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Bayesian methods for characterizing unknown parameters of material models

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ABSTRACT

A Bayesian framework is developed for characterizing the unknown parameters of probabilistic models for material properties. In this framework, the unknown parameters are viewed as random and described by their posterior distributions obtained from prior information and measurements of quantities of interest that are observable and depend on the unknown parameters. The proposed Bayesian method is applied to characterize an unknown spatial correlation of the conductivity field in the definition of a stochastic transport equation and to solve this equation by Monte Carlo simulation and stochastic reduced order models (SROMs). The Bayesian method is also employed to characterize unknown parameters of material properties for laser welds from measurements of peak forces sustained by these welds.

1. Introduction

Material properties at the fine scale vary randomly in space, *e.g.*, microstructural conductivity and mechanical properties of weld fusion zones. Mechanical systems are often subjected to actions that vary randomly in space and time, *e.g.*, pressure on the skin of aircrafts and features of most biological tissues. The determination of the response of these materials and systems involves solutions of equations with random coefficients, input, and end conditions, referred to as stochastic equations.

Monte Carlo simulation is the only general method for solving stochastic equations irrespective of their complexity. However, its use in applications encounters two obstacles. First, the method is computationally unfeasible if the time for calculating a single solution sample is excessive, especially when many samples are needed to construct reliable solution statistics. Second, the implementation of the method requires full probabilistic characterization of the random entries of these equations, which may not be available in many applications. This paper addresses the first concern by application of stochastic

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reduced-order models (SROMs) and it addresses the second through development of a Bayesian method for characterizing unknown parameters of material models.

It is assumed that the probability laws of the random entries of a stochastic equation have known functional forms but some of their parameters are unknown and unobservable, *e.g.*, parameters of spatial correlations of random field models for material microstructures. We develop a Bayesian framework in which the unknown parameters are viewed as random variables. The initial information on the unknown parameters is captured by prior distributions. Measurements of quantities of interest that are generated numerically and that depend on these parameters are used to update the prior distributions. Updated distributions, referred to as posterior distributions, summarize all available information on the unknown parameters. Stochastic equations depending on unknown parameters characterized by posterior distributions are hierarchical. They are classical stochastic equations that can be solved by existing methods if conditioned on these parameters.

We are not alone in employing a Bayesian framework in a mechanics application to inform a model with uncertain parameters. Applications span from heat conduction, to structural health monitoring, to structural dynamics, and include damage of composite materials such as concrete and fiber reinforced structures. Wang and Zabaras used a Bayesian approach for inverse heat conduction problems to ascertain uncertain material properties and boundary conditions [1]. Beck and Yuen use the approach to choose a class of models based on system response data for structural reliability applications [2]. Similarly, Grigoriu and Field use a Bayesian approach for model selection in a frame validation round-robin challenge problem [3]. Bogdanor *et al.* use a Bayesian approach to introduce uncertainty in initial material defects for multiscale modeling of failure in composites [4]. Vanik *et al.* use modal data to update model stiffness parameters for structural health monitoring [5]. Simeon et al. describe a Bayesian inference approach to model updating for material parameters in a reinforced concrete beam that used modal predictions and measurements to account for model and measurement uncertainty [6].

This is only a very brief survey of the literature and there are a multitude of other articles discussing the application of Bayes' theorem to mechanics problems that are naturally awash with uncertainty. In our work, we introduce the following novelties. First, the unknown model parameters are not observable and they need to be inferred from material properties at different scales, *e.g.*, the correlation parameter λ in the first example is inferred from measurement of apparent conductivity. Moreover, when our method is applied to an engineering problem with two variables simultaneously, we discover an unexpected non-uniqueness and we develop an explanation. Second, surrogate models based on SROMs [7] are used to solve stochastic differential equations (SDE) rather than brute force Monte Carlo simulation or approximate methods that cannot capture sample properties.

The essentials of the proposed method are outlined in the following section. The method is applied in subsequent sections to solve two stochastic problems. The first is a one-dimensional transport equation with random conductivity whose spatial correlation depends on an unknown parameter. Measurements of apparent conductivity are used to construct posterior distributions for the unknown correlation parameter. The second is a laser weld problem whose performance depends on various mechanical properties, some of which are assumed to be unknown. Measurements of peak weld loads are used to construct posterior distributions for these parameters.

2. Bayesian method

Suppose the probability laws of the random entries of a stochastic equation are defined up to a set of unknown parameters that are collected in a vector $\boldsymbol{\lambda}$. Conditional on $\boldsymbol{\lambda}$, the equation is a classical stochastic equation and can be solved by existing methods, *e.g.*, Monte Carlo simulation. It is assumed that $\boldsymbol{\lambda}$ cannot be observed directly. Quantities of interest that are observable and depend on $\boldsymbol{\lambda}$ are used to characterized this vector.

We develop a Bayesian framework for characterizing $\boldsymbol{\lambda}$. In this framework $\boldsymbol{\lambda}$ is viewed as a random vector denoted by $\boldsymbol{\Lambda}$. Information on the distribution of $\boldsymbol{\Lambda}$ is used to construct a prior density $f'(\boldsymbol{\lambda})$. If only the range of $\boldsymbol{\Lambda}$ is known, $f'(\boldsymbol{\lambda})$ is assumed to be uniform in this range. Since $\boldsymbol{\lambda}$ is unobservable, quantities of interest that can be measured and depend on $\boldsymbol{\lambda}$ are used to update $f'(\boldsymbol{\lambda})$ from:

$$f''(\boldsymbol{\lambda}) \propto f'(\boldsymbol{\lambda})\,\ell(\boldsymbol{\lambda} \mid \text{data}), \tag{1}$$

where $f''(\boldsymbol{\lambda})$ is the posterior density of $\boldsymbol{\Lambda}$, $\ell(\boldsymbol{\lambda}|\text{data})$ denotes the likelihood function of $\boldsymbol{\Lambda}$ corresponding to measurements of the selected quantity of interest, and the symbol $\propto$ means the ratio of the left- and right-hand sides of Eq. (1) is constant.

In this framework, the original stochastic equation becomes a hierarchical stochastic equation that can be solved in two steps. First, independent samples $\{\boldsymbol{\lambda}_i\}$ of $\boldsymbol{\Lambda}$ are generated from its posterior density $f''(\boldsymbol{\lambda})$. Second, solutions of the stochastic equation conditional on $\{\boldsymbol{\Lambda} = \boldsymbol{\lambda}_i\}$ can be obtained by existing methods for solving stochastic equations [7–13]. They can be subsequently used to find unconditional solution statistics. In Section 3, we illustrate the full implementation of this method for solving stochastic equations with uncertain parameters and develop statistics of quantiles of interest using Monte Carlo simulation and stochastic reduced-order models (SROM). In Section 4, we apply the Bayesian framework to a problem of practical relevance.