

Bayesian Large Model Calibration Using Simulation and Measured Data for Improved Predictions

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ABSTRACT

When utilizing large models containing numerous uncertain parameters, model calibration becomes a critical step in the analysis. Traditional methods of calibration involve adjusting uncertain parameters based on expert opinion or best estimates. While this traditional calibration may lead to better model predictions, it usually only yields better estimates for certain specific conditions. This drastically reduces the functionality of the model in question. Bayesian calibration is an alternative to traditional calibration methods which utilizes available information (simulation results and/or real world measured values) to iteratively refine uncertain parameters (either assumed or measured uncertainty) while considering not only parametric uncertainty, but also model, observational, and residual uncertainties at every step of the calibration process. Various methods have been previously developed for executing the calibration process, several of which can drastically reduce the computational expense of Bayesian calibration. A numerical example is included to illustrate the functionality of Bayesian calibration.

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INTRODUCTION

As computer processors continue to rapidly increase in power, widespread use of simulation has become standard best practice in both industry and academia. When considering the relatively cheap computational demand of doing a sufficiently large number of simulations, even when the system being modeled is extremely complex, it is clear why simulation has proliferated through such a majority of design and research. Even for simulations requiring several hours per run, the data collected from simulations is still incredibly cheaper to obtain than gathering data from laboratory testing or field measurements.

While the numerous advantages of simulation are inherently clear, there are several hidden dangers that can lead to dangerously misinformed decision making. Whenever simulation is utilized for analysis, there are certain specific steps that must be followed in order to ensure the simulation outputs are representative of the desired values. One of the crucial steps in any simulation is calibration, which is preconditioning the model such that the difference between the simulation outputs and measured data is minimized. Traditionally this calibration is done by adjusting uncertain input parameters based on expert opinion or the use of multivariable optimization algorithms. One major shortfall of expert opinion calibration is that it is subject to personal bias, and neither the expert opinion method nor the optimization method provides any quantification of uncertainty on the adjusted parameters and the output prediction. In other words, predictions arising from a traditionally calibrated system contain inherent uncertainties that are not quantified by the calibration process. This means that even a

“perfect” traditionally calibrated system will not quantify any form of confidence. Additionally, while calibration based on expert opinion or optimization generally leads to local minimum error between observed real world data and simulation results, the lack of uncertainty quantification means that there is no way of assessing whether the calibration leads to a more realistic prediction. It is possible that the data used to condition the system or the system itself contains errors, uncertainties and inadequacies which the calibration process may amplify for future “predictive” simulation outputs. In traditional calibration, there may be several combinations of calibration for a system that all lead to a common local minimum, but it is not possible to make or infer any probabilistic information regarding which of these calibration is closest to the “true” values desired for future simulations. At best, one could say that each of these calibrations is a possible best calibration.

One calibration strategy addressing most of the problems with traditional calibration is Bayesian calibration. Bayesian calibration is based on Bayes Theorem, which relates prior information with uncertainty to future information based on the likelihood of observed outputs from the system. In Bayesian calibration, all uncertain parameters are established by defining probability density functions (PDFs) based on the uncertainty associated with each parameter. These prior PDFs are updated by comparing the simulation predictions and real world observations by computing the likelihood of obtaining the real world observations from simulation based on the prior PDFs. This process essentially modifies the prior distributions that are most likely to account for discrepancies between real world data and simulation outputs. In this sense, Bayesian calibration

addresses the problem of traditional calibration in that the calibrated system is not merely one of several possible calibrations, but rather is the most probable calibration of the system, given the initial assessment of parameter uncertainty.

One important advantage of Bayesian calibration is that because it is integrally tied to uncertainty quantification, modeling and analysis, it allows for probabilistic analysis, risk assessment, and confidence interval determination of simulation results. This is incredibly significant for evaluating several designs to assess the best design based on decision maker's priorities. Traditional calibration techniques will rank the designs in a deterministic manner, but provide no indication of the relative advantages of any design over any other design. If Bayesian calibration is instead utilized, not only would the designs be ranked (based on mean values), but the distribution of each design allows the designer to choose a confidence level to rank these designs against each other. Or if the designer would rather rank the designs based on a design threshold, the probability that any design will surpass this threshold can be evaluated and used to rank designs. Clearly Bayesian calibration provides greatly increased flexibility in analysis and level of information compared with traditional calibration.

OVERVIEW

As previously stated, Bayesian calibration relates prior information with uncertainty to future information based on the likelihood of observed outputs from the system, based on Bayes Theorem. Specifically Bayesian calibration is updating the parameter, θ , prior uncertainty distribution $p(\theta)$ with the likelihood, $p(y|\theta)$, of observed data y as shown in Eq. (1).

$$p(\theta|y) \propto p(\theta) * p(y|\theta) \quad (1)$$

Bayes theorem allows for probabilistic modeling of both the uncertain parameter distribution and calibrated model predictions. This calibration procedure described by Kennedy and O'Hagan [4] (2001) allows for modeling the observed data, $y(x_i)$, as a function of the model residual variation and observation error, e_p , and the true process $\zeta(x_i)$ which is a function of the model inadequacy $\delta(x_i)$ and the computer model output $\eta(x_i, \theta)$ given known variable input parameters x_i and the uncertain calibration parameters θ as shown in Eq. (2).

$$y(x_i) = \zeta(x_i) + e_i = \eta(x_i, \theta) + \delta(x_i) + e_i \quad (2)$$

This formulation models $\eta(x_i, \theta)$ and $\zeta(x_i)$ as independent Gaussian processes and e_i is normally distributed as $N(0, \lambda)$.

METHODOLOGY

The basic steps for Bayesian calibration are:

1. Quantify all uncertainty for uncertain parameters by generating prior parameter distributions $p(\theta)$. This may require parameter screening for larger models as each additional uncertain

parameter modeled greatly increases the computational demand for each round of calibration.

2. Collect real world data $y(x_i)$ with measured known input parameters x_i
3. Calibrate prior parameter uncertainty distributions with the probability of observing data (Eq. (1))

The relative simplicity of Eq. (1) and (2) allows for direct programming for simulation. If sufficient data is available, a random subset of the data can be selected for each run of the simulation i and multiple subsets utilized to iteratively calibrate the model for the sampled subspace domain of the uncertain parameters. Each of these steps are explored in further detail in the following sections.

Uncertainty Quantification

Usually the most time consuming step of Bayesian calibration, uncertain parameter quantification often involves both expert opinion solicitation and literature review. When literature review produces a range of possible values and a likely value, a triangle distribution can be utilized to represent the probability density function (PDF) of the uncertain parameters. When only a range of possible values can be determined, a uniform distribution may be used [6].

Parameter Screening

As previously stated, if there are a sufficiently large number of uncertain parameters, parameter screening may be required to select a subset of the most influential uncertain parameters. Several screening techniques exist such as the Morris method which explores the effect of varying a single parameter at a time by breaking the specified parameter domain into a finite number of intervals. The effect of each variation in the parameter domain is totaled into a single representative sensitivity factor. A subset of the uncertain parameters with the greatest sensitivity factors are selected to be calibrated while all other uncertain parameters take assumed constant values.

Data Collection

Data collection is the most economically expensive step of Bayesian calibration and is a crucial step in any calibration method to model the systematic and random errors. Because model calibration seeks to utilize observed real world measurements to condition the model such that future model output can accurately predict real world outputs based on unobserved variable parameter values, and because the model is calibrated for the uncertain parameters' sampled domains, implementing an intelligent sampling strategy for uncertain parameter domain exploration is an important factor. Efficient sampling reduces the required amount of data and hence reduces the expense of this step in the calibration process. Once a sufficiently large sample size has been collected, a subset of data can be randomly selected for each simulation run in order to iteratively calibrate the model. Whenever data cannot be physically observed, data must be generated.

Calibration

Bayesian calibration is the step of utilizing the observed real world data to modify the most probable variable input parameters based upon the likelihood of observing the real world data with the model