Comparison of Surrogate Modeling and Sampling Strategies for Efficient Bayesian Model Calibration

Leon Riccius*, Iuri Rocha, Frans van der Meer

Delft University of Technology
Department of Civil Engineering and Geosciences
P.O.Box 5048, 2600GA, Delft, The Netherlands
l.f.riccius@tudelft.nl, i.rocha@tudelft.nl, f.p.vandermeer@tudelft.nl

ABSTRACT

In engineering mechanics, complex computational models, such as a finite element method (FEM) model, are used to simulate material behavior. These models usually feature a large number of parameters, especially if the material properties vary in space. An inverse problem must be solved to estimate the model parameters from experimental data. In the nonelastic regime, these inverse problems are typically non-linear, non-convex, and ill-posed but can be regularized elegantly by adopting a Bayesian approach. A naive application of Bayesian statistics to computational mechanics is infeasible. However, breakthroughs in Markov Chain Monte Carlo sampling and surrogate modeling make a Bayesian analysis applicable to a broader set of problems.

In Bayesian statistics, a prior distribution for the parameters is assumed and combined with a likelihood function that measures the fit of the model response and the observations. Following the Bayesian formalism, the posterior distribution for the parameters is obtained. Typically, the posterior distribution must be approximated due to the non-linear nature of the likelihood function, e.g., via sampling from the joint distribution of data and parameters. The bottleneck of the sampling effort is the evaluation of the expensive FEM model. The number of FEM model evaluations can be reduced by employing advanced sampling algorithms or training a cheap-to-evaluate surrogate model.

The use of surrogate models for Bayesian inference is increasingly common but mostly done based on ad hoc choices and rarely evaluated in a systematic manner. It is often not trivial to discern how the approximation error caused by the surrogate affects the performance of the sampler in targeting and optimally exploring the correct posterior distribution. We thoroughly analyze when a random walk sampling approach becomes prohibitively expensive and what benefits state-of-the-art (gradient-based) samplers offer. Further, we investigate how meta-models can facilitate the inference and how those meta-models can be combined with the various sampling techniques. While some of the aforementioned strategies have been investigated in isolation to some degree — through mathematical assessments of the various sampling algorithm's convergence rates on analytic functions, empirical studies of their performance on engineering problems, and comparative studies of the efficiency of different meta-modeling strategies — an investigation of their interplay is missing, which is addressed in our contribution. We demonstrate our findings on simple yet illustrative engineering mechanics problems with elasto-plastic materials.