Higher Order Quasi Monte-Carlo Integration in Uncertainty Quantification

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Abstract We review recent results on dimension-robust higher order convergence rates of Quasi-Monte Carlo Petrov-Galerkin approximations for response functionals of infinite-dimensional, parametric operator equations which arise in computational uncertainty quantification.

1 Introduction

Computational uncertainty quantification (UQ) for partial differential equations (PDEs) with uncertain distributed input data gives rise, upon uncertainty parametrization, to the task of numerical solution of parametric, deterministic operator equations. Due to the distributed nature of uncertain inputs, the number of parameters (and, hence, the dimension of the parameter spaces) in such UQ problems is infinite. The computation of response statistics corresponding to distributed uncertain inputs of PDEs involves, in addition, *numerical quadrature* of all possible 'uncertain scenarios', i.e., over the entire, infinite-dimensional parameter space.

This has lead to the widespread use of sampling, in particular Monte-Carlo (MC) and Markov-Chain Monte-Carlo (MCMC) methods, in the numerical treatment of these problems: MC methods afford convergence *rates* which are independent of the parameter dimension if the variance of the integrand can be bounded independently of the dimension (the computational *work* of MC methods, of course, increases linearly with the space dimension). This *dimension robustness* of MC methods is purchased at the cost of low order: the convergence rate of simple MC methods is,

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generically, limited to $1/2$: variance reduction and other devices can only reduced the constant, not the rate in the convergence bounds. At the same time, however, the *parametric regularity* required of integrand functions by MC methods is very moderate: mere square integrability with respect to a probability measure on the parameter space of the integrand functions is needed, and point evaluations of the integrand functions must be defined. In UQ for problems whose solutions exhibit propagation of singularities (as, eg., nonlinear hyperbolic conservation laws with random inputs, see eg. [14, 15] and the references there), this kind of regularity is the best that can generally be expected. In other applications, the parametric dependence of the response maps is considerably more regular: the solutions' dependence on the parameters is, in fact, *analytic*. This observation has been the basis for the widespread use of spectral- and polynomial chaos based numerical methods for approximating the parameter dependence in such problems (see eg. [1, 2, 9] and the references there).

Straightforward application of standard spectral techniques entails, however, the *curse of dimensionality*: the spectral- or even exponential convergence rate afforded by analytic parameter dependence is not realized in computational practice as soon as the number of parameters is just moderately large. High order numerical methods for infinite-dimensional problems require, therefore, a more refined analysis of analytic parameter dependence where, for dimension-independent convergence rates, the size of the domains of analyticity must increase with the problem dimension.

The purpose of the paper is to present recent advances in the analysis of higher order *Quasi Monte-Carlo (QMC)* methods, which were proposed initially in [3] (see also [6]), from [4, 5]. The presented results imply, for a particular type of analytic parameter dependence encountered for a large class of operator equations with random coefficients, dimension robust high order convergence rates, which are only limited by a certain sparsity measure of the uncertain input.

2 Affine Parametric Operator Equations

We present a model setting of affine parametric operator equations, and their Petrov-Galerkin (PG) discretizations, following the setting in [5]. We denote by $\mathscr{X}$ and $\mathscr{Y}$ two separable and reflexive Banach spaces over $\mathbb{R}$ (all results will hold with the obvious modifications also for spaces over $\mathbb{C}$) with (topological) duals $\mathscr{X}'$ and $\mathscr{Y}'$, respectively. By $\mathscr{L}(\mathscr{X},\mathscr{Y}')$, we denote the set of bounded linear operators $A : \mathscr{X} \to \mathscr{Y}'$. We consider *affine-parametric operator equations*: given $f \in \mathscr{Y}'$, for every $y \in U$ find $u(y) \in \mathscr{X}$ such that

$$A(y)\,u(y) = f \;. \tag{1}$$

For such parametrizations, the parametric operator $A(y)$ depends on y in an "*affine*" manner: there exists a sequence $\{A_j\}_{j \geq 0} \subset \mathscr{L}(\mathscr{X},\mathscr{Y}')$ such that

$$\forall y \in U : \quad A(y) = A_0 + \sum_{j \geq 1} y_j A_j \, . \tag{2}$$

After possibly rescaling, we restrict ourselves to the bounded (infinite-dimensional) parameter domain $U = [-\frac{1}{2}, \frac{1}{2}]^{\mathbb{N}}$. For every $f \in \mathscr{Y}'$ and for every $y \in U$, we solve the parametric operator equation (1), where the operator $A(y) \in \mathscr{L}(\mathscr{X}, \mathscr{Y}')$ is of affine parameter dependence, see (2). We associate with the A_j bilinear forms $\mathfrak{a}_j(\cdot, \cdot) : \mathscr{X} \times \mathscr{Y} \to \mathbb{R}$ via

$$\forall v \in \mathscr{X}, \, w \in \mathscr{Y} : \quad \mathfrak{a}_j(v, w) = {}_{\mathscr{Y}'}\langle A_j v, w \rangle_{\mathscr{Y}} \, , \quad j = 0, 1, 2, \ldots \, .$$

Similarly, for $y \in U$ we associate with the affine-parametric operator family $A(y)$ the parametric bilinear form $\mathfrak{a}(y; \cdot, \cdot) : \mathscr{X} \times \mathscr{Y} \to \mathbb{R}$ via

$$\forall v \in \mathscr{X}, \, w \in \mathscr{Y} : \quad \mathfrak{a}(y; v, w) = {}_{\mathscr{Y}'}\langle A(y) v, w \rangle_{\mathscr{Y}} \, .$$

In order for the sum in (2) to converge, we impose

Assumption 1 *The sequence $\{A_j\}_{j \geq 0} \subset \mathscr{L}(\mathscr{X}, \mathscr{Y}')$ in (2) satisfies:*

1. $A_0 \in \mathscr{L}(\mathscr{X}, \mathscr{Y}')$ is boundedly invertible, i.e., there exists $\mu_0 > 0$ such that

$$\inf_{0 \neq v \in \mathscr{X}} \sup_{0 \neq w \in \mathscr{Y}} \frac{\mathfrak{a}_0(v, w)}{\|v\|_{\mathscr{X}} \|w\|_{\mathscr{Y}}} \geq \mu_0 \, , \quad \inf_{0 \neq w \in \mathscr{Y}} \sup_{0 \neq v \in \mathscr{X}} \frac{\mathfrak{a}_0(v, w)}{\|v\|_{\mathscr{X}} \|w\|_{\mathscr{Y}}} \geq \mu_0 \, .$$

2. The fluctuation operators $\{A_j\}_{j \geq 1}$ are small with respect to A_0 in the following sense: there exists a constant $0 < \kappa < 2$ such that

$$\sum_{j \geq 1} \beta_{0,j} \leq \kappa < 2 \, , \quad where \quad \beta_{0,j} := \|A_0^{-1} A_j\|_{\mathscr{L}(\mathscr{X}, \mathscr{X})} \, , \quad j = 1, 2, \ldots \, . \tag{3}$$

Theorem 1 (cf. [17, Theorem 2]). *Under Assumption 1, for every realization $y \in U$ of the parameter vector, the affine parametric operator $A(y)$ given by (2) is boundedly invertible, uniformly with respect to y. In particular, for every $f \in \mathscr{Y}'$ and for every $y \in U$, the parametric operator equation*

$$find \quad u(y) \in \mathscr{X} : \quad \mathfrak{a}(y; u(y), w) = {}_{\mathscr{Y}'}\langle f, w \rangle_{\mathscr{Y}} \quad \forall w \in \mathscr{Y} \tag{4}$$

admits a unique solution $u(y)$ which satisfies the a-priori estimate

$$\|u(y)\|_{\mathscr{X}} \leq \frac{1}{\mu} \|f\|_{\mathscr{Y}'} \, , \quad with \quad \mu = (1 - \kappa/2) \mu_0 \, .$$

2.1 Single-level and multi-level algorithms

The Quantity of Interest (QoI) in our study is the expected value of a linear functional $G : \mathscr{X} \to \mathbb{R}$ of the solution u,

$$I(G(u)) = \int_U G(u(y)) \, dy.$$

In the following we discuss the approximation of the QoI by the algorithm $Q_{N,s}(G(u_s^h))$, where $Q_{N,s}$ is a quadrature rule (QMC rule) and u_s^h is the Petrov-Galerkin (PG) approximation of the dimension truncated problem, which means that the set of parameters $y \in U$ is restricted to y of the form $(y_1, y_2, \ldots, y_s, 0, 0, \ldots)$. The combined error of this *single-level algorithm* can be expressed as

$$
\begin{aligned}
I(G(u)) &- Q_{N,s}(G(u_s^h)) \\
&= \underbrace{I(G(u)) - I(G(u_s))}_{\text{truncation error}} + \underbrace{I(G(u_s)) - Q_{N,s}(G(u_s))}_{\text{integration error}} + \underbrace{Q_{N,s}(G(u_s - u_s^h))}_{\text{PG error}}, \quad (5)
\end{aligned}
$$

where 'PG error' stands for the Petrov-Galerkin discretization error. We discuss the three errors and the necessary background in the subsequent sections.

To reduce the computational cost required to achieve the same error, a novel *multi-level* algorithm was introduced and analyzed in [13]. It takes the form

$$Q_*^L(G(u)) := \sum_{\ell=0}^{L} Q_{s_\ell, N_\ell}(G(u_{s_\ell}^{h_\ell} - u_{s_{\ell-1}}^{h_{\ell-1}})) . \qquad (6)$$

In [13] the authors considered the case where each Q_{s_ℓ, N_ℓ} is a randomly shifted lattice rule with N_ℓ points in s_ℓ dimensions, and where $u_{s_{-1}}^{h_{-1}} := 0$, whereas in [5] the authors used an interlaced polynomial lattice rule.

It is well known [4] that under some assumptions the Petrov-Galerkin discretization error is of the form

$$\left| G(u(y)) - G(u^h(y)) \right| \leq C h^{t+t'} \|f\|_{\mathscr{X}_t'} \|G\|_{\mathscr{X}_{t'}'} . \qquad (7)$$

2.2 Parametric and spatial regularity of solutions

First we establish the regularity of the solution $u(y)$ of the parametric, variational problem (4) with respect to the parameter vector y. This is important for the analysis of the integration error using a QMC rule satisfying a dimension-independent error bound.

In the following, let $\mathbb{N}_0^{\mathbb{N}}$ denote the set of sequences $v = (v_j)_{j \geq 1}$ of non-negative integers v_j, and let $|v| := \sum_{j \geq 1} v_j$. For $|v| < \infty$, we denote the partial derivative of order v of $u(y)$ with respect to y by

$$\partial_y^v u(y) := \frac{\partial^{|v|}}{\partial_{y_1}^{v_1} \partial_{y_2}^{v_2} \cdots} u(y), \quad y \in U .$$

Theorem 2 (cf. [2, 10]). *Under Assumption 1, there exists a constant $C_0 > 0$ such that for every $f \in \mathscr{Y}'$ and for every $y \in U$, the partial derivatives of the parametric solution $u(y)$ of the parametric operator equation* (1) *with affine parametric, linear operator* (2) *satisfy the bounds*

$$\|\partial_y^\nu u(y)\|_{\mathscr{X}} \leq C_0 |\nu|! \beta_0^\nu \|f\|_{\mathscr{Y}'} \quad \text{for all } \nu \in \mathbb{N}_0^{\mathbb{N}} \text{ with } |\nu| < \infty ,$$

where $0! := 1$, $\beta_0^\nu := \prod_{j \geq 1} \beta_{0,j}^{\nu_j}$, *with $\beta_{0,j}$ as in* (3)*, and* $|\nu| = \sum_{j \geq 1} \nu_j$.

Spatial regularity is in *scales of smoothness spaces* $\{\mathscr{X}_t\}_{t \geq 0}$, $\{\mathscr{Y}_t\}_{t \geq 0}$, i.e.

$$\mathscr{X} = \mathscr{X}_0 \supset \mathscr{X}_1 \supset \mathscr{X}_2 \supset \cdots , \quad \mathscr{Y} = \mathscr{Y}_0 \supset \mathscr{Y}_1 \supset \mathscr{Y}_2 \supset \cdots , \quad \text{and}$$
$$\mathscr{X}' = \mathscr{X}_0' \supset \mathscr{X}_1' \supset \mathscr{X}_2' \supset \cdots , \quad \mathscr{Y}' = \mathscr{Y}_0' \supset \mathscr{Y}_1' \supset \mathscr{Y}_2' \supset \cdots .$$

For self-adjoint operators, usually $\mathscr{X}_t = \mathscr{Y}_t$.

Assumption 2 (see [5, Assumption 2]) *There exists $\bar{t} \geq 0$ such that*

1. *For every t, t' satisfying $0 \leq t, t' \leq \bar{t}$, we have*

$$\sup_{y \in U} \|A(y)^{-1}\|_{\mathscr{L}(\mathscr{Y}_{t'}, \mathscr{X}_t)} < \infty \quad \text{and} \quad \sup_{y \in U} \|(A^*(y))^{-1}\|_{\mathscr{L}(\mathscr{X}_{t'}', \mathscr{Y}_{t'})} < \infty . \quad (8)$$

   Moreover, there exist summability exponents $0 \leq p_0 \leq p_t \leq p_{\bar{t}} < 1$ such that

$$\sum_{j \geq 1} \|A_j\|_{\mathscr{L}(\mathscr{X}_t, \mathscr{Y}_{t'})}^{p_t} < \infty . \quad (9)$$

2. *Let $u(y) = (A(y))^{-1} f$ and $w(y) = (A^*(y))^{-1} G$. For $0 \leq t, t' \leq \bar{t}$, there exist constants $C_t, C_{t'} > 0$ such that for every $f \in \mathscr{Y}_t'$ and $G \in \mathscr{X}_{t'}'$ holds*

$$\sup_{y \in U} \|u(y)\|_{\mathscr{X}_t} \leq C_t \|f\|_{\mathscr{Y}_t'} \quad \text{and} \quad \sup_{y \in U} \|w(y)\|_{\mathscr{Y}_{t'}} \leq C_{t'} \|G\|_{\mathscr{X}_{t'}'} .$$

   Moreover, for every $0 \leq t \leq \bar{t}$ there exists a sequence $\beta_t = (\beta_{t,j})_{j \geq 1}$ satisfying

$$\sum_{j \geq 1} \beta_{t,j}^{p_t} < \infty ,$$

   such that for every $0 \leq t, t' \leq \bar{t}$ and for every $\nu \in \mathbb{N}_0^{\mathbb{N}}$ with $|\nu| < \infty$ we have

$$\sup_{y \in U} \|\partial_y^\nu u(y)\|_{\mathscr{X}_t} \leq C_t |\nu|! \beta_t^\nu \|f\|_{\mathscr{Y}_{t'}'},$$
$$\sup_{y \in U} \|\partial_y^\nu w(y)\|_{\mathscr{Y}_{t'}} \leq C_{t'} |\nu|! \beta_{t'}^\nu \|G\|_{\mathscr{X}_{t'}'} .$$

3. *The operators A_j are enumerated so that the sequence β_0 in* (3) *satisfies*

$$\beta_{0,1} \geq \beta_{0,2} \geq \cdots \geq \beta_{0,j} \geq \cdots . \quad (10)$$

2.3 Dimension truncation

We truncate the infinite sum in (2) to s terms and solve the corresponding opera-
tor equation (1) approximately using Galerkin discretization from two dense, one-
parameter families $\{\mathscr{X}^h\} \subset \mathscr{X}$, $\{\mathscr{Y}^h\} \subset \mathscr{Y}$ of subspaces of $\mathscr{X}$ and $\mathscr{Y}$: for $s \in \mathbb{N}$
and $y \in U$, we define

$$\mathfrak{a}_s(y;v,w) :=_{\mathscr{Y}'} \langle A^{(s)}(y)v,w \rangle_{\mathscr{Y}}, \quad \text{with} \quad A^{(s)}(y) := A_0 + \sum_{j=1}^{s} y_j A_j.$$

For $0 < h \le h_0$ and $y \in U$, the dimension truncated PG-solution is defined by

$$\text{find } u_s^h(y) \in \mathscr{X}^h: \quad \mathfrak{a}_s(y;u_s^h(y),w^h) =_{\mathscr{Y}'} \langle f,w^h \rangle_{\mathscr{Y}} \quad \forall w^h \in \mathscr{Y}^h. \tag{11}$$

By choosing $y = (y_1,\dots,y_s,0,0,\dots)$, the PG discretization error bound (7) remains
valid for the dimensionally truncated problem (11).

Theorem 3 (cf. [4, Theorem 2.6]). *Under Assumption 1, for every $f \in \mathscr{Y}'$, for every
$G \in \mathscr{X}'$, for every $y \in U$, for every $s \in \mathbb{N}$ and for every $h > 0$, the variational problem
(11) admits a unique solution $u_s^h(y)$ which satisfies*

$$|I(G(u^h)) - I(G(u_s^h))| \le C\|f\|_{\mathscr{Y}'} \|G\|_{\mathscr{X}'} \left(\sum_{j \ge s+1} \beta_{0,j} \right)^2$$

*for some constant $C > 0$ independent of f, G and of s where $\beta_{0,j}$ is defined in (3). In
addition, if (9) and (10) hold with $p_0 < 1$, then*

$$\sum_{j \ge s+1} \beta_{0,j} \le \min\left(\frac{1}{1/p_0 - 1}, 1 \right) \left(\sum_{j \ge 1} \beta_{0,j}^{p_0} \right)^{1/p_0} s^{-(1/p_0 - 1)}.$$

3 Quasi Monte-Carlo quadrature

In [12], Quasi-Monte Carlo rules of the form $Q_{N,s}(G(u_s^h)) = \frac{1}{N} \sum_{n=0}^{N-1} G(u_s^h(y_n - \frac{1}{2}))$,
where $y_n \in [0,1]^s$, have been used to approximate the dimension truncated integral
$I(G(u_s^h))$ (see also [11]). The rules considered therein are so-called randomly shifted
lattice rules. Using so-called "*product and order-dependent (POD) weights*" a con-
vergence rate of order $\mathcal{O}(N^{-\min(1/p_0 - 1, 1 - \delta)})$, for any $\delta > 0$, was shown.

   Noting that the integrand is actually analytic, the authors of [4] used *interlaced
polynomial lattice rules*, as introduced in [8] (which are a special type of higher
order digital net [3]), to obtain improved rates of convergence. The rules can be
constructed using the fast component-by-component approach of [16]. A new func-
tion space setting was introduced in [4] which uses Banach spaces and *smoothness
driven product and order dependent (SPOD) weights*.

Theorem 4 (cf. [4, Theorem 3.1]). *Let $s \geq 1$ and $N = b^m$ for $m \geq 1$ and prime b. Let $\gamma = (\gamma_j)_{j \geq 1}$ be a sequence of positive numbers, let $\overline{\gamma}_s = (\gamma_j)_{1 \leq j \leq s}$, and assume that*

$$\exists 0 < p \leq 1 : \quad \sum_{j=1}^{\infty} \gamma_j^p < \infty .$$

Define Suppose we have an integrand $F(y)$ whose partial derivatives satisfy

$$\forall \nu \in \{0, 1, \ldots, \alpha\}^s : \quad |(\partial_y^\nu F)(y)| \leq c |\nu|! \, \overline{\gamma}_s^\nu$$

for some constant $c > 0$. Then, an interlaced polynomial lattice rule of order α with N points can be constructed using a fast component-by-component algorithm, with cost $\mathcal{O}(\alpha s N \log N + \alpha^2 s^2 N)$ operations, such that

$$|I_s(F) - Q_{N,s}(F)| \leq C_{\alpha, \gamma, b, p} N^{-1/p} ,$$

where $C_{\alpha, \gamma, b, p} < \infty$ is a constant independent of s and N.

4 Combined error bound

In the case of the single level algorithm, the combined error (5) satisfies the following theorem.

Theorem 5 (cf. [4, Theorem 4.1]). *Under Assumption 1 and conditions* (8)*, $G \in \mathscr{X}_{t'}'$ and* (10)*, the integration error using an interlaced polynomial lattice rule of order $\alpha = \lfloor 1/p_0 \rfloor + 1$ with $N = b^m$ points (with b prime) in s dimensions, combined with a Petrov-Galerkin method in the domain D with one common subspace $\mathscr{X}^h$ with $M_h = \dim(\mathscr{X}^h)$ degrees of freedom and with linear cost $\mathcal{O}(M_h)$, satisfies*

$$|I(G(u)) - Q_{N,s}(G(u_s^h))| \leq \mathcal{O}\left(s^{-2(1/p_0 - 1)} + N^{-1/p_0} + h^{t+t'} \right) ,$$

where the constant is independent of s, h and N.

The multi-level algorithm additionally requires the Assumptions 2. The corresponding combined error bound using interlaced polynomial lattice rules is of the form (see [5, Theorem 3.4])

$$|I(G(u)) - Q_*^L(G(u_s^h))| \leq \mathcal{O}\left(s_L^{-2(1/p_0 - 1)} + h_L^{t+t'} + \sum_{\ell=0}^{L} N_\ell^{-1/p_t} \left(s_{\ell-1}^{-(1/p_0 - 1/p_t)} + h_{\ell-1}^{t+t'} \right) \right) .$$

The parameters s_ℓ and N_ℓ in (6) can be optimized using a Lagrange multiplier argument [13, 5], which, in most cases, yields an improvement compared to the single-level algorithm.

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