Active learning for optimizing drugs' doses and timing of administration in drug combinations studies

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Abstract:
In modern pharmaceutical studies, researchers have found that both the doses and time-of-administration of drug components have significant impacts on the treatment efficacy. Additionally, such drug combination studies often have constraints in practice, such as the minimum separation time and maximum number of drug components, which further complicates the analysis. To find the best drug combinations, simultaneous optimization of both the doses and time-of-administration of drugs is required, where one-shot experimental designs are often inefficient. In this work, we propose a new Gaussian process model and a novel active learning procedure for efficiently identify the optimal configurations for such experiments. The superiority of the proposed method is illustrated via a few simulations and a real case study.