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A Bayesian approach to multiscale inverse problems with on-the-fly scale determination

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A B S T R A C T

A Bayesian computational approach is presented to provide a multi-resolution estimate of an unknown spatially varying parameter from indirect measurement data. In particular, we are interested in spatially varying parameters with multiscale characteristics. In our work, we consider the challenge of not knowing the characteristic length scale(s) of the unknown a priori, and present an algorithm for on-the-fly scale determination. Our approach is based on representing the spatial field with a wavelet expansion. Wavelet basis functions are hierarchically structured, localized in both spatial and frequency domains and tend to provide sparse representations in that a large number of wavelet coefficients are approximately zero. For these reasons, wavelet bases are suitable for representing permeability fields with non-trivial correlation structures. Moreover, the intra-scale correlations between wavelet coefficients form a quadtree, and this structure is exploited to identify additional basis functions to refine the model. Bayesian inference is performed using a sequential Monte Carlo (SMC) sampler with a Markov Chain Monte Carlo (MCMC) transition kernel. The SMC sampler is used to move between posterior densities defined on different scales, thereby providing a computationally efficient method for adaptive refinement of the wavelet representation. We gain insight from the marginal likelihoods, by computing Bayes factors, for model comparison and model selection. The marginal likelihoods provide a termination criterion for our scale determination algorithm. The Bayesian computational approach is rather general and applicable to several inverse problems concerning the estimation of a spatially varying parameter. The approach is demonstrated with permeability estimation for groundwater flow using pressure sensor measurements.

1. Introduction

With advances in the computational sciences, practitioners are placing increasing reliance on complex physical models. These models have many unknown parameters that need to be inferred from experimental data. The identification of a

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spatially varying parameter, or a field, is often an important task. A typical example is the permeability estimation of the aquifer for subsurface flow [1]. The approach taken in the paper is, however, applicable to a large number of data-driven inverse problems arising in the physical sciences and engineering.

It is often the case that the spatially varying parameter must be recovered from limited data that is corrupted by noise. For these reasons, the Bayesian approach to inverse problems is preferred [2,3]. Moreover, the Bayesian approach allows us to incorporate prior knowledge into the model and provides a way of quantifying uncertainty in the solution.

Spatially varying parameters often belong to an infinite-dimensional space and intrinsically have multiscale characteristics [4]. In particular, permeability fields are essentially non-stationary with nontrivial correlation structures [5–8]. This significantly complicates forward uncertainty quantification analysis [9,10]. In the context of inverse analysis, the unknown field is often found by discretizing with a truncated spectral expansion and performing inference over a finite number of coefficients. In practice, the characteristic length scale of the unknown cannot be inferred directly from the observation data. The existing approaches tend to require strong assumptions about the scale of estimation, whereas we adopt a data-driven approach to choose a suitable model.

It is common practice to discretize the unknown parameter into a finite number of piecewise constant basis functions [11]. Standard models for spatial data, such as Gaussian processes and Markov random fields, may then be used to model the spatially varying parameter [4,12,13]. Whilst the Karhunen–Loève expansion may be used to construct an optimal basis, the covariance structure of the true permeability field is unknown [14]. A more recent approach uses a number of piecewise constant level sets [15]. Fourier basis functions have also been used to introduce a desired level of smoothness [16], however these parameterizations are not localized in both spatial and frequency domains. In choosing such parameterizations, strong assumptions are made about the field being inferred and these methods are generally not well-suited for fields with non-trivial correlation structures. Sparse interpolation schemes have also been used to parametrize the unknown property field [17]. For example, an adaptive Bayesian approach using a hierarchical sparse grid approximation to represent the unknown field was first presented in [18]. However, these methods tend to perform poorly on fields with sharp variations.

To this end, we parameterize the spatially varying parameter using a multi-resolution analysis [19]. Multi-resolution analysis has received a great deal of attention over the recent decades. The idea is to construct a wavelet expansion to capture localized structures over different length scales. Two significant applications of multi-resolution analysis include the discrete cosine transform and the discrete wavelet transform, used commonly for image compression [20,21]. For this reason, wavelet-bases are promising candidates for the parameterization of a spatially varying parameter with multiscale characteristics.

In parameterizing the spatially varying parameter, it is common practice to fix, a priori, either the length scale, number of length scales or the number of terms in a spectral expansion. In practice, it is not known a priori whether these restrictions are reasonable. We refer to this as the problem of 'scale determination' and recognize this as a model selection problem. Opting for a model of excessive complexity results in over-fitting and the task of inference becomes needlessly difficult. Conversely, an overly constrained model will not capture the most salient features. In the statistical literature, it is common practice to use the marginal likelihood to address the task of model selection [22].

Wavelet coefficients are hierarchical in nature and tend to be clustered around either 'high' or 'low' states [4]. Moreover, there are intra-scale correlations such that parent coefficients with small values are more likely to have children coefficients with small values. The hierarchical structure may be illustrated with a quadtree, which may be exploited when forming hierarchical models [23,24]. Additional insight can be gained by viewing wavelets on one scale as a correction to the representation at a coarser scale. Negligible wavelet coefficients therefore provide an indication that there are sufficient basis functions in the local region and that there would likely be a negligible contribution from the corresponding children wavelets. We use these ideas to develop an on-the-fly scale determination algorithm to adaptively refine the wavelet basis.

Bayesian inference is performed using the sequential Monte Carlo (SMC) [25–27] algorithm. SMC uses sequential importance sampling (SIS) to gradually move a particle approximation for an initial density, so that it becomes a particle approximation for a more complex, sometimes multi-modal, density. We use SMC for both Bayesian inference in a fixed model and for scale determination. In the latter case, we move a particle approximation from one posterior density to another and compare Bayes factors. When moving between posterior densities, the SMC method allows information from previous computations to be used efficiently. The SMC algorithm used in this paper is directly parallelizable.

In summary, the key contributions of this paper include the following in the context of Bayesian approaches to multiscale inverse problems:

- Application of multi-resolution analysis to multiscale inverse problems to obtain a hierarchical, wavelet-based representation of a spatially varying parameter.
- On-the-fly scale determination algorithm that provides an adaptive approach to model selection for our representation of the spatially varying parameter.

The rest of the paper is structured as follows. In Section 2, we present our method of parameterizing the spatially varying parameter, using a wavelet expansion. We first consider a fixed scale model, by fixing the truncation of the wavelet expansion. In Section 3, a Bayesian model for the fixed scale representation is presented. SMC is used to explore the resulting posterior densities. In Section 4, we address the issue of scale determination and propose an on-the-fly scale determination