OPTIMIZATION, CALIBRATION, AND UNCERTAINTY ANALYSIS
OF MULTIMODAL, COMPUTATIONALLY EXPENSIVE MODELS
WITH ENVIRONMENTAL APPLICATIONS

Abstract

Many important problems in engineering and science require optimization of computationally expensive (costly) functions. These applications include calibration of simulation model parameters to data and optimizing a design or operational plan to meet an economic objective. With costly functions (like nonlinear systems of PDEs, partial differential equations), this optimization is made difficult by the limited number of model simulations that can be done because each simulation takes a long time (e.g., an hour or more). The optimization problem is even more difficult if it has multiple local optima, thereby requiring a global optimization algorithm.

Our new algorithms use function approximation methods and experimental design to approximate the objective function based on previous costly function evaluations. In our optimization algorithm, function approximation is combined with metrics of locations of previous costly function evaluations to select iteratively the next costly function evaluation. The theorem for convergence to the global minimum will be described.

Numerical algorithm comparisons will be presented for test functions and for an environmentally based partial differential equation model that requires three hours to run for each simulation. This nonlinear model (based on fluid mechanics and chemical reactions) describes the fate and transport of water and pollutants in a groundwater aquifer. The optimization is used for calibration of the model by selecting the parameter values (decision variables) that best fit measured data from a military field site in Florida. The parameter surface is multimodal so this is a global optimization problem. The results indicate that a Regis and Shoemaker method generally gives better results for global optimization test problems and the environmental model than alternative methods when the number of model simulations is limited. It is especially effective at dimensions higher than six. Related parallel algorithms will also be briefly discussed.

Working with David Rupperts statistics group, we have also expanded the use of function approximation to Bayesian analysis of uncertainty for costly functions. In this NSF project, we are combining optimization for calibration with an assessment of the uncertainty in calibrated parameter estimates and in calibrated model output based on input data. Numerical results for an environmental PDE problem based on a hypothetical chemical spill demonstrated good accuracy and a 60-fold reduction in costly simulations over that required for conventional MCMC analysis for Bayesian uncertainty analysis.

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