.

備 註： Online live streaming through Cisco Webex will be available.

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.

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