COMMUNICATIONS IN COMPUTATIONAL PHYSICS
Vol. **6**, No. 4, pp. 826-847

Commun. Comput. Phys.
October 2009

A Stochastic Collocation Approach to Bayesian Inference in Inverse Problems

Youssef Marzouk[1,*] and Dongbin Xiu[2]

[1] *Department of Aeronautics & Astronautics, Massachusetts Institute of Technology, Cambridge, MA 02139, USA.*
[2] *Department of Mathematics, Purdue University, West Lafayette, IN 47907, USA.*

Received 27 August 2008; Accepted (in revised version) 18 February 2009

Communicated by Jan S. Hesthaven

Available online 12 March 2009

Abstract. We present an efficient numerical strategy for the Bayesian solution of inverse problems. Stochastic collocation methods, based on generalized polynomial chaos (gPC), are used to construct a polynomial approximation of the forward solution over the support of the prior distribution. This approximation then defines a surrogate posterior probability density that can be evaluated repeatedly at minimal computational cost. The ability to simulate a large number of samples from the posterior distribution results in very accurate estimates of the inverse solution and its associated uncertainty. Combined with high accuracy of the gPC-based forward solver, the new algorithm can provide great efficiency in practical applications. A rigorous error analysis of the algorithm is conducted, where we establish convergence of the approximate posterior to the true posterior and obtain an estimate of the convergence rate. It is proved that fast (exponential) convergence of the gPC forward solution yields similarly fast (exponential) convergence of the posterior. The numerical strategy and the predicted convergence rates are then demonstrated on nonlinear inverse problems of varying smoothness and dimension.

AMS subject classifications: 41A10, 60H35, 65C30, 65C50

Key words: Inverse problems, Bayesian inference, stochastic collocation, generalized polynomial chaos, uncertainty quantification.

1 Introduction

The indirect estimation of model parameters or inputs from observations constitutes an *inverse problem*. Such problems arise frequently in science and engineering, with applica-

*Corresponding author. *Email addresses:* `ymarz@mit.edu` (Y. Marzouk), `dxiu@purdue.edu` (D. Xiu)

tions ranging from subsurface and atmospheric transport to chemical kinetics. In practical settings, observations are inevitably noisy and may be limited in number or resolution. Quantifying the resulting *uncertainty* in inputs or parameters is then essential for predictive modeling and simulation-based decision-making.

The Bayesian approach to inverse problems [6,13,18,22,23] provides a foundation for inference from noisy and incomplete data, a natural mechanism for incorporating physical constraints and heterogeneous sources of information, and a quantitative assessment of uncertainty in the inverse solution. Indeed, the Bayesian setting casts the inverse solution as a *posterior* probability distribution over the model parameters or inputs. Though conceptually straightforward, this setting presents challenges in practice; the posterior probability distribution is typically not of analytical form and, especially in high dimensions, cannot be easily interrogated. Many numerical approaches have been developed in response, mostly seeking to approximate the posterior distribution or posterior expectations via samples [9]. These approaches require repeated solutions of the forward model; when the model is computationally intensive, e.g., specified by partial differential equations (PDEs), the Bayesian approach then becomes prohibitive.

Several efforts at accelerating Bayesian inference in inverse problems have appeared in recent literature; these have relied largely on reductions or surrogates for the forward model [3, 14, 17, 24], or instead have sought more efficient sampling from the posterior [4,5,11]. Recent work [17] used (generalized) polynomial chaos (gPC)-based stochastic Galerkin methods [8, 29] to propagate prior uncertainty through the forward model, thus yielding a polynomial approximation of the forward solution over the support of the prior. This approximation then entered the likelihood function, resulting in a posterior density that was inexpensive to evaluate. This scheme was used to infer parameters appearing nonlinearly in a transient diffusion equation, demonstrating exponential convergence to the true posterior and multiple order-of-magnitude speedup in posterior exploration via Markov chain Monte Carlo (MCMC). The gPC stochastic Galerkin approach has also been extended to Bayesian inference of spatially-distributed quantities, such as inhomogeneous material properties appearing as coefficients in a PDE [16].

An alternative to the stochastic Galerkin approach to uncertainty propagation is stochastic collocation [25,27]. A key advantage of stochastic collocation is that it requires only a finite number of uncoupled deterministic simulations, with no reformulation of the governing equations of the forward model. Also, stochastic collocation can deal with highly nonlinear problems that are challenging, if not impossible, to handle with stochastic Galerkin methods. A spectral representation may also be applied to arbitrary functionals of the forward solution; moreover, many methods exist for addressing high input dimensionality via efficient low-degree integration formulae or sparse grids. For an extensive discussion of gPC-based algorithms, see [26].

This paper extends the work of [17] by using gPC stochastic collocation to construct posterior surrogates for efficient Bayesian inference in inverse problems. We also conduct a rigorous error analysis of the gPC Bayesian inverse scheme. Convergence of the approximate posterior distribution to the true posterior distribution is established and