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[Qian Xiao](#)

Assistant Professor in Department of Statistics at University of Georgia

Title: Modeling and active learning for experiments with quantitative-sequence factors

Abstract: A new type of experiment that aims to determine the optimal quantities of a sequence of factors is eliciting considerable attention in medical science, bioengineering, and many other disciplines. Such studies require the simultaneous optimization of both quantities and sequence orders of several components which are called quantitative-sequence (QS) factors. Given the large and semi-discrete solution spaces in such experiments, efficiently identifying optimal or near-optimal solutions by using a small number of experimental trials is a nontrivial task. To address this challenge, we propose a novel active learning approach, called QS-learning, to enable effective modeling and efficient optimization for experiments with QS factors. QS-learning consists of three parts: a novel mapping-based additive Gaussian process (MaGP) model, an efficient global optimization scheme (QS-EGO), and a new class of optimal designs (QS-design). The theoretical properties of the proposed method are investigated, and optimization techniques using analytical gradients are developed. The performance of the proposed method is demonstrated via a real drug experiment on lymphoma treatment and several simulation studies.