Probabilistic Engineering Mechanics 43 (2016) 68–84

Contents lists available at ScienceDirect

Probabilistic Engineering Mechanics

journal homepage: www.elsevier.com/locate/probengmech

A unified framework for multilevel uncertainty quantification in Bayesian inverse problems

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ARTICLE INFO

Article history:
Received 26 September 2014
Received in revised form
25 June 2015
Accepted 4 September 2015
Available online 14 September 2015

Keywords:
Uncertainty quantification
Inverse problems
Bayesian inference
Hierarchical modeling
Probabilistic inversion
Borrowing strength
Markov chain Monte Carlo

ABSTRACT

In this paper a unified probabilistic framework for solving inverse problems in the presence of epistemic and aleatory uncertainty is presented. The aim is to establish a flexible theory that facilitates Bayesian data analysis in experimental scenarios as they are commonly met in engineering practice. Problems are addressed where learning about unobservable inputs of a forward model, e.g. reducing the epistemic uncertainty of fixed yet unknown parameters and/or quantifying the aleatory uncertainty of variable inputs, is based on processing response measurements. Approaches to Bayesian inversion, hierarchical modeling and uncertainty quantification are combined into a generic framework that eventually allows to interpret and accomplish this task as multilevel model calibration. A joint problem formulation, where quantities that are not of particular interest are marginalized out from a joint posterior distribution, or an intrinsically marginal formulation, which is based on an integrated likelihood function, can be chosen according to the inferential objective and computational convenience. Fully Bayesian probabilistic inversion, i.e. the inference the variability of unobservable model inputs across a number of experiments, is derived as a special case of multilevel inversion. Borrowing strength, i.e. the optimal estimation of experiment-specific unknown forward model inputs, is introduced as a means for combining information in inverse problems. Two related statistical models for situations involving finite or zero model/measurement error are devised. Multilevel-specific obstacles to Bayesian posterior computation via Markov chain Monte Carlo are discussed. The inferential machinery of Bayesian multilevel model calibration and its underlying flow of information are studied on the basis of a system from the domain of civil engineering. A population of identically manufactured structural elements serves as an exemplary system for examining different experimental settings from the standpoint of uncertainty quantification and reduction. In a series of tests the material variability throughout the ensemble of specimens, the entirety of specimen-specific material properties and the measurement error level are inferred under various uncertainties in the problem setup.

1. Introduction

Main characteristics and challenges of inverse problems in engineering sciences subsume the following issues. Firstly, the ever-growing complexity of physical modeling increases the computational expense of deterministic forward simulations. Secondly, uncertainty is omnipresent and calls for an adequate mathematical formalism of representation and management. Thirdly, since data are commonly scarce or prohibitively expensive to acquire, the available information has to be carefully handled. An abstract inverse problem statement thus reads as follows. By analyzing a limited amount of data the endeavor is to optimally learn about unknown forward model inputs that are subject to epistemic uncertainty and aleatory variability. This includes deducing fixed albeit unknown forward model parameters as well as hyperparameters that determine the distribution of variable model inputs. Such a universal formulation describes a class of inverse problems that has hardly been satisfactorily solved yet. Our goal is therefore to develop a rigorous and extensive framework for formulating and solving such inverse problems in support of data analysis for engineering systems. The focus of this research is on experimental situations as they are typically encountered in this field. We emphasize aspects of uncertainty quantification and information accumulation. In order to establish a sound conceptional and computational basis for solving those problems one has to complement ideas and techniques that have been developed in different academic disciplines and scientific communities so far. This involves inverse modeling, Bayesian statistics and uncertainty quantification. In the following we will shortly survey relevant theories and practices.

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http://dx.doi.org/10.1016/j.probengmech.2015.09.007
0266-8920/

In the first place we rely on the Bayesian approach to *classical inverse problems* [1,2]. When a physical theory or a computational solver relates physical parameters to measurable quantities, i.e. the *forward model*, classical inversion is the process of reasoning or inferring unknown yet physically fixed model parameters from recorded data [3,4]. Bayesian inference establishes a convenient probabilistic framework to accomplish this conventional type of parameter estimation and data assimilation. At least since the advent of the personal computer it is nowadays widely used in engineering applications [5,6]. The stochastic paradigm provides a natural mechanism for the regularization of ill-posed problems, however, it requires the specification of a prior and a noise model. *Hierarchical inversion* is an extension of the classical framework that allows to set parameters of the prior and the noise model in a data-informed manner [7,8]. While epistemic uncertainty is naturally incorporated, a shortcoming of these types of parameter estimation is that they do not account for aleatory variability.

In the second place *hierarchical statistical models* serve as the main tool for the analysis of complex systems. Those are systems that are hierarchically organized at multiple nested layers. Prominent instances include *random* and *mixed effects models* [9]. Historically those models were developed in social and biological sciences e.g. for purposes of educational research [10,11] and pharmacokinetics/dynamics [12,13]. Some recent reviews about the methods that were developed in these fields can be found in [14,15]. Hierarchical modeling can be viewed from a more frequentist [16,17] or a more Bayesian perspective [18,19]. At the present day it is mature area of research that establishes sort of an overarching theme in modern multidisciplinary statistics. Dedicated chapters can be found in numerous standard references for Bayesian modeling and inference [20,21]. A general observation is that hierarchical models may be complex in their probabilistic architecture whereas only little forward modeling takes place.

In the third place we respect the uncertainty taxonomy that is prevalent in risk assessment and decision making. According to this classification one distinguishes between epistemic and aleatory uncertainty [22,23]. On one side, *epistemic uncertainty* refers to the ignorance or lack of knowledge of the observer and analyst. By taking further evidence this type of uncertainty is reducible in principle. On the contrary, *aleatory uncertainty* or *variability* refers to a trait of the system under consideration. It is a structural randomness of irreducible character. Uncertainties can be accounted for in distinct mathematical frameworks and especially the representation of ignorance is the subject matter of ongoing debates [24,25]. Graphical statistical models such as *Bayesian probability networks* establish a powerful and widespread tool of uncertainty characterization [26,27]. In risk-based decision making Bayesian belief networks have been adopted for their strength and flexibility in uncertainty modeling [28,29] and their elegant mechanisms of information aggregation [30,31].

In the fourth place *probabilistic inverse problems* constitute a challenging class of inverse problems that is of theoretical and practical relevance alike. While classical inversion is concerned with estimating uncertain yet physically fixed parameters in a series of experiments, i.e. identifying an epistemically uncertain quantity, probabilistic inversion deals with inferring the distribution of such forward model inputs that vary throughout the experiments, i.e. quantifying their aleatory variability. Previously established approaches to this interesting type of problems with *latent/hidden variable* structure subsume various approximate solutions. A frequentist technique that is premised on the simulation of an explicitly marginalized likelihood is proposed in [32]. There are also attempts to compute approximate solutions based on variants of the expectation–maximization algorithm within a linearized Gaussian frame [33] or with the aid of Kriging surrogates [34]. A methodological review of this school of probabilistic inversion is found in [35]. These methods are only partly Bayesian and suffer from the deficiency of providing mere point estimates.

The potential of hierarchical models as instruments of statistical modeling and uncertainty quantification have barely been acknowledged for the purposes of inversion in a classical sense. Hierarchical and probabilistic inversion are first steps towards preparing the Bayesian framework for the treatment of more realistic experimental scenarios. These approaches do not fully exhaust the inferential machinery of hierarchical models and the probability logic of Bayesian networks, though. In this contribution we thus aim at bridging that gap by developing a coherent Bayesian framework for managing uncertainties in such undertakings. By drawing on the statistical theory of hierarchical models, we cast inversion under parameter uncertainty and variability as *Bayesian multilevel calibration*. This embeds a joint and a marginal problem formulation of Bayesian inference under uncertainty, both of which can be numerically solved with plain vanilla or specialized Markov chain Monte Carlo methods.

This new formulation of *multilevel inversion* is especially well-adapted to the challenges that engineers are frequently faced with. It naturally allows for sophisticated uncertainty modeling which comprises both epistemic and aleatory uncertainty. The inclusion of the former is straightforward whereas the introduction of the latter is an extension to classical parameter estimation. It also promotes a pervasive “blackbox” point of view on the forward model. While this is inevitable in many complex applications, it is not readily compliant with traditional hierarchical models. Previously established strategies of enhanced uncertainty quantification, e.g. hierarchical and probabilistic inversion, emerge as special cases of the proposed general problem formulation. This also offers the opportunity to cope with probabilistic inversion within a fully Bayesian setting. Beyond these extensions some fundamentally new possibilities are suggested. Based on the probabilistic calculus of multilevel models, we develop a novel formulation of multilevel inversion in the zero-noise and “perfect” data limit. The statistical effect of “borrowing strength” or “optimal combination of information” is transferred and applied to inverse problems.

The paper is organized as follows. In Section 2 we will elaborate a general Bayesian framework for the treatment of uncertainty and variability in inverse problems. This is followed by a discussion about Bayesian inference in the context of multilevel inversion in Section 3. Thereafter Section 4 will provide an extension of the framework that will allow for handling “perfect” data. Probabilistic inversion and borrowing strength will be placed in context in Sections 5 and 6, respectively. Dedicated Bayesian computations based on Markov chain Monte Carlo are reviewed in Section 7. Lastly in Section 8 we will conduct a selection of numerical case studies, where by considering various experimental situations and uncertainty setups the very potential and the computational challenges of the devised modeling paradigm will become transparent.

2. Bayesian multilevel modeling

Due to the lack of a unified terminology, we define a *hierarchical* or *multilevel model* as “an overall system model that is hierarchically composed of deterministic and stochastic submodels”. Important types of submodels comprise physical models of the deterministic system components (Section 2.1), prior descriptions of parameter uncertainty and variability (Section 2.2) and residual representations of forward model prediction errors (Section 2.3). From these submodels we will assemble a generic Bayesian multilevel model (Section 2.4). This will represent the overall system under consideration including its deterministic and probabilistic aspects.