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Sparse Quadrature Approach to Bayesian Inverse Problems

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Sparse Quadrature Approach to Bayesian Inverse Problems

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(joint work with Claudia Schillings)

We consider the parametric deterministic formulation of Bayesian inverse problems with distributed parameter uncertainty from infinite dimensional, separable Banach spaces X, with uniform prior probability measure on space X of all uncertainties. Under the assumption of given observation data δ subject to additive observation noise $\eta \sim N(0, \Gamma)$ with positive covariance Γ, an infinite-dimensional version of Bayes' formula has been shown in [14].

For problems with uncertain, distributed parameters $u \in X$ (which could be a diffusion coefficient, elastic moduli in solid mechanics, shape of the domain D of definition of the physical problem [1], kinetic parameters in stoichiometric models of reaction-systems in biological systems [4, 7], permeability in porous media or optimal control of uncertain systems [9]), we develop a practical, adaptive computational algorithm for the efficient approximation of the infinite-dimensional integrals with respect to the Bayesian posterior (conditional on given data δ) μ^δ which arise in Bayes' formula in [14].

The Bayesian posterior μ^δ is shown to admit a representation in terms of a (generalized) polynomial chaos expansion in the (countably many) coordinates y_j which parametrize the uncertainty. We prove that if the uncertain datum $u \in X$ admits the (norm-convergent in X) expansion

$$u = \langle u \rangle + \sum_{j \geq 1} y_j \psi_j(x)$$

with $|y_j| \leq 1$ and with $(\|\psi_j\|_X)_{j\geq 1} \in \ell^p(\mathbb{N})$ for some $0 < p < 1$, then the solution $q(u) = (A(u))^{-1} f$ of the parametric operator equation will depend holomorphically on the parameters y_j, with precise control of the domain of holomorphy [3, 8, 5, 1, 9]. In two-scale limits of homogenization theory, these domains are independent of physical scale parameters [8].

We prove, generalizing [13], that the holomorphic dependence on the parameters y_j of the forward solution of the above problems implies p-sparsity of the polynomial chaos expansion for the parametric forward solution $q(u) = (A(u))^{-1} f$ and also for the density function of derivative of the Bayesian posterior μ^δ with respect to the prior μ_0, conditional on given data δ.

The proof of the p-sparsity in [12, 10] is based on verification of holomorphic dependence of the polynomial chaos representation for the density of the Bayesian posterior with respect to the prior, following the proofs in the linear, elliptic diffusion problems in [3, 13].

Based on this sparsity result, dimension independent convergence rates of best N-term approximations of the parametric forward map as well as of the parametric density of the Bayesian posterior with respect to uniform prior follows from Stechkin's lemma.

We propose a deterministic, adaptive algorithm inspired by [6] and analogous to the adaptive interpolation methods in [2] and the references there. The proposed algorithm determines iteratively, and depending on the observation data δ and the observation noise variance Γ a sequence of quadrature dimensions and quadrature orders.

Convergence rates for the adaptive Smolyak quadrature approximation are shown, computationally, to coincide with the best N term approximation rates of the Bayesian posterior density which, in turn [12, 10] depend only on the sparsity class (characterized in turn by the summability exponent $p \in (0,1)$ of the uncertain distributed parameter $u \in X$.

Convergence rates are obtained in [12, 10] via monotone L^∞ N-term approximations of the posterior density from [2]. The resulting rates $1/p - 1$ are larger than the rate $1/2$ afforded by Monte-Carlo methods and their variants (notably MCMC) for $p < 2/3$ when stated in terms of the number N of (numerical) solutions of the forward problems which are necessary in the quadrature algorithm.

Applications with verified holomorphic dependence include high-dimensional parametric initial value problems [4], semilinear elliptic equations [5, 1] with uncertain differential operators, parabolic evolution problems with uncertain operators [1], elliptic multiscale problems with uncertain coefficients [8] and from biological systems sciences [7], as well as optimal control of uncertain systems [9], and problems with uncertain shape [1].

Numerical examples are presented for diffusion problems with uncertain diffusion coefficient from [12], [10], and for large, parametric systems of initial value problems from stoichiometric models for biological systems with mass-action kinetics from [4, 7]. Computational savings with respect to adaptivity in the forward solver are indicated. Here, we present numerical experiments based on the parametric, parabolic initial boundary-value problem

$$\begin{aligned} \partial_t q(t,x) - \operatorname{div}(u(x)\nabla q(t,x)) = f(t,x) \quad (t,x) \in T \times D\,, \\ q(0,x) = 0 \quad x \in D\,, \\ q(t,0) = q(t,1) = 0 \quad t \in T\,, \end{aligned}$$

with $f(t,x) = 100 \cdot tx$, $D = (0,1)$ and $T = (0,1)$. The uncertain coefficient u is parametrized as $u(x,y) = \bar{a} + \sum_{j=1}^{128} y_j \psi_j$, where $\bar{a} = 1$ and $\psi_j = \alpha_j \chi_{D_j}$ with $D_j = [(j-1)\frac{1}{128}, j\frac{1}{128}]$, $\boldsymbol{y} = (y_j)_{j=1,\dots,128}$ and $\alpha_j = \frac{0.6}{j^\zeta}$, $\zeta = 3$. Figure 1 shows the convergence behavior of the adaptive Smolyak algorithm for the approximation of the normalization constant considering a variation of the number of observation points as well as of the observational noise.

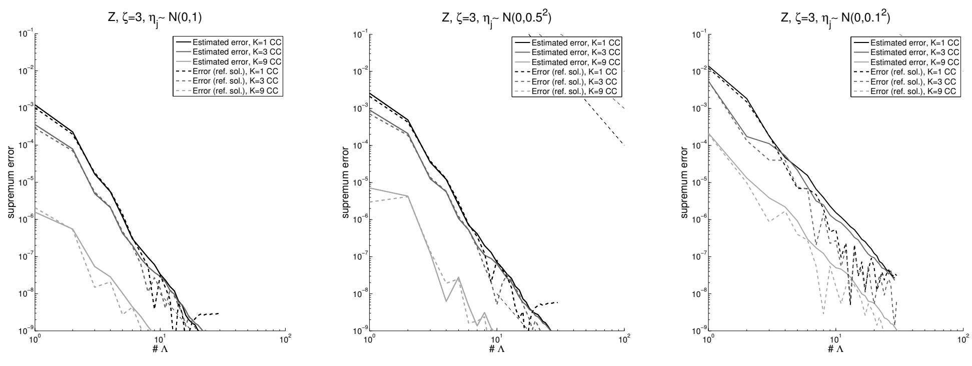

FIGURE 1. Comparison of the estimated error and actual error of the normalization constant $Z = \mathbb{E}^{\mu^\delta}[1]$ with respect to the cardinality $\#\Lambda$ of the index sets Λ_N (Clenshaw-Curtis quadrature) with $K = 1,3,9$ (number of observation points), $\eta \sim \mathcal{N}(0,1)$ (l.), $\eta \sim \mathcal{N}(0,0.5^2)$ (m.), $\eta \sim \mathcal{N}(0,0.1^2)$ (r.).

A detailed discussion of the numerical experiments for the parametric, parabolic evolution problem with random coefficients can be found in [10]. The numerical experiments indicate that, as the observation noise with variance $\Gamma \to 0$, growth of the constants in the Smolyak quadrature error estimates. In [11], we present an asymptotic analysis and prove $C \sim \exp(b/\Gamma)$ for some constants $b, C > 0$. We also show in [11] that the Bayesian estimate admits a finite limit in the case $\Gamma \to 0$, and propose regularization of the integrand functions arising in the computation of the conditional expectation.

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