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Comment

Max D. Morris

The authors have provided an interesting and readable account of a statistical approach to the problem of approximating an unknown, deterministic computer model. The approximation of unknown functions, of at least a few arguments, has received considerable attention in other specialty areas of mathematics, but is relatively new to statistics. A statistical approach brings a unique potential for dealing with uncertainty in the problem. In particular, it can lead to measures of quality for each prediction, and a structure on which to base the design of efficient experiments. Techniques which are relevant for approximating computer models are particularly timely, because the scientific and technical professions are quickly becoming reliant upon these as research tools, and this manuscript reports some of the first serious efforts to make statistics relevant to these activities.

THE CLASSICAL APPROACH

At the end of Section 3, the authors give their basic argument for treating this problem statistically: "Modeling a computer code as if it were a realization of a stochastic process . . . gives a basis for the quantification of uncertainty . . ." Following this, Section 4 outlines their strategy which seems clearly classical (as opposed to Bayesian) in form; it is what a classical statistician would do if the computer model actually had been generated as a realization of the stochastic process. While this strategy does provide a mathematical structure for dealing with uncertainty, classical statisticians who like to motivate their analyses with fictional accounts of random sampling and hypothetical replays of an experiment may find this an uncomfortable setting. After all, unless one randomizes the experimental design, there will not be a credible frequentist probability structure in this problem.

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(My own usual preference for classical procedures is heavily dependent on credible frequentist models. In this problem, the Bayesian approach seems somewhat more direct to me.)

A classical statistician, in order to proceed, will need to be more pragmatic, by saying that a credible frequentist model is unnecessary so long as the method works. The first test of whether the method works is whether it produces good approximations to computer models. These authors, and others they have referenced, have assembled a body of evidence that indicates that this and similar methods have the potential to produce good approximations. The second test, which should be of particular concern to statisticians, is whether it produces good (useful, dependable, meaningful?) measures of uncertainty. Passing this second test will be important if we are to take seriously any claims of quantified prediction uncertainty or design optimality. It is encouraging that the mean square errors of prediction calculated in the example of Section 6 seem to behave as we would hope.

CHOICE OF CORRELATION FUNCTION

As the authors point out in Section 4, the hopes of the pragmatic classical statistician will be pinned on the supposition that the computational model "though deterministic, may resemble a sample path of a (suitably chosen) stochastic process . . ." So, choosing a suitable stochastic process, presumably one for which y would be a "typical" realization, becomes an issue. This is particularly true for preliminary design purposes (before data are taken from which a correlation structure can be estimated). Some guidelines for this selection process are well-known; the authors note that $p = 2$ processes produce smoother realizations than $p = 1$ processes. Also, a tentative value of θ must be chosen for preliminary design purposes; the authors use $\theta = 2$ in the example of Section 6.

When selecting a process in several dimensions, some attention should probably be paid to the degree of interaction among inputs for typical realizations.