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Stochastic Collocation via l_1-Minimisation on Low Discrepancy Point Sets with Application to Uncertainty Quantification

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Abstract. Various numerical methods have been developed in order to solve complex systems with uncertainties, and the stochastic collocation method using ℓ_1-minimisation on low discrepancy point sets is investigated here. Halton and Sobol' sequences are considered, and low discrepancy point sets and random points are compared. The tests discussed involve a given target function in polynomial form, high-dimensional functions and a random ODE model. Our numerical results show that the low discrepancy point sets perform as well or better than random sampling for stochastic collocation via ℓ_1-minimisation.

AMS subject classifications: 41A10, 60H35, 65N35

Key words: Stochastic collocation, Quasi-Monte Carlo sequence, low discrepancy point sets, Legendre polynomials, ℓ_1-minimisation.

1. Introduction

In recent years, the field of Uncertainty Quantification (UQ) has received intense attention, and various numerical methods have been developed for complex systems with uncertainties. One approach is to consider the input data as random variables, or random fields with known covariance structures, so the underlying challenge is the approximation of target quantities of interest that depend on a large number of random variables. A traditional approach is the Monte Carlo method, where one first generates a number of random realisations for the prescribed random inputs and then utilises existing deterministic solvers for each realisation — e.g. see Ref. [11] and the references therein. However, the convergence of the Monte Carlo method is relatively slow.

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Stochastic collocation based on generalised polynomial chaos (gPC) is another popular approach in the computation of UQ. It is an easily implemented non-intrusive method, and leads naturally to the solution of uncoupled deterministic problems — cf. Refs. [21, 22, 26, 27] and references therein for more detail. The key step is to determine the coefficients of the gPC expansion for the solution, for which there are two major approaches — one based on interpolation and the other on regression. It is a challenge to deal with high dimensional random spaces where the number of collocation points grows fast, known as *the curse of dimensionality*.

Compressive sensing (also known as compressed sampling) in signal processing has recently been introduced to stochastic collocation methods for UQ and some key properties are obtained, such as the probability under which the sparse random response function can be recovered [9, 19]. Compressive sensing (CS) deals with insufficient information about the target function, as is the case in many practical UQ problems. For instance, solutions to linear elliptic partial differential equations with high-dimensional random coefficients admit sparse representations with respect to the gPC basis under some mild conditions [5, 28]. Using CS, one can employ arbitrary nodal sets with an arbitrary number of nodes, which can be helpful in practical computation.

Theoretical analysis indicates that a good nodal array is of great importance to guarantee the design matrix with an acceptable restricted isometry constant (RIC) in the CS approach [23]. Rauhut and Ward [23, 24] investigated the recovery of expansions that are sparse in a univariate Legendre polynomial basis, and Yan *et al.* [35] extended their work to focus on the recoverability of stochastic solutions in high-dimensional random spaces, via ℓ_1-minimisation in a Legendre basis with random sampling. Hampton & Doostan [15] discussed convergence analysis and sampling strategies to recover a sparse stochastic function in both Hermite and Legendre gPC expansions for the ℓ_1-minimisation problem. Although random sampling methods have been used widely in the CS framework, a judicious deterministic choice of points may provide several advantages over randomly generated points. Xu & Zhou [34] presented deterministically constructed "Weil points" to recover sparse Chebyshev polynomials, and they removed the so called "failure probability". However, unlike the least-squares framework for UQ applications where low discrepancy points have been tested [4, 12, 20], stochastic collocation via CS by the Quasi-Monte Carlo method is rarely considered in the literature.

Here we emphasise the recoverability of stochastic solutions in high-dimensional random spaces, with evaluations at low discrepancy point sets. To facilitate practical implementation, we consider the case of uniform density and employ orthogonal multi-dimensional Legendre polynomials as basis functions. Random sets and the low discrepancy point sets, especially Halton and Sobol' sequences, are compared numerically in some case examples. The numerical tests show that both Halton and Sobol' sequences perform better than random sampling for low dimensional problems, and Halton sequences perform best. Furthermore, the QMC points and the random points show similar convergence properties in higher dimensions.

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A brief introduction to the stochastic collocation approach is given in Section 2, and we mainly discuss the ℓ_1-minimisation method for stochastic collocation in Section 3. In Section 4, we give the main existing results on different sampling methods. Section 5 introduces the low discrepancy point sets that is our main focus in this article. Our numerical results comparing the random points and the low discrepancy points are presented in Section 6, and our conclusions are in Section 7.

2. Stochastic Collocation Method

In this section, we closely follow Refs. [21, 35] to provide a basic introduction to the stochastic collocation method, with our main focus on our mathematical model in Uncertainty Quantification.

Let $Z = (Z_1, \cdots, Z_d) \in \mathbb{R}^d$, $d \geq 1$ be a set of (independent) random variables modelling the random inputs for a partial differential equation (PDE), such that

$$\begin{cases} \mu_t(x,t,Z) = \boldsymbol{L}(\mu)\,, & D \times (0,T] \times I_Z\,, \\ \boldsymbol{B}(\mu) = 0\,, & \partial D \times [0,T] \times I_Z\,, \\ \mu = \mu_0\,, & D \times \{t=0\} \times I_Z\,, \end{cases} \tag{2.1}$$

where $\boldsymbol{L}$ denotes a (nonlinear) differential operator and $\boldsymbol{B}$ is a boundary condition operator, $I_Z = \prod_{i=1}^d I_i \subseteq \mathbb{R}^d$, $d \geq 1$ is the range of Z, $D \in \mathbb{R}^k$ for $k = 1, 2$ or 3 denotes the physical domain and the time $T > 0$. We equip Z with a distribution function $\rho(z) = Prob(Z \leq z)$ where $z \in \mathbb{R}^d$ is real, and let $\rho_i(z_i) = Prob(Z_i \leq z_i)$, $z_i \in \mathbb{R}$ be the marginal distribution function for each component of Z. We assume that the random variables $\{Z_i\}_{i=1}^d$ are mutually independent, so obviously $\rho(z) = \prod_{i=1}^d \rho_i(z_i)$. For simplicity, we assume that I_Z is bounded, and with a proper scaling we confine ourselves to a hypercube — i.e. $Z \in [-1,1]^d$, $d \geq 1$.

2.1. Generalised polynomial chaos

The generalised Polynomial Chaos method (gPC) in Refs. [14,32] involves the strategy of approximating the Z-dependence of $\mu(x,t,Z)$ from (2.1) by a Z-polynomial. To this end, one may first define a one-dimensional orthogonal polynomial space. Thus for each $i = 1, \cdots, d$, let $\{\phi_{m,i}\}_{m=0}^{k_i}$ be a set of m^{th}-order orthogonal polynomials with respect to the variable z_i satisfying the orthogonality condition

$$\int_{I_i} \phi_{m,i}(z_i)\phi_{n,i}(z_i)\rho_i(z_i)dz_i = \delta_{mn}\,. \tag{2.2}$$

Then the one-dimensional orthogonal polynomial spaces with respect to the measure $\rho_i(z_i)dz_i$ in I_i is defined as

$$W^{i,k_i} := \text{span}\Big\{\phi_{0,i}, \cdots, \phi_{k_i,i}\Big\}\,, \quad i = 1, \cdots, d\,.$$

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The type of orthogonal polynomials $\{\phi_{m,i}\}$ for $i = 1, \cdots, d$ in (2.2) is determined by the probability density function $\rho_i(z_i)$ — e.g. Hermite polynomials are associated with the Gaussian distribution, Legendre polynomials with the uniform distribution, etc. See Ref. [32] for a detailed discussion of these correspondences and their resulting computational efficiency.

Here we use Legendre polynomials, and the corresponding d-variate orthogonal polynomial space in I_Z is defined as

$$W_P^d := \text{span}\left\{ \prod_{i=1}^{d} \phi_{k_i,i} : \mathbf{k} \in \mathbb{P}_0^d, |\mathbf{k}| \leq P \right\}, \qquad \dim(W_P^d) = \frac{(P+d)!}{P!d!} := M ,$$

where $\mathbf{k} = (k_1, \cdots, k_d)$ is a multi-index with $|\mathbf{k}| = \sum_{i=1}^{d} k_i$. Let $\Phi_{\mathbf{m}}$ be the d-variate orthonormal polynomials from W_P^d, constructed as products of a sequence of univariate polynomials in each of the directions z_i, $i = 1, \cdots, d$ — i.e.

$$\Phi_{\mathbf{m}}(z) = \phi_{m_1,1}(z_1) \cdots \phi_{m_d,d}(z_d), \quad m_1 + \cdots + m_d \leq P .$$

Obviously, we have

$$\mathbb{E}[\Phi_{\mathbf{m}} \Phi_{\mathbf{n}}] = \int_\Gamma \Phi_{\mathbf{m}}(z) \Phi_{\mathbf{n}}(z) \rho(z) dz = \delta_{\mathbf{mn}} ,$$

where $\delta_{\mathbf{mn}} = \delta_{m_1 n_1} \cdots \delta_{m_d n_d}$ is the d-dimensional delta function and $\mathbb{E}$ is the expectation operator. Upon choosing a proper ordering scheme for the multi-index, one can order the multi-dimensional polynomials via a single index — e.g. see Ref. [31]. Then

$$\mathbb{E}[\Phi_m \Phi_n] = \int_\Gamma \Phi_m(z) \Phi_n(z) \rho(z) dz = \delta_{mn} , \quad 1 \leq m, n \leq M ,$$

where each single-index m corresponds uniquely to a multi-index $(m_1, \cdots, m_d)$.

Other classical polynomial spaces based on W^{i,k_i} typically considered in practice include the following.

- *Tensor-product (TP) polynomial space:*

  $$T_P^d := \text{span}\left\{ \prod_{i=1}^{d} \phi_{k_i,i} : \mathbf{k} \in \mathbb{P}_0^d, \max_{i=1,\cdots,d} k_i \leq P \right\}, \quad \dim(T_P^d) = (P+1)^d := M ,$$

  where $\mathbf{k} = (k_1, \cdots, k_d)$ is the multi-index.
- *Hyperbolic cross (HC) polynomial space:*

  $$H_P^d := \text{span}\left\{ \prod_{i=1}^{d} \phi_{k_i,i} : \mathbf{k} \in \mathbb{P}_0^d, \prod_{i=1}^{d} (k_i + 1) \leq P + 1 \right\} ,$$

  where $\mathbf{k} = (k_1, \cdots, k_d)$ is the multi-index. The dimension of H_P^d has the upper bound [20]

  $$\dim(H_P^d) \leq \lfloor (P+1)(1 + \log(P+1))^{d-1} \rfloor .$$

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Here we mainly focus on the *total degree polynomial space* W_P^d, and some simple numerical tests on TP and HC polynomial spaces — cf. Section 6. A gPC method involves finding an approximation of $\mu(x,t;Z)$ in W_P^d defined as

$$\mu_M(x,t;Z) = \sum_{m=1}^{M} \mu_m(x,t)\Phi_m(Z)\ , \quad M = \frac{(P+d)!}{P!d!}\ ,$$

where

$$\mu_m(x,t) = \mathbb{E}[u(x,t;Z)\Phi_m(Z)] = \int_\Gamma u(x,t;z)\Phi_m(z)\pi(z)dz \tag{2.3}$$

are the expansion coefficients.

3. Stochastic Collocation via ℓ_1-Minimisation

The determination of $\mu_m(x,t)$ in Eq. (2.3) poses the main difficulty in the gPC method, and one way to proceed is a collocation scheme. In the stochastic collocation method, a set of nodes $\Theta_N = \{z^{(j)}\}_{j=1}^N \subset I_Z$ (where $N \geq 1$ is the number of nodes) is chosen, and for each $j = 1,\cdots,N$ a deterministic problem (2.1) is solved at the node $z^{(j)}$ to obtain $\mu^{(j)} \triangleq \mu(x,t,z^{(j)})$:

$$\begin{cases} \mu_t(x,t,z^{(j)}) = \boldsymbol{L}(\mu)\ , & D\times(0,T]\ , \\ \boldsymbol{B}(\mu) = 0\ , & \partial D\times[0,T]\ , \\ \mu = \mu_0\ , & D\times\{t=0\}\ . \end{cases} \tag{3.1}$$

After the pairings $(z^{(j)},\mu^{(j)})$, $j=1,\cdots,N$ are obtained, the task is to construct a function $\omega(Z)$, which usually resides in a proper polynomial space in term of Z such that $\omega(z^{(j)}) = \mu^{(j)}$ for all $j=1,\cdots,N$ that leads to a (polynomial) interpolation problem. Thus the stochastic collocation method is equivalent to solving N deterministic problems (3.1) at each nodal point $z^{(j)}$, $j=1,\cdots,N$. With increasing stochastic dimension or polynomial degree, the total number of nodes increases rapidly, so the scheme becomes highly undesirable because obtaining function values at the nodes is typically expensive for complex systems. The key issue for this approach is therefore the selection of the minimal number of support nodes to achieve a good approximation — and here we adopt the idea of compressed sampling to do so.

Let $\{z^{(n)}\}_{n=1}^N$ be *i.i.d.* samples of Z, and $\{\mu(z^{(n)})\}_{n=1}^N$ the corresponding realisations of the stochastic function $\mu(x,t,z)$. In the stochastic collocation approach, the interpolation condition of $\mu_M(z^{(n)}) = \mu(z^{(n)})$, $n=1,\cdots,N$ results in the following problem:

$$\mathbf{Ac} = \mathbf{u}\ , \tag{3.2}$$

where $\mathbf{c} = (c_1,\cdots,c_M)^T \in \mathbb{R}^M$ is the coefficient vector to be determined in the gPC expansion (2.3), $\mathbf{u} = (\mu(z^{(1)}),\cdots,\mu(z^{(N)}))^T \in \mathbb{R}^N$ is the vector of samples of $\mu(Z)$, and $\mathbf{A} \in \mathbb{R}^{N\times M}$ is the measurement matrix with the entries

$$\mathbf{A}_{nm} = \Phi_m(z^{(n)})\ , \quad n=1,\cdots,N,\ \ m=1,\cdots,M\ . \tag{3.3}$$

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We prefer to use a minimal number N of samples, less than the cardinality of the polynomial space for the approximation M, so the system (3.2) becomes under-determined and has infinitely many solutions. One approach to circumvent this difficulty is to employ sparse reconstruction and seek a solution $\mathbf{c}$ with the minimum number of nonzero terms. This can be formulated as the optimisation problem

$$\mathbf{P}_0 : argmin\|\mathbf{c}\|_0 \quad subject\ to \quad \mathbf{Ac} = \mathbf{u}\ , \tag{3.4}$$

where $\|\mathbf{c}\|_0 := \#\{m : c_m \neq 0\}$ is the ℓ_0-norm on the vectors. A vector is called s-sparse if $\|\mathbf{c}\|_0 \leq s$, and in general the problem (3.4) is NP-hard to compute. To overcome this combinatoric complexity, various tractable alternatives have been developed, most notably the ℓ_1-minimisation problem that in our context is

$$\mathbf{P}_1 : argmin\|\mathbf{c}\|_1 \quad subject\ to \quad \mathbf{Ac} = \mathbf{u}\ . \tag{3.5}$$

The advantage of this $\mathbf{P}_1$ formulation is that it is a convex problem, so computational solvers for convex problems may be leveraged [36, 37]. Moreover, the interpolation condition $\mathbf{Ac} = \mathbf{u}$ can be relaxed to $\|\mathbf{Ac} - \mathbf{u}\| \leq \epsilon$ for some tolerance value ϵ, since in practice the approximation $\mathbf{u}$ may not be exact or may be corrupted by noise. This leads to the Basis Pursuit Denoising form:

$$\mathbf{P}_{1,\epsilon} : argmin\|\mathbf{c}\|_1 \quad subject\ to \quad \|\mathbf{Ac} - \mathbf{u}\| \leq \epsilon,$$

where the tolerance ϵ can be identified via cross validation. Ref. [9] and references therein discuss this Basis Pursuit Denoising form to solve PDE with random inputs. We focus on the traditional ℓ_1-minimisation (3.5) here. The stochastic collocation method for (2.1) thus consists of the following steps:

1. Choose a random nodal set $\{z^{(n)}\}_{n=1}^N$ in space I_Z.
2. For each $n = 1, \cdots, N$, solve (3.1) with fixed parameter set $z^{(n)} = (z_1^{(n)}, \cdots, z_d^{(n)})$ using an accurate numerical scheme, to obtain its solution $\mu(z^{(n)})$.
3. Evaluate the approximate gPC expansion coefficients via ℓ_1-minimisation

$$\tilde{\mathbf{c}} = \arg\min_{\mathbf{c}\in\mathbb{R}^M} \|\mathbf{c}\|_1\ , \quad \text{subject to} \quad \mathbf{Ac} = \mathbf{u}\ . \tag{3.6}$$

4. Finally, construct the M^{th}-order gPC approximation

$$\mu_M(Z) = \sum_{m=1}^{M} \tilde{c}_m \Phi_m(Z)\ . \tag{3.7}$$

The choice of the nodal sets and computation of the measure matrix $\mathbf{A}$ are the pre-processing steps, and the evaluation of gPC coefficients (3.6) and reconstruction of the approximate gPC expression (3.7) are post-processing steps. The compressive sensing (CS) results show that a sparse vector $\mathbf{c}$ can be recovered successfully from $\mathbf{Ac} = \mathbf{u}$ via ℓ_1-minimisation with high probability, provided that $\mathbf{A}$ satisfies a restricted isometry property(RIP) condition. We summarise some existing results in the next section.

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4. Existing Results

The error of the best s-term approximation of a coefficient vector $\mathbf{c} \in \mathbb{R}^M$ in the ℓ^p-norm is defined as

$$\sigma_{s,p}(\mathbf{c}) = \inf_{\|\mathbf{y}\|_0 \le s} \|\mathbf{y} - \mathbf{c}\|_p \ ,$$

where $\|\mathbf{c}\|_p = (\sum_{m=1}^M |c_m|^p)^{1/p}$, $1 \le p < \infty$. Clearly, $\sigma_{s,p}(\mathbf{c}) = 0$ if $\mathbf{c}$ is s-sparse — i.e. $\|\mathbf{c}\|_0 \le s$. Let $\mathbf{A}$ be an $N \times M$ matrix, and define the restricted isometry constant (RIC) $\delta_s < 1$ to be the smallest positive number such that the inequality

$$(1 - \delta_s)\|\mathbf{c}\|_2^2 \le \|\mathbf{A}\mathbf{c}\|_2^2 \le (1 + \delta_s)\|\mathbf{c}\|_2^2$$

holds for all $\mathbf{c} \in \mathbb{R}^M$ satisfying $\|\mathbf{c}\|_0 \le s$. If this inequality holds, the matrix $\mathbf{A}$ is said to satisfy the s-restricted isometry property with restricted isometry constant δ_s [2, 3]. Now, we are ready to state the following sparse recovery theorem for RIP matrices.

Theorem 4.1 (cf. Refs. [2,3,23]). *Let $\mathbf{A} \in \mathbb{R}^{N\times M}$ be a matrix with RIC such that $\delta_s \le 0.307$. For a given $\tilde{\mathbf{c}} \in \mathbb{R}^M$, let $\mathbf{c}^\#$ be the solution of the ℓ_1-minimisation*

$$argmin\|\mathbf{c}\|_1 \quad subject\ to \quad \mathbf{A}\mathbf{c} = \mathbf{A}\tilde{\mathbf{c}} \ . \tag{4.1}$$

Then the reconstruction error satisfies

$$\|\mathbf{c}^\# - \tilde{\mathbf{c}}\|_2 \le C\frac{\sigma_{s,1}(\tilde{c})}{\sqrt{s}}$$

for some constant $C > 0$ that depends only on δ_s. In particular, if $\tilde{\mathbf{c}}$ is s-sparse then reconstruction is exact — i.e. $\mathbf{c}^\# = \tilde{\mathbf{c}}$.

This theorem indicates that a good nodal array will lead to a design matrix $\mathbf{A}$ with an acceptable RIC so that Theorem 4.1 may be invoked for convergence.

4.1. Random sampling

Random sampling is one popular method to solve the sparse recovery problem. The recovery of expansions that are sparse in a univariate Legendre polynomial basis was investigated in Refs. [23,24], where the analysis relies strongly on RIP results from bounded orthonormal polynomial systems as summarised in the following theorem.

Theorem 4.2 (cf. Ref. [23]). *Let $\{\Phi_m\}$ be a bounded orthonormal system — i.e.*

$$\sup_m \|\Phi_m\|_\infty = \sup_m \sup_z |\Phi_m(z)| \le L$$

for some constant $L \ge 1$. Let $\mathbf{A} \in \mathbb{R}^{N\times M}$ be the interpolation matrix with entries

$$\left\{a_{n,m} = \Phi_m(z^{(n)})\right\}_{1\le m\le M, 1\le n\le N} \ ,$$

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where the points $\{z^{(n)}\}_{1\leq n\leq N}$ *are i.i.d. samples drawn from a one-dimensional uniform measure, and that there is* $\delta > 0$ *such that*

$$N > C\,\delta^{-2}L^2 s\log^3(s)\log(M)\ .$$

Then with probability at least $1 - M^{-\gamma log^3(s)}$, *the RIC of* $(1/\sqrt{N})\mathbf{A}$ *satisfies* $\delta_s \leq \delta$. *(Here the* $C, \gamma > 0$ *are universal constants.)*

In Ref. [24] this theorem was used to provide the recoverability result for one-dimensional sparse Legendre polynomial expansions with randomly generated samples, and then extended in Ref. [35] to high-dimensional problems for both the original ℓ_1-minimisation and the preconditioned ℓ_1-minimisation. Theoretical analysis shows that if $\{z^{(n)}\}_{1\leq n\leq N}$ is a set of *i.i.d.* random samples drawn from the uniform measure, in order to guarantee with high probability that the solution $\mathbf{c}^{\#}$ to the ℓ_1-minimisation problem (4.1) is within a factor of the best s-term error

$$Pr\left[\|\mathbf{c}^{\#} - \tilde{\mathbf{c}}\|_2 \leq \frac{C\sigma_s(\tilde{\mathbf{c}})_1}{\sqrt{s}}\right] \geq 1 - M^{-\gamma\log^3(s)}$$

we need $N > 3^P s\log^3(s)\log(M)$, where the constants C and γ are universal.

4.2. Deterministic sampling

Deterministic CS sampling is well studied for the recovery of sparse trigonometric polynomials [1, 6, 17, 18, 33]. In Ref. [34], the authors propose using Weil points to recover sparse Chebyshev polynomials, as theoretically ℓ_1-minimisation can recover s-sparse Chebyshev polynomials provided that the number of the Weil samples scales quadratically with the sparsity s — i.e. $N \sim C(\Lambda)s^2$. The constant $C(\Lambda)$ differs for different polynomial spaces(W_P^d, T_P^d, H_P^d). Numerically, the Weil points provide performance similar to random Chebyshev samples, although the Weil estimates obtained are not optimal in the sense that the number of sample points N are required to scale quadratically on the sparsity s.

5. ℓ_1-Minimisation with Low Discrepancy Points

We now proceed to discuss low discrepancy points and their application in the CS framework for UQ applications, based on the existing main results quoted in the previous section. Let us first introduce the notion of discrepancy, which measures the maximal deviation between the empirical distribution of a sequence and the uniform distribution — cf. also Refs. [8, 10] for surveys on the discrepancy of sequences and applications.

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Definition 5.1 (Discrepancy — cf. Ref. [16])**.** Let $S = \{x_1, \cdots, x_N\}$ be a finite set of real numbers in $[0,1)^d$. Then the discrepancy of the given set S is defined as

$$D_N(S) := \sup_{J \in [0,1)^d} \left| \frac{1}{N} \sum_{n=1}^{N} \chi_J(x_n) - \lambda_S(J) \right| ,$$

where $\chi_J(x)$ denotes the characteristic function of J defined as

$$\chi_J(x) = \begin{cases} 1 , & x \in J , \\ 0 , & x \notin J , \end{cases}$$

and $\lambda_S(J)$ is the d-dimensional Lebesgue measure.

If $(x_n)_{n \in \mathbb{N}}$ is an infinite sequence of points, we associate to it the sequence of discrepancies $D_N(\{x_1, \cdots, x_N\})$. So $D_N(x_n)$ denotes the discrepancy of the initial segment $\{x_1, \cdots, x_N\}$ of the infinite sequence. Sequences that have discrepancy $\mathcal{O}((\log N)^d / N)$ are called low discrepancy sequences. We consider two well known examples of multidimensional low discrepancy sequences and point sets — viz. Halton and Sobol' sequences [7, 16].

Definition 5.2 (Radical inverse function — cf. Ref. [7])**.** For integers $i \geq 0$ and $b \geq 2$, we define the radical inverse function $\psi_b(i)$ as follows: if

$$i = \sum_{a=1}^{\infty} i_a b^{a-1}$$

where $i_a \in \{0, 1, \cdots, b-1\}$, then

$$\psi_b(i) := \sum_{a=1}^{\infty} \frac{i_a}{b^a}$$

— i.e. if $i = (\cdots i_2 i_1)_b$ denotes the base b representation of i, then $\psi_b(i) := (0.i_1 i_2 \cdots)_b$.

Example 5.1 (Halton sequence — cf. Ref. [7])**.** If $p_1, p_2, \cdots, p_d$ denotes the first d prime numbers, the Halton sequence $x_1, x_2, \cdots$ in d dimensions is

$$x_n = (\psi_{p_1}(n), \psi_{p_2}(n), \cdots, \psi_{p_d}(n)), \quad n = 1, 2, \cdots .$$

Nets and sequences provide another method for obtaining well distributed point sets in the unit cube $[0,1)^d$. The (t, m, d)-net concept is based on subdividing the unit cube into intervals, and placing points in the cube such that each interval of a certain size and shape contains the correct number of points [7].

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Definition 5.3 ((t,m,d)-net)**.** Let $t \geq 0$, $m \geq 1$, $d \geq 1$ and $b \geq 2$ be integers with $t \leq m$. A (t,m,d)-net in base b is a point set S consisting of b^m points in $[0,1)^d$ such that every elementary interval of the form

$$\prod_{j=1}^{d} \left[\frac{a_j}{b^{s_j}}, \frac{a_j+1}{b^{s_j}} \right)$$

for each $s_j \geq 0$, $0 \leq a_j < b^{s_j}$ and $s_1 + s_2 + \cdots + s_d = m - t$ contains exactly b^t points of S.

Definition 5.4 ((t,d)-sequence — cf. Ref. [7])**.** Let $t \geq 0$ and $d \geq 1$ be integers. A (t,d)-sequence in base b is a sequence of points $S = (\mathbf{t}_0, \mathbf{t}_1, \cdots)$ in $[0,1)^d$ such that for any integers $m > t$ and $\ell \geq 0$ every block of b^m points

$$\mathbf{t}_{\ell b^m}, \cdots, \mathbf{t}_{(\ell+1)b^m-1}$$

in the sequence P forms a (t,m,d)-net in base b.

Now suppose b is a prime and let $\mathbb{Z}_b := \{0, 1, \cdots, b-1\}$ denote the equivalence classes of integers modulo b. Let $\mathbb{Z}_b[x]$ denote the set of polynomials over the finite field $\mathbb{Z}_b$.

Example 5.2 (Sobol' sequence — cf. Ref. [25])**.** A Sobol' sequence is a (t,d)-sequence in base $b = 2$, where t is a non-decreasing function of s. As discussed in Refs. [7, 25], Sobol' sequences are digital (t,d)-sequences with

$$t = \sum_{j=1}^{d} (e_j - 1) \ ,$$

where e_j is the degree of the polynomial p_j and $p_1, \cdots, p_d \in \mathbb{Z}_2[x]$ denote distinct primitive polynomials ordered according to their degree, defined as

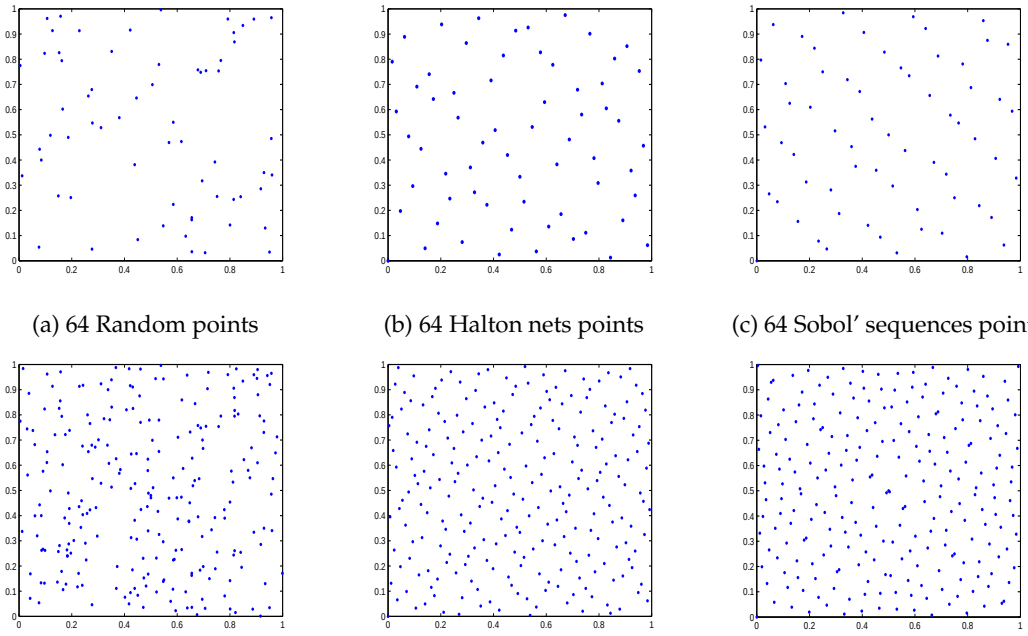
$$p_j(x) = x^{e_j} + a_{1,j}x^{e_j-1} + a_{2,j}x^{e_j-2} + \cdots + a_{e_j-1,j}x + 1 \quad for\, 1 \leq j \leq s \ ,$$

where $a_{j,k} \in \mathbb{Z}_b$.

In Fig. 1, we compare the point distributions of the three sampling methods for the 2-dimensional case: at the top, the chosen number of points is 64; and at the bottom there are 240. Evidently, low discrepancy points distribute more homogeneously than random samples.

Remark 5.1. The QMC points presented are asymptotically uniformly distributed and thus suitable for sampling Legendre problems, orthogonal with respect to the uniform measure. In UQ applications, one could be interested in other types of polynomial expansions, where some suitable transformation to transfer uniform QMC points to fit the desired measure (a so-called "change of measure") could be used.

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(a) 64 Random points (b) 64 Halton nets points (c) 64 Sobol' sequences points

(d) 240 random points (e) 240 Halton nets points (f) 240 Sobol' sequences points

Figure 1: Comparison of random sampling, Halton sequences and Sobol' sequences.

6. Numerical Tests

We now present some numerical examples we considered to compare how random samples perform versus the low discrepancy point sets with different kinds of points in ℓ_1 minimisation. We randomly generated a set of coefficients with corresponding sparsity, and then recovered the coefficient for both low dimension $d = 2$ and high dimension $d = 10$. Some classical test functions were considered, as originals to be approximated by the ℓ_1-minimisation. Finally, an ODE problem provided a performance comparison for the various point sets in the ℓ_1-minimisation.

For implementation of the ℓ_1 minimisation, we employed available tools such as the Spectral Projected Gradient algorithm (SPGL1) [30] implemented in the MATLAB package SPGL1 [29]. We performed the numerical tests for the three options — viz. random sampling and Halton and Sobol' sequences, respectively denoted "Uniform", "Halton" and "Sobol" in the figures. We conducted three groups of tests, and in particular TD spaces, TP spaces and HC spaces for the first two cases.

6.1. Benchmark test: fixed sparsity

For the three polynomial spaces (TD, TP and HC) detailed in Section 2, we assumed that the target exact function has the polynomial form $u(Z) = \sum_{m=1}^{M} \tilde{c}_m \Phi_m(Z)$

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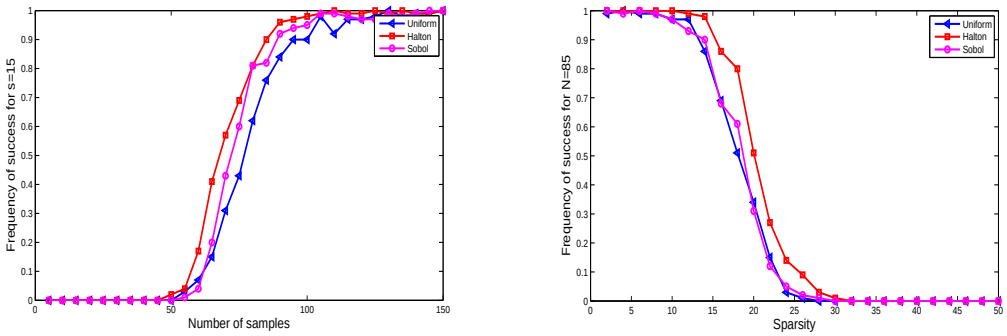


Figure 2: $d = 2$, $P = 20$, $d < P$, $M = 231$, TD Space. Left: reconstruction successful probability vs. number of sample points N, with $s = 15$. Right: reconstruction successful probability vs. sparsity s, with $N = 85$.

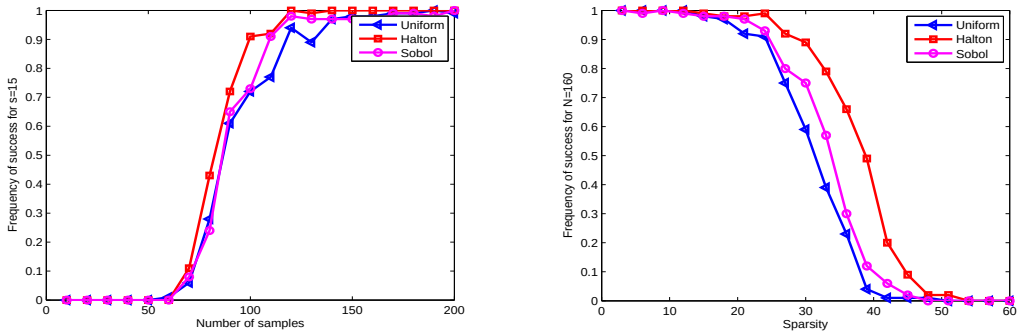


Figure 3: $d = 2$, $P = 20$, $d < P$, $M = 441$, TP Space. Left: reconstruction successful probability vs. number of sample points N, with $s = 15$. Right: reconstruction successful probability vs. sparsity s, with $N = 160$.

with $\|\tilde{\mathbf{c}}\|_0 = s$, and attempted to recover this vector $\tilde{\mathbf{c}}$. For a given sparsity level s, we fixed s coefficients of the polynomial but kept the other coefficients zero. The values of the s nonzero coefficients were drawn as *i.i.d.* samples from a standard normal distribution, and we examined the frequency of successful recoveries from 100 trials of the algorithms. A recovery was considered successful when the resulting coefficient vector $\mathbf{c}$ satisfied $\|\mathbf{c} - \tilde{\mathbf{c}}\|_\infty \leq 10^{-3}$.

The first test was for a low dimensional case $d = 2$. The left-hand plots of Figs. 2, 3 and 4 show the recovery rate for sparse Legendre polynomials with fixed sparsity s as a function of the number of sample points in the TD, TP and HC polynomial spaces, respectively. The right-hand plots show the recovery results for sparse Legendre polynomials, as a function of the sparsity level s. Evidently, both Halton and Sobol' sequences perform better than random sampling, and the Halton sequence seems the best for this two-dimensional case.

The second test was for a higher dimensional case $d = 10$. When the dimension d exceeds P, the number of basis functions grows too fast for the *tensor-product polynomial space*, so in our computation we avoided this space and concentrated on the

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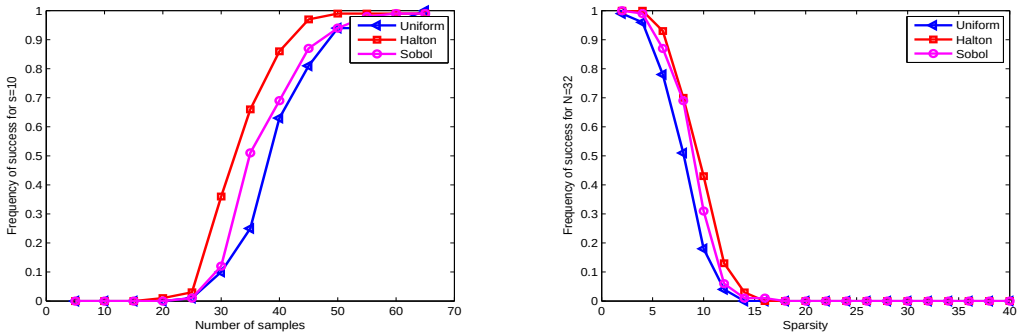


Figure 4: $d = 2$, $P = 20$, $d < P$, $M = 70$, HC Space. Left: reconstruction successful probability vs. number of sample points N, with $s = 15$. Right: reconstruction successful probability vs. sparsity s, with $N = 32$.

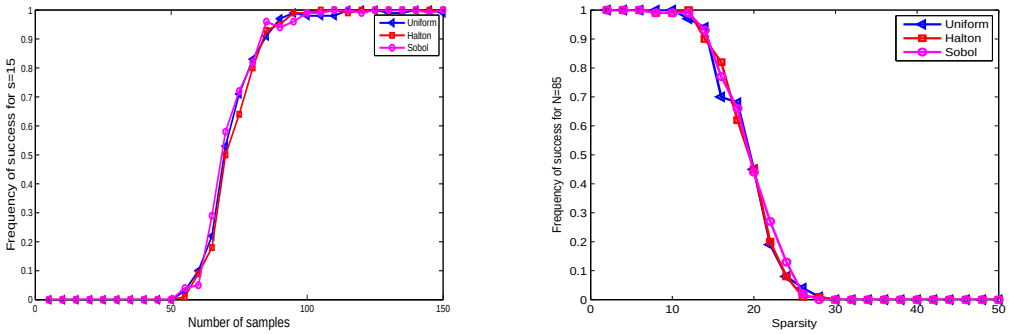


Figure 5: $d = 10$, $P = 3$, $d > P$, $M = 286$, TD Space. Left: reconstruction successful probability vs. number of sample points N, with $s = 15$. Right: reconstruction successful probability vs. sparsity s, with $N = 85$.

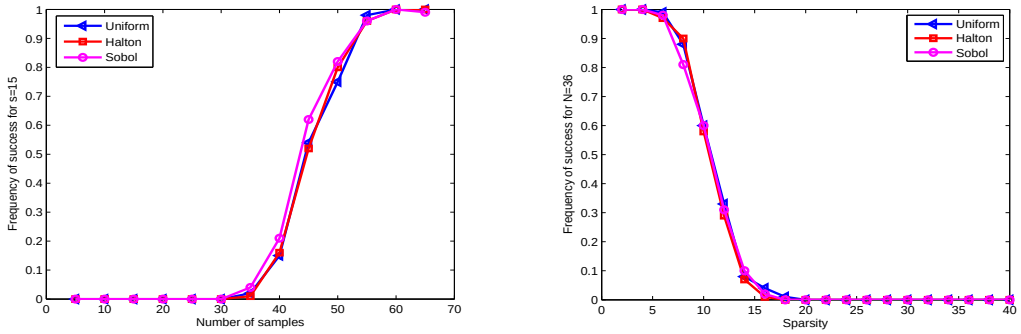


Figure 6: $d = 10$, $P = 3$, $d > P$, $M = 76$, HC Space. Left: reconstruction successful probability vs. number of sample points N, with $s = 10$. Right: reconstruction successful probability vs. sparsity s, with $N = 36$.

TD and HC polynomial spaces. The left-hand plot of Fig. 5 for TD spaces shows the recovery rate for sparse Legendre polynomials (with $s = 15$, $d = 10$, and $M = 286$) as

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a function of the number of sample points. In the right-hand plot, the recovery results for sparse Legendre polynomials (with $N = 85$, $d = 10$, and $M = 286$) as a function of sparsity level s are shown. The numerical treatment was the same for HC spaces when at high dimension, and Fig. 6 shows the recovery results. It is seen that the three kinds of design points have very similar performance in this case.

6.2. Approximation of the test functions

We chose a *total-degree polynomial space* and used ℓ_1 minimisation to approximate the three test functions

$$f_1(x) = \exp\left(-\sum_{i=1}^{d}\left(c_i^2(x_i-\omega_i)^2\right)\right),$$
$$f_2(x) = \exp\left(-\sum_{i=1}^{d} c_i|x_i-\omega_i|\right),$$
$$f_3(x) = \frac{1}{\sum_{i=1}^{d}\omega_i + c_i x_i},$$

where x is an d-dimensional vector in $[-1,1]^d$. Here ω acts as a shift parameter, unless otherwise stated we chose $\omega_i = 0.5$, $i = 1,\cdots,d$ and consider two c_i values that determine the effective dimensionality of the function — viz. $c_i = \exp(-6i/d)$ and $c_i = 1/2^{i+1}$. Both $d = 2$ and $d = 10$ were investigated, and in particular the convergence with respect to the following l_2 error:

$$\varepsilon_{\ell^2} = \left(\frac{1}{M}\sum_{k=1}^{M}\left|f(x^{(k)}) - g(x^{(k)})\right|^2\right)^{1/2},$$

where f and g are the exact test function and its approximation obtained with the ℓ_1 minimisation algorithm, respectively. In all of the following examples, the points number adopted was $M = 1000$.

For the low dimensional case $d = 2$ and TD spaces, the error between the exact test function and the recovery results is shown in Fig. 7, where it appears that all of the sampling methods can recovery the true function to some extent. However, the Halton sequence produces the smallest error and the fastest decline speed, and so achieves the best effective approximation of the original test function. Moreover, we observe that the approximation using Sobol points is also better than random sampling, so that in the low-dimensional case the low discrepancy points are better than random sampling. This is consistent with the results in the Benchmark test above.

For the high dimensional case $d = 10$, Fig. 8 shows that when the number of point is less than 10 all three sampling methods cannot achieve good approximations, although increasing the number of points considerably improves the approximation. Thus when the number is high enough the variation in the approximation error slows

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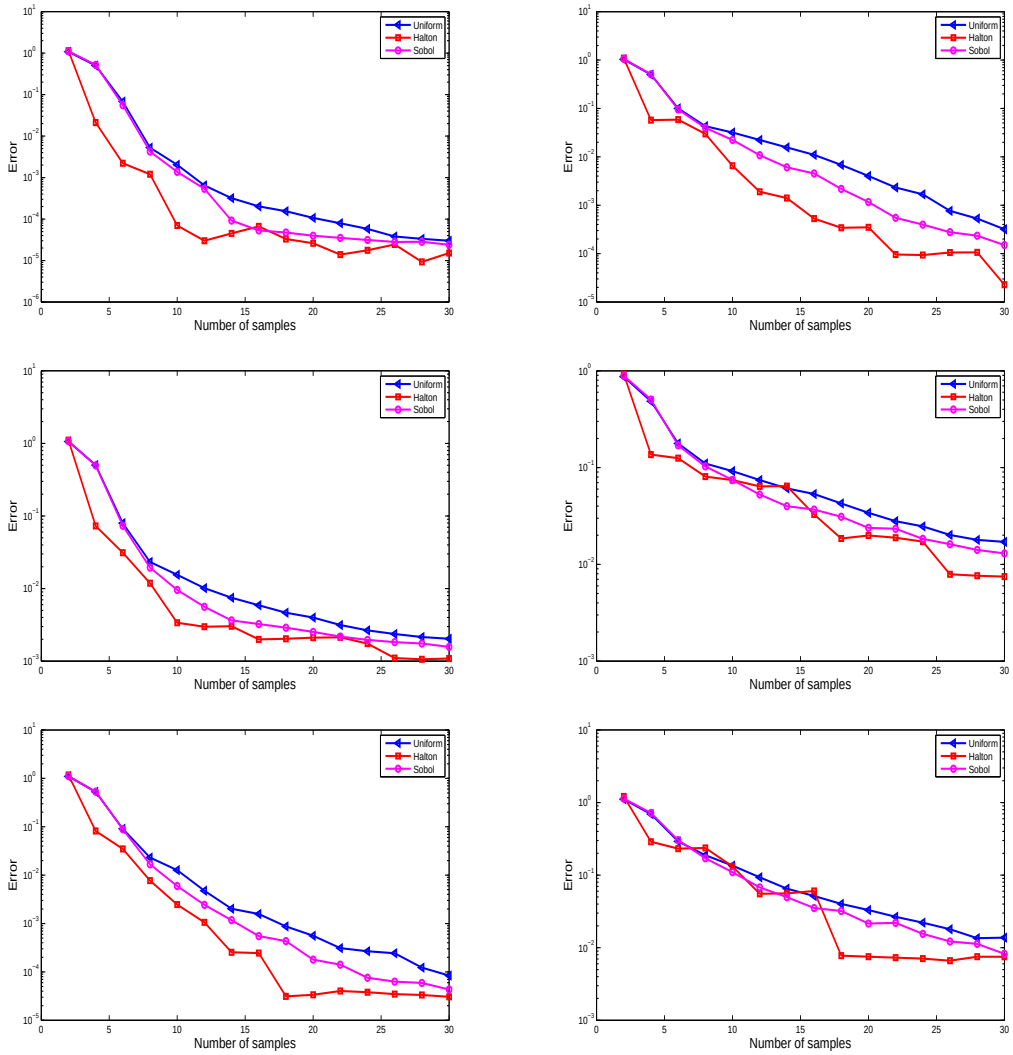


Figure 7: Samples vs. approximate error, when $d = 2$, $P = 10$, TD Space. Top: $f_1(x)$, Middle: $f_2(x)$, Bottom: $f_3(x)$. Left: $c_i = \exp(-6i/d)$, Right: $c_i = 1/2^{i+1}$.

and approaches a stable value. In addition to these common features, Halton points are slightly superior than other two sets.

We also considered two other types of polynomial spaces — viz. *tensor-product polynomial space* and *hyperbolic cross polynomial space*. The third test function was selected to test the performance of the different sampling point sets. Fig. 9 for the low dimensional case $d = 2$ shows that quasi-Monte-Carlo points are better than random point sets, and in particular the Halton points produce the best approximation. For the high dimensional case $d = 10$, Fig. 10 shows that the three sampling methods produce similar results when the number of points is high enough.

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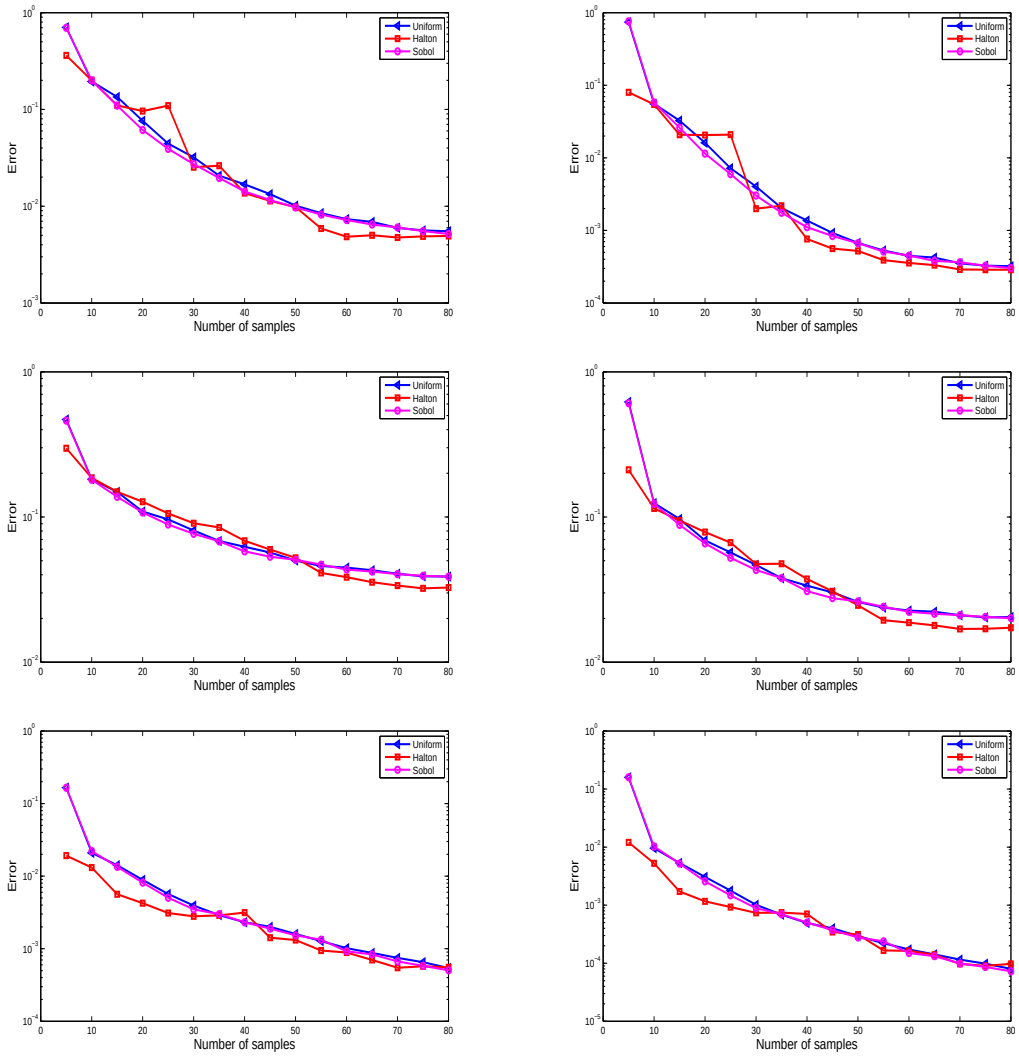


Figure 8: Samples vs. approximate error, when $d = 10$, $P = 3$, TD Space. Top: $f_1(x)$, Middle: $f_2(x)$, Bottom: $f_3(x)$. Left: $c_i = \exp(-6i/d)$, Right: $c_i = 1/2^{i+1}$.

6.3. A random ODE model: Genetic toggle switch

We considered a random ODE model known as the genetic toggle switch applicable to Escherichia coli [13], defined by the system of ODE

$$\frac{d\mu}{dt} = \frac{\alpha_1}{1+\nu^\beta} - \mu\,, \qquad \frac{d\nu}{dt} = \frac{\alpha_2}{1+\omega^\gamma} - \nu, \qquad \omega = \frac{\mu}{(1+[IPTG]/\kappa)^\eta}\,,$$

where α_1, α_2, β, γ, η, κ are parameters and $[IPTG]$ is an input that controls the behaviour of the steady state solution. One can refer to [12] for more details.

We randomly chose the parameters α_2, β and the vector form $\boldsymbol{\alpha} = \langle \boldsymbol{\alpha} \rangle (1 + \sigma x)$

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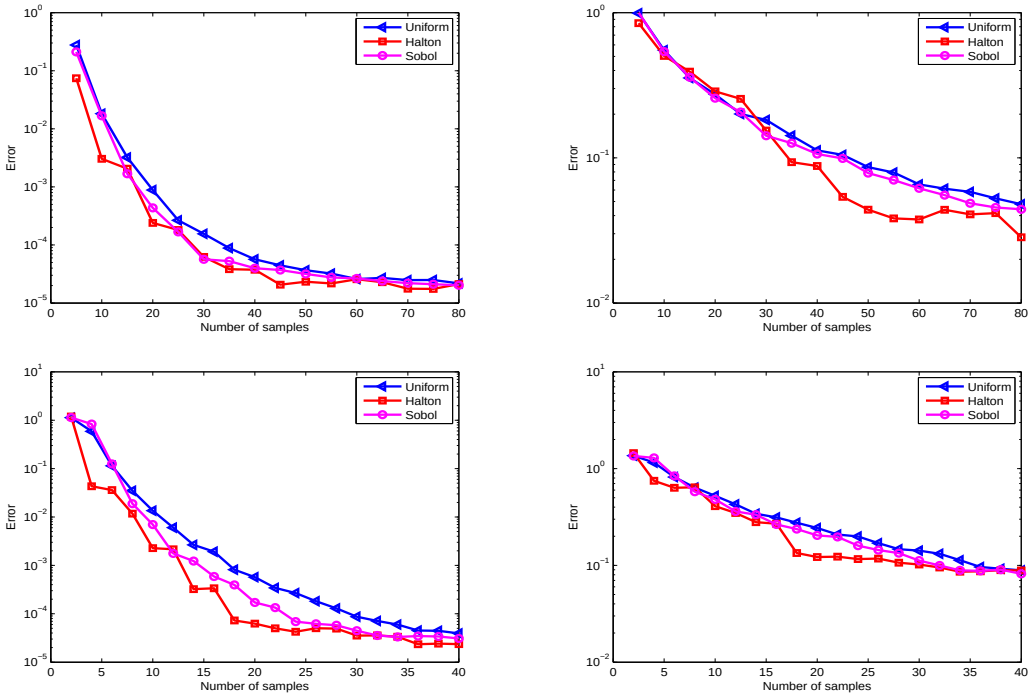


Figure 9: Samples vs. approximate error for $f_3(x)$, Top: *tensor-product polynomial space* and $d = 2$, $P = 10$, Bottom: *hyperbolic cross polynomial space* and $d = 2$, $P = 20$. Left: $c_i = \exp(-6i/d)$, Right: $c_i = 1/2^{i+1}$.

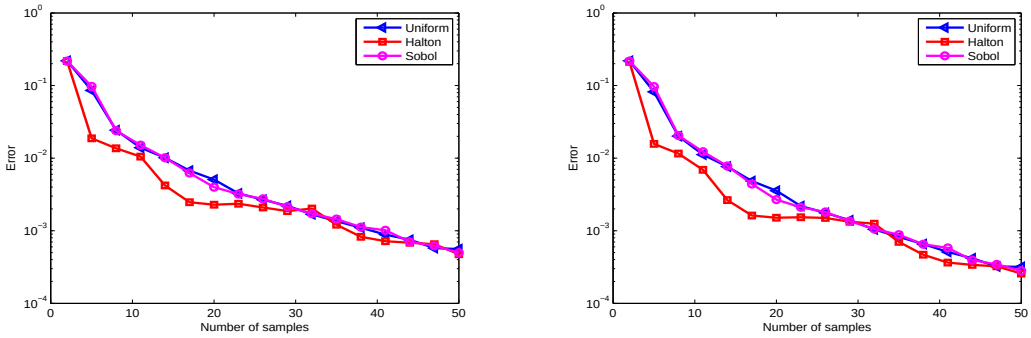


Figure 10: Samples vs. approximate error for $f_3(x)$, when $d = 10$, $P = 3$, HC Space. Left: $c_i = \exp(-6i/d)$, Right: $c_i = 1/2^{i+1}$.

where $\langle \boldsymbol{\alpha} \rangle = (15.6, 2.5)$ are the expectation values, and uniformly distributed random variables $x = (x_1, x_2)$ with $x_i \in [-1, 1]$, $i = 1, 2$. A 10% variation was introduced during the computation — i.e. we chose $\sigma = 0.1$. Corresponding to the uniform distribution, the gPC basis consisted of Legendre polynomials. We employed a 4th-order Runge-Kutta deterministic solver, and the Monte Carlo method with 1000 samples to get the exact solutions. In Fig. 11, we show the convergence properties of the stochas-

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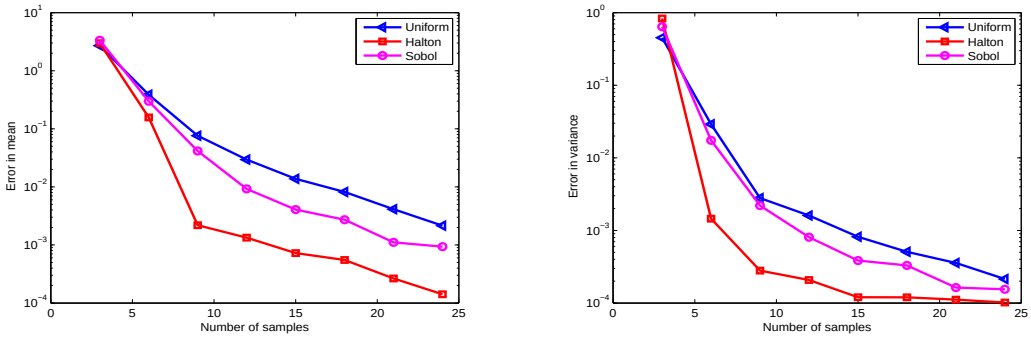


Figure 11: Samples vs. approximate error, for the ODE problem, where $d = 2$, $P = 10$. Left: error in mean, Right: error in variance.

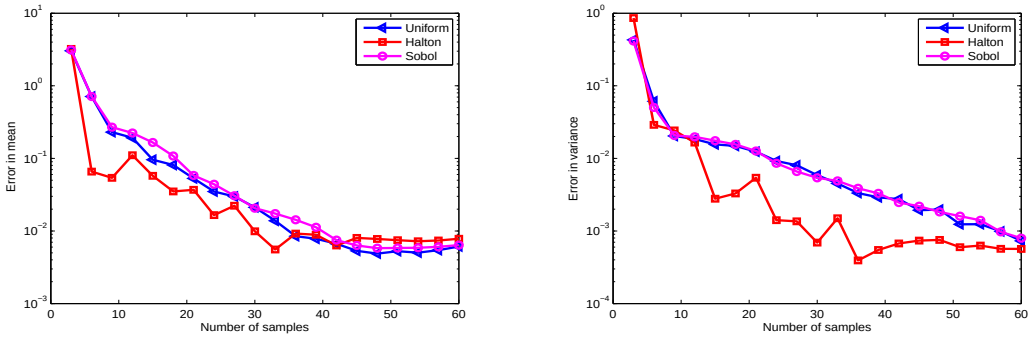


Figure 12: Samples vs. approximate error, for the ODE problem, where $d = 6$, $P = 3$. Left: the mean value of the error, Right: the variance of the error.

tic collocation ℓ_1-minimisation approach with respect to the number of points for the different sampling approaches. It is seen that the Halton sequence is again the best choice for approximating the solution.

Subsequently, we adopted the parameters $\boldsymbol{\alpha} = \langle \boldsymbol{\alpha} \rangle (1 + \sigma x)$ where

$$\langle \boldsymbol{\alpha} \rangle = (156.25, 15.6, 2.5, 1.0, 2.0015, 2.9618 \times 10^{-5}) ,$$

and as before set $\sigma = 0.1$ and assumed that x is a random vector uniformly distributed in $[-1, 1]^6$ with independent components. The random space was then six-dimensional, and in that sense the high dimensional situation. The convergence rates are shown in Fig. 12.

From these two tests, we observe that when the number of points is low none of the three sample methods achieve an acceptable approximation. However, with an increased number of point's each method gradually produced an improved approximation. In the first test for example, when the dimension is as low as 2 the ℓ_1-minimisation with Halton points achieves a high convergence rate; and even when the dimension is 6 (that we may view as high dimension), in Fig. 12 we see that the

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approach with Halton points also realises a fast approximation, as do the Sobol' sequence and random sampling.

7. Conclusion

The numerical comparison between different nodal points for the stochastic collocation method via ℓ_1 minimisation has been considered, with three kinds of nodal points — viz. random sampling, the Halton sequence and the Sobol' sequence. It was shown numerically that low discrepancy nodes provide better convergence for low dimensional problems, when the Halton sequence proved the most efficient. For high dimensional problems, the three kinds of nodes produced similar performance. Low discrepancy point sets thus seem to be a good choice for stochastic collocation methods via ℓ_1 minimisation. Finally, we remark that theoretical analysis for stochastic collocation methods via CS based on QMC points will be considered in future work.

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