

Dimension Truncation in QMC for Affine-Parametric Operator Equations

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Research Report No. 2017-03

January 2017

Latest revision: August 2017

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Abstract An application of quasi-Monte Carlo methods of significant recent interest in the MCQMC community is the quantification of uncertainties in partial differential equation models. Uncertainty quantification for both forward problems and Bayesian inverse problems leads to high-dimensional integrals that are well-suited for QMC approximation. One of the approximations required in a general formulation as an affine-parametric operator equation is the truncation of the formally infinite-parametric operator to a finite number of dimensions. To date, a numerical study of the available theoretical convergence rates for this error have to the author's knowledge not been published. We present novel results for a selection of model problems, the computation of which has been enabled by recently developed, higher-order QMC methods based on interlaced polynomial lattice rules. Surprisingly, the observed rates are one order better in the case of integration over the parameters than the commonly cited theory suggests; a proof of this higher rate is included, resulting in a theoretical statement consistent with the observed numerics.

1 Introduction

An important application of quasi-Monte Carlo methods that has been of interest to the MCQMC community in recent years is the quantification of uncertainties in partial differential equation (PDE) models which depend on uncertain inputs, see e.g. [2, 5, 6, 7, 14, 15, 16, 18] to name but a few. The goal of computation is usually the mathematical expectation of a goal functional which depends on the solution to the PDE, corresponding to an integral over the uncertain inputs. Especially in the case where distributed uncertain inputs are considered, the problems often involve high-dimensional input parameter vectors, with the corresponding expectations being

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integrals over high-dimensional spaces. This fits naturally into a quasi-Monte Carlo framework, and various advances have been achieved in this field in recent years.

A large class of such problems can be formulated as so-called affine-parametric operator equations, for which many general theoretical results are available. These equations are formulated based on infinite parameter sequences, each corresponding to a realization of the uncertain input. In order to make computations feasible, a truncation to finitely many parameters is inevitable, and introduces an error into the computation. This error is called the *dimension truncation error*, and its study is the subject of this article.

Bounds on the dimension truncation error in this context are known [5, 15, 16], but to the author's knowledge, no numerical evidence has been published to support their sharpness. One reason for this may be that obtaining conclusive measurements is computationally very intensive, requiring approximations of integrals in a high number of dimensions to possibly very high accuracy, where each evaluation additionally involves an approximation of the solution to the operator equation by some numerical method, also with high precision. We fill this gap by providing measurements of this error for selected PDE test problems, where we apply a recently introduced higher-order quasi-Monte Carlo method based on interlaced polynomial lattice (IPL) rules [5, 11, 13] to attain the required accuracy in the approximation of the involved integral at reasonable cost. Combined with evaluation on a massively parallel computer system, approximations with sufficient accuracy are obtained in reasonable time.

Remarkably, the measured convergence rate of the error of an integral over the parameters in terms of the truncation dimension s is found to be one order higher than the current theoretical results as stated in e.g. [5, 7, 15, 16, 18]. This prompted a more detailed investigation into this convergence rate, and a proof of this higher rate is given below in Section 3 under some minor additional assumptions on the probability measure which are often fulfilled in practice. The higher rate shown here is due to a sharper analysis of the error, which was prompted by the reported numerical results.

We continue now by stating the setting of affine-parametric operator equations and present in Section 3 our main result, a novel estimate of the dimension truncation error which improves the known convergence rate by one order. In order to measure this error and verify the predicted rate, the higher-order QMC method used in the experiments is briefly mentioned in Section 4. Results supporting sharpness of the derived rate are then given in Section 5.

2 Affine-Parametric Operator Equations

Let \mathcal{X} , \mathcal{Y} denote two separable Banach spaces with norms $\|\cdot\|_{\mathcal{X}}$, $\|\cdot\|_{\mathcal{Y}}$ and duals \mathcal{X}' , \mathcal{Y}' , respectively. We denote by $\mathbf{y} = (y_1, y_2, \dots)$ a sequence of parameters taking values in $U = [-1/2, 1/2]^{\mathbb{N}}$, i.e. the set of sequences with entries $y_j \in [-1/2, 1/2]$. For each $\mathbf{y} \in U$, we denote by $A(\mathbf{y})$ a bounded linear operator from \mathcal{X} to \mathcal{Y}' ,

i.e. $A(\mathbf{y}) \in \mathcal{L}(\mathcal{X}, \mathcal{Y}')$. In the following, we denote by ${}_{\mathcal{Y}'}\langle \cdot, \cdot \rangle_{\mathcal{Y}}$ the duality pairing in \mathcal{Y} . Then, for a given deterministic forcing function $f \in \mathcal{Y}'$ we seek for $\mathbf{y} \in U$ a solution $q(\mathbf{y}) \in \mathcal{X}$ to the problem

$$A(\mathbf{y})q(\mathbf{y}) = f \quad \text{in } \mathcal{Y}'. \quad (1)$$

In the following, we will assume the operator $A(\mathbf{y})$ to depend on the y_j in an affine manner. More specifically, for a *nominal operator* A_0 and a sequence of *fluctuation operators* $(A_j)_{j \geq 1}$ we assume $A(\mathbf{y})$ to be of the form

$$A(\mathbf{y}) = A_0 + \sum_{j \geq 1} y_j A_j. \quad (2)$$

We now state some assumptions on $(A_j)_{j \geq 0}$ that are required for the well-posedness of (1) with $A(\mathbf{y})$ given by (2), or for the dimension truncation statements in Section 3.

Assumption 1. *Assume that the nominal operator $A_0 \in \mathcal{L}(\mathcal{X}, \mathcal{Y}')$ is boundedly invertible. Additionally, assume that the fluctuation operators $(A_j)_{j \geq 1}$ are small wrt. A_0 , i.e. there exists a $\kappa < 2$ such that for the sequence $\mathbf{b} = (b_1, b_2, \dots)$, defined by $b_j := \|A_0^{-1} A_j\|_{\mathcal{L}(\mathcal{X})}$ it holds that $\|\mathbf{b}\|_{\ell^1(\mathbb{N})} := \sum_{j \geq 1} b_j \leq \kappa < 2$, cp. [18, Ass. 2].*

Assumption 2. *Assume that there exists $0 < p < 1$ such that for $\mathbf{b} = (b_j)_{j \geq 1}$ from Assumption 1 it holds that $\mathbf{b} \in \ell^p(\mathbb{N})$, i.e. $\sum_{j \geq 1} b_j^p < \infty$.*

Assumption 3. *Assume the fluctuation operators $(A_j)_{j \geq 1}$ to be arranged such that $\mathbf{b} = (b_j)_{j \geq 1}$ from Assumption 1 is non-increasing.*

Proposition 1 ([18, Thm. 2]). *Under Assumption 1, for every parameter sequence $\mathbf{y} \in U = [-1/2, 1/2]^{\mathbb{N}}$ the parametric operator $A(\mathbf{y})$ is boundedly invertible. Furthermore, for any $\mathbf{y} \in U$ and any $f \in \mathcal{Y}'$, the weak parametric equation*

$${}_{\mathcal{Y}'}\langle A(\mathbf{y})q(\mathbf{y}), v \rangle_{\mathcal{Y}} = {}_{\mathcal{Y}'}\langle f, v \rangle_{\mathcal{Y}}, \quad \forall v \in \mathcal{Y}$$

admits a unique solution $q(\mathbf{y})$ and there holds the a-priori estimate

$$\sup_{\mathbf{y} \in U} \|q(\mathbf{y})\|_{\mathcal{X}} \leq C \|f\|_{\mathcal{Y}'},$$

where $C > 0$ is a constant independent of f .

Often, a quantity of interest (QoI) depending on the solution $q(\mathbf{y})$ is to be computed. We consider here as QoI a linear goal functional $G \in \mathcal{X}'$, and assume given a product probability measure $\boldsymbol{\mu}(\mathbf{y}) = \prod_{j \geq 1} \mu_j(y_j)$ on U . The goal of computation is the mathematical expectation

$$\mathbb{E}[G(q)] = \int_U G(q(\mathbf{y})) \boldsymbol{\mu}(d\mathbf{y}). \quad (3)$$

Examples of the goal functional G are point evaluation of the solution, or an average over (a subset of) the spatial domain. The following statement on the parametric

regularity of the solution, i.e. a bound on the partial derivatives of $q(\mathbf{y})$ with respect to the y_j , will be required for the higher-order quasi-Monte Carlo method to be presented in Section 4.

Proposition 2 ([5, Thm. 2.2]). *Let $\mathcal{F} = \{\mathbf{v} \in \mathbb{N}_0^{\mathbb{N}} : |\mathbf{v}| := \sum_{j \geq 1} v_j < \infty\}$ denote the set of finitely supported multiindices and denote by $\partial_{\mathbf{y}}^{\mathbf{v}}$ partial derivatives of order v_j with respect to coordinate y_j and let $q(\mathbf{y})$ be the solution to (1) with $A(\mathbf{y})$ as in (2) satisfying Assumption 1. Then, there exists a constant $C > 0$ and a sequence $\boldsymbol{\beta}$ satisfying Assumption 2 such that for all $f \in \mathcal{Y}^1$ and every $\mathbf{y} \in U$ it holds that*

$$\forall \mathbf{v} \in \mathcal{F} : \quad \|\partial_{\mathbf{y}}^{\mathbf{v}} q(\mathbf{y})\|_{\mathcal{X}} \leq C |\mathbf{v}|! \boldsymbol{\beta}^{\mathbf{v}} := C \left(\sum_{j \geq 1} v_j \right)! \prod_{j \geq 1} \beta_j^{v_j}.$$

2.1 Approximation

In order to obtain a computable approximation to (3), three approximations are required: (i) dimension truncation of the affine-parametric operator from (2), (ii) Petrov-Galerkin discretization of the equation (1) based on the dimensionally truncated operator, and (iii) quasi-Monte Carlo approximation of the integral over $\mathbf{y} \in U$.

We denote by $A^s(\mathbf{y}) = A(y_1, \dots, y_s, 0, \dots)$ the dimensionally truncated operator, and by $q^s(\mathbf{y})$ the solution to (1) based on $A^s(\mathbf{y})$. Petrov-Galerkin discretization yields for fixed $\mathbf{y} \in U$ a discrete solution $q_h^s(\mathbf{y})$ approximating $q^s(\mathbf{y})$, where the discretization parameter h usually signifies the maximal meshwidth when using the finite element method. The third and final approximation is replacing the integral over U by an N -point QMC quadrature rule with point set $\mathcal{P}_N = \{\mathbf{y}^{(0)}, \dots, \mathbf{y}^{(N-1)}\} \subset [0, 1]^s$, yielding the full approximation

$$\mathbb{E}[G(q)] = \int_U G(q(\mathbf{y})) \boldsymbol{\mu}(\mathrm{d}\mathbf{y}) \quad \approx \quad \frac{1}{N} \sum_{n=0}^{N-1} G(q_h^s(\mathbf{y}^{(n)} - \mathbf{1}/2)). \quad (4)$$

By the triangle inequality, we can write the total error $E_{s,h,N}$ as

$$\begin{aligned} E_{s,h,N} &= \left| \int_U G(q(\mathbf{y})) \boldsymbol{\mu}(\mathrm{d}\mathbf{y}) - \frac{1}{N} \sum_{n=0}^{N-1} G(q_h^s(\mathbf{y}^{(n)} - \mathbf{1}/2)) \right| \\ &\leq \left| \int_U G(q_h^s(\mathbf{y})) \boldsymbol{\mu}(\mathrm{d}\mathbf{y}) - \frac{1}{N} \sum_{n=0}^{N-1} G(q_h^s(\mathbf{y}^{(n)} - \mathbf{1}/2)) \right| \\ &\quad + \left| \int_U G(q^s(\mathbf{y})) - G(q_h^s(\mathbf{y})) \boldsymbol{\mu}(\mathrm{d}\mathbf{y}) \right| + \left| \int_U G(q(\mathbf{y})) - G(q^s(\mathbf{y})) \boldsymbol{\mu}(\mathrm{d}\mathbf{y}) \right|. \quad (5) \end{aligned}$$

The dimension truncation error is the last term in (5), which we will bound in the following section and approximate computationally in Section 5. In order to do the latter, we must still rely on an approximation of the form (4), in principle choosing

N and h large and small enough, respectively, to ensure that the first two errors are negligible. We comment more on the choice of these values in Section 5 below.

3 Dimension Truncation Error Estimates

We begin by recalling existing estimates on the dimension truncation error pointwise in \mathbf{y} , i.e. $\|q(\mathbf{y}) - q^s(\mathbf{y})\|_{\mathcal{X}}$. Then, we detail in Theorem 1 a novel result which gives a statement on the convergence of the error of the integral $|\int_U G(q(\mathbf{y}) - q^s(\mathbf{y})) d\mathbf{y}|$ in the truncation dimension s , improving upon known bounds.

Proposition 3. *For every $f \in \mathcal{Y}'$, $\mathbf{y} \in U$, $s \in \mathbb{N}$, denote by $q^s(\mathbf{y})$ the solution to a problem of the form $A^s(\mathbf{y})q^s(\mathbf{y}) = f$ with $A^s(\mathbf{y}) = A(y_1, \dots, y_s, 0, \dots)$. Let Assumptions 1 and 2 hold, and assume additionally that μ_j is such that $\int_U y_j \mu_j(dy_j) = 0$ for all $j \geq 1$. Then, for a constant $C > 0$ which is independent of s and f it holds that*

$$\forall \mathbf{y} \in U : \quad \|q(\mathbf{y}) - q^s(\mathbf{y})\|_{\mathcal{X}} \leq C \|f\|_{\mathcal{Y}'} s^{-1/p+1}. \quad (6)$$

Proof. See e.g. [1, 5, 15]. \square

We now make the following additional assumption on the measure μ , noting that the first part holds in particular for all symmetric distributions.

Assumption 4. *Assume that $\mu(\mathbf{y}) = \prod_{j \geq 1} \mu_j(y_j)$ is a product probability measure and that the factor measures μ_j on the parameters y_j are such that for all $j \geq 1$ it holds that $\int_{-1/2}^{1/2} y_j \mu_j(dy_j) = 0$ and $\int_{-1/2}^{1/2} y_j^k \mu_j(dy_j) \leq C_k < \infty$ for all integers $k \geq 2$.*

In [15], the bound $|\int_U q(\mathbf{y}) - q^s(\mathbf{y}) d\mathbf{y}| \leq C s^{-2(1/p-1)}$ was shown for equations of the type considered here under Assumption 2 and $\int_{-1/2}^{1/2} y_j \mu(dy_j) = 0$, which we improve here to $\mathcal{O}(s^{-2/p+1})$, which is one order better. We begin by proving the following Lemma.

Lemma 1. *Let $A^s(\mathbf{y})$ denote the operator $A(\mathbf{y})$ of the form (2) truncated after dimension s , i.e. $A^s(\mathbf{y}) = A(y_1, \dots, y_s, 0, \dots)$. Assume Assumptions 1 and 3. Then, for sufficiently large s it holds that*

$$\sup_{\mathbf{y} \in U} \|(A^s(\mathbf{y}))^{-1}(A(\mathbf{y}) - A^s(\mathbf{y}))\|_{\mathcal{L}(\mathcal{X})} \leq \frac{1}{2 - \kappa} \sum_{j > s} b_j < 1. \quad (7)$$

Proof. We have $\|(A^s)^{-1}(A - A^s)\|_{\mathcal{L}(\mathcal{X})} \leq \|(A^s)^{-1}A_0\|_{\mathcal{L}(\mathcal{X})} \|A_0^{-1}(A - A^s)\|_{\mathcal{L}(\mathcal{X})}$, which we bound individually. For the first factor, Assumption 1 implies that for all $\mathbf{y} \in U$ it holds that $\|A_0^{-1}A^s\|_{\mathcal{L}(\mathcal{X})} \leq \sum_{j=1}^s y_j \|A_0^{-1}A_j\|_{\mathcal{L}(\mathcal{X})} < 1$, implying with the Neumann series the bound

$$\|(A^s)^{-1}A_0\|_{\mathcal{L}(\mathcal{X})} = \|(A_0^{-1}A^s)^{-1}\|_{\mathcal{L}(\mathcal{X})} \leq \frac{1}{1 - \frac{1}{2} \sum_{j=1}^s b_j} \leq \frac{1}{1 - \frac{1}{2} \|\mathbf{b}\|_{\ell^1(\mathbb{N})}}. \quad (8)$$

For the second factor, we have

$$\|A_0^{-1}(A - A^s)\|_{\mathcal{L}(\mathcal{X})} = \|A_0^{-1} \sum_{j>s} y_j A_j\|_{\mathcal{L}(\mathcal{X})} \leq \frac{1}{2} \sum_{j>s} \|A_0^{-1} A_j\|_{\mathcal{L}(\mathcal{X})} = \frac{1}{2} \sum_{j>s} b_j.$$

Combining these two bounds and recalling $\|\mathbf{b}\|_{\ell^1(\mathbb{N})} \leq \kappa$ yields the first inequality. The bound is less than 1 for sufficiently large s since $\mathbf{b} \in \ell^1(\mathbb{N})$ and the b_j are assumed in Assumption 3 to be non-increasing. \square

Theorem 1. *For every $s \in \mathbb{N}$, denote by $q^s(\mathbf{y})$ the solution to a problem of the form $A^s q^s = f$ with A^s as in (2) where $\mathbf{y} = (y_1, \dots, y_s, 0, \dots)$. Let Assumptions 1 to 4 hold. Then, for any $s \in \mathbb{N}$, $f \in \mathcal{X}'$ and $G \in \mathcal{X}'$ there exists a constant $C > 0$ which is independent of s , f and G such that*

$$\left| \int_U G(q(\mathbf{y}) - q^s(\mathbf{y})) \boldsymbol{\mu}(\mathbf{d}\mathbf{y}) \right| \leq C \|G\|_{\mathcal{X}'} \|f\|_{\mathcal{X}'} s^{-2/p+1}. \quad (9)$$

Proof. Assumption 1 implies bounded invertibility of $A(\mathbf{y})$ and $A^s(\mathbf{y})$ for any $\mathbf{y} \in U$, thus we can write (omitting the argument \mathbf{y} for legibility) $A = A^s + A - A^s = A^s(I + (A^s)^{-1}(A - A^s))$. We aim to write the inverse of A given in this form as a Neumann series, which is justified for suitably large s by Lemma 1. Thus, we have

$$A^{-1} = (I + (A^s)^{-1}(A - A^s))^{-1} (A^s)^{-1} = \sum_{k \geq 0} (-(A^s)^{-1}(A - A^s))^k (A^s)^{-1}.$$

Fubini's theorem, together with linearity of G and of the integral then implies

$$\begin{aligned} \int_U G(q(\mathbf{y}) - q^s(\mathbf{y})) \boldsymbol{\mu}(\mathbf{d}\mathbf{y}) &= \int_U G((A^{-1} - (A^s)^{-1})f) \boldsymbol{\mu}(\mathbf{d}\mathbf{y}) \\ &= \int_U G\left(\sum_{k \geq 1} \left(-\sum_{j>s} y_j (A^s)^{-1} A_j\right)^k q^s\right) \boldsymbol{\mu}(\mathbf{d}\mathbf{y}) \\ &= \sum_{k \geq 1} (-1)^k \int_U G\left(\left(\sum_{j>s} y_j (A^s)^{-1} A_j\right)^k q^s\right) \boldsymbol{\mu}(\mathbf{d}\mathbf{y}). \quad (10) \end{aligned}$$

We assume now additionally Assumptions 2 and 3. Then, using a similar approach as in [15], we obtain for $k' \in \mathbb{N}$ and a constant $C_{f,G} > 0$ the bound

$$\begin{aligned} \left| \sum_{k \geq k'} (-1)^k \int_U G\left(\left(\sum_{j>s} y_j (A^s)^{-1} A_j\right)^k q^s\right) \boldsymbol{\mu}(\mathbf{d}\mathbf{y}) \right| & \quad (11) \\ \leq C \|G\|_{\mathcal{X}'} \|f\|_{\mathcal{X}'} \sup_{\mathbf{y} \in U} \sum_{k \geq k'} \|(A^s)^{-1}(A - A^s)\|_{\mathcal{L}(\mathcal{X})}^k & \leq C_{f,G} s^{k'(-1/p+1)}. \end{aligned}$$

The above gives a bound for the remainder of the sum over k , starting at term k' ; our goal now is to bound the terms up to k' by a better estimate. To this end, we use linearity of G and the integral, as well as the identity $(\sum_{j>s} y_j (A^s)^{-1} A_j)^k = \sum_{\boldsymbol{\eta} \in \{j>s\}^k} \prod_{i=1}^k (y_{\eta_i} (A^s)^{-1} A_{\eta_i})$, which respects the generally non-commutative nature

of the operators. Denoting by $U_s = [-1/2, 1/2]^s$ the truncated parameter domain and setting $\boldsymbol{\mu}_s(\mathbf{y}_s) := \prod_{j=1}^s \mu_j(y_j)$ we obtain

$$\begin{aligned} & \int_U G\left(\left(\sum_{j>s} y_j (A^s)^{-1} A_j\right)^k q^s\right) \boldsymbol{\mu}(\mathbf{d}\mathbf{y}) \\ &= \sum_{\boldsymbol{\eta} \in \{j>s\}^k} \int_U G\left(\left(\prod_{i=1}^k y_{\eta_i}\right) \prod_{i=1}^k ((A^s)^{-1} A_{\eta_i}) q^s\right) \boldsymbol{\mu}(\mathbf{d}\mathbf{y}) \\ &= \sum_{\boldsymbol{\eta} \in \{j>s\}^k} \int_U \left(\prod_{i=1}^k y_{\eta_i}\right) \boldsymbol{\mu}(\mathbf{d}\mathbf{y}) \int_{U_s} G\left(\prod_{i=1}^k ((A^s)^{-1} A_{\eta_i}) q^s\right) \boldsymbol{\mu}_s(\mathbf{d}\mathbf{y}_s). \end{aligned}$$

It is important to note that the functional G in the last statement is applied to an expression that depends only on the first s dimensions (through A^s and q^s), allowing the integral with respect to y_j for $j > s$ to be separated out. See also the proof of [10, Prop. 8] for a similar argument. For any $\boldsymbol{\eta} \in \{j > s\}^k$ it holds that

$$\begin{aligned} & \int_U G\left(\left(\prod_{i=1}^k y_{\eta_i}\right) \prod_{i=1}^k ((A^s)^{-1} A_{\eta_i}) q^s\right) \boldsymbol{\mu}(\mathbf{d}\mathbf{y}) \\ &= \int_U \int_{U_s} \left(\prod_{i=1}^k y_{\eta_i}\right) G\left(\prod_{i=1}^k ((A^s)^{-1} A_{\eta_i}) q^s\right) \boldsymbol{\mu}_s(\mathbf{d}\mathbf{y}_s) \boldsymbol{\mu}(\mathbf{d}\mathbf{y}) \\ &= \int_U \left(\prod_{i=1}^k y_{\eta_i}\right) \int_{U_s} G\left(\prod_{i=1}^k ((A^s)^{-1} A_{\eta_i}) q^s\right) \boldsymbol{\mu}_s(\mathbf{d}\mathbf{y}_s) \boldsymbol{\mu}(\mathbf{d}\mathbf{y}) \\ &= \int_U \left(\prod_{i=1}^k y_{\eta_i}\right) \boldsymbol{\mu}(\mathbf{d}\mathbf{y}) \int_{U_s} G\left(\prod_{i=1}^k ((A^s)^{-1} A_{\eta_i}) q^s\right) \boldsymbol{\mu}_s(\mathbf{d}\mathbf{y}_s). \end{aligned}$$

We will now introduce various definitions required below: let $\mathbf{v}(\boldsymbol{\eta}) := (\#\{i = 1, \dots, k : \eta_i = j\})_{j \geq 1}$, i.e. $v_j(\boldsymbol{\eta}) \in \{0, \dots, k\}$ for $j \geq 1$, define the support of a multi-index $\mathbf{v} \in \mathcal{F}$ by $\text{supp}(\mathbf{v}) := \{j \in \mathbb{N} : v_j \neq 0\}$ and let $\#S$ denote the cardinality of a set S . Note that $\min \text{supp} \mathbf{v}(\boldsymbol{\eta}) > s$ as well as $\# \text{supp}(\mathbf{v}(\boldsymbol{\eta})) \leq k$ for $\boldsymbol{\eta} \in \{j > s\}^k$ as in the sums above. Thus, for every such $\boldsymbol{\eta}$ we can write $\prod_{i=1}^k y_{\eta_i} = \prod_{j>s} y_j^{v_j(\boldsymbol{\eta})} = \mathbf{y}^{\mathbf{v}(\boldsymbol{\eta})}$, where the product is over a finite set since $\mathbf{v}(\boldsymbol{\eta})$ is finitely supported.

Assumption 4 now directly implies that all terms where $v_j = 1$ for at least one $j > s$ are zero. For $k = 1$, $v_j \in \{0, 1\}$ for all $j > s$, thus all terms contain at least one exponent equal to 1 and are zero. We consider in the following $k \geq 2$, and aim to rewrite the sum over $\boldsymbol{\eta}$ as a sum over the set $\mathcal{F}_{k,s} := \{\mathbf{v} \in \mathcal{F} : |\mathbf{v}| = k, \min \text{supp}(\mathbf{v}) > s, v_j \neq 1 \forall j\}$. For all $\mathbf{v} \in \mathcal{F}_{k,s}$ it holds that $\# \text{supp}(\mathbf{v}) \leq k/2$, since the smallest nonzero element is 2, and we have the condition $|\mathbf{v}| = k$. We define $c_{\mathbf{v}} := \left| \int_U \mathbf{y}^{\mathbf{v}} \boldsymbol{\mu}(\mathbf{d}\mathbf{y}) \right|$, which, since $\# \text{supp}(\mathbf{v}) \leq k/2$ and recalling the definition of C_k from Assumption 4 fulfills $c_{\mathbf{v}} \leq \prod_{j \in \text{supp}(\mathbf{v})} C_{v_j} \leq (\max_{j>s} C_{v_j})^{k/2}$. Defining $C_{f,G} := \|G\|_{\mathcal{X}'} \|f\|_{\mathcal{Y}'}$ and writing $\boldsymbol{\mu}_{\{1:s\}}(\mathbf{y}) = \prod_{j=1}^s \mu_j(y_j)$, we have

$$\begin{aligned}
& \left| \sum_{\boldsymbol{\eta} \in \{j>s\}^k} \int_U \left(\prod_{j>s} y_j^{v_j(\boldsymbol{\eta})} \right) \boldsymbol{\mu}(\mathbf{d}\mathbf{y}) \int_{U_s} G \left(\prod_{i=1}^k ((A^s)^{-1} A_{\eta_i}) q^s \right) \boldsymbol{\mu}_{\{1:s\}}(\mathbf{d}\mathbf{y}) \right| \\
& \leq C_{f,G} \sum_{\boldsymbol{\eta} \in \{j>s\}^k} c_{\mathbf{v}(\boldsymbol{\eta})} \int_{U_s} \prod_{i=1}^k \|((A^s)^{-1} A_{\eta_i})\|_{\mathcal{L}(\mathcal{X})} \boldsymbol{\mu}_{\{1:s\}}(\mathbf{d}\mathbf{y}) \\
& = C_{f,G} \sum_{\mathbf{v} \in \widetilde{\mathcal{F}}_{k,s}} \binom{k}{\mathbf{v}} c_{\mathbf{v}} \int_{U_s} \prod_{j>s} \|((A^s)^{-1} A_j)\|_{\mathcal{L}(\mathcal{X})}^{v_j} \boldsymbol{\mu}_{\{1:s\}}(\mathbf{d}\mathbf{y}).
\end{aligned}$$

We bound $\sup_{\mathbf{y} \in U} \|(A^s)^{-1} A_j\|_{\mathcal{L}(\mathcal{X})} \leq (1 - \kappa/2)^{-1} b_j =: \widetilde{b}_j$ similar to (8) and $\binom{k}{\mathbf{v}} c_{\mathbf{v}} \leq c_k := (\max_{j>s} C_{v_j})^{k/2} k!$. Let $\widetilde{\mathcal{F}}_{k,s} := \{\mathbf{v} \in \mathcal{F} : |\mathbf{v}|_{\infty} \leq k, \mathbf{v} \neq \mathbf{0}, \min \text{supp}(\mathbf{v}) > s, v_j \neq 1 \forall j\}$, where we observe that $\widetilde{\mathcal{F}}_{k,s} \supset \mathcal{F}_{k,s}$, which yields with $\widetilde{b}_j \geq 0$ for all $j \geq 1$

$$C_{f,G} \sum_{\mathbf{v} \in \mathcal{F}_{k,s}} \binom{k}{\mathbf{v}} c_{\mathbf{v}} \int_{U_s} \prod_{j>s} \|((A^s)^{-1} A_j)\|_{\mathcal{L}(\mathcal{X})}^{v_j} \boldsymbol{\mu}_{\{1:s\}}(\mathbf{d}\mathbf{y}) \leq c_k C_{f,G} \sum_{\mathbf{v} \in \widetilde{\mathcal{F}}_{k,s}} \prod_{j>s} \widetilde{b}_j^{v_j}.$$

We now rewrite the sum over $\widetilde{\mathcal{F}}_{k,s}$ as the product of a sum, since we notice that every element of the set $\widetilde{\mathcal{F}}_{k,s}$ (resulting in a term $\widetilde{\mathbf{b}}^{\mathbf{v}}$) corresponds to one term of the product $\prod_{j>s} (1 + \sum_{\ell=2}^k \widetilde{b}_j^{\ell})$, with the exception of the additional term 1 (corresponding to $\mathbf{v} = \mathbf{0}$, which is excluded in $\widetilde{\mathcal{F}}_{k,s}$), that we subtract. Defining $\widehat{b}_j^2 := \widetilde{b}_j^2 (1 - \widetilde{b}_j)^{-1}$, it holds that $(\widehat{b}_j)_{j \geq 1} \in \ell^p(\mathbb{N})$ and $\widehat{b}_j < 1$ for all $j > s$ for suitably large s . The first term in parenthesis below can thus be rewritten using basic properties of the geometric series,

$$\begin{aligned}
\sum_{\mathbf{v} \in \widetilde{\mathcal{F}}_{k,s}} \widetilde{\mathbf{b}}^{\mathbf{v}} &= \prod_{j>s} \left(1 + \sum_{\ell=2}^k \widetilde{b}_j^{\ell} \right) - 1 = \prod_{j>s} \left(1 + \widetilde{b}_j^2 \frac{1 - \widetilde{b}_j^{k-1}}{1 - \widetilde{b}_j} \right) - 1 \leq \prod_{j>s} \left(1 + \widehat{b}_j^2 \right) - 1 \\
&= \exp \left(\sum_{j>s} \log(1 + \widehat{b}_j^2) \right) - 1 \leq C \sum_{j>s} \widehat{b}_j^2 \leq \frac{C}{1 - s^{-2/p+1}} s^{-2/p+1}. \quad (12)
\end{aligned}$$

We recall the Neumann series (10), for which the $k = 1$ term is zero, and split it into a sum over $k = 2, \dots, k' - 1 < \infty$, where each term is bounded from above by (12) times the constants $c_k C_{f,G} < \infty$, and a remainder with $k \geq k'$ for which we use (11). For each $p < 1$, the choice $k' = k'(p) = \lceil (2-p)/(1-p) \rceil < \infty$ ensures that the remainder converges at least as rapidly as the estimate $s^{-2/p+1}$. Collecting terms then yields the statement. \square

For fast decay of the sequence \mathbf{b} from Assumption 2, i.e. for small values of p , the convergence rate of the dimension truncation error of the integral from Theorem 1 can be quite high. Balancing the required finite element and quadrature approximation errors with the possibly very small values of the dimension truncation error would result in a large number of samples, and consequently a large amount of work, even for moderate s . A standard Monte Carlo method converging like $N^{-1/2}$ in the number

of samples N is thus not feasible, as the number of required samples is much too large. A QMC method converging at rate 1 is better, but for small p is still not accurate enough to allow these computations to be executed in a reasonable amount of time.

Other approaches may converge more quickly, for example adaptive Smolyak or sparse grid-type quadrature methods [12, 17]. However, these are inherently serial, and the computational cost due to the involved internal bookkeeping overhead also increases rapidly if high accuracies are required. Thus, the only method known to the author to perform well enough (in terms of convergence rate and amenability to parallel implementation) for such measurements to be performed for a large range of values of $0 < p < 1$ and in high enough dimension to yield conclusive results is the higher-order QMC method of [5, 13] based on interlaced polynomial lattice rules, which we now briefly describe.

4 Interlaced Polynomial Lattice Rules

For the presentation of interlaced polynomial lattice (IPL) rules, we require some definitions and notation. A polynomial lattice rule (without interlacing for the moment) is an equal-weight quadrature rule with $N = b^m$ points for some prime number b and positive integer m , and is given by a *generating vector* whose components are polynomials of degree less than m over the finite field \mathbb{Z}_b . Let $\mathbb{Z}_b[x]$ denote the set of all polynomials over \mathbb{Z}_b , i.e. polynomials of the form $\sum_{k=0}^{m-1} \xi_k x^k$ with $\xi_k \in \mathbb{Z}_b$. Then, the generating vector is denoted by $\mathbf{q} \in (\mathbb{Z}_b[x])^s$ with $\mathbf{q} = (q_j(x))_{j=1}^s$. We associate with each integer $n = 0, \dots, b^m - 1$ a polynomial $n(x) = \sum_{k=0}^{m-1} \xi_k x^k$, where ξ_k are the digits of n in base b , that is $n = \xi_0 + \xi_1 b + \xi_2 b^2 + \dots + \xi_{m-1} b^{m-1}$. To obtain points in $[0, 1]^s$ from the generating vector \mathbf{q} , we require the mapping $v_m: \mathbb{Z}_b(x^{-1}) \rightarrow [0, 1)$ which is given for any integer w by

$$v_m \left(\sum_{k=w}^{\infty} \xi_k x^{-k} \right) = \sum_{k=\max(1,w)}^m \xi_k b^{-k}.$$

For an irreducible polynomial $P \in \mathbb{Z}_b[x]$ of degree equal to m , the j -th component of the n -th point of the point set $\mathcal{P}_N = \{\mathbf{y}^{(0)}, \dots, \mathbf{y}^{(N-1)}\}$ is given by

$$(\mathbf{y}^{(n)})_j = v_m \left(\frac{n(x)q_j(x)}{P(x)} \right), \quad n = 0, \dots, N-1, \quad j = 1, \dots, s.$$

To obtain orders of convergence higher than one, we require an additional interlacing step. To this end, we denote the digit interlacing function of $\alpha \in \mathbb{N}$ points as $D_\alpha: [0, 1)^\alpha \rightarrow [0, 1)$,

$$D_\alpha(x_1, \dots, x_\alpha) = \sum_{a=1}^{\infty} \sum_{j=1}^{\alpha} \xi_{j,a} b^{-j-(a-1)\alpha},$$

where $\xi_{j,a}$ is the a -th digit in the expansion of the j -th point $x_j \in [0, 1)$ in base b^{-1} , $x_j = \xi_{j,1}b^{-1} + \xi_{j,2}b^{-2} + \dots$. For vectors in αs dimensions, digit interlacing is defined block-wise and denoted by $\mathcal{D}_\alpha: [0, 1)^{\alpha s} \rightarrow [0, 1)^s$ with

$$\mathcal{D}_\alpha(x_1, \dots, x_{\alpha s}) = (D_\alpha(x_1, \dots, x_\alpha), D_\alpha(x_{\alpha+1}, \dots, x_{2\alpha}), \dots, D_\alpha(x_{(s-1)\alpha+1}, \dots, x_{s\alpha})).$$

For a generating vector $\mathbf{q} \in (\mathbb{Z}_b[x])^{\alpha s}$ containing α components for each of the s dimensions, the interlaced polynomial lattice point set is $\mathcal{D}_\alpha(\widetilde{\mathcal{P}}_N) \subset [0, 1)^s$, where $\widetilde{\mathcal{P}}_N \subset [0, 1)^{\alpha s}$ denotes the (classical) polynomial lattice point set in αs dimensions with generating vector \mathbf{q} . For more details on this method, see e.g. [5, 11, 13]. The following proposition states the higher order rates that are obtainable under suitable sparsity assumptions of the form stated in Proposition 2.

Proposition 4 ([5, Thm. 3.1]). *For $m \geq 1$ and a prime number b , denote by $N = b^m$ the number of QMC points. Let $s \geq 1$ and $\boldsymbol{\beta} = (\beta_j)_{j \geq 1}$ be a sequence of positive numbers, and let $\boldsymbol{\beta}_s = (\beta_j)_{1 \leq j \leq s}$ denote the first s terms of $\boldsymbol{\beta}$. Assume that $\boldsymbol{\beta} \in \ell^p(\mathbb{N})$ for some $p \in (0, 1)$.*

If there exists a $c > 0$ such that for $\alpha := \lfloor 1/p \rfloor + 1$ a function F satisfies

$$\forall \mathbf{v} \in \{0, 1, \dots, \alpha\}^s, \forall s \in \mathbb{N}: \quad |(\partial_{\mathbf{y}}^{\mathbf{v}} F)(\mathbf{y})| \leq c |\mathbf{v}|! \boldsymbol{\beta}_s^{\mathbf{v}}, \quad (13)$$

then an interlaced polynomial lattice (IPL) rule of order α with N points can be constructed in $\mathcal{O}(\alpha s N \log N + \alpha^2 s^2 N)$ operations, such that for the quadrature error it holds that

$$|I_s(F) - \mathcal{Q}_{N,s}(F)| \leq C_{\alpha, \boldsymbol{\beta}, b, p, F} N^{-1/p}, \quad (14)$$

where the constant $C_{\alpha, \boldsymbol{\beta}, b, p, F} < \infty$ is independent of s and N .

5 Experiments

We consider three different examples that fit into the affine-parametric framework, and measure the dimension truncation error for each one, both for the pointwise case and for the integral case. For the latter, we verify in all three cases that the bound from Theorem 1 corresponds to the measured rates, for various values of the fluctuation summability exponent p . The results thus give concrete evidence supporting the sharpness of both estimates. Below, we specify the fluctuation decay rate $\zeta > 1$, which implies p -summability for any $p > 1/\zeta$. Using the limiting value $p = 1/\zeta$, we expect the dimension truncation convergence rate $s^{-\zeta+1}$ for the pointwise case and rate $s^{-2\zeta+1}$ for the integral case, cf. Proposition 3 and Theorem 1, respectively. For the computations of the pointwise error, we use the parameter value $\mathbf{y} = e^{-2} \mathbf{1} = e^{-2}(1, 1, \dots) \in U$.

5.1 Example 1: Test Integrand

The first example is designed to serve as a simplified test case that does not require finite element discretization, since the operator equation simplifies to an algebraic equation, see also [11, Eq. 18]. We seek to approximate the integral over $U = [-1/2, 1/2]^N$ of the “solution” $q(\mathbf{y})$ which is given in this case by

$$q(\mathbf{y}) = \left(1 + \sum_{j \geq 1} y_j c_j\right)^{-1}, \quad c_j = \sigma j^{-\zeta}, \quad \sigma = 0.1. \quad (15)$$

We thus circumvent the finite element discretization error, but must still ensure that the QMC error is small enough. For a rough estimate of the number of QMC points $N = 2^m$, consider decay rate ζ and truncation dimension $s = 2^\beta$ for some $\beta > 1$. Then, by Theorem 1 the dimension truncation error is of order $s^{-2\zeta+1} = 2^{(-2\zeta+1)\beta}$. By Proposition 4, the QMC error converges like $N^{-\zeta} = 2^{-m\zeta}$. Assuming the constants in the error estimates to be equal, we thus require $2^{-m\zeta} < 2^{(-2\zeta+1)\beta}$, implying $m > (2 - 1/\zeta)\beta$. For $s = 1024$ we have $\beta = 10$ and obtain with $\zeta = 2$ the condition $m > 15$. Below, we use $m = 18$, which suffices for the considered values of ζ up to 3 and yields clear measurements of the integral dimension truncation error.

For this example, since no finite element solver is needed and efficiency is not such an issue, the implementation was conducted in Python with the higher-order QMC rules applied with the `pyQMC` library, see [8]. The required generating vectors were obtained by fast CBC construction [11] and are available at [8] under the heading “Standard SPOD Weights”. For the computations below, we used the parameters $\alpha = 2$, $C = 0.1$, and $\theta = 0.2$. The reference approximations in $s = 1024$ dimensions with an IPL rule based on $N = 2^{18}$ points are given for $\zeta = 1.5, 2, 2.5, 3$ by 1.0010038828766668, 1.0009035434306022, 1.0008655151823671, and 1.0008491110838873, respectively.

As shown in the results in Figure 1, the expected convergence rates can be clearly observed in both cases. We note that this example additionally allows straightforward computation of the integrals in (10) for arbitrary k , allowing verification of the individual estimates in the proof.

5.2 Example 2: Diffusion Equation in One Dimension

We formulate here a model diffusion equation in spatial dimension $d = 1, 2$ for use in this and the next example. Denoting by $D \subset \mathbb{R}^d$ a bounded domain, for any $\mathbf{y} \in U$ we seek $q(\cdot, \mathbf{y}) \in \mathcal{X} = \mathcal{Y} = H_0^1(D)$ such that

$$-\nabla \cdot (u(x, \mathbf{y}) \nabla q(x, \mathbf{y})) = f(x) \text{ in } D, \quad q(x, \mathbf{y}) = 0 \text{ on } \partial D, \quad (16)$$

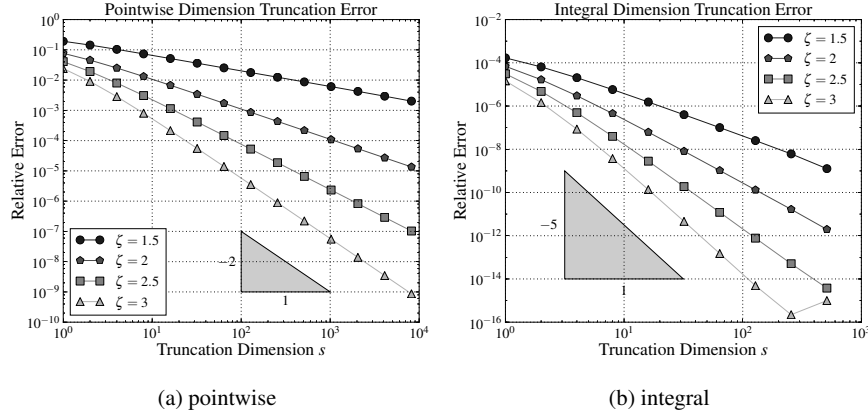


Fig. 1: Dimension truncation error for the test integrand (15). (a) pointwise dimension truncation error $|q(\mathbf{y}) - q^s(\mathbf{y})|$ for $\mathbf{y} = e^{-2}\mathbf{1}$ with $q(\mathbf{y})$ approximated by a reference value in $s = 2^{15}$ dimensions, with expected rate $-\zeta + 1$. (b) integral dimension truncation error $|\int_U q(\mathbf{y}) - q^s(\mathbf{y}) d\mathbf{y}|$ with reference dimension $s = 1024$ and expected rate $-2\zeta + 1$. Higher-order QMC based on IPL rules was used with $N = 2^{18}$ points. The expected rates are clearly observed in both cases.

where $u(x, \mathbf{y}) \in \mathbb{R}$ denotes for each \mathbf{y} a spatially varying diffusion coefficient. It is well-known that the following assumption implies that there exists a unique solution to (16) for any sequence $\mathbf{y} \in U$.

Assumption 5 (Uniform ellipticity). *There exist constants $u^-, u^+ > 0$ such that for all $\mathbf{y} \in U$ and for almost every $x \in D$ it holds that $0 < u^- \leq u(x; \mathbf{y}) \leq u^+$.*

An affine-parametric partial differential equation is obtained for example by the following choice of coefficient parametrization,

$$u(x; \mathbf{y}) = u_0 + \sum_{j \geq 1} y_j \psi_j(x), \quad x \in D, \mathbf{y} \in U. \quad (17)$$

In the one-dimensional case we use the parametric basis functions $\psi_{2j}(x) = (2j)^{-\zeta} \sin(j\pi x)$ and $\psi_{2j-1}(x) = (2j-1)^{-\zeta} \cos(j\pi x)$.

For simplicity of implementation, we compute the convergence of the pointwise dimension truncation error by applying a linear goal functional $G \in \mathcal{X}'$ and observing with Proposition 3 that

$$|G(q(\mathbf{y})) - G(q^s(\mathbf{y}))| \leq \|G\|_{\mathcal{X}'} \|q - q^s\|_{\mathcal{X}} \leq C \|G\|_{\mathcal{X}'} \|f\|_{\mathcal{Y}'} s^{-1/p+1}.$$

We choose as goal functional integration over the spatial domain D , $G(q(\mathbf{y})) = \int_D q(x, \mathbf{y}) dx$ and set $f(x) = 10x$. Finite element discretization with standard piecewise linear finite elements on an equidistant mesh of $D = [0, 1]$ with meshwidth h is used. Since no exact solution is available, we resort to using a reference solution with

truncation dimension chosen to be twice the number of dimensions in the most precise measurement, see the caption of Figure 2 for details. The finite element meshwidth was the same for all computations and chosen to be $h = 2^{-18}$. Note that this is not sufficient to completely remove the finite element error; in the plots below, we consider convergence of $\int_U G(q_h^s(\mathbf{y})) \, d\mathbf{y}$ to $\int_U G(q_h(\mathbf{y})) \, d\mathbf{y}$, for fixed h . In this case, we can use the same generating vectors as for Example 1 but with $m = 20$.

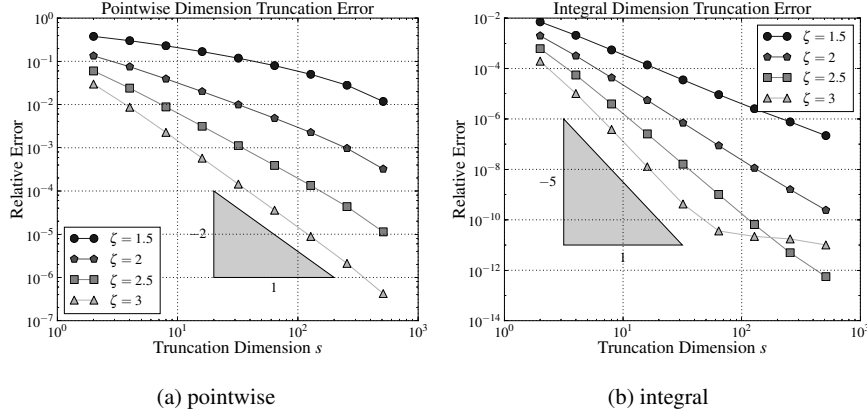


Fig. 2: Dimension truncation error for the diffusion equation with $d = 1$. (a) pointwise dimension truncation error $|q_h(\mathbf{y}) - q_h^s(\mathbf{y})|$ for $\mathbf{y} = e^{-2}\mathbf{1}$ with $q_h(\mathbf{y})$ approximated by a reference value in $s = 2^{15}$ dimensions, with expected rate $-\zeta + 1$. (b) integral dimension truncation error $|\int_U q_h(\mathbf{y}) - q_h^s(\mathbf{y}) \, d\mathbf{y}|$ with reference dimension $s = 1024$ and expected rate $-2\zeta + 1$. The expected rates are clearly observed in both cases.

5.3 Example 3: Diffusion Equation in Two Dimensions

We consider here again (16) as in Example 2, but in two spatial dimensions, requiring a different choice of fluctuation basis, see also related experiments in [3, 4]. The parametrization is given in terms of the eigenfunctions of the Dirichlet Laplacian on $D = (0, 1)^2$, where we choose the fluctuations $\psi_j(x) = (k_{1,j}^2 + k_{2,j}^2)^{-\zeta} \sin(\pi k_{1,j} x_1) \sin(\pi k_{2,j} x_2)$ by reordering the tuples $(k_{1,j}, k_{2,j}) \in \mathbb{N}^2$ such that $(\|\psi_j(x)\|_{L^\infty(D)})_{j \geq 1}$ is non-increasing. Choosing the deterministic right-hand side $f(x) = 100x_1$ results in an affine-parametric PDE satisfying Assumption 2 with $p > 1/\zeta$. The pointwise dimension truncation error is again computed by considering a goal functional as detailed in Example 2 above, where this time we choose as goal functional the integral over $\tilde{D} = (1/2, 1)^2 \subset D$, i.e. $G(q(\mathbf{y})) = \int_{\tilde{D}} q(x, \mathbf{y}) \, dx$.

For spatial discretization, we use a tensor product mesh with nodes obtained from the Cartesian product of equidistant nodes on $(0, 1)$, with standard piecewise bilinear finite element basis functions. The one-dimensional meshwidth is 2^{-6} ,

resulting in $\mathcal{O}(2^{12})$ degrees of freedom. In this example and the previous one, a C++ implementation was used for efficiency reasons. The IPL rules were applied using the `gMLQMC` library [9] and the evaluation was conducted on the Piz Daint HPC system of CSCS with up to 1440 parallel processes. The generating vectors used here are available at [8] under the heading ‘‘SPOD Weights for 2d Diffusion Equation’’.

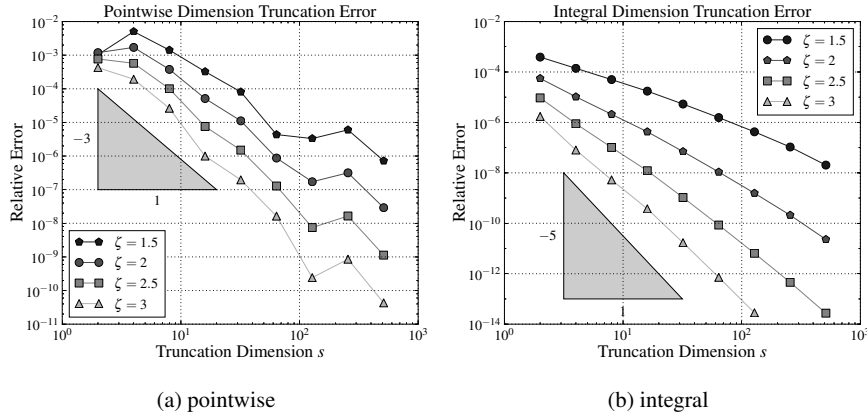


Fig. 3: Dimension truncation error for the diffusion equation with $d = 2$. (a) pointwise dimension truncation error $|q_h(\mathbf{y}) - q_h^s(\mathbf{y})|$ for $\mathbf{y} = e^{-2}\mathbf{1}$ with $q_h(\mathbf{y})$ approximated by a reference value in $s = 2^{15}$ dimensions, with expected rate $-\zeta + 1$. (b) integral dimension truncation error $|\int_U q_h(\mathbf{y}) - q_h^s(\mathbf{y}) d\mathbf{y}|$ with reference dimension $s = 1024$ and expected rate $-2\zeta + 1$. The expected rate is clearly observed in (b), while in (a) the rate seems to be one order better than expected.

6 Conclusions

We consider the error committed by truncating countably affine-parametric operator equations to a finite number of terms, and prove the convergence rate $s^{-2/p+1}$ where s is the truncation dimension and $p < 1$ the summability of the sequence of fluctuation operator norms, improving on the rate $s^{2(-1/p+1)}$ for the case of integration over a sequence of parameters. Numerical experiments verify this rate for a test integrand and two PDE examples, in one and two spatial dimensions, using up to $s = 1024$ parametric dimensions. Measurements of the pointwise dimension truncation error are also given, confirming the established theory.

Acknowledgements This work is supported by the Swiss National Science Foundation (SNSF) under project number SNF149819 and by the Swiss National Supercomputing Centre (CSCS) under Project ID d41.

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