

# Tractability of Halton sequence based QMC quadrature for elliptic PDEs with lognormal diffusion

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## Model Problem

Let  $(\Omega, \mathcal{F}, P)$  be a complete probability space and  $D \subset \mathbb{R}^n$  a domain in  $n = 2, 3$  dimensions. We consider the stochastic diffusion problem

$$\begin{aligned} \text{find } u(\omega) \in H_0^1(D) \text{ such that for almost all } \omega \in \Omega \\ - \operatorname{div}(a(\omega)\nabla u(\omega)) = f \text{ in } D. \end{aligned}$$

The logarithm of the diffusion coefficient is supposed to be a centered Gaussian field which can be represented by a Karhunen-Loève expansion

$$\kappa(\mathbf{x}, \omega) := \log(a(\mathbf{x}, \omega)) = \sum_{k=1}^{\infty} \sqrt{\lambda_k} \varphi_k(\mathbf{x}) \psi_k(\omega).$$

## Assumptions:

- ▶ The functions  $\{\varphi_k\}_k \subset L^\infty(D)$  are pairwise  $L^2(D)$ -orthonormal,
- ▶ the sequence

$$\gamma_k := \sqrt{\lambda_k} \|\varphi_k\|_{L^\infty(D)}$$

satisfies  $\{\gamma_k\}_k \in \ell^1(\mathbb{N})$ ,

- ▶ the random variables  $\{\psi_k\}_k$  are independent, standard normally distributed, i.e.  $\psi_k \sim \mathcal{N}(0, 1)$ .

In practice the Karhunen-Loève expansion is appropriately truncated after  $m$  terms.

## Parametrized problem

The last assumption implies that the pushforward measure  $\mathbb{P}_\psi := \mathbb{P} \circ \psi$  is given by the joint density function

$$\rho(\mathbf{y}) := \prod_{k=1}^m \rho(y_k), \quad \text{where} \quad \rho(y) := \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{y^2}{2}\right).$$

Thus the parametrized and truncated diffusion coefficient is

$$\kappa(\mathbf{x}, \mathbf{y}) := \sum_{k=1}^m \sqrt{\lambda_k} \varphi_k(\mathbf{x}) y_k \quad \text{and} \quad a(\mathbf{x}, \mathbf{y}) := \exp(\kappa(\mathbf{x}, \mathbf{y}))$$

for all  $\mathbf{x} \in D$  and  $\mathbf{y} = (y_1, y_2, \dots, y_m) \in \mathbb{R}^m$ .

The corresponding parametrized problem is

$$\text{find } u \in L^2_\rho(\mathbb{R}^m; H_0^1(D)) \text{ such that}$$

$$- \operatorname{div}(a(\mathbf{x}, \mathbf{y}) \nabla u(\mathbf{x}, \mathbf{y})) = f(\mathbf{x}) \text{ in } D \text{ for all } \mathbf{y} \in \mathbb{R}^m.$$

Note that the diffusion coefficient  $a$  is not uniformly elliptic in  $\mathbf{y}$ .  
But the diffusion coefficient satisfies

$$0 < a_{\min}(\mathbf{y}) := \operatorname{ess\,inf}_{\mathbf{x} \in D} a(\mathbf{x}, \mathbf{y}) \leq \operatorname{ess\,sup}_{\mathbf{x} \in D} a(\mathbf{x}, \mathbf{y}) =: a_{\max}(\mathbf{y}) < \infty$$

for all  $\mathbf{y} \in \mathbb{R}^m$ . Thus for every fixed  $\mathbf{y} \in \mathbb{R}^m$  the problem

$$- \operatorname{div}(a(\mathbf{x}, \mathbf{y}) \nabla u(\mathbf{x}, \mathbf{y})) = f(\mathbf{x}) \text{ in } D$$

$$u(\mathbf{x}, \mathbf{y}) = 0 \text{ on } \partial D$$

is elliptic and admits a unique solution  $u(\cdot, \mathbf{y}) \in H_0^1(D)$  with

$$\|u(\cdot, \mathbf{y})\|_{H^1(D)} \lesssim \frac{1}{a_{\min}(\mathbf{y})} \|f\|_{L^2(D)}.$$

We will not compute an approximation of the solution itself. Instead we consider the computations of statistical quantities of the solution, like its moments. This means that we have to approximate high-dimensional integrals of the form

$$\mathcal{M}_\rho(u)(\mathbf{x}) := \int_{\mathbb{R}^m} u^p(\mathbf{x}, \mathbf{y}) \rho(\mathbf{y}) \, d\mathbf{y}.$$

QMC quadrature rules use classically points in the hypercube  $[0, 1]^m$ . Hence we transform the integral:

$$\int_{\mathbb{R}^m} u^p(\mathbf{x}, \mathbf{y}) \rho(\mathbf{y}) \, d\mathbf{y} = \int_{[0,1]^m} u^p(\mathbf{x}, \Phi^{-1}(\mathbf{z})) \, d\mathbf{z},$$

where  $\Phi^{-1}(\mathbf{z})$  denotes the inverse of the  $m$ -dimensional cumulative normal distribution.

## QMC quadrature

A QMC quadrature rule for  $v \in L^1([0, 1]^m; X)$ , where  $X$  is a Banach space of functions defined on  $D$ , is of the form

$$(\mathbf{Q}v)(\mathbf{x}) = \frac{1}{N} \sum_{i=1}^N v(\mathbf{x}, \xi_i).$$

Here  $N$  denotes the number of *samples* and  $\xi_i \in \mathbb{R}^m$  is one *sample point*. In contrast to the MC quadrature, where the set of sample points is chosen randomly, QMC quadrature constructs the sample points. One classical construction was developed by Halton.



## Halton sequence

Let  $b_1, \dots, b_m$  denotes the first  $m$  prime numbers. The  $m$ -dimensional *Halton sequence* is given by

$$\xi_i = [h_{b_1}(i), \dots, h_{b_m}(i)]^T, \quad i = 0, 1, 2, \dots,$$

where  $h_{b_j}(i)$  denotes the  $i$ -th element of the *van der Corput sequence* with respect to  $b_j$ . That is, if  $i = \dots c_3 c_2 c_1$  (in radix  $b_j$ ), then  $h_{b_j}(i) = 0.c_1 c_2 c_3 \dots$  (in radix  $b_j$ ).

The Halton sequence belongs to the class of *low discrepancy* sequences.

## Koksma-Hlawka-inequality

For a function  $v \in W_{\text{mix}}^{1,1}([0, 1]^m; H_0^1(D))$ , i.e.

$$\|v\|_{W_{\text{mix}}^{1,1}([0,1]^m; H^1(D))} := \sum_{\|\mathbf{q}\|_{\infty} \leq 1} \int_{[0,1]^m} \|\partial_{\mathbf{y}}^{\mathbf{q}} v(\mathbf{y})\|_{H^1(D)} \, d\mathbf{y} < \infty,$$

the error of QMC quadrature can be estimated by

$$\|(\mathbf{I} - \mathbf{Q})v\|_{H^1(D)} \lesssim \mathcal{D}_{\infty}^*(\Xi) \|v\|_{W_{\text{mix}}^{1,1}([0,1]^m; H^1(D))}.$$

The  $L^{\infty}$ -star discrepancy  $\mathcal{D}_{\infty}^*(\Xi)$  of the set of sample points  $\Xi = \{\xi_1, \dots, \xi_N\} \subset [0, 1]^m$  is defined by

$$\mathcal{D}_{\infty}^*(\Xi) := \sup_{\mathbf{t} \in [0,1]^m} \left| \text{Vol}([0, \mathbf{t}]) - \frac{1}{N} \sum_{i=1}^N \mathbb{1}_{[0, \mathbf{t}]}(\xi_i) \right|.$$

There arise two main problems:

- ▶ The function  $u(\mathbf{x}, \Phi^{-1}(\mathbf{z}))$  does not belong to  $W_{\text{mix}}^{1,1}([0, 1]^m; H_0^1(D))$  since it is unbounded at the boundary of  $[0, 1]^m$ .
- ▶ The  $L^\infty$ -star discrepancy of *low discrepancy* sequences is bounded by  $\mathcal{O}(N^{-1} \log^m N)$ . Thus, even if the integrand belongs to  $W_{\text{mix}}^{1,1}([0, 1]^m; H_0^1(D))$ , the cost for QMC quadrature to reach a certain accuracy may grow exponentially in the dimension  $m$ . If we observe such a behaviour then the method is called *intractable*.

In the following we show that the QMC quadrature with Halton points is *polynomial tractable* for our model problem, under certain decay properties of the series  $\{\gamma_k\}_k$ . Polynomial tractable means that we achieve a convergence order  $\mathcal{O}(N^{-s} m^q)$  for some  $s, q > 0$ .

## Convergence analysis

- ▶ The Halton sequence avoids the region around the boundary of the hypercube. More precisely there exists a constant  $r \in [1, 2]$  such that  $\Xi \subset K_N$  with  $K_N := [\varepsilon_N, 1 - \varepsilon_N]^m$  and  $\varepsilon_N = CN^{-r}$ .
- ▶ The derivatives of the solution  $u$  satisfy

$$\|\partial_{\mathbf{y}}^{\alpha} u(\cdot, \mathbf{y})\|_{H^1(D)} \leq |\alpha|! \left( \frac{\gamma}{\log 2} \right)^{|\alpha|} \sqrt{\frac{a_{\max}(\mathbf{y})}{a_{\min}(\mathbf{y})}} \|u(\cdot, \mathbf{y})\|_{H^1(D)}.$$

The first property means that the QMC quadrature introduces a truncation error since it does not reflect the behaviour of the integrand in  $[0, 1]^m \setminus K_N$ .

Let now  $\hat{u}(\mathbf{x}, \mathbf{z}) := u(\mathbf{x}, \Phi^{-1}(\mathbf{z}))$ . For  $\mathbf{z} \in (0, 1)^m \setminus K_N$  we replace  $\hat{u}$  by its low variation extension  $\hat{u}_{\text{ext}}$ , i.e.

$$\hat{u}_{\text{ext}}(\mathbf{z}) := \hat{u}(\mathbf{z}_0) + \sum_{\|\alpha\|_\infty=1} \int_{[(\mathbf{z}_0)_\alpha, (\mathbf{z})_\alpha]} \mathbb{1}_{\mathbf{y} \vee_\alpha \mathbf{z}_0 \in K_N} \partial^\alpha \hat{u}(\mathbf{y} \vee_\alpha \mathbf{z}_0) d(\mathbf{y})_\alpha.$$

Given a vector  $\mathbf{z} \in \mathbb{R}^m$ , with  $(\mathbf{z})_\alpha \in \mathbb{R}^{\|\alpha\|_1}$  we mean the vector obtained by omitting every entry  $z_i$  for which  $\alpha_i = 0$ . For two vectors  $\mathbf{y}, \mathbf{z} \in \mathbb{R}^m$  we define  $\mathbf{y} \vee_\alpha \mathbf{z} := (y_i^{\alpha_i} z_i^{(1-\alpha_i)})_{i=1}^m$ . The anchor point  $\mathbf{z}_0$  is an arbitrary element of  $K_N$ . In the following we will assume that  $\mathbf{z}_0 = [1/2, \dots, 1/2]^\top$ . For  $\mathbf{y} \in K_N$  we set  $\hat{u}_{\text{ext}}(\mathbf{z}) = \hat{u}(\mathbf{z})$ .

We split the integration error into three parts:

$$\begin{aligned} \|(\mathbf{I} - \mathbf{Q})\hat{u}\|_{H^1(D)} &\leq \|\mathbf{I}(\hat{u} - \hat{u}_{\text{ext}})\|_{H^1(D)} \\ &\quad + \|\mathbf{Q}(\hat{u} - \hat{u}_{\text{ext}})\|_{H^1(D)} + \|(\mathbf{I} - \mathbf{Q})\hat{u}_{\text{ext}}\|_{H^1(D)}. \end{aligned}$$

The second term vanishes since  $\hat{u}|_{K_N} = \hat{u}_{\text{ext}}|_{K_N}$ . For the first term we have to estimate  $\|\hat{u}(\cdot, \mathbf{z}) - \hat{u}_{\text{ext}}(\cdot, \mathbf{z})\|_{H^1(D)}$ .

It holds for a multiindex  $\alpha$  with  $\|\alpha\|_\infty = 1$ :

$$\begin{aligned} \|\partial_z^\alpha u(\cdot, \Phi^{-1}(z))\|_{H^1(D)} &= \left\| \partial_y^\alpha u(\cdot, \Phi^{-1}(z)) \prod_{k=1}^m (\partial_{z_k} \Phi^{-1}(z_k))^{\alpha_k} \right\|_{H^1(D)} \\ &\leq \left| \prod_{k=1}^m (\partial_{z_k} \Phi^{-1}(z_k))^{\alpha_k} \right| \|\partial_y^\alpha u(\cdot, \Phi^{-1}(z))\|_{H^1(D)}. \end{aligned}$$

Furthermore we find

$$\partial_z \Phi^{-1}(z) = \mathcal{O}(\min(z, 1-z)^{-1-\delta/2}) \quad \text{for every } \delta > 0$$

and

$$\exp(c\Phi^{-1}(z)) = \mathcal{O}(\min(z, 1-z)^{-\delta/2}) \quad \text{for } c \in \mathbb{R} \text{ and every } \delta > 0.$$

Since  $\Phi^{-1}(1/2) = 0$  and

$$\begin{aligned} \sqrt{\frac{\alpha_{\max}(\Phi^{-1}(\mathbf{z}))}{\alpha_{\min}(\Phi^{-1}(\mathbf{z}))^3}} &\leq \exp\left(\sum_{k=1}^m 2\gamma_k |\Phi^{-1}(z_k)|\right) \\ &\lesssim \prod_{k=1}^m (\min(z_k, 1 - z_k))^{-\delta_k/2} \end{aligned}$$

we can prove that

$$\begin{aligned} \|\partial_{\mathbf{z}}^{\alpha} \hat{u}(\cdot, \mathbf{z} \vee_{\alpha} \mathbf{z}_0)\|_{H^1(D)} &\lesssim |\alpha|! \left(\frac{\gamma}{\log 2}\right)^{|\alpha|} \|f\|_{L^2(D)} \\ &\quad \prod_{k=1}^m \left(\min(z_k, 1 - z_k)\right)^{-1 - \delta_k} \alpha_k. \end{aligned}$$



Since

$$\hat{u}(\mathbf{z}) - \hat{u}_{\text{ext}}(\mathbf{z}) = \sum_{\|\alpha\|_{\infty}=1} \int_{[(z_0)_{\alpha}, (\mathbf{z})_{\alpha}]} \mathbb{1}_{\mathbf{y} \vee_{\alpha} \mathbf{z}_0 \notin K_N} \partial^{\alpha} \hat{u}(\mathbf{y} \vee_{\alpha} \mathbf{z}_0) d(\mathbf{y})_{\alpha},$$

we can establish with the above estimation on the derivative that

$$\begin{aligned} & \|\hat{u}(\cdot, \mathbf{z}) - \hat{u}_{\text{ext}}(\cdot, \mathbf{z})\|_{H^1(D)} \\ & \lesssim \|f\|_{L^2(D)} \prod_{k=1}^m \left(1 + \frac{k\gamma_k}{\delta_k}\right) \prod_{k=1}^m \min\{z_k, 1 - z_k\}^{-\delta_k} \end{aligned}$$

holds for all  $\mathbf{z} \in [0, 1]^m \setminus K_N$ .

Thus, it holds for the first term in the error splitting

$$\begin{aligned}
 & \|\mathbf{I}(\hat{u} - \hat{u}_{\text{ext}})\|_{H^1(D)} \\
 & \leq \int_{(0,1)^m \setminus K_N} \|\hat{u}(\cdot, \mathbf{z}) - \hat{u}_{\text{ext}}(\cdot, \mathbf{z})\|_{H^1(D)} \, d\mathbf{z} \\
 & \lesssim \|f\|_{L^2(D)} \int_{(0,1)^m \setminus [\varepsilon_N, 1 - \varepsilon_N]^m} \prod_{k=1}^m \min\{z_k, 1 - z_k\}^{-\delta_k} \, d\mathbf{z} \prod_{k=1}^m \left(1 + \frac{k\gamma_k}{\delta_k}\right) \\
 & \leq \|f\|_{L^2(D)} 2^m \sum_{k=1}^m \int_0^{\varepsilon_N} z_k^{-\delta_k} \, dz_k \prod_{i=1, i \neq k}^m \int_0^{1/2} z_i^{-\delta_i} \, dz_i \prod_{k=1}^m \left(1 + \frac{k\gamma_k}{\delta_k}\right) \\
 & \leq \|f\|_{L^2(D)} 2^m \sum_{k=1}^m \varepsilon_N^{1-\delta_k} 2^{-m+1} 2^{\sum_{k=1}^m \delta_k} \prod_{k=1}^m \left[ \left(1 + \frac{k\gamma_k}{\delta_k}\right) \left(\frac{1}{1-\delta_k}\right) \right] \\
 & \lesssim \|f\|_{L^2(D)} m N^{r(\max_{k=1, \dots, m} \delta_k - 1)} \prod_{k=1}^m \left[ \left(1 + \frac{k\gamma_k}{\delta_k}\right) \left(\frac{1}{1-\delta_k}\right) 2^{\delta_k} \right].
 \end{aligned}$$

The aim to proof tractability is to find an error bound, which grows at most polynomially in  $m$ . Thus we have to treat the product in the above estimate carefully. Since we can choose arbitrary  $\delta_k > 0$  we can assume that  $\delta_k \sim k^{-1-\varepsilon}$  for some  $\varepsilon > 0$ . Then it holds

$$\prod_{k=1}^m 2^{\delta_k} \leq 2^{\sum_{k=1}^m \delta_k} < \infty \quad \text{and} \quad \prod_{k=1}^m \frac{1}{1 - \delta_k} < \infty.$$

Both terms can be bounded independent of  $m$ . If we furthermore assume that  $\gamma_k \lesssim k^{-2-\tilde{\varepsilon}}\delta_k$  for  $\tilde{\varepsilon} > 0$  then

$$\prod_{k=1}^m \left( 1 + \frac{k\gamma_k}{\delta_k} \right) \leq \prod_{k=1}^m (1 + k^{-1-\varepsilon}) < \infty$$

is also bounded independent of  $m$ .

Finally, we bound the third term  $\|(\mathbf{I} - \mathbf{Q})\hat{u}_{\text{ext}}\|_{H^1(D)}$ . Therefore we define the centered discrepancy for a given set of  $N$  sample points  $\Xi \subset \mathbb{R}^m$  and a point  $\mathbf{z} \in \mathbb{R}^m$  by

$$\mathcal{D}^c(\mathbf{z}, \Xi) := \prod_{k=1}^m (-z_k + \mathbb{1}_{\{z_k > 1/2\}}) - \frac{1}{N} \sum_{\xi \in \Xi} \prod_{k=1}^m (\mathbb{1}_{\{z_k > 1/2\}} - \mathbb{1}_{\{z_k > \xi_k\}}).$$

We further denote by  $(\Xi)_\alpha$  the projection of  $\Xi$  given by  $(\Xi)_\alpha := \{(\xi)_\alpha, \xi \in \Xi\}$ . Then it holds

$$\begin{aligned} \|(\mathbf{I} - \mathbf{Q})\hat{u}_{\text{ext}}\|_{H^1(D)} &\leq \sum_{\|\alpha\|_\infty=1} \int_{[0,1]^{|\alpha|}} \|\partial_{\mathbf{z}}^\alpha \hat{u}_{\text{ext}}(\cdot, \mathbf{z} \vee_\alpha \mathbf{z}_0)\|_{H^1(D)} \mathbf{d}(\mathbf{z})_\alpha \\ &\quad \cdot \sup_{(\mathbf{z}_\alpha) \in [0,1]^{|\alpha|}} \mathcal{D}^c((\mathbf{z})_\alpha, (\Xi)_\alpha). \end{aligned}$$

We introduce weights  $w_k$ ,  $k = 1, \dots, m$  and define product weights corresponding to an multiindex  $\alpha$  as  $w_\alpha := \prod_{k=1}^m w_k^{\alpha_k}$ . Multiplying and dividing by these weights yields

$$\begin{aligned}
 & \|(\mathbf{I} - \mathbf{Q})\hat{u}_{\text{ext}}\|_{H^1(D)} \\
 & \leq \sum_{\|\alpha\|_\infty=1} w_\alpha^{-1/2} \int_{[0,1]^{|\alpha|}} \left\| \partial_{\mathbf{z}}^\alpha \hat{u}_{\text{ext}}(\cdot, \mathbf{z} \vee_\alpha \mathbf{z}_0) \right\|_{H^1(D)} \mathbf{d}(\mathbf{z})_\alpha \\
 & \quad \cdot w_\alpha^{1/2} \sup_{(\mathbf{z}_\alpha) \in [0,1]^{|\alpha|}} \mathcal{D}^c((\mathbf{z})_\alpha, (\Xi)_\alpha) \\
 & \leq \sup_{\|\alpha\|=1} w_\alpha^{-1/2} \int_{[0,1]^{|\alpha|}} \left\| \partial_{\mathbf{z}}^\alpha \hat{u}_{\text{ext}}(\cdot, \mathbf{z} \vee_\alpha \mathbf{z}_0) \right\|_{H^1(D)} \mathbf{d}(\mathbf{z})_\alpha \\
 & \quad \cdot \sum_{\|\alpha\|_\infty=1} w_\alpha^{1/2} \sup_{(\mathbf{z}_\alpha) \in [0,1]^{|\alpha|}} \mathcal{D}^c((\mathbf{z})_\alpha, (\Xi)_\alpha)
 \end{aligned}$$

If we choose the weights as  $w_k = \frac{4k^2\gamma_k^2}{\delta_k^2 \log^2 2}$  we are able to show

$$\begin{aligned} & \sup_{\|\alpha\|=1} w_\alpha^{-1/2} \int_{[0,1]^{|\alpha|}} \left\| \partial_{\mathbf{z}}^\alpha \hat{u}_{\text{ext}}(\cdot, \mathbf{z} \vee_\alpha \mathbf{z}_0) \right\|_{H^1(D)} d(\mathbf{z})_\alpha \\ & \lesssim N^r \sum_{k=1}^m \delta_k \|f\|_{L^2(D)}. \end{aligned}$$

If moreover  $\gamma_k$  satisfies for  $\hat{\varepsilon} > 0$

$$\gamma_k \lesssim \frac{\delta_k \log 2}{4} k^{-3-\hat{\varepsilon}}$$

then we can achieve the discrepancy bound

$$\sum_{\|\alpha\|_\infty=1} w_\alpha^{1/2} \sup_{(\mathbf{z}_\alpha) \in [0,1]^{|\alpha|}} \mathcal{D}^c((\mathbf{z})_\alpha, (\Xi)_\alpha) \lesssim N^{-1+\tilde{\delta}}.$$

## Theorem

The QMC quadrature rule  $\mathbf{Q}$  using  $N$  Halton points satisfies

$$\|(\mathbf{I} - \mathbf{Q})\hat{u}\|_{H^1(D)} \lesssim \|f\|_{L^2(D)} \left( mN^{r(\max_{k=1, \dots, m} \delta_k - 1)} + N^{-1 + \tilde{\delta} + r \sum_{k=1}^m \delta_k} \right),$$

for an arbitrarily chosen  $\tilde{\delta} > 0$  and  $0 < \delta_k \lesssim k^{-1-\varepsilon}$  for some  $\varepsilon > 0$ ,  
 under the condition that the sequence  $\{\gamma_k\}_k$  fulfills  
 $\gamma_k \lesssim \frac{\delta_k \log 2}{4} k^{-3-\hat{\varepsilon}}$  for some  $\hat{\varepsilon} > 0$ .