Bayesian Design of Experiments via Gaussian Process Emulation

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ABSTRACT:
The design of any experiment is implicitly Bayesian, with prior knowledge being used informally to aid decisions such as which factors to vary and the choice of plausible causal relationships between the factors and measured responses. Bayesian methods allow uncertainty in these decisions to be incorporated into design selection through prior distributions that encapsulate information available from scientific knowledge or previous experimentation. Further, a design may be explicitly tailored to the aim of the experiment through a decision-theoretic approach with an appropriate loss function.

When designing experiments for nonlinear parametric models, finding a Bayesian optimal design is typically analytically intractable and often computational infeasible. The expected loss usually involves an intractable and high dimensional integral. We will present methodology for mitigating the computational expense of design through combining an application of Gaussian Process (GP) regression models with a cyclic descent (coordinate exchange) optimisation algorithm. We adopt methodology from the field of computer experiments and build a GP emulator for the expected loss. The methods allow optimal designs to be found for previously infeasible problems. We will describe the methodology and demonstrate it on a variety of examples.