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Uncertainty quantification in complex systems using approximate solvers

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ABSTRACT

Scientists have come to recognize the stochastic aspects inherent in several physical systems and processes and seek ways to quantify the probabilistic characteristics of their behavior. Their analysis tools are usually restricted to elaborate legacy codes which have been developed over a long period of time and are generally well-tested. They do not however include any stochastic components and their alteration is commonly impossible or ill-advised. Hence, the only feasible solution for uncertainty quantification is through Monte Carlo stochastic simulation.

The latter allows the analyst to use existing legacy codes as black boxes. A series of "independent" runs are performed from which the stochastic features of the response can be extracted. More often than not, in systems of practical interest , each of these runs can last for several hours or days. Despite significant progress in advanced Monte Carlo methodologies ([4]), it is critically important to reduce the required number of runs as much as possible or equivalently construct estimators that are most informative about the response characteristic given a fixed number of runs.

One approach that has been largely unexplored is to use computationally inexpensive, approximate solvers and combine the information they provide with a few, carefully selected runs of the full, exact model ([3]). In mechanics problems for example where finite elements are commonly used, such approximate solvers can be readily constructed by considering coarser discretizations of the domain of interest or even performing fewer iterations if an iterative solver is used. Naturally the solutions produced will not be as accurate but nevertheless contain information about the true response. As it will be shown it suffices that the approximate solutions are correlated with the exact even if, in absolute terms, they are significantly different. Such an approach can be employed even in cases where no accurate computational model exists but rather we have to rely on experiments in order to collect the necessary information about the system. Since conducting experiments can be costly and time consuming it is desirable to minimize them by making use of approximate computational models that might be available.

In this paper we investigate Bayesian alternatives to classical Monte Carlo methods for evaluating integrals that correspond to quantiles (e.g. failure probabilities in reliability analysis) or moments of the

response ([1]). In particular we seek to solve a regression problem that establishes the connection between the response values from the approximate and exact solver. This is achieved using a flexible, non-parametric Bayesian model that employs a very efficient Sequential Monte Carlo inference algorithm ([2]). An added advantage of this approach is that prior knowledge or expertise of the analyst regarding the relationship between approximate and exact solvers can be readily incorporated in the prior distributions. Once this relation is established, the posterior distribution can be readily used to obtain estimates and confidence intervals on the integrals of interest. These can in turn be used to actively and adaptively improve the accuracy of the regression by performing runs of the expensive solver in regions that contribute most significantly to these uncertainties. An interesting extension involves using more than one approximate solvers simultaneously in order to improve the accuracy of the regression model. This resembles mixtures of experts models that are commonly used in various statistical applications, as each approximate solver provides some, generally incomplete, information about the exact model which is then aggregated in order to obtain the best possible estimate. Several numerical examples are presented.

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