Quasi-Monte Carlo methods for Bayesian shape inversion

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Part I: Quasi-Monte Carlo methods

High-dimensional numerical integration

$$\int_{[0,1]^s} f(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y} \approx \sum_{i=1}^{n} w_i f(\boldsymbol{t}_i)$$

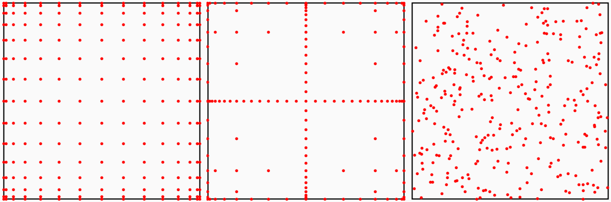


Figure 1: Tensor product grid, sparse grid, Monte Carlo nodes (not QMC rules)

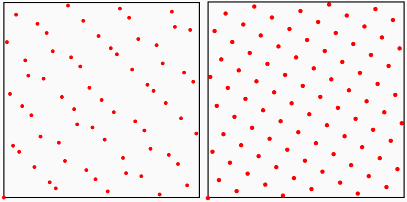


Figure 2: Sobol′ points, lattice rule (examples of QMC rules)

Quasi-Monte Carlo (QMC) methods are a class of equal weight cubature rules

$$\int_{[0,1]^s} f(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y} \approx \frac{1}{n}\sum_{i=1}^{n} f(\boldsymbol{t}_i),$$

where $(\boldsymbol{t}_i)_{i=1}^n$ is an ensemble of *deterministic* nodes in $[0,1]^s$.

The nodes $(\boldsymbol{t}_i)_{i=1}^n$ are NOT random!! Instead, they are *deterministically chosen*.

QMC methods exploit the smoothness and anisotropy of an integrand in order to achieve better-than-Monte Carlo rates.

Lattice rules

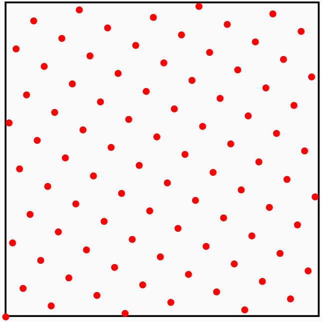
Rank-1 lattice rules

$$Q_{s,n}(f) = \frac{1}{n} \sum_{i=1}^{n} f(\boldsymbol{t}_i)$$

have the points

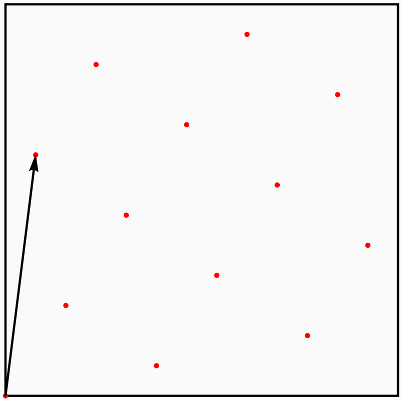
$$\boldsymbol{t}_i = \mathrm{mod}\left(\frac{i\boldsymbol{z}}{n}, 1\right), \quad i \in \{1, \dots, n\},$$

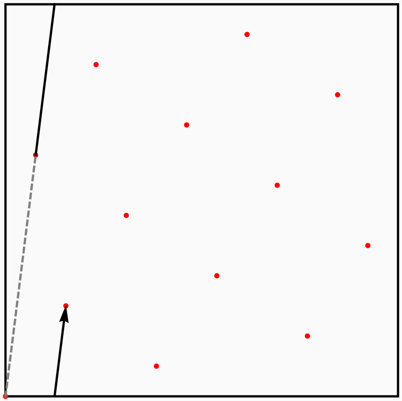
where the entire point set is determined by the *generating vector* $\boldsymbol{z} \in \mathbb{N}^s$, with all components *coprime* to n.

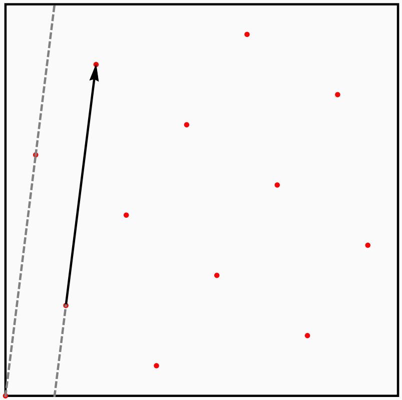


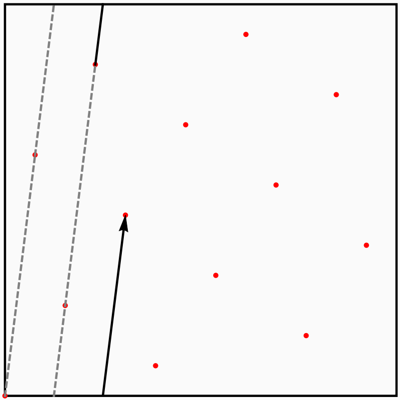
Lattice rule with $\boldsymbol{z} = (1, 55)$ and $n = 89$ nodes in $[0, 1]^2$

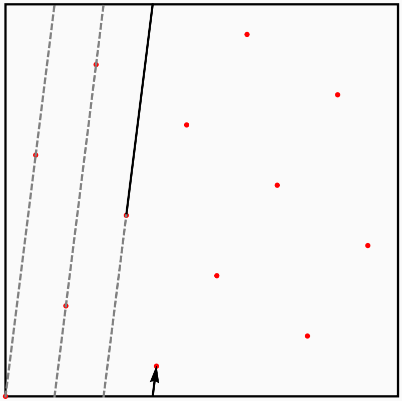
The quality of the lattice rule is determined by the choice of $\boldsymbol{z}$.

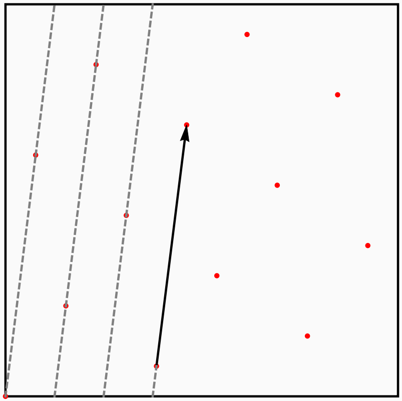


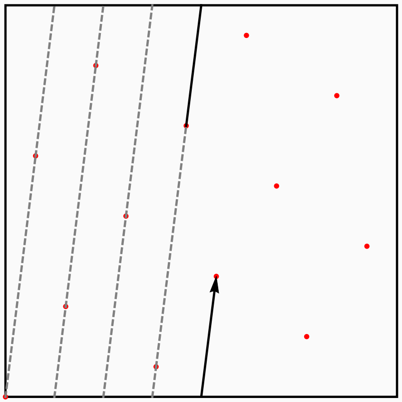


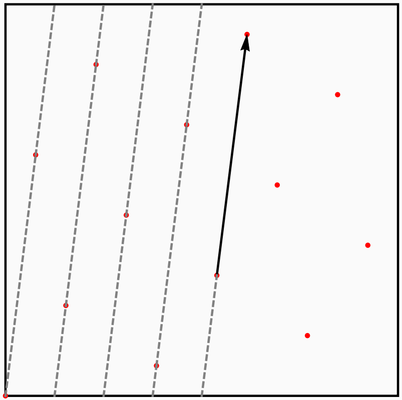


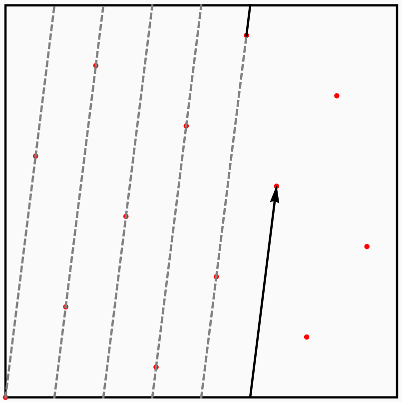


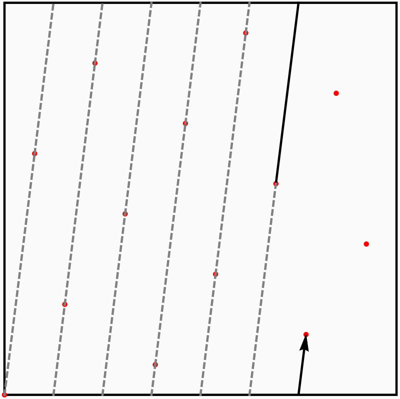


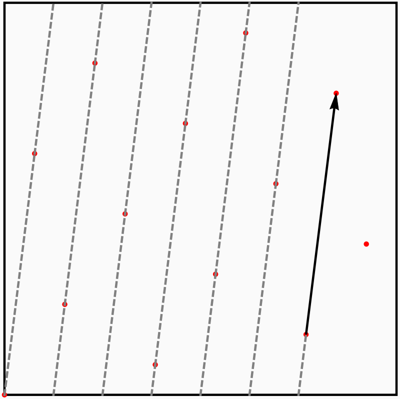


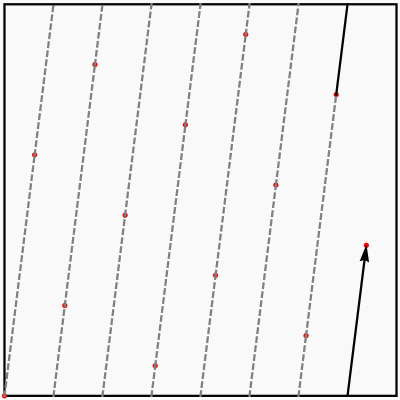












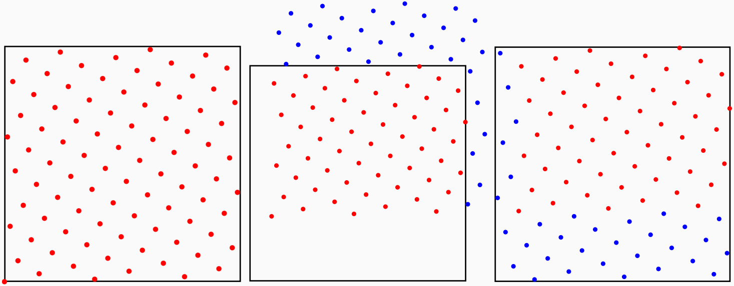
Randomly shifted lattice rules

Shifted rank-1 lattice rules have points

$$\boldsymbol{t}_i = \mathrm{mod}\left(\frac{i\boldsymbol{z}}{n} + \boldsymbol{\Delta}, 1\right), \quad i \in \{1, \ldots, n\}.$$

$\boldsymbol{\Delta} \in [0, 1)^s$ is the shift

Use a number of random shifts for error estimation.



Lattice rule shifted by $\boldsymbol{\Delta} = (0.1, 0.3)$.

Let $\boldsymbol{\Delta}^{(r)}$, $r = 1, \ldots, R$, be independent random shifts drawn from $U([0,1]^s)$ and define

$$Q_{s,n}^{(r)}(f) := \frac{1}{n} \sum_{i=1}^{n} f(\mathrm{mod}(\boldsymbol{t}_i + \boldsymbol{\Delta}^{(r)}, 1)). \text{ (QMC rule with 1 random shift)}$$

Then

$$\overline{Q}_{s,n}(f) = \frac{1}{R} \sum_{r=1}^{R} Q_{s,n}^{(r)} f \qquad \text{(QMC rule with } R \text{ random shifts)}$$

is an unbiased estimator of $I_s(f)$.

Let $f:[0,1]^s \to \mathbb{R}$ be sufficiently smooth.

Error bound (one random shift):

$$|I_s(f) - Q_{s,n}^{\mathbf{\Delta}}(f)| \leq e_{s,n,\gamma}^{\mathbf{\Delta}}(\boldsymbol{z})\|f\|_{\boldsymbol{\gamma}}.$$

R.M.S. error bound (shift-averaged):

$$\sqrt{\mathbb{E}_{\mathbf{\Delta}}[|I_s(f) - \overline{Q}_{s,n}(f)|^2]} \leq e_{s,n,\boldsymbol{\gamma}}^{\mathrm{sh}}(\boldsymbol{z})\|f\|_{\boldsymbol{\gamma}}.$$

We consider weighted Sobolev spaces with dominating mixed smoothness, equipped with norm

$$\|f\|_{\boldsymbol{\gamma}}^2 = \sum_{\mathfrak{u}\subseteq\{1,\ldots,s\}} \frac{1}{\gamma_{\mathfrak{u}}} \int_{[0,1]^{|\mathfrak{u}|}} \left(\int_{[0,1]^{s-|\mathfrak{u}|}} \frac{\partial^{|\mathfrak{u}|} f}{\partial \boldsymbol{y}_{\mathfrak{u}}}(\boldsymbol{y}) \, \mathrm{d}\boldsymbol{y}_{-\mathfrak{u}} \right)^2 \mathrm{d}\boldsymbol{y}_{\mathfrak{u}}$$

and (squared) worst case error

$$P(\boldsymbol{z}) := e_{s,n,\boldsymbol{\gamma}}^{\mathrm{sh}}(\boldsymbol{z})^2 = \frac{1}{n} \sum_{k=0}^{n-1} \sum_{\varnothing\neq\mathfrak{u}\subseteq\{1,\ldots,s\}} \gamma_{\mathfrak{u}} \prod_{j\in\mathfrak{u}} \omega\left(\left\{\frac{kz_j}{n}\right\}\right)$$

where $\omega(x) = x^2 - x + \frac{1}{6}$.

CBC algorithm (Sloan, Kuo, Joe 2002)

The idea of the *component-by-component* (CBC) algorithm is to find a good generating vector $\boldsymbol{z} = (z_1, \dots, z_s)$ by proceeding as follows:

1. Set $z_1 = 1$;
2. With z_1 fixed, choose z_2 to minimize error criterion $P(z_1, z_2)$;
3. With z_1 and z_2 fixed, choose z_3 to minimize error criterion $P(z_1, z_2, z_3)$

   $\vdots$

Efficient implementation using FFT (QMC4PDE, QMCPy, etc.) if the weights have certain structure – typically, product-and-order dependent (POD) weights are used in practice.

Theorem (CBC error bound)
Let $n = 2^k$ be the number of lattice points. The generating vector $\boldsymbol{z} \in \mathbb{N}^s$ constructed by the CBC algorithm, minimizing the squared shift-averaged worst-case error $[e^{\mathrm{sh}}_{s,n,\boldsymbol{\gamma}}(\boldsymbol{z})]^2$ for the weighted unanchored Sobolev space in each step, satisfies

$$[e^{\mathrm{sh}}_{s,n,\boldsymbol{\gamma}}(\boldsymbol{z})]^2 \leq \left(\frac{2}{n} \sum_{\varnothing \neq \mathfrak{u} \subseteq \{1,\ldots,s\}} \gamma_{\mathfrak{u}}^{\lambda} \left(\frac{2\zeta(2\lambda)}{(2\pi^2)^{\lambda}}\right)^{|\mathfrak{u}|}\right)^{1/\lambda} \quad \text{for all } \lambda \in (1/2, 1],$$

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

Remarks:

- Optimal rate of convergence $\mathcal{O}(n^{-1+\delta})$ in weighted Sobolev spaces, independently of s under an appropriate condition on the weights.
- Cost of algorithm for POD weights is $\mathcal{O}(s\, n \log n + s^2\, n)$ using FFT.

Significance: Suppose that $f \in H_{s,\boldsymbol{\gamma}}$ for all $\boldsymbol{\gamma} = (\gamma_{\mathfrak{u}})_{\mathfrak{u} \subseteq \{1,\ldots,s\}}$. Then for any given sequence of weights $\boldsymbol{\gamma}$, we can use the CBC algorithm to obtain a generating vector satisfying the error bound

$$\sqrt{\mathbb{E}_{\boldsymbol{\Delta}} |I_s f - Q_{s,n}^{\boldsymbol{\Delta}} f|^2} \leq \left(\frac{2}{n} \sum_{\varnothing \neq \mathfrak{u} \subseteq \{1,\ldots,s\}} \gamma_{\mathfrak{u}}^{\lambda} \left(\frac{2\zeta(2\lambda)}{(2\pi^2)^{\lambda}} \right)^{|\mathfrak{u}|} \right)^{1/(2\lambda)} \|f\|_{s,\boldsymbol{\gamma}} \tag{1}$$

for all $\lambda \in (1/2, 1]$. We can use the following strategy:

- For a given integrand f, estimate the norm $\|f\|_{s,\boldsymbol{\gamma}}$.
- Find weights $\boldsymbol{\gamma}$ which minimize the error bound (1).
- Using the optimized weights $\boldsymbol{\gamma}$ as input, use the CBC algorithm to find a generating vector which satisfies the error bound (1).

Part II: Parameterization of input uncertainty

Consider the elliptic PDE problem:

$$\begin{cases} -\nabla \cdot \big(a(\boldsymbol{x})\nabla u(\boldsymbol{x})\big) = f(\boldsymbol{x}) & \text{for } \boldsymbol{x} \in D, \\ +\text{boundary conditions.} \end{cases}$$

In practice, one or several of the material/system parameters may be uncertain or incompletely known and modeled as random fields:

- PDE coefficient a may be uncertain;
- Source term f may be uncertain;
- Boundary conditions may be uncertain;
- The domain D itself may be uncertain (main topic of this talk).

In forward uncertainty quantification, one is interested in assessing how uncertainties in the inputs of a mathematical model affect the output.

In inverse uncertainty quantification, one is typically interested in computing the statistics for the posterior distribution of unknown model parameters conditioned on measurements of the system response.

Background

A popular model in the literature: the uniform and affine model.

Let $(\Omega, \mathcal{A}, \mathbb{P})$ be a probability space. For $\boldsymbol{x} \in D$ and $\omega \in \Omega$,

$$a(\boldsymbol{x}, \omega) = \bar{a}(\boldsymbol{x}) + \sum_{j=1}^{s} Y_j(\omega)\psi_j(\boldsymbol{x}), \quad Y_j \text{ i.i.d. uniform on } [-\tfrac{1}{2}, \tfrac{1}{2}].$$

Computing $\mathbb{E}[u(\boldsymbol{x}, \cdot)]$ (or some quantity of interest $\mathbb{E}[G(u)]$) using

- Rank-1 lattice cubature rules with random shifts
  $\Rightarrow$ dimension-independent cubature error $\mathcal{O}(n^{-1+\varepsilon})$ at best.
  (Kuo, Schwab, Sloan 2012)
- Interlaced polynomial lattice rules
  $\Rightarrow$ higher order dimension-independent convergence $\mathcal{O}(n^{-1/p})$ for $0 < p < 1$ (p is a summability exponent s.t. $(\|\psi_j\|_{L^\infty})_{j\geq 1} \in \ell^p$).
  (Dick, Kuo, Le Gia, Nuyens, Schwab 2014)

Gevrey regular random inputs

Chernov and Lê (2024a and 2024b) observed that the input random field can be much more general while retaining dimension-independent QMC convergence rates for the PDE response. It is enough that the input random field satisfies a certain parametric regularity bound.

Identifying $y_j \equiv Y_j(\omega)$ as parameters, the parametric coefficient $a\colon D \times [-\frac{1}{2}, \frac{1}{2}]^s \to \mathbb{R}$ is called Gevrey regular if it satisfies

$$\|\partial_{\boldsymbol{y}}^{\boldsymbol{\nu}} a(\cdot, \boldsymbol{y})\|_{L^\infty(D)} \leq C(|\boldsymbol{\nu}|!)^\delta \boldsymbol{b}^{\boldsymbol{\nu}} \quad \text{for all } \boldsymbol{\nu} \in \mathbb{N}_0^s,\ \boldsymbol{y} \in [-\tfrac{1}{2}, \tfrac{1}{2}]^s$$

for some constant $C > 0$ and Gevrey parameter $\delta \geq 1$.

Here, we use multi-index notation

$$\partial_{\boldsymbol{y}}^{\boldsymbol{\nu}} = \prod_{j=1}^s \frac{\partial^{\nu_j}}{\partial y_j^{\nu_j}}, \quad \boldsymbol{b}^{\boldsymbol{\nu}} = \prod_{j=1}^s b_j^{\nu_j}, \quad |\boldsymbol{\nu}| = \sum_{j=1}^s \nu_j,$$

Part III: Domain uncertainty quantification for elliptic PDEs

Consider the Poisson problem

$$\begin{cases} -\Delta u(\boldsymbol{x}, \omega) = f(\boldsymbol{x}) & \text{for } \boldsymbol{x} \in D(\omega), \\ u(\boldsymbol{x}, \omega) = 0 & \text{for } \boldsymbol{x} \in \partial D(\omega), \end{cases}$$

where the bounded domain $D(\omega) \subset \mathbb{R}^d$, $d \in \{2, 3\}$, is assumed to be *uncertain*.

Domain mapping method: Let $D_{\mathrm{ref}} \subset \mathbb{R}^d$, $d \in \{2, 3\}$, be a fixed reference domain. Define perturbation field $\boldsymbol{V}(\omega) \colon \overline{D_{\mathrm{ref}}} \to \mathbb{R}^d$, which we assume is given explicitly.

Uncertain domains studied by many authors in the literature: Harbrecht, Peters, Siebenmorgen, Schwab, Zech...

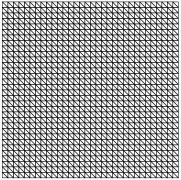


Figure 3: Reference domain

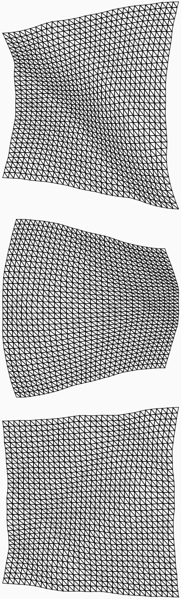


Figure 4: Three realizations of the random domain

Parameterization of domain uncertainty

Let $U := [-\frac{1}{2}, \frac{1}{2}]^s$ and let $\boldsymbol{V}\colon \overline{D_{\mathrm{ref}}} \times U \to \mathbb{R}^d$ be a vector field such that

$$\|\partial_{\boldsymbol{y}}^{\boldsymbol{\nu}} \boldsymbol{V}(\cdot, \boldsymbol{y})\|_{W^{1,\infty}(D_{\mathrm{ref}})} \leq C(|\boldsymbol{\nu}|!)^{\delta} \boldsymbol{b}^{\boldsymbol{\nu}} \quad \text{for all } \boldsymbol{\nu} \in \mathbb{N}_0^s,\ \boldsymbol{y} \in U.$$

for some $C > 0$ and $\delta \geq 1$.

In consequence, the Jacobian matrix $J(\cdot, \boldsymbol{y})\colon D_{\mathrm{ref}} \to \mathbb{R}^{d \times d}$ of vector field $\boldsymbol{V}$ satisfies

$$\|\partial_{\boldsymbol{y}}^{\boldsymbol{\nu}} J(\cdot, \boldsymbol{y})\|_{L^{\infty}(D_{\mathrm{ref}})} \leq C(|\boldsymbol{\nu}|!)^{\delta} \boldsymbol{b}^{\boldsymbol{\nu}} \quad \text{for all } \boldsymbol{\nu} \in \mathbb{N}_0^s,\ \boldsymbol{y} \in U.$$

The family of *admissible domains* $\{D(\boldsymbol{y})\}_{\boldsymbol{y} \in U}$ is parameterized by

$$D(\boldsymbol{y}) := \boldsymbol{V}(D_{\mathrm{ref}}, \boldsymbol{y}), \quad \boldsymbol{y} \in U,$$

and we define the *hold-all domain* by setting

$$\mathcal{D} := \bigcup_{\boldsymbol{y} \in U} D(\boldsymbol{y}).$$

Assumptions

The reference domain $D_{\mathrm{ref}} \subset \mathbb{R}^d$, $d \in \{2,3\}$, is bounded with Lipschitz boundary.

(A1) For each $\boldsymbol{y} \in U$, $\boldsymbol{V}(\cdot,\boldsymbol{y})\colon \overline{D_{\mathrm{ref}}} \to \mathbb{R}^d$ is an invertible, twice continuously differentiable vector field.

(A2) For some $C_0 > 0$, there holds

$$\|\boldsymbol{V}(\cdot,\boldsymbol{y})\|_{\mathcal{C}^2(\overline{D_{\mathrm{ref}}})} \leq C_0 \quad \text{and} \quad \|\boldsymbol{V}^{-1}(\cdot,\boldsymbol{y})\|_{\mathcal{C}^2(\overline{D(\boldsymbol{y})})} \leq C_0 \quad \text{for all } \boldsymbol{y} \in U.$$

(A3) There exist constants $0 < \sigma_{\min} \leq 1 \leq \sigma_{\max} < \infty$ such that

$$\sigma_{\min} \leq \min \sigma(J(\boldsymbol{x},\boldsymbol{y})) \leq \max \sigma(J(\boldsymbol{x},\boldsymbol{y})) \leq \sigma_{\max} \quad \text{for all } \boldsymbol{x} \in D_{\mathrm{ref}},\ \boldsymbol{y} \in U,$$

where $\sigma(J(\boldsymbol{x},\boldsymbol{y}))$ denotes the set of all singular values of matrix $J(\boldsymbol{x},\boldsymbol{y})$,

(A5) There holds $\sum_{j\geq 1} b_j^p < \infty$ for some $p \in (0,1)$.

The variational formulation of the model problem can be stated as follows: for $\boldsymbol{y} \in U$, find $u(\cdot, \boldsymbol{y}) \in H_0^1(D(\boldsymbol{y}))$ such that

$$\int_{D(\boldsymbol{y})} \nabla u(\boldsymbol{x}, \boldsymbol{y}) \cdot \nabla v(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} = \int_{D(\boldsymbol{y})} f(\boldsymbol{x}) \, v(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} \quad \forall v \in H_0^1(D(\boldsymbol{y})), \quad (2)$$

where $f : \mathcal{D} \to \mathbb{R}$ is assumed to satisfy $\|\partial^{\boldsymbol{\nu}} f\|_{L^\infty(\mathcal{D})} \leq C(|\boldsymbol{\nu}|!)^\delta \boldsymbol{\rho}^{\boldsymbol{\nu}}$.

We can transport the variational formulation (2) to the reference domain by a change of variable. Let us define

$$A(\boldsymbol{x}, \boldsymbol{y}) := (J(\boldsymbol{x}, \boldsymbol{y})^{\mathrm{T}} J(\boldsymbol{x}, \boldsymbol{y}))^{-1} \det J(\boldsymbol{x}, \boldsymbol{y})$$
$$f_{\mathrm{ref}}(\boldsymbol{x}, \boldsymbol{y}) := f(V(\boldsymbol{x}, \boldsymbol{y})) \det J(\boldsymbol{x}, \boldsymbol{y}),$$

for $\boldsymbol{x} \in D_{\mathrm{ref}}$, $\boldsymbol{y} \in U$. Then we can recast the problem (2) on the reference domain as follows: for $\boldsymbol{y} \in U$, find $\widehat{u}(\cdot, \boldsymbol{y}) \in H_0^1(D_{\mathrm{ref}})$ such that

$$\int_{D_{\mathrm{ref}}} \big(A(\boldsymbol{x}, \boldsymbol{y}) \nabla \widehat{u}(\boldsymbol{x}, \boldsymbol{y})\big) \cdot \nabla \widehat{v}(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} = \int_{D_{\mathrm{ref}}} f_{\mathrm{ref}}(\boldsymbol{x}, \boldsymbol{y}) \, \widehat{v}(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} \quad \forall \widehat{v} \in H_0^1(D_{\mathrm{ref}}). \quad (3)$$

The solutions to problems (2) and (3) are connected to one another via

$$u(\cdot, \boldsymbol{y}) = \widehat{u}\big(\boldsymbol{V}^{-1}(\cdot, \boldsymbol{y}), \boldsymbol{y}\big) \quad \Leftrightarrow \quad \widehat{u}(\cdot, \boldsymbol{y}) = u\big(\boldsymbol{V}(\cdot, \boldsymbol{y}), \boldsymbol{y}\big), \quad \boldsymbol{y} \in U.$$

Theorem (Djurdjevac–K–Schillings–Zepernick 2024+)
There holds for all $\boldsymbol{y} \in U$ and all multi-indices $\boldsymbol{\nu} \neq \mathbf{0}$ that

$$\|\partial_{\boldsymbol{y}}^{\boldsymbol{\nu}} \widehat{u}(\cdot, \boldsymbol{y})\|_{H_0^1(D_{ref})} \leq c_1\, c_2^{|\boldsymbol{\nu}|} (|\boldsymbol{\nu}|!)^{\delta} \boldsymbol{b}^{\boldsymbol{\nu}},$$

where

$$c_1 = \frac{|D_{\rm ref}|^{1/2} C_{D_{\rm ref}} \sigma_{\max}^d 2^{1-\delta} C}{\sigma_{\min}^d ((d^2)!)^{\delta}} \left(1 + C C_{D_{\rm ref}} \left(\frac{\sigma_{\max}}{\sigma_{\min}}\right)^d\right),$$

$$c_2 = \sigma_{\min}^{-4} C^5 \max\left\{(d^2!)^{\delta}, \frac{\sigma_{\max}^d}{\sigma_{\min}^{d-1}}\right\} \max\{1, \|\boldsymbol{\rho}\|_{\ell^{1/\delta}}\} 2^{\delta d^2 + 6\delta + 2},$$

with $C_{D_{ref}}$ denoting the Poincaré constant of D_{ref} and $|D_{\rm ref}| = \int_{D_{\rm ref}} \mathrm{d}\boldsymbol{x}$.

Plugging the above into the QMC error bound suggests choosing the (POD) weights

$$\gamma_{\mathfrak{u}} := \left((|\mathfrak{u}|!)^{\delta} \prod_{j \in \mathfrak{u}} \frac{c_2 b_j}{\sqrt{2\zeta(2\lambda)/(2\pi^2)^{\lambda}}}\right)^{\frac{2}{1+\lambda}} \quad \text{for } \mathfrak{u} \subset \{1, \ldots, s\},$$

and by setting $\lambda := \frac{p}{2-p}$ if $p \in (\frac{2}{3}, \frac{1}{\delta})$ and $\lambda = \frac{1}{2-2\varepsilon}$ for arbitrary $\varepsilon \in (0, \frac{1}{2})$ if $p \in (0, \min\{\frac{2}{3}, \frac{1}{\delta}\}]$, $p \neq \frac{1}{\delta}$, we obtain QMC convergence rate $\sqrt{\mathbb{E}_{\boldsymbol{\Delta}} \|I_s(\widehat{u}) - Q_{s,n,\boldsymbol{\Delta}}(\widehat{u})\|_{L^2(D_{\rm ref})}^2} = \mathcal{O}(n^{\max\{-\frac{1}{p} + \frac{1}{2}, -1+\varepsilon\}})$ where the implied coefficient can be shown to be independent of the dimension s.

We endow the unknown parameter $\boldsymbol{y}$ with the uniform prior distribution $\mathcal{U}([-\frac{1}{2}, \frac{1}{2}]^s)$ and consider the mathematical measurement model

$$\boldsymbol{\delta} = \mathcal{G}(\boldsymbol{y}) + \boldsymbol{\eta},$$

where $\boldsymbol{\delta} \in \mathbb{R}^k$ are the measurements, $\boldsymbol{\eta} \sim \mathcal{N}(0, \Gamma)$ is k-dimensional additive Gaussian noise with covariance matrix $\Gamma \in \mathbb{R}^{k \times k}$, $\boldsymbol{\eta}$ is assumed to be independent of the process generating the observations, and $\mathcal{G} \colon U \to \mathbb{R}^k$ is the parameter-to-observation map which we define as $\mathcal{G}(\boldsymbol{y}) = \mathcal{O}(\widehat{u}(\cdot, \boldsymbol{y}))$ with $\mathcal{O} \in H^{-1}(D_{\mathrm{ref}})$.

Bayes' formula can be used to express the distribution of the unknown parameter conditioned on the measurements via the posterior distribution

$$\pi(\boldsymbol{y}|\boldsymbol{\delta}) = \frac{\pi(\boldsymbol{\delta}|\boldsymbol{y})\pi(\boldsymbol{y})}{Z(\boldsymbol{\delta})} = \frac{\mathrm{e}^{-\frac{1}{2}\|\boldsymbol{\delta} - \mathcal{G}(\boldsymbol{y})\|^2_{\Gamma^{-1}}}}{\int_{[-\frac{1}{2}, \frac{1}{2}]^s} \mathrm{e}^{-\frac{1}{2}\|\boldsymbol{\delta} - \mathcal{G}(\boldsymbol{y})\|^2_{\Gamma^{-1}}} \,\mathrm{d}\boldsymbol{y}}, \quad \boldsymbol{y} \in [-\tfrac{1}{2}, \tfrac{1}{2}]^s.$$

As the reconstruction of the unknown domain, we consider

$$\boldsymbol{V}^{\delta}(\boldsymbol{x}, \boldsymbol{y}) := \mathbb{E}[\boldsymbol{V}(\boldsymbol{x}, \cdot)|\delta] = \frac{Z'(\boldsymbol{\delta})}{Z(\boldsymbol{\delta})},$$

$$Z'(\boldsymbol{\delta}) := \int\limits_{[-\frac{1}{2}, \frac{1}{2}]^s} \boldsymbol{V}(\boldsymbol{x}, \boldsymbol{y}) \mathrm{e}^{-\frac{1}{2}\|\boldsymbol{\delta} - \mathcal{G}(\boldsymbol{y})\|^2_{\Gamma^{-1}}} \,\mathrm{d}\boldsymbol{y}, \quad Z(\boldsymbol{\delta}) := \int\limits_{[-\frac{1}{2}, \frac{1}{2}]^s} \mathrm{e}^{-\frac{1}{2}\|\boldsymbol{\delta} - \mathcal{G}(\boldsymbol{y})\|^2_{\Gamma^{-1}}} \,\mathrm{d}\boldsymbol{y}.$$

Theorem (Djurdjevac–K–Orteu–Schillings 2024+)
There holds for all $\boldsymbol{y} \in U$ *and all multi-indices* $\boldsymbol{\nu} \neq \mathbf{0}$ *that*

$$\left|\partial_{\boldsymbol{y}}^{\boldsymbol{\nu}} \mathrm{e}^{-\frac{1}{2}\|\boldsymbol{\delta}-\mathcal{G}(\boldsymbol{y})\|_{\Gamma^{-1}}^{2}}\right| \leq c_3 c_4^{|\boldsymbol{\nu}|} (|\boldsymbol{\nu}|!)^{\delta} \boldsymbol{b}^{\boldsymbol{\nu}},$$

where

$$c_3 = \frac{1}{2} \cdot 3.47^{k}, \quad c_4 = 2 c_1 c_2 \lambda_{\min}(\Gamma)^{-1/2}.$$

Theorem (Djurdjevac–K–Orteu–Schillings 2024+)
There holds for all $\boldsymbol{y} \in U$ *and all multi-indices* $\boldsymbol{\nu} \neq \mathbf{0}$ *that*

$$\left|\partial_{\boldsymbol{y}}^{\boldsymbol{\nu}} \left(\boldsymbol{V}(\boldsymbol{x}, \boldsymbol{y}) \mathrm{e}^{-\frac{1}{2}\|\boldsymbol{\delta}-\mathcal{G}(\boldsymbol{y})\|_{\Gamma^{-1}}^{2}}\right)\right| \leq c_5 c_6^{|\boldsymbol{\nu}|} ((|\boldsymbol{\nu}|+1)!)^{\delta} \boldsymbol{b}^{\boldsymbol{\nu}},$$

where $c_5 = C c_3$ *and* $c_6 = \max\{1, c_4\}$.

We want to apply QMC to approximate both the numerator and denominator of the ratio estimator $\frac{Z'}{Z}$.

The ratio estimator satisfies the following bound:

$$\begin{aligned}\left|\frac{Z'}{Z}-\frac{Z_n'}{Z_n}\right|=\left|\frac{Z'Z_n-Z_n'Z}{ZZ_n}\right|&=\left|\frac{Z'Z_n-Z'Z+Z'Z-Z_n'Z}{ZZ_n}\right|\\&\leq\frac{|Z'||Z-Z_n|}{|ZZ_n|}+\frac{|Z'-Z_n'|}{|Z_n|}\\&\lesssim|Z-Z_n|+|Z'-Z_n'|,\end{aligned}$$

meaning that we can simply use the larger derivative bound to inform our choice of weights:

$$\gamma_{\mathfrak{u}}:=\left(((|\mathfrak{u}|+1)!)^{\delta}\prod_{j\in\mathfrak{u}}\frac{c_6 b_j}{\sqrt{2\zeta(2\lambda)/(2\pi^2)^{\lambda}}}\right)^{\frac{2}{1+\lambda}}\quad\text{for }\mathfrak{u}\subset\{1,\ldots,s\},$$

where we set $\lambda:=\frac{p}{2-p}$ if $p\in(\frac{2}{3},\frac{1}{\delta})$ and $\lambda=\frac{1}{2-2\varepsilon}$ for arbitrary $\varepsilon\in(0,\frac{1}{2})$ if $p\in(0,\min\{\frac{2}{3},\frac{1}{\delta}\}]$, $p\neq\frac{1}{\delta}$. We obtain QMC convergence rate $\sqrt{\mathbb{E}_{\boldsymbol{\Delta}}\left|\frac{Z'}{Z}-\frac{Z'_{n,\boldsymbol{\Delta}}}{Z_{n,\boldsymbol{\Delta}}}\right|^2}=\mathcal{O}(n^{\max\{-\frac{1}{p}+\frac{1}{2},-1+\varepsilon\}})$ where the implied coefficient can be shown to be independent of the dimension s.

Numerical experiments

Let $D_{\mathrm{ref}} = \{\boldsymbol{x} \in \mathbb{R}^2 \mid x_1^2 + x_2^2 \leq 1\}$ and consider the perturbation field

$$\boldsymbol{V}(\boldsymbol{x}, \boldsymbol{y}) = a(\boldsymbol{x}, \boldsymbol{y})\boldsymbol{x}, \quad \boldsymbol{x} \in D_{\mathrm{ref}},\ \boldsymbol{y} \in [-\tfrac{1}{2}, \tfrac{1}{2}]^s,$$

where

$$a(\boldsymbol{x}, \boldsymbol{y}) := 1 + \sum_{j=1}^{s} j^{-2.1} \sin(3j\,\mathrm{atan2}(x_1, x_2) + \pi)\mathrm{e}^{-(\frac{1}{2}+y_j)^{-1}}.$$

with $s = 100$. We fix $f(\boldsymbol{x}) = 10\sin(x_1 x_2) - 5\cos^2(x_1 + x_2)$.

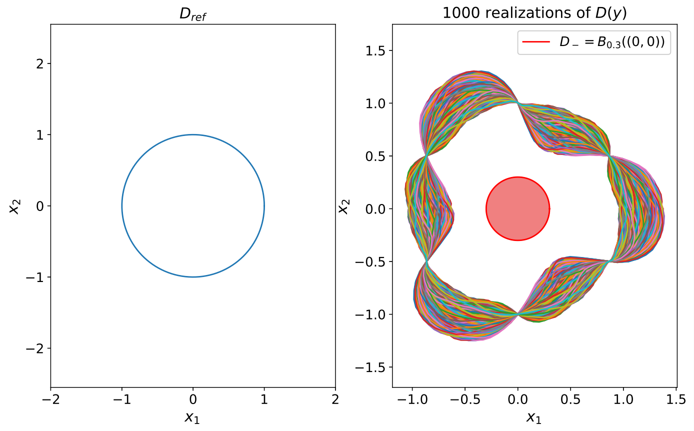
Thus the reference domain in this case is the unit disk, and the uncertain boundary is the curve defined by the radial transformation $r = 1 + \sum_{j=1}^{s} j^{-2.1} \sin(3j\,\theta + \pi)\mathrm{e}^{-(\frac{1}{2}+y_j)^{-1}}$ for each realization of $\boldsymbol{y}$.

The reconstruction is obtained by solving the PDE problem over the transported domain using piecewise linear FEM with mesh size $h = 2^{-5}$.

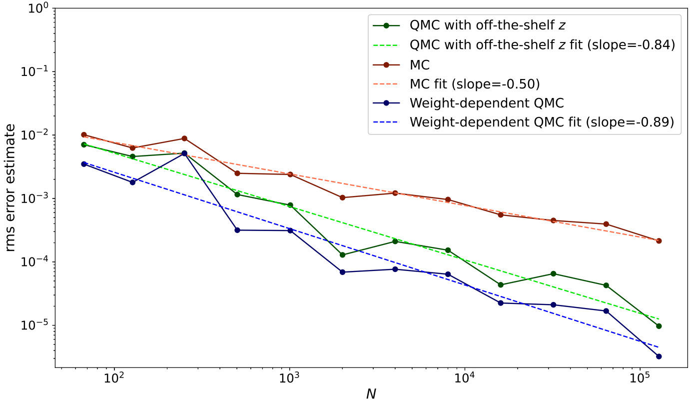
To assess the convergence behavior, we first consider the observation operator

$$\mathcal{O}\colon H_0^1(\mathcal{D}) \to \mathbb{R}, \quad u \mapsto \int_{D_-} u(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x},$$

where $D_- = B_{0.3}((0,0)) \subset \bigcap_{\boldsymbol{y}\in[-\frac{1}{2},\frac{1}{2}]^{100}} D(\boldsymbol{y})$. The observations were generated using a finer FE mesh ($h = 2^{-6}$) and the measurements were contaminated with 10% relative Gaussian noise.



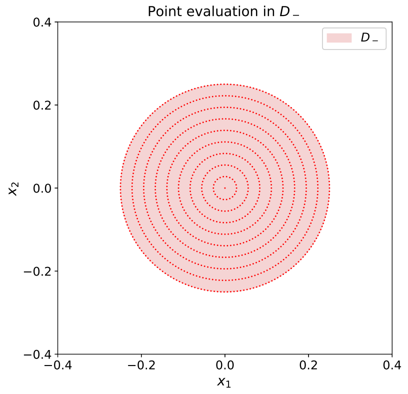
QMC convergence of V^{δ}



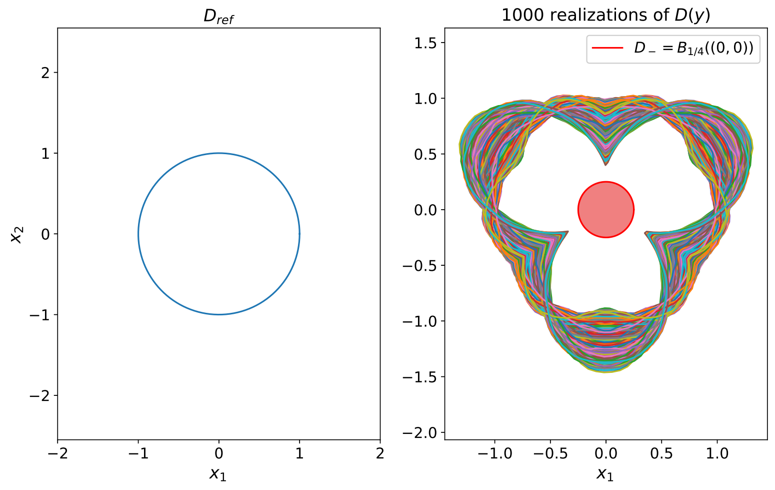
Next, we consider reconstructing the domain shape based on measurements. Here, we consider the observation operator

$$\mathcal{O}(u(\cdot,\boldsymbol{y})) = [u(\boldsymbol{x}_1,\boldsymbol{y}),\ldots,u(\boldsymbol{x}_k,\boldsymbol{y})]^{\mathrm{T}},$$

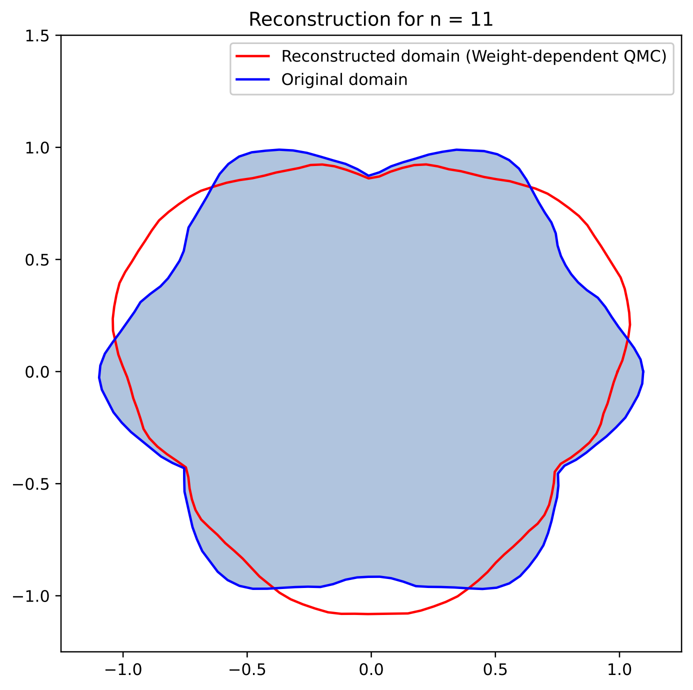
where the PDE solution is sampled over a point set belonging to D_- (below). The observations were generated using a finer FE mesh ($h = 2^{-6}$) and contaminated with 5% relative Gaussian noise.

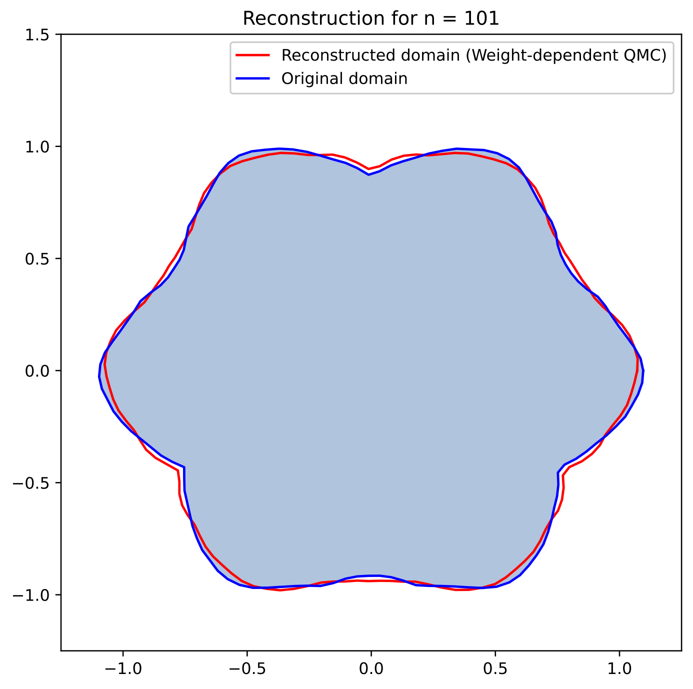


First, we generate the ground truth domain as a realization of the random field with $s = 200$ terms. Then we compute the reconstruction using $s = 20$ terms.

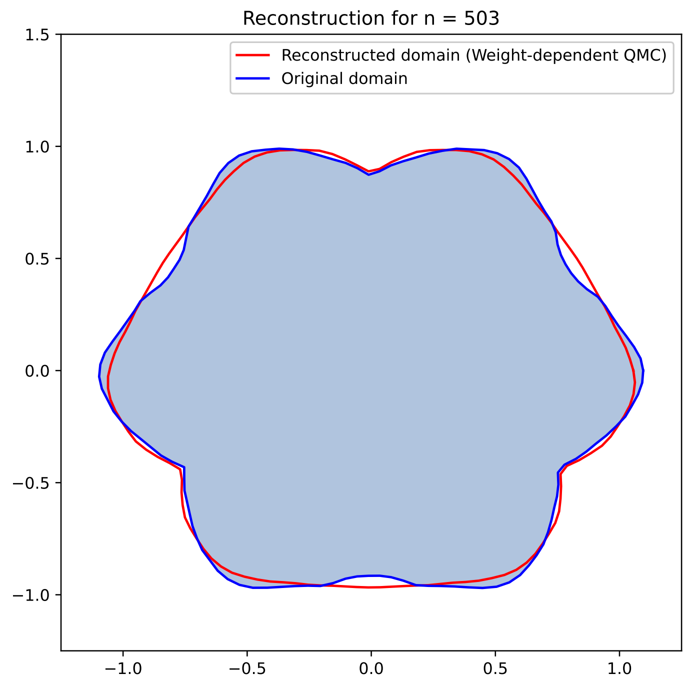


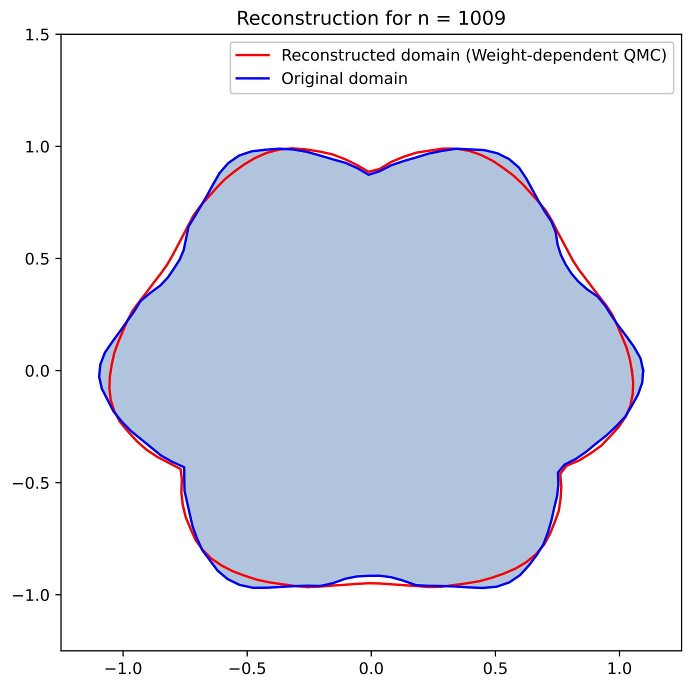
$$a(\boldsymbol{x}, \boldsymbol{y}) := 1 + 1.2 \sum_{j=1}^{s} j^{-2.1} \sin(3j\, \mathrm{atan2}(x_1, x_2) - \pi/2) \mathrm{e}^{-(\frac{1}{2} + y_j)^{-1}}$$


Reconstruction for n = 11
Reconstructed domain (Weight-dependent QMC)
Original domain
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.0
−0.5
0.0
0.5
1.0

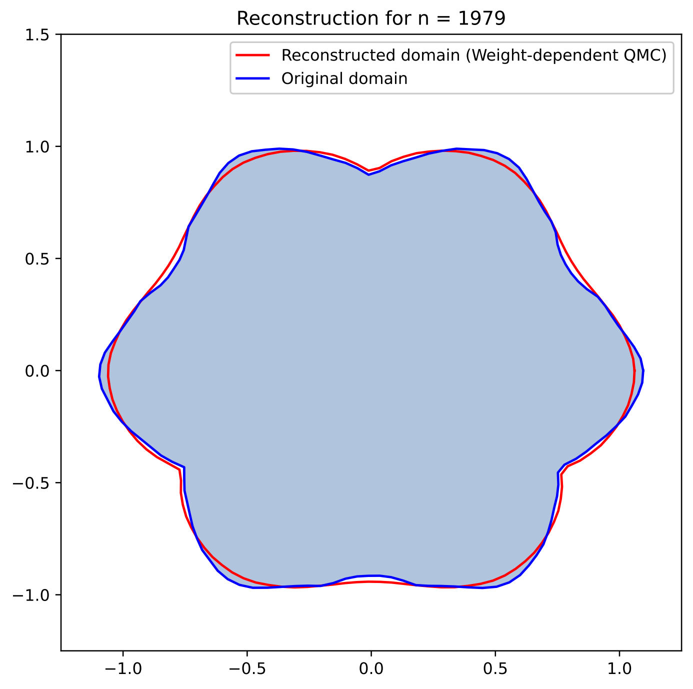


Reconstruction for n = 101
Reconstructed domain (Weight-dependent QMC)
Original domain
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.0
−0.5
0.0
0.5
1.0


Reconstruction for n = 503
Reconstructed domain (Weight-dependent QMC)
Original domain
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.0
−0.5
0.0
0.5
1.0

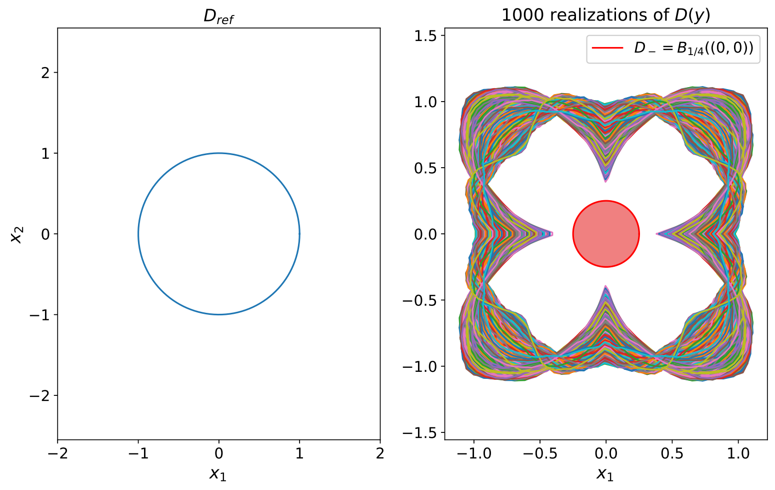


Reconstruction for n = 1009
Reconstructed domain (Weight-dependent QMC)
Original domain
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.0
−0.5
0.0
0.5
1.0

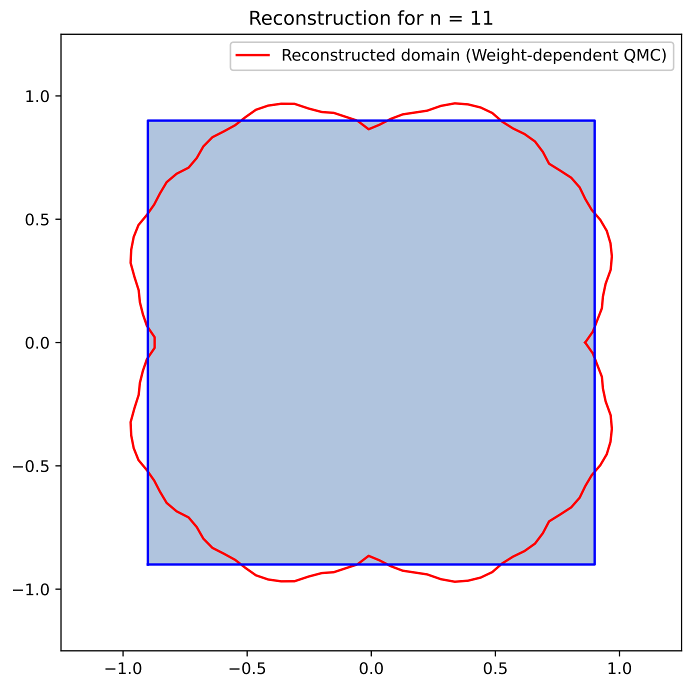


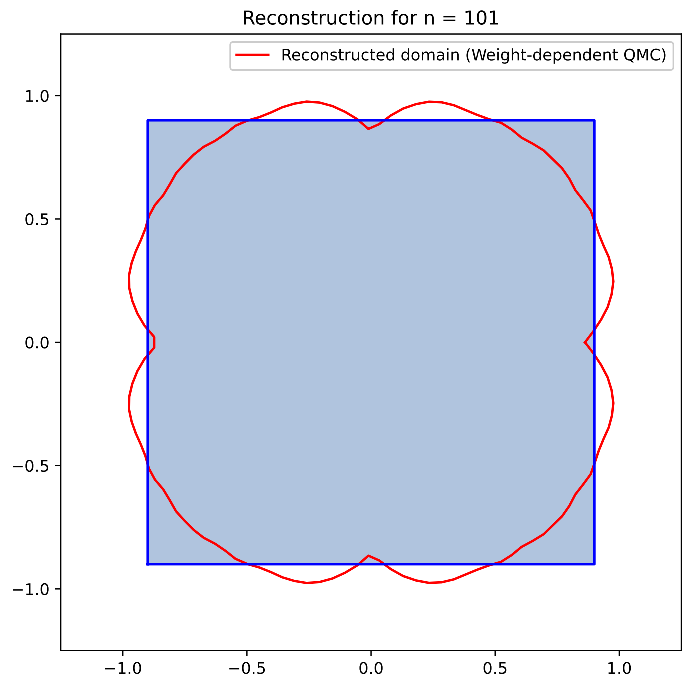
Reconstruction for n = 1979
Reconstructed domain (Weight-dependent QMC)
Original domain
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.0
−0.5
0.0
0.5
1.0

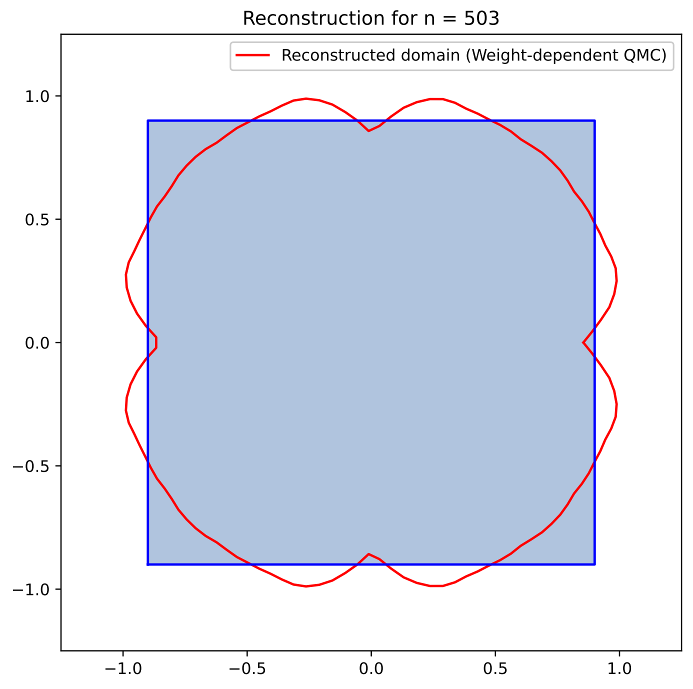
Finally, we consider the problem of reconstructing a domain which lies outside the range of our parameterization. The reconstruction is computed using $s = 100$ terms.

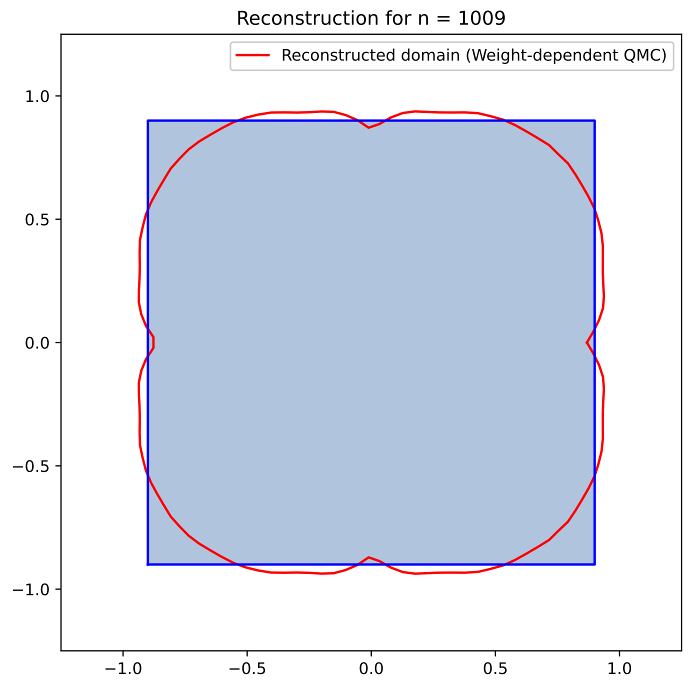


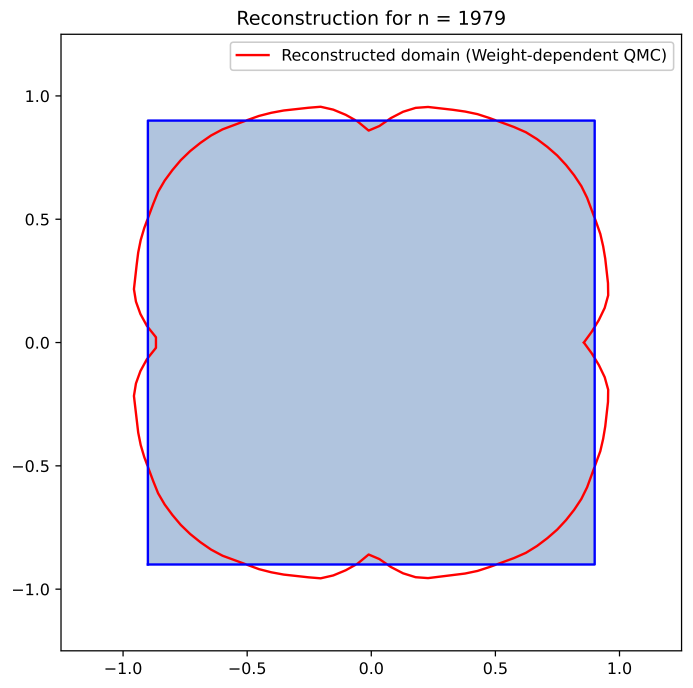
$$a(\boldsymbol{x}, \boldsymbol{y}) := 1 + 1.2 \sum_{j=1}^{s} j^{-2.1} \sin(4j \, \mathrm{atan2}(x_1, x_2) - \pi/2) \mathrm{e}^{-(\frac{1}{2} + y_j)^{-1}}$$


Reconstruction for n = 11
Reconstructed domain (Weight-dependent QMC)
1.0
0.5
0.0
−0.5
−1.0
−1.0
−0.5
0.0
0.5
1.0


Reconstruction for n = 101
Reconstructed domain (Weight-dependent QMC)
1.0
0.5
0.0
−0.5
−1.0
−1.0
−0.5
0.0
0.5
1.0


Reconstruction for n = 503
Reconstructed domain (Weight-dependent QMC)
1.0
0.5
0.0
−0.5
−1.0
−1.0
−0.5
0.0
0.5
1.0


Reconstruction for n = 1009
Reconstructed domain (Weight-dependent QMC)
1.0
0.5
0.0
−0.5
−1.0
−1.0
−0.5
0.0
0.5
1.0


Reconstruction for n = 1979
Reconstructed domain (Weight-dependent QMC)
1.0
0.5
0.0
−0.5
−1.0
−1.0
−0.5
0.0
0.5
1.0

Conclusions

- Modeling the uncertain domains using Gevrey regular parameterizations leads to dimension-independent QMC convergence rates when computing high-dimensional integrals over the posterior.
- Gevrey regular random fields cover a wider range of potential parameterizations for uncertain domains than those covered by affine and uniform models.
- The method could be extended to simultaneous recovery of the domain shape and diffusion coefficient a.

Thank you for your attention!

Some QMC resources

Surveys on QMC for PDE problems:

- J. Dick, F. Y. Kuo, and I. H. Sloan. High-dimensional integration: The quasi-Monte Carlo way. Acta Numer. **22**:133–288, 2013.
- 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.
- F. Y. Kuo and D. Nuyens. Application of quasi-Monte Carlo methods to PDEs with random coefficients – An overview and tutorial. MCQMC 2016 proceedings, pp. 53–71, 2018.

Software:

- F. Y. Kuo and D. Nuyens. QMC4PDE software. `https://people.cs.kuleuven.be/~dirk.nuyens/qmc4pde/`
- D. Nuyens. Magic point shop. `https://people.cs.kuleuven.be/~dirk.nuyens/qmc-generators/`
- F. Y. Kuo. Lattice rule generating vectors. `https://web.maths.unsw.edu.au/~fkuo/lattice/index.html`
- R. N. Gantner. Tools for Higher-Order Quasi-Monte Carlo. `www.sam.math.ethz.ch/HOQMC/`
- F. J. Hickernell et al. QMCPy. `https://arxiv.org/abs/2102.07833`