Uncertainty Quantification and Quasi-Monte Carlo

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Today's lecture follows the survey article

F. Y. Kuo and D. Nuyens. Application of quasi-Monte Carlo methods to elliptic PDEs with random diffusion coefficients - a survey of analysis and implementation. *Found. Comput. Math.* **16**:1631–1696, 2016. arXiv version: https://arxiv.org/abs/1606.06613

Introduction: transformation to the unit cube

Consider the (univariate) integral

$$\int_{-\infty}^{\infty} g(y)\phi(y)\,\mathrm{d}y,$$

where $\phi\colon \mathbb{R} \to \mathbb{R}_{\geq 0}$ is a univariate probability density function, i.e., $\int_{-\infty}^{\infty} \phi(y)\,\mathrm{d}y = 1$. How do we transform the integral into $[0,1]$?

Let $\Phi\colon \mathbb{R} \to [0,1]$ denote the cumulative distribution function of ϕ, defined by $\Phi(y) := \int_{-\infty}^{y} \phi(t)\,\mathrm{d}t$ and let $\Phi^{-1}\colon [0,1] \to \mathbb{R}$ denote its inverse. Then we use the change of variables

$$x = \Phi(y) \quad \Leftrightarrow \quad y = \Phi^{-1}(x)$$

to obtain

$$\int_{-\infty}^{\infty} g(y)\phi(y)\,\mathrm{d}y = \int_0^1 g(\Phi^{-1}(x))\,\mathrm{d}x = \int_0^1 f(x)\,\mathrm{d}x,$$

where $f := g \circ \Phi^{-1}$ is the transformed integrand.

Actually, we can multiply and divide by any other probability density function $\widetilde{\phi}$ and then map to $[0, 1]$ using its inverse cumulative distribution function $\widetilde{\Phi}^{-1}$:

$$\begin{aligned}
\int_{-\infty}^{\infty} g(y)\phi(y)\,\mathrm{d}y &= \int_{-\infty}^{\infty} \frac{g(y)\phi(y)}{\widetilde{\phi}(y)}\widetilde{\phi}(y)\,\mathrm{d}y \\
&= \int_{-\infty}^{\infty} \widetilde{g}(y)\widetilde{\phi}(y)\,\mathrm{d}y \qquad\qquad (\widetilde{g}(y) := \tfrac{g(y)\phi(y)}{\widetilde{\phi}(y)}) \\
&= \int_0^1 \widetilde{g}(\widetilde{\Phi}^{-1}(x))\,\mathrm{d}x = \int_0^1 \widetilde{f}(x)\,\mathrm{d}x. \quad (\widetilde{f} := \widetilde{g} \circ \widetilde{\Phi}^{-1})
\end{aligned}$$

Ideally we would like to use a density function which leads to an easy integrand in the unit cube. (Compare this with *importance sampling* for the Monte Carlo method.)

This transformation can be generalized to s dimensions in the following way. If we have a product of univariate densities, then we can apply the mapping Φ^{-1} *componentwise*

$$\boldsymbol{y} = \Phi^{-1}(\boldsymbol{x}) = [\Phi^{-1}(x_1), \ldots, \Phi^{-1}(x_s)]^{\mathrm{T}}$$

to obtain

$$\int_{\mathbb{R}^s} g(\boldsymbol{y}) \prod_{j=1}^{s} \phi(y_j) \, \mathrm{d}\boldsymbol{y} = \int_{(0,1)^s} g(\Phi^{-1}(\boldsymbol{x})) \, \mathrm{d}\boldsymbol{x} = \int_{(0,1)^s} f(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x}.$$

(Of course, dividing and multiplying by a product of arbitrary probability density functions would work here as well!)

Lognormal model

Let $D \subset \mathbb{R}^d$, $d \in \{2, 3\}$, be a bounded Lipschitz domain. In the "lognormal" case, we assume that the parameter $\boldsymbol{y}$ is distributed in $\mathbb{R}^{\mathbb{N}}$ according to the product Gaussian measure $\mu_G = \bigotimes_{j=1}^{\infty} \mathcal{N}(0, 1)$. The parametric coefficient $a(\boldsymbol{x}, \boldsymbol{y})$ now takes the form

$$a(\boldsymbol{x}, \boldsymbol{y}) := a_0(\boldsymbol{x}) \exp\left(\sum_{j=1}^{\infty} y_j \psi_j(\boldsymbol{x})\right), \quad \boldsymbol{x} \in D, \ \boldsymbol{y} \in \mathbb{R}^{\mathbb{N}}, \tag{1}$$

where $a_0 \in L^\infty(D)$ with $a_0(\boldsymbol{x}) > 0$, $\boldsymbol{x} \in D$.

A coefficient of the form (1) can arise from the Karhunen–Loève (KL) expansion in the case where $\log(a)$ is a stationary Gaussian random field with a specified mean and a covariance function.

Example

Consider a Gaussian random field with an isotropic *Matérn covariance* $\mathrm{Cov}(\boldsymbol{x}, \boldsymbol{x}') := \rho_\nu(|\boldsymbol{x} - \boldsymbol{x}'|)$, with

$$\rho_\nu(r) := \sigma^2 \frac{2^{1-\nu}}{\Gamma(\nu)} \left(2\sqrt{\nu}\frac{r}{\lambda_C}\right)^\nu K_\nu\left(2\sqrt{\nu}\frac{r}{\lambda_C}\right),$$

where Γ is the gamma function and K_ν is the modified Bessel function of the second kind. The parameter $\nu > 1/2$ is a smoothness parameter, σ^2 is the variance, and λ_C is the correlation length scale.

If $\{(\lambda_j, \xi_j)\}_{j=1}^\infty$ is the sequence of eigenvalues and eigenfunctions of the covariance operator $(\mathcal{C}f)(\boldsymbol{x}) := \int_D \rho_\nu(|\boldsymbol{x} - \boldsymbol{x}'|) f(\boldsymbol{x}')\,\mathrm{d}\boldsymbol{x}'$, i.e., $\mathcal{C}\xi_j = \lambda_j \xi_j$, where we assume that $\lambda_1 \geq \lambda_2 \geq \cdots$ and the eigenfunctions are normalized s.t. $\|\xi_j\|_{L^2(D)} = 1$, then we can set $\psi_j(\boldsymbol{x}) := \sqrt{\lambda_j}\xi_j(\boldsymbol{x})$ in (1) to obtain the KL expansion for this Gaussian random field.

Lognormal model: let $D \subset \mathbb{R}^d$, $d \in \{2,3\}$, be a bounded Lipschitz domain, and let $f \in H^{-1}(D)$. Let $\psi_j \in L^\infty(D)$ and $b_j := \|\psi_j\|_{L^\infty}$ for $j \in \mathbb{N}$ such that $\sum_{j=1}^\infty b_j < \infty$, and set

$$U_{\boldsymbol{b}} := \left\{ \boldsymbol{y} \in \mathbb{R}^{\mathbb{N}} : \sum_{j=1}^{\infty} b_j |y_j| < \infty \right\}.$$

Consider the problem of finding, for all $\boldsymbol{y} \in U$, $u(\cdot, \boldsymbol{y}) \in H_0^1(D)$ such that

$$\int_D a(\boldsymbol{x}, \boldsymbol{y}) \nabla u(\boldsymbol{x}, \boldsymbol{y}) \cdot \nabla v(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} = \langle f, v \rangle_{H^{-1}(D), H_0^1(D)} \quad \text{for all } v \in H_0^1(D),$$

where the diffusion coefficient is assumed to have the parameterization

$$a(\boldsymbol{x}, \boldsymbol{y}) := a_0(\boldsymbol{x}) \exp\left(\sum_{j=1}^{\infty} y_j \psi_j(\boldsymbol{x}) \right), \quad \boldsymbol{x} \in D, \ \boldsymbol{y} \in U_{\boldsymbol{b}},$$

where $a_0 \in L^\infty(D)$ is such that $a_0(\boldsymbol{x}) > 0$, $\boldsymbol{x} \in D$.

Standing assumptions for the lognormal model

(B1) We have $a_0 \in L^\infty(D)$ and $\sum_{j=1}^\infty b_j < \infty$.

(B2) For every $\boldsymbol{y} \in U_{\boldsymbol{b}}$, the expressions $a_{max}(\boldsymbol{y}) := \max_{\boldsymbol{x}\in\overline{D}} a(\boldsymbol{x},\boldsymbol{y})$ and $a_{\min}(\boldsymbol{y}) := \min_{\boldsymbol{x}\in\overline{D}} a(\boldsymbol{x},\boldsymbol{y})$ are well-defined and satisfy $0 < a_{\min}(\boldsymbol{y}) \leq a(\boldsymbol{x},\boldsymbol{y}) \leq a_{\max}(\boldsymbol{y}) < \infty$.

(B3) $\sum_{j=1}^\infty b_j^p < \infty$ for some $p \in (0,1)$.

Remark: Note that in the lognormal case, $a(\boldsymbol{x},\boldsymbol{y})$ can take values which are arbitrarily close to 0 or arbitrarily large. Thus, the best we can do is to find $\boldsymbol{y}$-dependent lower and upper bounds $a_{\min}(\boldsymbol{y})$ and $a_{\max}(\boldsymbol{y})$. This will lead to a $\boldsymbol{y}$-dependent *a priori* bound and, consequently, $\boldsymbol{y}$-dependent parametric regularity bounds. This will make the QMC analysis more involved, leading one to consider "special" weighted, unanchored Sobolev spaces.

Clearly, the diffusion coefficient $a(\boldsymbol{x}, \boldsymbol{y})$ blows up for certain values of $\boldsymbol{y} \in \mathbb{R}^{\mathbb{N}}$ (think of $y_j = b_j^{-1}$), but the PDE problem is well-defined in the parameter set $U_{\boldsymbol{b}}$ which turns out to be of full measure in $(\mathbb{R}^{\mathbb{N}}, \mathcal{B}(\mathbb{R}^{\mathbb{N}}), \mu_G)$.

Lemma

There holds $U_{\boldsymbol{b}} \in \mathcal{B}(\mathbb{R}^{\mathbb{N}})$, where $\mathcal{B}$ denotes the Borel σ-algebra and $\mu_G(U_{\boldsymbol{b}}) = 1$.

Proof. See Lemma 2.28 in "Sparse tensor discretizations of high-dimensional parametric and stochastic PDEs" by Ch. Schwab and C. J. Gittelson (2011). □

The previous lemma implies that

$$I(F) := \int_{\mathbb{R}^{\mathbb{N}}} F(\boldsymbol{y})\,\mu_G(\mathrm{d}\boldsymbol{y}) = \int_{U_{\boldsymbol{b}}} F(\boldsymbol{y})\,\mu_G(\mathrm{d}\boldsymbol{y}).$$

Thus, it is sufficient to restrict our parametric regularity analysis to $\boldsymbol{y} \in U_{\boldsymbol{b}}$, for which $a(\boldsymbol{x}, \boldsymbol{y})$ (and hence $u(\boldsymbol{x}, \boldsymbol{y})$) are well-defined.

Let $G \in H^{-1}(D)$, our (dimensionally-truncated) integral quantity of interest can thus be written as

$$\begin{aligned} I_s(G(u_s)) := \int_{\mathbb{R}^s} G(u_s(\cdot, \boldsymbol{y})) \prod_{j=1}^{s} \phi(y_j)\,\mathrm{d}\boldsymbol{y} &= \int_{(0,1)^s} G(u(\Phi^{-1}(\boldsymbol{w})))\,\mathrm{d}\boldsymbol{w} \\ &\approx \frac{1}{n} \sum_{i=1}^{n} G(u(\Phi^{-1}(\boldsymbol{t}_i))) \\ &=: Q_{n,s}(G(u(\cdot, \Phi^{-1}(\cdot)))), \end{aligned}$$

where $Q_{n,s}$ represents a QMC rule over an s-dimensional point set $\{\boldsymbol{t}_i\}_{i=1}^{n} \subset (0,1)^s$.

Akin to the uniform case, we have a total error decomposition of the form

$$\begin{aligned} |I(G(u)) - Q_{n,s}(G(u_{s,h}))| \leq |I(G(u - u_h))| \\ + |I(G(u_h) - G(u_{s,h}))| \\ + |I_s(G(u_{s,h})) - Q_{n,s}(G(u_{s,h}))|. \end{aligned}$$

We focus on the QMC error, but briefly mention the corresponding dimension truncation and finite element error results below. For further details, see Graham, Kuo, Nichols, Scheichl, Schwab, Sloan (2015).

- If $D \subset \mathbb{R}^2$ is a bounded convex polyhedron, $f \in L^2(D)$, $G \in L^2(D)'$, and $a(\cdot, \boldsymbol{y})$ is Lipschitz for all $\boldsymbol{y} \in U_{\boldsymbol{b}}$, then the finite element error satisfies $\mathbb{E}[G(u - u_h)] = \mathcal{O}(h^2)$. (Similar result holds for $D \subset \mathbb{R}^3$.)
- For the Matérn covariance with $\nu > d/2$, there holds

$$|I(G(u_h)) - I(G(u_{s,h}))| = \mathcal{O}(s^{-\chi}), \quad 0 < \chi < \frac{\nu}{d} - \frac{1}{2}.$$

  There has been some recent work on generalizing this result, cf., e.g., Guth and Kaarnioja (2024): https://arxiv.org/abs/2209.06176

Let us focus on the QMC error

$$\int_{\mathbb{R}^s} G(u_{s,h}(\cdot,\boldsymbol{y}))\,\mathrm{d}\boldsymbol{y} - \frac{1}{n}\sum_{k=1}^{n} G(u_{s,h}(\cdot,\Phi^{-1}(\boldsymbol{t}_k))).$$

In this setting, we have

$$I_s(F) := \int_{\mathbb{R}^s} F(\boldsymbol{y})\prod_{j=1}^{s}\phi(y_j)\,\mathrm{d}\boldsymbol{y} = \int_{(0,1)^s} F(\Phi^{-1}(\boldsymbol{w}))\,\mathrm{d}\boldsymbol{w}$$

and the randomly shifted QMC rules

$$Q_{n,s}^{(r)}(F) = \frac{1}{n}\sum_{k=1}^{n} F(\Phi^{-1}(\{\boldsymbol{t}_k + \boldsymbol{\Delta}_r\})),$$

$$\overline{Q}_{n,R}(F) := \frac{1}{R}\sum_{r=1}^{R} Q_{n,s}^{(r)}(F),$$

where we have R independent random shifts $\boldsymbol{\Delta}_1,\ldots,\boldsymbol{\Delta}_R$ drawn from $\mathcal{U}([0,1]^s)$, $\boldsymbol{t}_k := \{\frac{k\boldsymbol{z}}{n}\}$, with generating vector $\boldsymbol{z} \in \mathbb{N}^s$.

Function space setting

Kuo, Sloan, Wasilkowski, Waterhouse (2010): It turns out that the appropriate function space for unbounded integrands is a "special" weighted, unanchored Sobolev space equipped with the norm

$$\|F\|_{s,\gamma} = \Bigg[\sum_{\mathfrak{u}\subseteq\{1:s\}} \frac{1}{\gamma_{\mathfrak{u}}} \int_{\mathbb{R}^{|\mathfrak{u}|}} \left(\int_{\mathbb{R}^{s-|\mathfrak{u}|}} \frac{\partial^{|\mathfrak{u}|}}{\partial \boldsymbol{y}_{\mathfrak{u}}} F(\boldsymbol{y}) \Bigg(\prod_{j\in\{1:s\}\setminus\mathfrak{u}} \phi(y_j) \Bigg) \,\mathrm{d}\boldsymbol{y}_{-\mathfrak{u}} \right)^2 \times \Bigg(\prod_{j\in\mathfrak{u}} \varpi_j^2(y_j) \Bigg) \,\mathrm{d}\boldsymbol{y}_{\mathfrak{u}} \Bigg]^{1/2}$$

where we have the weights

$$\varpi_j^2(y) := \exp(-2\alpha_j|y_j|), \quad \alpha_j > 0.$$

Brief idea: We're interested in functions of the form $g(\boldsymbol{y}) = f(\Phi^{-1}(\boldsymbol{y}))$, where $f \in \mathcal{F}$. Now there exists an isometric space $\mathcal{G}$ of functions s.t.

$$f \in \mathcal{F} \quad \Leftrightarrow \quad g = f(\Phi^{-1}(\cdot)) \in \mathcal{G} \text{ and } \|f\|_{\mathcal{F}} = \|g\|_{\mathcal{G}}.$$

If $\mathcal{F}$ is a RKHS with kernel $K_{\mathcal{F}}$, then $\mathcal{G}$ is a RKHS with kernel $K_{\mathcal{G}}(\boldsymbol{x},\boldsymbol{y}) = K_{\mathcal{F}}(\Phi^{-1}(\boldsymbol{x}),\Phi^{-1}(\boldsymbol{y}))$. Thus the core idea is to investigate Sobolev spaces over unbounded domains which can be mapped isomorphically onto weighted Sobolev spaces over $(0,1)^s$.

Theorem (Graham, Kuo, Nichols, Scheichl, Schwab, Sloan (2015))

Let F belong to the special weighted space over $\mathbb{R}^s$ with weights $\boldsymbol{\gamma}$, with ϕ being the standard normal density, and the weight functions ϖ_j defined as above. A randomly shifted lattice rule in s dimensions with n being a prime power can be constructed by a CBC algorithm such that

$$\sqrt{\mathbb{E}_{\boldsymbol{\Delta}}|I_s F - Q_{n,s}^{\boldsymbol{\Delta}} F|^2} \leq \left(\frac{2}{n} \sum_{\emptyset \neq \mathfrak{u} \subseteq \{1:s\}} \gamma_{\mathfrak{u}}^{\lambda} \prod_{j \in \mathfrak{u}} \varrho_j(\lambda) \right)^{1/(2\lambda)} \|F\|_{s,\boldsymbol{\gamma}},$$

where $\lambda \in (1/2, 1]$ and

$$\varrho_j(\lambda) = 2 \left(\frac{\sqrt{2\pi} \exp(\alpha_j^2/\eta_*)}{\pi^{2-2\eta_*}(1-\eta_*)\eta_*} \right)^{\lambda} \zeta(\lambda + \tfrac{1}{2}) \quad \text{and} \quad \eta_* = \frac{2\lambda - 1}{4\lambda},$$

with $\zeta(x) := \sum_{k=1}^{\infty} k^{-x}$ denoting the Riemann zeta function for $x > 1$.

The steps for QMC analysis are the same as in the uniform case: (1) estimate $\|\cdot\|_{s,\boldsymbol{\gamma}}$ for a given integrand (2) find weights $\boldsymbol{\gamma}$ which minimize the upper bound (3) plug the weights into the new error bound and estimate the constant (which ideally can be bounded independently of s).

Applying the theory in practice

Let us consider the parametric regularity of

$$\int_D a(\boldsymbol{x},\boldsymbol{y})\nabla u(\boldsymbol{x},\boldsymbol{y})\cdot\nabla v(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} = \langle f, v\rangle_{H^{-1}(D),H_0^1(D)} \quad \text{for all } v\in H_0^1(D),$$

where $a(\boldsymbol{x},\boldsymbol{y}) := a_0(\boldsymbol{x})\exp\big(\sum_{j=1}^\infty y_j\psi_j(\boldsymbol{x})\big)$ and $f\in H^{-1}(D)$.

Our strategy will be to obtain a parametric regularity bound for

$$\|\sqrt{a(\cdot,\boldsymbol{y})}\nabla\partial^{\boldsymbol{\nu}}u(\cdot,\boldsymbol{y})\|_{L^2(D)},$$

that is, we find a *sharp* estimate $\partial^{\boldsymbol{\nu}}u(\cdot,\boldsymbol{y})$ in the *energy norm*, and then use the coercivity of the problem to bound this from below by

$$\begin{aligned}\|\sqrt{a(\cdot,\boldsymbol{y})}\nabla\partial^{\boldsymbol{\nu}}u(\cdot,\boldsymbol{y})\|_{L^2(D)} &\geq \sqrt{a_{\min}(\boldsymbol{y})}\|\nabla\partial^{\boldsymbol{\nu}}u(\cdot,\boldsymbol{y})\|_{L^2(D)}\\ &= \sqrt{a_{\min}(\boldsymbol{y})}\|\partial^{\boldsymbol{\nu}}u(\cdot,\boldsymbol{y})\|_{H_0^1(D)}.\end{aligned}$$

(Compare with task 1 of Exercise 2, where we used a similar technique to obtain a better constant for Céa's lemma!)

Lemma

$$\|\sqrt{a(\cdot,\boldsymbol{y})}\nabla\partial^{\boldsymbol{\nu}}u(\cdot,\boldsymbol{y})\|_{L^2(D)}\leq \Lambda_{|\boldsymbol{\nu}|}\boldsymbol{b}^{\boldsymbol{\nu}}\frac{\|f\|_{H^{-1}(D)}}{\sqrt{a_{\min}(\boldsymbol{y})}},$$

where $(\Lambda_k)_{k=0}^{\infty}$ *are the* ordered Bell numbers *defined by the recursion*

$$\Lambda_0:=1\quad \textit{and}\quad \Lambda_k:=\sum_{\ell=1}^{k}\binom{k}{\ell}\Lambda_{k-\ell},\quad k\geq 1.$$

Proof. By induction with respect to the order of the multi-indices. The case $|\boldsymbol{\nu}|=0$ is resolved by observing that

$$\begin{aligned}\|a(\cdot,\boldsymbol{y})^{1/2}\nabla u(\cdot,\boldsymbol{y})\|_{L^2(D)}^2=\int_D a(\boldsymbol{x},\boldsymbol{y})|\nabla u(\boldsymbol{x},\boldsymbol{y})|^2\,\mathrm{d}\boldsymbol{x}&=\int_D f(\boldsymbol{x})u(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\\ &\leq \|f\|_{H^{-1}(D)}\|u(\cdot,\boldsymbol{y})\|_{H_0^1(D)}\\ &\leq \frac{\|f\|_{H^{-1}(D)}}{\sqrt{a_{\min}(\boldsymbol{y})}}\|a(\cdot,\boldsymbol{y})^{1/2}\nabla u(\cdot,\boldsymbol{y})\|_{L^2(D)}\end{aligned}$$

Next, let $\boldsymbol{\nu} \in \mathscr{F} \setminus \{\mathbf{0}\}$ be such that the claim has been proved for all multi-indices with order $< |\boldsymbol{\nu}|$. By exploiting the fact that

$$\left\| \frac{\partial^{\boldsymbol{m}} a(\cdot, \boldsymbol{y})}{a(\cdot, \boldsymbol{y})} \right\|_{L^\infty(D)} = \left\| \prod_{j \geq 1} \psi_j(\cdot)^{\nu_j} \right\|_{L^\infty(D)} \leq \boldsymbol{b}^{\boldsymbol{\nu}},$$

we obtain (using the Leibniz product rule)

$$\begin{aligned} &\sum_{\boldsymbol{m} \leq \boldsymbol{\nu}} \binom{\boldsymbol{\nu}}{\boldsymbol{m}} \int_D \partial^{\boldsymbol{m}} a(\boldsymbol{x}, \boldsymbol{y}) \nabla \partial^{\boldsymbol{\nu}-\boldsymbol{m}} u(\boldsymbol{x}, \boldsymbol{y}) \cdot \nabla v(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} = 0 \\ \Leftrightarrow \quad & \int_D a(\boldsymbol{x}, \boldsymbol{y}) \nabla \partial^{\boldsymbol{\nu}} u(\boldsymbol{x}, \boldsymbol{y}) \cdot \nabla v(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} \\ & \quad = - \sum_{\mathbf{0} \neq \boldsymbol{m} \leq \boldsymbol{\nu}} \binom{\boldsymbol{\nu}}{\boldsymbol{m}} \int_D \underbrace{\partial^{\boldsymbol{m}} a(\boldsymbol{x}, \boldsymbol{y})}_{= \frac{\partial^{\boldsymbol{m}} a(\boldsymbol{x}, \boldsymbol{y})}{a(\boldsymbol{x}, \boldsymbol{y})} a(\boldsymbol{x}, \boldsymbol{y})} \nabla \partial^{\boldsymbol{\nu}-\boldsymbol{m}} u(\boldsymbol{x}, \boldsymbol{y}) \cdot \nabla v(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x}. \end{aligned}$$

Testing against $v = \partial^{\boldsymbol{\nu}} u$ yields...

$$\|a^{1/2}(\cdot,\boldsymbol{y})\nabla\partial^{\boldsymbol{\nu}}u(\cdot,\boldsymbol{y})\|_{L^2(D)}^2 = \int_D a(\boldsymbol{x},\boldsymbol{y})|\nabla u(\boldsymbol{x},\boldsymbol{y})|^2\,\mathrm{d}\boldsymbol{x}$$

$$\leq \sum_{\boldsymbol{0}\neq\boldsymbol{m}\leq\boldsymbol{\nu}} \binom{\boldsymbol{\nu}}{\boldsymbol{m}} \int_D \left|\frac{\partial^{\boldsymbol{m}}a(\boldsymbol{x},\boldsymbol{y})}{a(\boldsymbol{x},\boldsymbol{y})}\right| a(\boldsymbol{x},\boldsymbol{y})\nabla\partial^{\boldsymbol{\nu}-\boldsymbol{m}}u(\boldsymbol{x},\boldsymbol{y})\cdot\nabla\partial^{\boldsymbol{\nu}}u(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}\boldsymbol{x}$$

$$\leq \sum_{\boldsymbol{0}\neq\boldsymbol{m}\leq\boldsymbol{\nu}} \binom{\boldsymbol{\nu}}{\boldsymbol{m}} \boldsymbol{b}^{\boldsymbol{m}}\|a^{1/2}(\cdot,\boldsymbol{y})\nabla\partial^{\boldsymbol{\nu}-\boldsymbol{m}}u(\cdot,\boldsymbol{y})\|_{L^2(D)}\|a^{1/2}(\cdot,\boldsymbol{y})\nabla\partial^{\boldsymbol{\nu}}u(\cdot,\boldsymbol{y})\|_{L^2(D)}$$

leading to the recurrence relation

$$\|a^{1/2}(\cdot,\boldsymbol{y})\nabla\partial^{\boldsymbol{\nu}}u(\cdot,\boldsymbol{y})\|_{L^2(D)} \leq \sum_{\boldsymbol{0}\neq\boldsymbol{m}\leq\boldsymbol{\nu}} \binom{\boldsymbol{\nu}}{\boldsymbol{m}} \boldsymbol{b}^{\boldsymbol{m}}\|a^{1/2}(\cdot,\boldsymbol{y})\nabla\partial^{\boldsymbol{\nu}-\boldsymbol{m}}u(\cdot,\boldsymbol{y})\|_{L^2(D)}$$

By our induction hypothesis,
$\|a^{1/2}(\cdot,\boldsymbol{y})\nabla\partial^{\boldsymbol{\nu}-\boldsymbol{m}}u(\cdot,\boldsymbol{y})\|_{L^2(D)} \leq \Lambda_{|\boldsymbol{\nu}|-|\boldsymbol{m}|}\boldsymbol{b}^{\boldsymbol{\nu}-\boldsymbol{m}}\frac{\|f\|_{H^{-1}(D)}}{\sqrt{a_{\min}(\boldsymbol{y})}}$. This results in...

$$
\begin{aligned}
\|a^{1/2}(\cdot,\boldsymbol{y})\nabla\partial^{\boldsymbol{\nu}}u(\cdot,\boldsymbol{y})\|_{L^2(D)} &\le \sum_{\mathbf{0}\neq\boldsymbol{m}\le\boldsymbol{\nu}}\binom{\boldsymbol{\nu}}{\boldsymbol{m}}\boldsymbol{b}^{\boldsymbol{m}}\|a^{1/2}(\cdot,\boldsymbol{y})\nabla\partial^{\boldsymbol{\nu}-\boldsymbol{m}}u(\cdot,\boldsymbol{y})\|_{L^2(D)} \\
&\le \boldsymbol{b}^{\boldsymbol{\nu}}\frac{\|f\|_{H^{-1}(D)}}{\sqrt{a_{\min}(\boldsymbol{y})}}\sum_{\mathbf{0}\neq\boldsymbol{m}\le\boldsymbol{\nu}}\binom{\boldsymbol{\nu}}{\boldsymbol{m}}\Lambda_{|\boldsymbol{\nu}|-|\boldsymbol{m}|} \\
&= \boldsymbol{b}^{\boldsymbol{\nu}}\frac{\|f\|_{H^{-1}(D)}}{\sqrt{a_{\min}(\boldsymbol{y})}}\sum_{\ell=1}^{|\boldsymbol{\nu}|}\Lambda_{|\boldsymbol{\nu}|-\ell}\sum_{\substack{|\boldsymbol{m}|=\ell\\ \boldsymbol{m}\le\boldsymbol{\nu}}}\binom{\boldsymbol{\nu}}{\boldsymbol{m}} \\
&= \boldsymbol{b}^{\boldsymbol{\nu}}\frac{\|f\|_{H^{-1}(D)}}{\sqrt{a_{\min}(\boldsymbol{y})}}\sum_{\ell=1}^{|\boldsymbol{\nu}|}\Lambda_{|\boldsymbol{\nu}|-\ell}\binom{|\boldsymbol{\nu}|}{\ell} \\
&= \boldsymbol{b}^{\boldsymbol{\nu}}\frac{\|f\|_{H^{-1}(D)}}{\sqrt{a_{\min}(\boldsymbol{y})}}\Lambda_{|\boldsymbol{\nu}|}. \quad \square
\end{aligned}
$$

A bound for Λ_k

The ordered Bell numbers have the following simple upper bound.

Lemma (Beck, Tempone, Nobile, Tamellini (2012))

$$\Lambda_k \leq \frac{k!}{(\log 2)^k}$$

Proof. By definition $\Lambda_k = \sum_{\ell=1}^k \binom{k}{\ell} \Lambda_{k-\ell} = \sum_{\ell=1}^k \frac{k!}{\ell!} \frac{\Lambda_{k-\ell}}{(k-\ell)!}$, $\Lambda_0 = 1$. Define $f_k := \frac{\Lambda_k}{k!}$; then clearly

$$f_k = \sum_{\ell=1}^k \frac{f_{k-\ell}}{\ell!}, \quad f_0 = f_1 = 1.$$

We prove by induction that $f_k \leq \alpha^k$ for some $\alpha \geq 1$. The base steps $k = 0, 1$ hold for all $\alpha \geq 1$ due to $f_0 = f_1 = 1$. Thus we assume that the claim holds for $f_1, \ldots, f_{k-1}$.

$$f_k = \sum_{\ell=1}^{k} \frac{f_{k-\ell}}{\ell!} \le \sum_{\ell=1}^{k} \frac{\alpha^{k-\ell}}{\ell!} = \alpha^k \sum_{\ell=1}^{k} \frac{\alpha^{-\ell}}{\ell!} \le \alpha^k (\mathrm{e}^{\frac{1}{\alpha}} - 1) \le \alpha^k,$$

where the last step holds provided that

$$\begin{aligned} \mathrm{e}^{\frac{1}{\alpha}} - 1 \le 1 \quad &\Leftrightarrow \quad \mathrm{e}^{\frac{1}{\alpha}} \le 2 \\ &\Leftrightarrow \quad \frac{1}{\alpha} \le \log 2 \\ &\Leftrightarrow \quad \alpha \ge \frac{1}{\log 2}. \end{aligned}$$

Thus $f_k \le \alpha^k$ for all $\alpha \ge \frac{1}{\log 2} (> 1)$. We get the sharpest bound by taking $\alpha = \frac{1}{\log 2}$, which yields

$$\Lambda_k = k! f_k \le \frac{k!}{(\log 2)^k}$$

as desired. □

Proposition

$$\|\partial^{\boldsymbol{\nu}} u(\cdot,\boldsymbol{y})\|_{H_0^1(D)} \le \frac{\|f\|_{H^{-1}(D)}}{\min_{\boldsymbol{x}\in\overline{D}} a_0(\boldsymbol{x})} \frac{|\boldsymbol{\nu}|!}{(\log 2)^{|\boldsymbol{\nu}|}} \boldsymbol{b}^{\boldsymbol{\nu}} \prod_{j\ge 1} \exp(b_j|y_j|)$$

Proof. From the previous discussion, we have that

$$\begin{aligned}
\sqrt{a_{\min}(\boldsymbol{y})}\|\nabla\partial^{\boldsymbol{\nu}} u(\cdot,\boldsymbol{y})\|_{L^2(D)} &\le \|\sqrt{a(\cdot,\boldsymbol{y})}\nabla\partial^{\boldsymbol{\nu}} u(\cdot,\boldsymbol{y})\|_{L^2(D)} \\
&\le \Lambda_{|\boldsymbol{\nu}|}\boldsymbol{b}^{\boldsymbol{\nu}} \frac{\|f\|_{H^{-1}(D)}}{\sqrt{a_{\min}(\boldsymbol{y})}} \\
&\le \frac{|\boldsymbol{\nu}|!}{(\log 2)^{|\boldsymbol{\nu}|}} \boldsymbol{b}^{\boldsymbol{\nu}} \frac{\|f\|_{H^{-1}(D)}}{\sqrt{a_{\min}(\boldsymbol{y})}}
\end{aligned}$$

$$\Rightarrow \quad \|\partial^{\boldsymbol{\nu}} u(\cdot,\boldsymbol{y})\|_{H_0^1(D)} \le \frac{\|f\|_{H^{-1}(D)}}{a_{\min}(\boldsymbol{y})} \frac{|\boldsymbol{\nu}|!}{(\log 2)^{|\boldsymbol{\nu}|}} \boldsymbol{b}^{\boldsymbol{\nu}}.$$

The claim follows by observing that

$$\frac{1}{a_{\min}(\boldsymbol{y})} = \frac{1}{\min_{\boldsymbol{x}\in\overline{D}}\left(a_0(\boldsymbol{x})\exp(\sum_{j\ge 1} y_j\psi_j(\boldsymbol{x}))\right)} \le \frac{\exp(\sum_{j\ge 1}|y_j|\|\psi_j\|_{L^\infty(D)})}{\min_{\boldsymbol{x}\in\overline{D}} a_0(\boldsymbol{x})}.$$

$\square$

Estimating the special weighted Sobolev norm

Let $G \in H^{-1}(D)$. Then

$$
\begin{aligned}
&\|G(u)\|_{s,\gamma}^2 \\
&= \sum_{\mathfrak{u}\subseteq\{1:s\}} \frac{1}{\gamma_{\mathfrak{u}}} \int_{\mathbb{R}^{|\mathfrak{u}|}} \bigg(\int_{\mathbb{R}^{s-|\mathfrak{u}|}} \frac{\partial^{|\mathfrak{u}|}}{\partial \boldsymbol{y}_{\mathfrak{u}}} G(u(\cdot,\boldsymbol{y})) \prod_{j\not\in\mathfrak{u}} \phi(y_j)\,\mathrm{d}\boldsymbol{y}_{-\mathfrak{u}} \bigg)^2 \prod_{j\in\mathfrak{u}} \varpi_j^2(y_j)\,\mathrm{d}\boldsymbol{y}_{\mathfrak{u}} \\
&\lesssim \sum_{\mathfrak{u}\subseteq\{1:s\}} \frac{(|\mathfrak{u}|!)^2}{\gamma_{\mathfrak{u}}} \bigg(\prod_{j\in\mathfrak{u}} \frac{b_j}{\log 2} \bigg)^2 \int_{\mathbb{R}^s} \prod_{j=1}^{s} \exp(2b_j|y_j|) \prod_{j\not\in\mathfrak{u}} \phi(y_j) \prod_{j\in\mathfrak{u}} \varpi_j^2(y_j)\,\mathrm{d}\boldsymbol{y} \\
&= \sum_{\mathfrak{u}\subseteq\{1:s\}} \frac{(|\mathfrak{u}|!)^2}{\gamma_{\mathfrak{u}}} \bigg(\prod_{j\in\mathfrak{u}} \frac{b_j}{\log 2} \bigg)^2 \bigg(\prod_{j\not\in\mathfrak{u}} \underbrace{\int_{\mathbb{R}} \exp(2b_j|y_j|)\phi(y_j)\,\mathrm{d}y_j}_{=2\exp(2b_j^2)\Phi(2b_j)} \bigg) \\
&\qquad\qquad \times \bigg(\prod_{j\in\mathfrak{u}} \int_{\mathbb{R}} \exp(2b_j|y_j|)\varpi_j^2(y_j)\,\mathrm{d}y_j \bigg)
\end{aligned}
$$

Multiplying and dividing the summand by $\prod_{j\in\mathfrak{u}} 2\exp(2b_j^2)\Phi(2b_j)$ yields...

$$
\begin{aligned}
&\|G(u)\|_{s,\boldsymbol{\gamma}}^2 \\
&\quad \le \sum_{\mathfrak{u}\subseteq\{1:s\}} \frac{(|\mathfrak{u}|!)^2}{\gamma_{\mathfrak{u}}} \bigg(\prod_{j=1}^{s} 2\exp(2b_j^2)\Phi(2b_j) \bigg) \\
&\qquad \times \bigg(\prod_{j\in\mathfrak{u}} \frac{b_j^2}{2(\log 2)^2 \exp(2b_j^2)\Phi(2b_j)} \int_{\mathbb{R}} \exp(2b_j|y_j|)\varpi_j^2(y_j)\,\mathrm{d}y_j \bigg).
\end{aligned}
$$

Recall that $\varpi_j^2(y_j) = \exp(-2\alpha_j|y_j|)$. If $\alpha_j > b_j$, then

$$
\textstyle\int_{\mathbb{R}} \exp(2b_j|y_j|)\varpi_j^2(y_j)\,\mathrm{d}y_j = \frac{1}{\alpha_j - b_j}
$$

and we obtain

$$
\begin{aligned}
&\|G(u)\|_{s,\boldsymbol{\gamma}}^2 \\
&\quad \le \sum_{\mathfrak{u}\subseteq\{1:s\}} \frac{(|\mathfrak{u}|!)^2}{\gamma_{\mathfrak{u}}} \bigg(\prod_{j=1}^{\infty} 2\exp(2b_j^2)\Phi(2b_j) \bigg) \\
&\qquad \times \bigg(\prod_{j\in\mathfrak{u}} \frac{b_j^2}{2(\log 2)^2 \exp(2b_j^2)\Phi(2b_j)(\alpha_j - b_j)} \bigg).
\end{aligned}
$$

The remainder of the argument follows by similar reasoning as the uniform setting: the error criterion is minimized by choosing the weights

$$\gamma_{\mathfrak{u}} = \left(|\mathfrak{u}|! \prod_{j\in\mathfrak{u}} \frac{b_j}{\sqrt{2}(\log 2)\exp(b_j^2)\sqrt{\Phi(2b_j)(\alpha_j - b_j)\varrho_j(\lambda)}}\right)^{2/(1+\lambda)} \tag{2}$$

for $\mathfrak{u} \subseteq \{1 : s\}$, with

$$\lambda = \begin{cases} \frac{1}{2-2\delta} \text{ for arbitrary } \delta \in (0, 1/2) & \text{if } p \in (0, 2/3], \\ \frac{p}{2-p} & \text{if } p \in (2/3, 1). \end{cases}$$

The resulting bound can be minimized with respect to the parameters α_j. This corresponds to minimizing $\varrho_j(\lambda)^{1/\lambda}/(\alpha_j - b_j)$ with respect to α_j, which yields

$$\alpha_j = \frac{1}{2}\left(b_j + \sqrt{b_j^2 + 1 - \frac{1}{2\lambda}}\right).$$

We obtain the overall cubature error rate $\mathcal{O}(n^{\max\{-1/p+1/2,-1+\delta\}})$ independently of the dimension s. Thus using the weights (2) as inputs to a (fast) CBC algorithm produces a QMC rule with a dimension independent convergence rate in the lognormal setting!