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ScienceDirect
Comput. Methods Appl. Mech. Engrg. 327 (2017) 147–172
Computer methods in applied mechanics and engineering
www.elsevier.com/locate/cma

Hessian-based adaptive sparse quadrature for infinite-dimensional Bayesian inverse problems☆

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Available online 24 August 2017

Highlights

- We proposed a new Hessian-based adaptive sparse quadrature to compute infinite-dimensional integrals with respect to the posterior distribution in the context of Bayesian inverse problems with Gaussian prior.
- Moreover, we established that under certain assumptions, the convergence rate of the adaptive sparse quadrature is dimension independent, thus breaking the curse of dimensionality.
- Furthermore, we proved that the convergence can be much faster than Monte Carlo type of methods, given that the integrand is sufficiently smooth.
- Finally, we demonstrated the dimension-independent and fast convergence for both linear inverse problems and nonlinear inverse problems.

Abstract

In this work we propose and analyze a Hessian-based adaptive sparse quadrature to compute infinite-dimensional integrals with respect to the posterior distribution in the context of Bayesian inverse problems with Gaussian prior. Due to the concentration of the posterior distribution in the domain of the prior distribution, a prior-based parametrization and sparse quadrature may fail to capture the posterior distribution and lead to erroneous evaluation results. By using a parametrization based on the Hessian of the negative log-posterior, the adaptive sparse quadrature can effectively allocate the quadrature points according to the posterior distribution. A dimension-independent convergence rate of the proposed method is established under certain assumptions on the Gaussian prior and the integrands. Dimension-independent and faster convergence than $O(N^{-1/2})$ is demonstrated for a linear as

☆ We wish to dedicate this article to Professor J. Tinsley Oden in appreciation of his foundational work in computational science, engineering, and mathematics over the last half century, and for his leadership and vision in this field. This work was supported by DARPA's EQUiPS program under contract number W911NF-15-2-0121, National Science Foundation grants CBET-1508713 and ACI-1550593, and DOE grants DE-SC0010518 and DE-SC0009286.

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http://dx.doi.org/10.1016/j.cma.2017.08.016
0045-7825/Published by Elsevier B.V.

well as a nonlinear inverse problem whose posterior distribution can be effectively approximated by a Gaussian distribution at the MAP point.
Published by Elsevier B.V.

MSC: 65C20; 65D30; 65D32; 65N12; 65N15; 65N21

Keywords: Infinite-dimensional Bayesian inverse problems; Curse of dimensionality; Hessian-based adaptive sparse quadrature; Sparse grid; Gaussian prior; Dimension-independent convergence analysis

1. Introduction

In many practical applications, a quantity of interest (QoI) predicted by a mathematical model of a physical system may be stochastic rather than deterministic due to uncertainties arising from inadequate knowledge of input parameters that characterize material properties, computational geometries, initial and boundary conditions, source terms, etc. Solution of an inverse problem will reduce these uncertainties based on available observational data on some system outputs, leading to more reliable computational predictions of the QoI. In a Bayesian framework, the solution of the inverse problem entails the computation of the posterior probability distribution of the uncertain input parameter conditioned on (possibly) noisy observational data of the system output. A prior probability distribution, based on experts' belief, is prescribed for the uncertain input parameter. Then, the posterior distribution of the uncertain parameter can be formally obtained by the Radon–Nikodym derivative by Bayes' theorem [1]. Once the posterior distribution is known, one is often interested in evaluating the statistical moments of the QoI (e.g., expectation and variance) with respect to the posterior distribution for the assessment, design, control and optimization of the system.

We consider the case of a spatially heterogeneous uncertain parameter, i.e., a spatially correlated random field with a prescribed bounded covariance between any two points of the physical domain. This setting makes the uncertain parameter infinite-dimensional, which naturally leads to an infinite-dimensional integration problem for the evaluation of the statistical moments of the QoI with respect to the posterior distribution. Several computational challenges are commonly faced for such integration problems. Traditional deterministic integration methods face the curse of dimensionality, i.e., the computational complexity grows exponentially fast with respect to the parameter dimension so that only a limited number of dimensions can be resolved. On the other hand stochastic integration methods such as Monte Carlo (MC) or Markov-chain Monte Carlo (MCMC) do not depend on the parameter dimension but on the variance of the QoI; however the convergence of the quadrature errors, $O(N^{-1/2})$ with N quadrature samples [2], is often very slow. In addition, the posterior distribution, unlike the prior distribution, is usually not explicitly available but rather is implicitly represented by means of the Bayes Theorem and becomes rather concentrated in the parameter space when the observational data are very informative and thus is difficult to sample efficiently. Finally, when the system is modeled by partial differential equations (PDE) in complex geometries, evaluation of the QoI at each quadrature sample require a full PDE solve that can involve expensive large-scale computations, so that only a small number of samples can be computed.

We tackle these computational challenges by exploiting the *intrinsic sparsity* of the integration problem with respect to the posterior distribution and the *structure* of the inverse problem. By sparsity, we mean that the QoI has markedly different sensitivity in different parameter dimensions under the posterior distribution; in other words, the dependence of the QoI on different parameter dimensions is rather anisotropic with suitable parametrization of the uncertain parameter, so that we can identify the most sensitive dimensions and allocate most of the computational effort in these dimensions [3–8]. By structure, we mean that high-order derivatives of the parameter-to-observable map with respect to the parameter at the maximum a posteriori (MAP) point, in particular the Hessian, describe the inherent structure of the manifold of the posterior distribution about the MAP point, which is especially useful when the posterior distribution is relatively concentrated at the MAP point due to informative observational data [9–12]. To exploit these opportunities and to make the solution of the infinite-dimensional Bayesian inverse problem computationally feasible, here we develop a novel Hessian-based adaptive sparse quadrature for integration of a QoI with respect to the posterior distribution.

More specifically, we consider a Gaussian distribution in a Hilbert space as the prior distribution for the uncertain parameter, where the covariance operator is given by a fractional power of a second order elliptic differential operator. We then compute the MAP point by solving an optimization problem using a Lagrangian variational approach and an