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Bayesian Adaptive Spline Surfaces: An Emulator Made For Sensitivity Analysis

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For models that are even slightly expensive to evaluate, many global sensitivity methods can be difficult to use. Accurate estimation of Sobol indices or delta indices can require many thousands to millions of model evaluations. While methods like derivative-based global sensitivity metrics allow the user to bound Sobol indices with very limited model runs, these bounds are not always small enough to be practical. Further, the practitioner is often faced with the "given data" scenario, where they have been given a set of model evaluations and they cannot further design more evaluations. Various approximations to sensitivity indices exist for the "given data" scenario, but accuracy can be a challenge.

Emulator-based sensitivity analysis is a frequent solution to these problems. The practitioner uses a reasonable number of model evaluations (or "given data") to train a statistical surrogate, or emulator, of the more expensive model of interest. Assuming sufficient emulator accuracy, the practitioner can then perform sensitivity analysis of the emulator (which is cheap to evaluate) to approximate sensitivity analysis of the model of interest. For example, Figure 1 shows accuracy of emulator-based delta sensitivity compared to the standard approach. Many classes of emulators exist, including Gaussian processes, basis function approaches, polynomial chaos, tree-based models, and neural networks, and some of these are nicely suited for use for sensitivity analysis problems. In this talk, I will describe in detail one emulator that I have found especially useful: Bayesian adaptive spline surfaces (BASS).

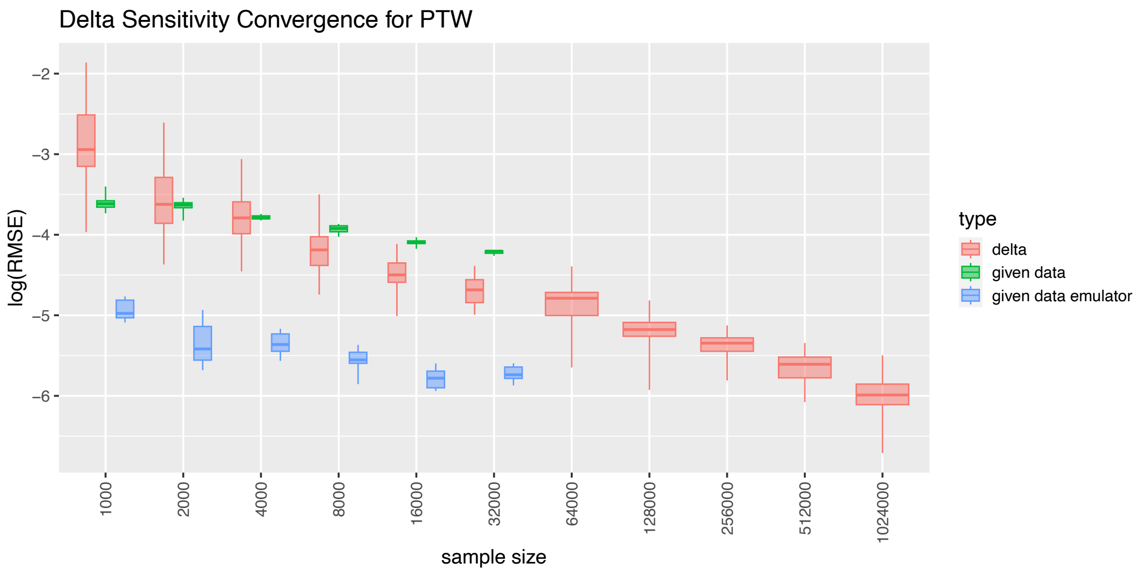

Figure 1: Convergence of three different approaches to calculating delta sensitivity indices for a material strength model called PTW. The emulator approach with given data achieves greater accuracy than the given data approach of python's SALib (with the same given data).

BASS [1-3] is a Bayesian version of Friedman's multivariate adaptive regression splines (MARS). Given training data, the response is modeled as a linear combination of tensor product spline basis functions. The variables and interactions involved in the basis functions, as well as the spline knots and the number of basis functions, are learned in a fully Bayesian framework. This emulator works well in practice: it is relatively fast, accurate, and scalable [4]. In addition, the form of the basis functions simplifies many sensitivity analysis tasks. For example, the Sobol indices can be calculated analytically for main effects, total effects, and all interactions under many input distribution assumptions, including truncated Gaussian mixtures. Tools in R (BASS package [1]) and python (pyBASS) allow for this kind of analysis to be performed routinely.

Recent work has also demonstrated that the active subspace is also available in closed form for BASS [5], and that, with a particular input dependence structure, Shapley effects are also analytical. Of course, all of these sensitivity metrics could be approximated using sampling for any number of emulators, but sampling-free formulations simplify many aspects of their use. Additionally, the error distribution of BASS can be generalized for use for robust regression, quantile regression, and other forms of flexible-likelihood regression, and the sensitivity metrics mentioned above can still be calculated analytically [6]. Figure 2 demonstrates how sensitivity changes with quantile for a stochastic epidemiology model [6].

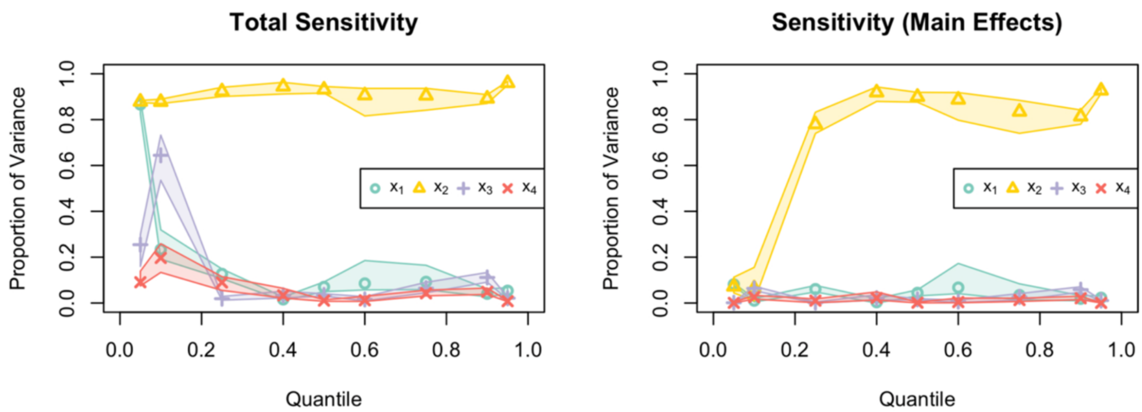

Figure 2: 80% posterior intervals for the Sobol indices of a stochastic SIR model as a function of response quantile. Low quantiles are sensitive to all inputs and their two-way interactions (not shown), but sensitivity in the large quantiles is dominated by x2.

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