Closed-loop automatic experimentation for optimisation

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Automated experimental systems, involving minimal human intervention, are becoming more popular and common, providing economical and fast data collection. We discuss some statistical issues around the design of experiments and data modelling for such systems. Our application is to “closed-loop” optimisation of chemical processes, where automation of reaction synthesis, chemical analysis and statistical design and modelling increases lab efficiency and allows 24/7 use of equipment.

Our approach uses nonparametric regression modelling, specifically Gaussian process regression, to allow flexible and robust modelling of potentially complex relationships between reaction conditions and measured responses. A Bayesian approach is adopted to uncertainty quantification, facilitated through computationally efficient Sequential Monte Carlo algorithms for the approximation of the posterior predictive distribution. We propose a new criterion, Expected Gain in Utility (EGU), for optimisation of a noisy response via fully-sequential design of experiments, and we compare the performance of EGU to extensions of the Expected Improvement criterion, which is popular for optimisation of deterministic functions. We also show how the modelling and design can be adapted to identify, and then down-weight, potentially outlying observations to obtain a more robust analysis.

Joint work with Tim Waite (University of Manchester, UK)