Surrogate Optimization for Nonlinear and Global Optimization of Computationally Expensive Simulation Models

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Optimization and uncertainty analyses used in conjunction with complex simulation models are important for making predictions based on observations and for finding optimal designs or policies. Global Optimization and uncertainty analysis typically require a very large number of simulations, often thousands or tens of thousands. However, this approach is not feasible for computationally expensive simulation models that arise in many engineering and science applications.

Our approach to create more efficient methods for this analysis is to iteratively approximate the objective function $f(x)$ to create a response surface or "**surrogate model**" upon which sampling can be done to significantly reduce the number of expensive simulations required. It is this use of previously evaluated points $f(x_i)$ to build the surrogate model that is responsible for great savings in computational time. All of our methods are derivative-free and can be applied to systems of nonlinear partial differential equations as well as to other multimodal functions (including "blackbox functions).

I will review surrogate local and global methods (serial and parallel) and present some applications to several large simulation models that solve systems of PDEs based on field data and discuss some of their theoretical properties. Some of these applications require one or two hours per simulation, so it is important the optimization be able to find the global minimum with relatively few simulations. We compare the results with our algorithms (past and recently improved) to other alternative methods including surrogate approaches like EGO as well as non-surrogate optimization approaches. These applications are for groundwater contamination and for geologic carbon sequestration, but success on these would support the likelihood of success on other simulations models involving nonlinear PDE's. One of our methods Stochastic RBF is being incorporated into a DOE software package for optimizing simulation models based on nonlinear PDE's.

This talk is based primarily on research done jointly with R. Regis, Yilun Wang, Aman Singh, Antoine Espinet, and S. Wild

Prof. Shoemaker is currently giving a special topics course on Surrogate Optimization, CEE6205 or ORIE 7391, (variable credit) , Tu.-Thurs, 3:00-4:05, Rm 162 Hollister, Spring 2011.