Quasi-Monte Carlo for Bayesian inverse problems governed by PDEs

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Part I: Quasi-Monte Carlo methods

High-dimensional numerical integration

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

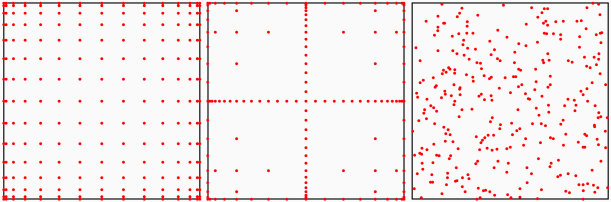


Figure 1: Tensor product grid, sparse grid, Monte Carlo nodes (not QMC rules)

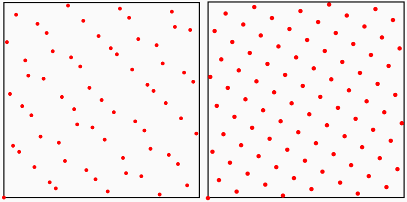


Figure 2: Sobol′ points, lattice rule (examples of QMC rules)

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

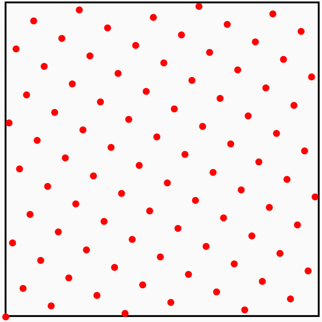
Rank-1 lattice rules

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

have the points

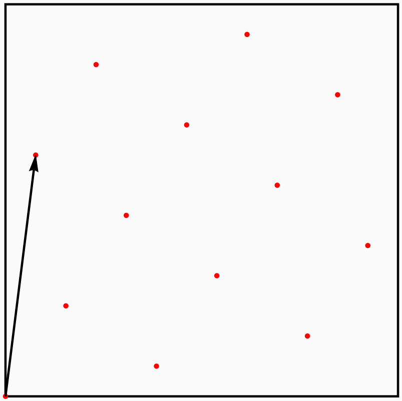
$$\boldsymbol{t}_i = \mathrm{mod}\left(\frac{i\boldsymbol{z}}{n}, 1\right), \quad i \in \{1, \ldots, n\},$$

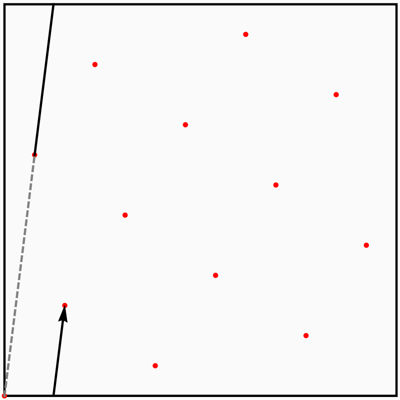
where the entire point set is determined by the *generating vector* $\boldsymbol{z} \in \mathbb{N}^s$, with all components *coprime* to n.

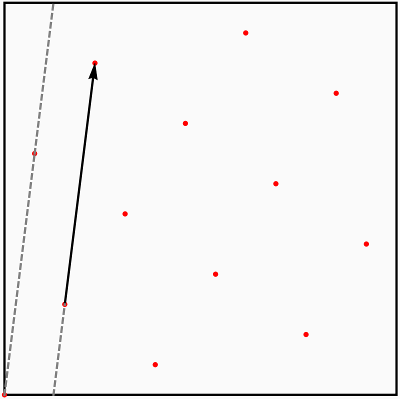


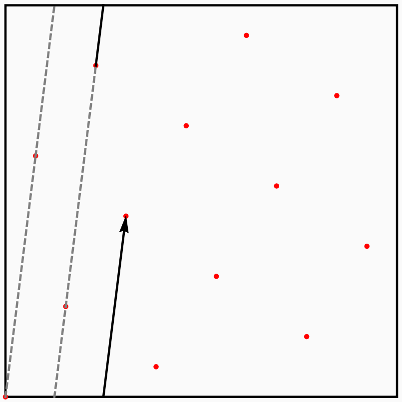
Lattice rule with $\boldsymbol{z} = (1, 55)$ and $n = 89$ nodes in $[0, 1]^2$

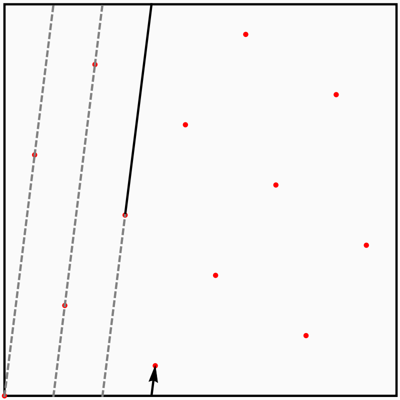
The quality of the lattice rule is determined by the choice of $\boldsymbol{z}$.

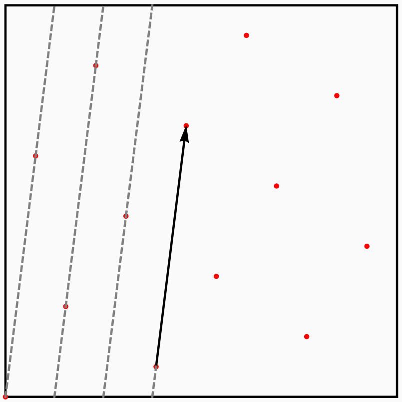


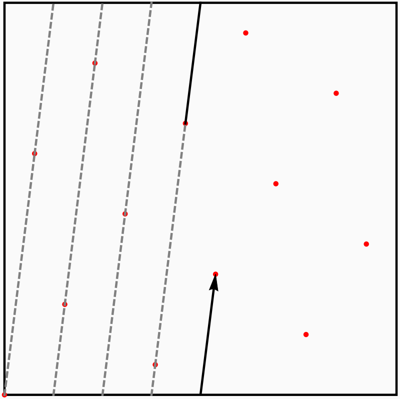


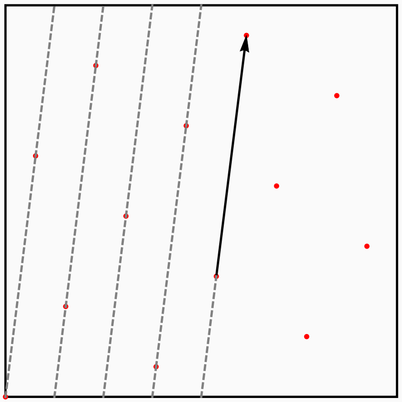


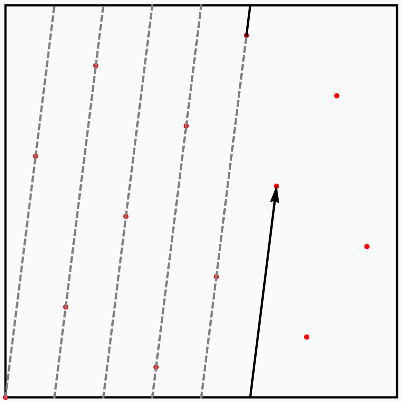


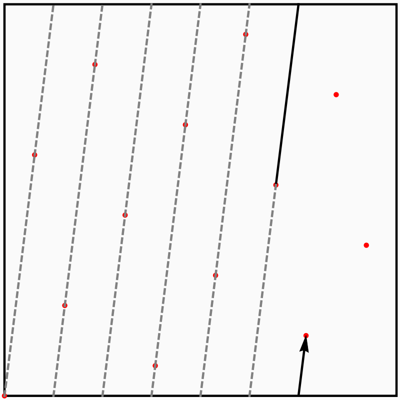


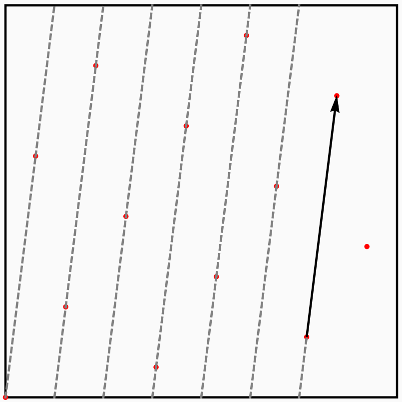


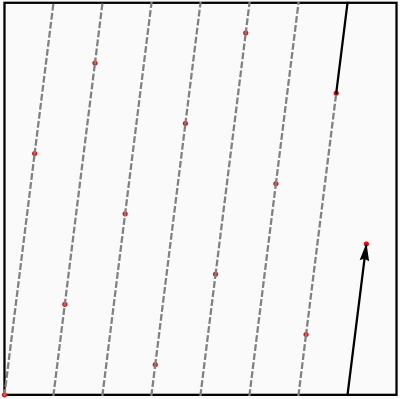












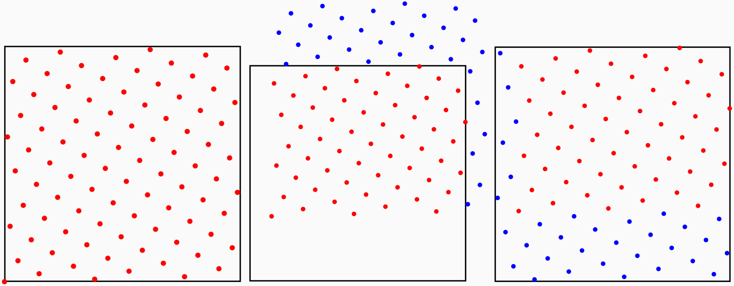
Randomly shifted lattice rules

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

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

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):

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

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

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

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 $\boldsymbol{z} = (z_1, \ldots, z_s)$ 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

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

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

Remarks:

- Optimal rate of convergence $\mathcal{O}(n^{-1+\varepsilon})$ 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:

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

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.

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 $\omega \in \Omega$,

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

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

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

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

Here, we use multi-index notation

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

$$\boldsymbol{\nu}! = \prod_{j\geq 1} \nu_j, \quad \binom{\boldsymbol{\nu}}{\boldsymbol{m}} = \prod_{j\geq 1} \binom{\nu_j}{m_j}.$$

Part III: Application to Bayesian inverse problems

We consider a mathematical measurement model

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

where $\boldsymbol{\delta} \in \mathbb{R}^k$ are the measurements, $\boldsymbol{y} \in U \subset \mathbb{R}^s$ the unknown, $\boldsymbol{\eta} \sim \mathcal{N}(0, \Gamma)$ is k-dimensional additive Gaussian noise with covariance matrix $\Gamma \in \mathbb{R}^{k \times k}$, $\boldsymbol{\eta}$ is assumed to be independent of $\boldsymbol{y}$, and $G\colon U \to \mathbb{R}^k$ is the parameter-to-observation map.

The likelihood of $\boldsymbol{\delta}$, given $\boldsymbol{y}$, is

$$\pi(\boldsymbol{\delta}|\boldsymbol{y}) \propto \exp\left(-\frac{1}{2}(\boldsymbol{\delta} - G(\boldsymbol{y}))^{\mathrm{T}}\Gamma^{-1}(\boldsymbol{\delta} - G(\boldsymbol{y}))\right) = \exp\left(-\frac{1}{2}\|\boldsymbol{\delta} - G(\boldsymbol{y})\|^2_{\Gamma^{-1}}\right).$$

If $\boldsymbol{y}$ has the prior density $\pi(\boldsymbol{y})$, then Bayes' formula can be used to obtain the posterior density of $\boldsymbol{y}$, given $\boldsymbol{\delta}$, as

$$\pi(\boldsymbol{y}|\boldsymbol{\delta}) = \frac{\pi(\boldsymbol{\delta}|\boldsymbol{y})\pi(\boldsymbol{y})}{Z(\boldsymbol{\delta})}, \quad Z(\boldsymbol{\delta}) = \int_U \pi(\boldsymbol{\delta}|\boldsymbol{y})\pi(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y}.$$

We can obtain information about the unknown parameter $\boldsymbol{y}$ given some indirect observations $\boldsymbol{\delta}$ by computing the statistics of the posterior distribution.

Assumptions about the forward model:

A1 The forward mapping satisfies

$$\|\partial_{\boldsymbol{y}}^{\boldsymbol{\nu}} G(\boldsymbol{y})\| \leq C_0(|\boldsymbol{\nu}|!)^{\beta} \boldsymbol{b}^{\boldsymbol{\nu}},$$

where $\boldsymbol{b} := (b_j)_{j\geq 1} \in \ell^p$ are nonnegative real numbers for some $p \in (0,1)$ and $C_0, \beta \geq 1$.

A2 $U = [-\frac{1}{2}, \frac{1}{2}]^s$ and $\pi(\boldsymbol{y}) = 1$ for $\boldsymbol{y} \in U$ and 0 otherwise.

A3 There exists $0 < \mu_{\min} \leq 1$ such that $\lambda_{\min}(\Gamma) \geq \mu_{\min}$.

Example

Model problem: Let $D \subset \mathbb{R}^d$, $d \in \{1,2,3\}$, be a nonempty and bounded Lipschitz domain and $z \in H^{-1}(D)$. For each $\boldsymbol{y} \in U$, there exists a weak solution $u(\cdot, \boldsymbol{y}) \in H_0^1(D)$ to

$$\begin{cases} -\nabla \cdot (a(\boldsymbol{x}, \boldsymbol{y}) \nabla u(\boldsymbol{x}, \boldsymbol{y})) = z(\boldsymbol{x}), & \boldsymbol{x} \in D,\ \boldsymbol{y} \in U, \\ u(\boldsymbol{x}, \boldsymbol{y}) = 0, & \boldsymbol{x} \in \partial D,\ \boldsymbol{y} \in U, \end{cases}$$

where we assume that $\boldsymbol{y} = (y_j)_{j=1}^s$ i.i.d. uniformly distributed in $[-1/2, 1/2]$,

$$a(\boldsymbol{x}, \boldsymbol{y}) = a_0(\boldsymbol{x}) + \sum_{j=1}^{s} y_j \psi_j(\boldsymbol{x}), \quad \boldsymbol{x} \in D,\ \boldsymbol{y} \in [-1/2, 1/2]^s,$$

with $a_0 \in L^\infty(D)$ and $\psi_j \in L^\infty(D)$, $j \geq 1$, such that $0 < a_{\min} \leq a(\boldsymbol{x}, \boldsymbol{y}) \leq a_{\max} < \infty$ for all $\boldsymbol{x} \in D$, $\boldsymbol{y} \in [-1/2, 1/2]^s$.

Then $G(\boldsymbol{y}) := \mathcal{O}(u(\cdot, \boldsymbol{y}))$, where $\mathcal{O} \colon H_0^1(D) \to \mathbb{R}^k$ is bounded and linear, satisfies A1 with $b_j := \|\psi_j\|_{L^\infty(D)} / a_{\min}$.

We are interested in conditional mean estimators of the form

$$\hat{\boldsymbol{F}} = \mathbb{E}_{\pi(\cdot|\boldsymbol{\delta})}[\boldsymbol{F}(\boldsymbol{y})] = \int_U \boldsymbol{F}(\boldsymbol{y})\pi(\boldsymbol{y}|\boldsymbol{\delta})\,\mathrm{d}\boldsymbol{y} = \frac{\int_U \boldsymbol{F}(\boldsymbol{y})\pi(\boldsymbol{\delta}|\boldsymbol{y})\pi(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y}}{\int_U \pi(\boldsymbol{\delta}|\boldsymbol{y})\pi(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y}} =: \frac{Z'}{Z},$$

where $\boldsymbol{F}\colon U \to \mathbb{R}^L$ is some quantity of interest.

For example, if $\boldsymbol{F}(\boldsymbol{y}) = \boldsymbol{y}$, then $\hat{\boldsymbol{F}}$ is the posterior mean.

- We want to use QMC to approximate the numerator and denominator of this ratio estimator.
- For the design of efficient QMC cubature rules, we need to characterize the parametric regularity of integrands corresponding to both the numerator and denominator, provided that $\boldsymbol{F}$ is sufficiently smooth (e.g., belonging to a Gevrey class).

Theorem
There holds for all $\boldsymbol{y} \in U$ and all multi-indices $\boldsymbol{\nu} \neq \mathbf{0}$ that

$$\left|\partial_{\boldsymbol{y}}^{\boldsymbol{\nu}} \mathrm{e}^{-\frac{1}{2}\|\boldsymbol{\delta}-G(\boldsymbol{y})\|_{\Gamma^{-1}}^2}\right| \leq C_1 C_2^{|\boldsymbol{\nu}|}(|\boldsymbol{\nu}|!)^{\beta} \boldsymbol{b}^{\boldsymbol{\nu}},$$

where

$$C_1 = \frac{1}{2^{\beta}} \cdot 3.47^k, \quad C_2 = 2^{\beta} \frac{C_0}{\sqrt{\lambda_{\min}}}.$$

Proof (idea): The integrand can be expressed as a composition of functions

$$(f \circ h)(\boldsymbol{y}),$$

where $f(\boldsymbol{x}) = \mathrm{e}^{-\boldsymbol{x}^{\mathrm{T}}\boldsymbol{x}/2}$ and $h(\boldsymbol{y}) = \Gamma^{-1/2}(\boldsymbol{\delta} - G(\boldsymbol{y}))$.

Cramér's inequality: $|\partial_{\boldsymbol{x}}^{\boldsymbol{\nu}} \mathrm{e}^{-\boldsymbol{x}^{\mathrm{T}}\boldsymbol{x}/2}| \leq \sqrt{\boldsymbol{\nu}!}$ for all $\boldsymbol{x} \in \mathbb{R}^k$ and $\boldsymbol{\nu} \in \mathbb{N}_0^k$.

We already know from the regularity bound of the forward problem that $\|\partial_{\boldsymbol{y}}^{\boldsymbol{\nu}} h(\boldsymbol{y})\| \leq \frac{C_0}{\sqrt{\mu_{\min}}}(|\boldsymbol{\nu}|!)^{\beta} \boldsymbol{b}^{\boldsymbol{\nu}}$ for $\boldsymbol{\nu} \neq \mathbf{0}$.

We use the multivariate chain rule (Faà di Bruno's formula) to put everything together.

Faà di Bruno's formula (recursive version; Savits 2006):

$$\partial_{\boldsymbol{y}}^{\boldsymbol{\nu}} f(h(\boldsymbol{y})) = \sum_{\substack{1\le|\boldsymbol{\lambda}|\le|\boldsymbol{\nu}|\\ \boldsymbol{\lambda}\in\mathbb{N}_0^k}} \partial_{\boldsymbol{x}}^{\boldsymbol{\lambda}} f(\boldsymbol{x})\Big|_{\boldsymbol{x}=G(\boldsymbol{y},\cdot)} \kappa_{\boldsymbol{\nu},\boldsymbol{\lambda}}(\boldsymbol{y}), \quad \boldsymbol{\nu}\neq\boldsymbol{0},$$

where the sequence $(\kappa_{\boldsymbol{\nu},\boldsymbol{\lambda}})$ depends only on h via

$\kappa_{\boldsymbol{\nu},\boldsymbol{0}} \equiv \delta_{\boldsymbol{\nu},\boldsymbol{0}}$,

$\kappa_{\boldsymbol{\nu},\boldsymbol{\lambda}} \equiv 0 \quad$ if $|\boldsymbol{\nu}| < |\boldsymbol{\lambda}|$ or $\boldsymbol{\lambda} \not\geq \boldsymbol{0}$ (i.e., if $\boldsymbol{\lambda}$ contains negative entries),

$$\kappa_{\boldsymbol{\nu}+\boldsymbol{e}_j,\boldsymbol{\lambda}}(\boldsymbol{y}) = \sum_{\ell\in\mathrm{supp}(\boldsymbol{\lambda})} \sum_{\boldsymbol{0}\le\boldsymbol{m}\le\boldsymbol{\nu}} \binom{\boldsymbol{\nu}}{\boldsymbol{m}} \partial_{\boldsymbol{y}}^{\boldsymbol{m}+\boldsymbol{e}_j}[h(\boldsymbol{y})]_\ell \kappa_{\boldsymbol{\nu}-\boldsymbol{m},\boldsymbol{\lambda}-\boldsymbol{e}_\ell}(\boldsymbol{y}) \quad \text{otherwise.}$$

Since $\|\partial_{\boldsymbol{y}}^{\boldsymbol{\nu}} h(\boldsymbol{y})\| \le \frac{C_0}{\sqrt{\mu_{\min}}}(|\boldsymbol{\nu}|!)^\beta \boldsymbol{b}^{\boldsymbol{\nu}}$, we obtain the following *uniform* bound.

Lemma
For all $1 \le |\boldsymbol{\lambda}| \le |\boldsymbol{\nu}|$, there holds

$$|\kappa_{\boldsymbol{\nu},\boldsymbol{\lambda}}(\boldsymbol{y})| \le \left(\frac{C_0}{\sqrt{\mu_{\min}}}\right)^{|\boldsymbol{\nu}|} \left(\frac{|\boldsymbol{\nu}|!(|\boldsymbol{\nu}|-1)!}{\boldsymbol{\lambda}!(|\boldsymbol{\nu}|-|\boldsymbol{\lambda}|)!(|\boldsymbol{\lambda}|-1)!}\right)^\beta \boldsymbol{b}^{\boldsymbol{\nu}}.$$

Proof.
By induction w.r.t. the order of the multi-index $\boldsymbol{\nu}$. □

For the present problem, we obtain

$$
\begin{aligned}
&|\partial_{\boldsymbol{y}}^{\boldsymbol{\nu}} \mathrm{e}^{-\frac{1}{2}\|\boldsymbol{y}-G(\boldsymbol{y})\|_{\Gamma^{-1}}^2}| \\
&\leq \left(\frac{C_0}{\sqrt{\mu_{\min}}}\right)^{|\boldsymbol{\nu}|} \\
&\quad \times \sum_{\substack{1\leq|\boldsymbol{\lambda}|\leq|\boldsymbol{\nu}|\\ \boldsymbol{\lambda}\in\mathbb{N}_0^k}} |\partial_{\boldsymbol{x}}^{\boldsymbol{\lambda}} \mathrm{e}^{-\boldsymbol{x}^{\mathrm{T}}\boldsymbol{x}/2}|\Big|_{\boldsymbol{x}=\Gamma^{-1/2}(\boldsymbol{y}-G(\boldsymbol{y}))} \left(\frac{|\boldsymbol{\nu}|!(|\boldsymbol{\nu}|-1)!}{\boldsymbol{\lambda}!(|\boldsymbol{\nu}|-|\boldsymbol{\lambda}|)!(|\boldsymbol{\lambda}|-1)!}\right)^{\beta} \boldsymbol{b}^{\boldsymbol{\nu}} \\
&\leq \left(\frac{C_0}{\sqrt{\mu_{\min}}}\right)^{|\boldsymbol{\nu}|} \boldsymbol{b}^{\boldsymbol{\nu}} (|\boldsymbol{\nu}|!)^{\beta}((|\boldsymbol{\nu}|-1)!)^{\beta} \sum_{\substack{1\leq|\boldsymbol{\lambda}|\leq|\boldsymbol{\nu}|\\ \boldsymbol{\lambda}\in\mathbb{N}_0^k}} \left(\frac{\sqrt{\boldsymbol{\lambda}!}}{\boldsymbol{\lambda}!(|\boldsymbol{\nu}|-|\boldsymbol{\lambda}|)!(|\boldsymbol{\lambda}|-1)!}\right)^{\beta}.
\end{aligned}
$$

It remains to estimate the multi-index sum, but fortunately this is not too difficult:

$$
\begin{aligned}
&\sum_{\substack{1\le|\boldsymbol{\lambda}|\le|\boldsymbol{\nu}|\\ \boldsymbol{\lambda}\in\mathbb{N}_0^k}} \left(\frac{\sqrt{\boldsymbol{\lambda}!}}{\boldsymbol{\lambda}!(|\boldsymbol{\nu}|-|\boldsymbol{\lambda}|)!(|\boldsymbol{\lambda}|-1)!}\right)^{\beta} \\
&= \sum_{\ell=1}^{|\boldsymbol{\nu}|} \left(\frac{1}{(|\boldsymbol{\nu}|-\ell)!(\ell-1)!}\right)^{\beta} \sum_{\substack{\boldsymbol{\lambda}\in\mathbb{N}_0^k\\ |\boldsymbol{\lambda}|=\ell}} \left(\frac{1}{\sqrt{\boldsymbol{\lambda}!}}\right)^{\beta} \\
&\le \left(\sum_{\ell=1}^{|\boldsymbol{\nu}|} \left(\frac{1}{(|\boldsymbol{\nu}|-\ell)!(\ell-1)!}\right)^{\beta}\right) \underbrace{\left(\sum_{\lambda=0}^{\infty} \frac{1}{\sqrt{\lambda!}}\right)}_{=3.469506}{}^{k} \\
&\le 3.47^k \left(\sum_{\ell=1}^{|\boldsymbol{\nu}|} \frac{1}{(|\boldsymbol{\nu}|-\ell)!(\ell-1)!}\right)^{\beta} = 3.47^k \cdot \frac{2^{\beta|\boldsymbol{\nu}|-\beta}}{((|\boldsymbol{\nu}|-1)!)^{\beta}},
\end{aligned}
$$

where we made use of $\sum_k a_k \le \left(\sum_k a_k^{1/\beta}\right)^{\beta}$ for $a_k \ge 0$ and $\beta \ge 1$ as well as the summation identity $\sum_{\ell=1}^{\nu} \frac{1}{(\nu-\ell)!(\ell-1)!} = \frac{2^{\nu-1}}{(\nu-1)!}$.

This yields the desired result. $\square$

Theorem
Suppose that the quantity of interest $\boldsymbol{F}\colon U \to \mathbb{R}^L$ satisfies

$$\|\partial_{\boldsymbol{y}}^{\boldsymbol{\nu}} \boldsymbol{F}(\boldsymbol{y})\| \leq C_0(|\boldsymbol{\nu}|!)^{\beta} \boldsymbol{b}^{\boldsymbol{\nu}}.$$

There holds for all $\boldsymbol{y} \in U$ and all multi-indices $\boldsymbol{\nu} \neq \boldsymbol{0}$ that

$$\left|\partial_{\boldsymbol{y}}^{\boldsymbol{\nu}}\left(\boldsymbol{F}(\boldsymbol{y})\mathrm{e}^{-\frac{1}{2}\|\boldsymbol{\delta}-G(\boldsymbol{y})\|_{\Gamma^{-1}}^2}\right)\right| \leq C_0 C_1 C_2^{|\boldsymbol{\nu}|}((|\boldsymbol{\nu}|+1)!)^{\beta} \boldsymbol{b}^{\boldsymbol{\nu}}.$$

Proof. By the Leibniz product rule:

$$\left|\partial_{\boldsymbol{y}}\left(\boldsymbol{F}(\boldsymbol{y})\mathrm{e}^{-\frac{1}{2}\|\boldsymbol{\delta}-G(\boldsymbol{y})\|_{\Gamma^{-1}}^2}\right)\right| = \left|\sum_{\boldsymbol{m}\leq\boldsymbol{\nu}} \binom{\boldsymbol{\nu}}{\boldsymbol{m}} \partial_{\boldsymbol{y}}^{\boldsymbol{\nu}-\boldsymbol{m}} \boldsymbol{F}(\boldsymbol{x},\boldsymbol{y}) \partial^{\boldsymbol{m}} \mathrm{e}^{-\frac{1}{2}\|\boldsymbol{\delta}-G(\boldsymbol{y})\|_{\Gamma^{-1}}^2}\right|$$

$$\leq \sum_{\boldsymbol{m}\leq\boldsymbol{\nu}} \binom{\boldsymbol{\nu}}{\boldsymbol{m}} C_0((|\boldsymbol{\nu}|-|\boldsymbol{m}|)!)^{\beta} \boldsymbol{b}^{\boldsymbol{\nu}-\boldsymbol{m}} C_1 C_2^{|\boldsymbol{m}|}(|\boldsymbol{m}|!)^{\beta} \boldsymbol{b}^{\boldsymbol{m}}$$

$$\leq C_0 C_1 C_2^{|\boldsymbol{\nu}|} \boldsymbol{b}^{\boldsymbol{\nu}} \sum_{\boldsymbol{m}\leq\boldsymbol{\nu}} \binom{\boldsymbol{\nu}}{\boldsymbol{m}} ((|\boldsymbol{\nu}|-|\boldsymbol{m}|)!)^{\beta} (|\boldsymbol{m}|!)^{\beta}$$

$$\leq \cdots \leq C_0 C_1 C_2^{|\boldsymbol{\nu}|} \boldsymbol{b}^{\boldsymbol{\nu}} ((|\boldsymbol{\nu}|+1)!)^{\beta}. \quad \square$$

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:

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

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

$$\gamma_{\mathfrak{u}} := \left(((|\mathfrak{u}|+1)!)^{\beta}\prod_{j\in\mathfrak{u}}\frac{C_2 b_j}{\sqrt{2\zeta(2\lambda)/(2\pi^2)^{\lambda}}}\right)^{\frac{2}{1+\lambda}} \quad \text{for } \mathfrak{u}\subset\{1,\ldots,s\},$$

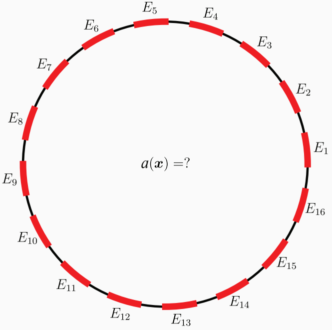
where we set $\lambda := \frac{p}{2-p}$ if $p \in (\frac{2}{3}, \frac{1}{\beta})$ and $\lambda = \frac{1}{2-2\varepsilon}$ for arbitrary $\varepsilon \in (0, \frac{1}{2})$ if $p \in (0, \min\{\frac{2}{3}, \frac{1}{\beta}\}]$, $p \neq \frac{1}{\beta}$. We obtain QMC convergence rate $\sqrt{\mathbb{E}_{\boldsymbol{\Delta}}\left|\frac{Z'}{Z}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

Application 1: Electrical impedance tomography

Electrical impedance tomography

Use measurements of current and voltage collected at electrodes covering part of the boundary to infer the interior conductivity of an object/body.

$$\begin{cases} \nabla \cdot (a \nabla u) = 0 & \text{in } D, \\ a \frac{\partial u}{\partial \boldsymbol{n}} = 0 & \text{on } \partial D \setminus \bigcup_{k=1}^{L} \overline{E_k}, \\ u + z_k a \frac{\partial u}{\partial \boldsymbol{n}} = \mathcal{U}_k & \text{on } E_k,\ k \in \{1, \ldots, L\}, \\ \int_{E_k} a \frac{\partial u}{\partial \boldsymbol{n}} \, \mathrm{d}S = I_k, & k \in \{1, \ldots, L\}, \end{cases}$$



Model specifics

- $D \subset \mathbb{R}^d$, $d \in \{1,2,3\}$ nonempty physical domain with Lipschitz boundary, $y \in U := [-1/2, 1/2]^s$.
- Assumptions on a:
  1. $a(\cdot, \boldsymbol{y}) \in L^\infty(D)$ for all $\boldsymbol{y} \in U$.
  2. There exist constants $C_a, \sigma \geq 1$ and a sequence $\boldsymbol{\rho} = (\rho_j)_{j\geq 1} \in \ell^p(\mathbb{N})$, $p \in (0,1)$, of non-negative real numbers such that
  $$\|\partial_{\boldsymbol{y}}^{\boldsymbol{\nu}} a(\cdot, \boldsymbol{y})\|_{L^\infty(D)} \leq C_a (|\boldsymbol{\nu}|!)^\beta \boldsymbol{\rho}^{\boldsymbol{\nu}} \quad \text{for all } \boldsymbol{\nu} \in \mathbb{N}_0^s \text{ and } \boldsymbol{y} \in U.$$
  3. There exist positive constants $a_{\min}$ and $a_{\max}$ such that
  $$0 < a_{\min} \leq a(\boldsymbol{x}, \boldsymbol{y}) \leq a_{\max} < \infty \quad \text{for all } \boldsymbol{x} \in D \text{ and } \boldsymbol{y} \in U.$$
- $\{E_k\}_{k=1}^L$, $L \geq 2$, open, nonempty, connected subsets of D s.t. $\overline{E}_i \cap \overline{E}_j = \varnothing$ for $i \neq j$
- Quotient Hilbert space $\mathcal{H} := (H^1(D) \oplus \mathbb{R}^L)/\mathbb{R}$ with the norm
$$\|(v, V)\|_{\mathcal{H}}^2 := \int_D |\nabla v|^2 \, \mathrm{d}\boldsymbol{x} + \sum_{k=1}^L \int_{E_k} (v - V_m)^2 \, \mathrm{d}S, \quad (v, V) \in \mathcal{H}.$$
- Contact impedances $\{z_m\}_{m=1}^M$ satisfy $0 < \varsigma_- \leq z_m \leq \varsigma_+ < \infty \; \forall\, m$.

Forward problem

For $\boldsymbol{y} \in U$ find the electromagnetic potential $u(\cdot, \boldsymbol{y})$ and the potentials on the electrodes $\mathcal{U}(\boldsymbol{y})$ such that the model equations hold.

Variational formulation: Find $(u(\cdot, \boldsymbol{y}), \mathcal{U}(\boldsymbol{y})) \in \mathcal{H}$ such that

$$\int_D a(\cdot, \boldsymbol{y}) \nabla u(\cdot, \boldsymbol{y}) \cdot \nabla v \,\mathrm{d}\boldsymbol{x} + \sum_{m=1}^{L} \frac{1}{z_m} \int_{E_m} (u(\cdot, \boldsymbol{y}) - \mathcal{U}_m(\boldsymbol{y}))(v - V_m) \,\mathrm{d}S = \sum_{m=1}^{L} I_m V_m$$

for all $(v, V) \in \mathcal{H}$.

Lemma

Let $\boldsymbol{\nu} \in \mathscr{F}$ and $\boldsymbol{y} \in U$. Then there exists a constant $C = C_{D,E} \geq 1$ s.t.

$$\|(u(\cdot, \boldsymbol{y}), \mathcal{U}(\boldsymbol{y})\|_{\mathcal{H}} \leq \frac{C_{D,E}|I|}{\min\{a_{\min}, \varsigma_+^{-1}\}} \quad \textit{for all } \boldsymbol{y} \in U,$$

and, moreover,

$$\|\partial^{\boldsymbol{\nu}}(u(\cdot, \boldsymbol{y}), \mathcal{U}(\boldsymbol{y}))\|_{\mathcal{H}} \leq C_u(|\boldsymbol{\nu}|!)^{\beta} \boldsymbol{b}^{\boldsymbol{\nu}},$$

where $C_u = \frac{C_{D,E}|I|}{\min\{a_{\min}, \varsigma_+^{-1}\}}$ *and* $b_j := \big(1 + \frac{C_a}{\min\{a_{\min}, \varsigma_+^{-1}\}}\big)\rho_j$.

This fits into our theoretical framework!

Inverse problem

Assume there are some voltage measurements taken at the L electrodes placed on the boundary of the computational domain D corresponding to the observation operator $G \colon U \to \mathbb{R}^L$

$$G(\boldsymbol{y}) := [\mathcal{U}_1(\boldsymbol{y}), \ldots, \mathcal{U}_L(\boldsymbol{y})]^{\mathrm{T}}.$$

Consider the problem of finding an unknown $\boldsymbol{y} \in U$ using the data $\boldsymbol{\delta} \in \mathbb{R}^L$, where $\boldsymbol{y}$ and $\boldsymbol{\delta}$ are related by the equation

$$\boldsymbol{\delta} = \mathcal{O}(\boldsymbol{y}) + \boldsymbol{\eta}.$$

- $\boldsymbol{\eta} \in \mathbb{R}^L$ Gaussian observational noise in $\boldsymbol{\delta}$, let $\boldsymbol{y}, \boldsymbol{\delta}, \boldsymbol{\eta}$ to be random variables independent of each other

Parameter estimation

To reconstruct $a(\cdot, \boldsymbol{y})$ with the unknown parameter $\boldsymbol{y} \in [-1/2, 1/2]^s$, we consider the estimator

$$\hat{a}(\boldsymbol{x}) = \frac{\int_{[-1/2,1/2]^s} a(\boldsymbol{x}, \boldsymbol{y})\, \pi(\boldsymbol{\delta}|\boldsymbol{y})\pi(\boldsymbol{y})\, \mathrm{d}\boldsymbol{y}}{\int_{[-1/2,1/2]^s} \pi(\boldsymbol{\delta}|\boldsymbol{y})\pi(\boldsymbol{y})\, \mathrm{d}\boldsymbol{y}}.$$

Bayes' formula:

$$\pi(\boldsymbol{y}|\boldsymbol{\delta}) = \frac{\pi(\boldsymbol{\delta}|\boldsymbol{y})\pi(\boldsymbol{y})}{Z(\boldsymbol{\delta})}, \quad \pi(\boldsymbol{\delta}|\boldsymbol{y}) \propto \mathrm{e}^{-\frac{1}{2}\|\boldsymbol{\delta} - G(\boldsymbol{y})\|^2_{\Gamma^{-1}}},$$

where $\pi(\boldsymbol{y})$ denotes the prior density of $\boldsymbol{y}$, here $\boldsymbol{y} \sim \mathcal{U}([-1/2, 1/2]^s)$, and $\pi(\boldsymbol{\delta}|\boldsymbol{y})$ the likelihood of $\boldsymbol{\delta}$ given $\boldsymbol{y}$.

Numerical experiment

Generate synthetic measurement data $\boldsymbol{\delta}$ using the parametrization

$$a(\boldsymbol{x}, \boldsymbol{y}) = \exp\left(\sum_{j=1}^{20} y_j \psi_j(\boldsymbol{x})\right), \quad \boldsymbol{x} \in D,\ \boldsymbol{y} \in [-1/2, 1/2]^{20},$$

with

$$\psi_j(\boldsymbol{x}) := \frac{5}{(k_j^2 + \ell_j^2)^2} \sin(\tfrac{1}{14}\pi k_j x_1) \sin(\tfrac{1}{14}\pi \ell_j x_2)$$

where the sequence $(k_j, l_j)_{j \geq 1}$ is an ordering of the elements of $\mathbb{N} \times \mathbb{N}$.

The measurements were contaminated by 10% relative Gaussian noise.

Reconstruction

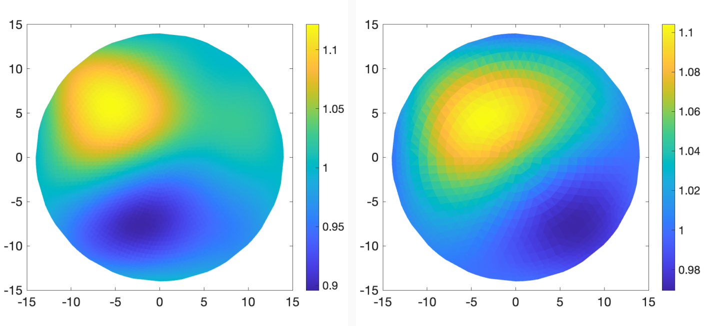
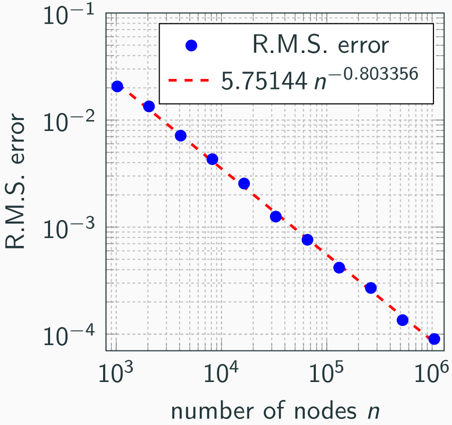


Figure 3: Randomly generated ground truth conductivity field on the left, reconstruction corresponding to noisy voltage measurements on the right. The reconstruction corresponds to $n = 2^{20}$ QMC nodes with a single random shift.

Error plot

R.M.S. errors for the reconstruction corresponding to the reconstruction with $R = 16$ random shifts plotted alongside the corresponding least squares fits.



Application 2: Bayesian shape inversion

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, Multerer, Siebenmorgen, Schwab, Gantner, Zech...

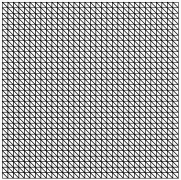


Figure 4: Reference domain

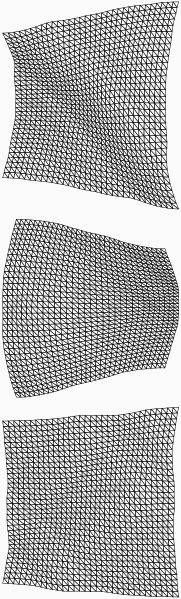


Figure 5: Three realizations of the random domain

Model specifics

- Fixed reference domain $D_{\mathrm{ref}} \subset \mathbb{R}^d$, $d \in \{2,3\}$ is a nonempty physical domain with Lipschitz boundary.
- The family of admissible domains $D(\boldsymbol{y}) := \boldsymbol{V}(D_{\mathrm{ref}}, \boldsymbol{y})$ for $\boldsymbol{y} \in U := [-1/2, 1/2]^s$. Hold-all domain $\mathcal{D} = \bigcup_{\boldsymbol{y} \in U} D(\boldsymbol{y})$.
- Assumptions on $\boldsymbol{V}$:
  1. $\boldsymbol{V}(\cdot, \boldsymbol{y})\colon \overline{D_{\mathrm{ref}}} \to \overline{D(\boldsymbol{y})}$ is a $\mathcal{C}^2$-diffeomorphism for all $\boldsymbol{y} \in U$.
  2. There exist constants $C_{\boldsymbol{V}}, \beta \geq 1$ and a sequence $\boldsymbol{b} = (b_j)_{j \geq 1} \in \ell^p(\mathbb{N})$, $p \in (0,1)$, of non-negative real numbers such that

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

  3. There exist positive constants $0 < \sigma_{\min} \leq 1 \leq \sigma_{\max}$ such that

$$0 < \sigma_{\min} \leq \min \sigma(D\boldsymbol{V}(\boldsymbol{x}, \boldsymbol{y})) \leq \max \sigma(D\boldsymbol{V}(\boldsymbol{x}, \boldsymbol{y})) \leq \sigma_{\max} < \infty$$

     for all $\boldsymbol{x} \in D$ and $\boldsymbol{y} \in U$, with $\sigma(M)$ denoting the set of singular values of matrix M.

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 $\|\partial^{\boldsymbol{\nu}} f\|_{L^\infty(\mathcal{D})} \le C_{\boldsymbol{V}} (|\boldsymbol{\nu}|!)^{\beta} \boldsymbol{\rho}^{\boldsymbol{\nu}}$.

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

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

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
There holds for all $\boldsymbol{y} \in U$ and all multi-indices $\boldsymbol{\nu} \neq \mathbf{0}$ that

$$\|\partial_{\boldsymbol{y}}^{\boldsymbol{\nu}} \widehat{u}(\cdot, \boldsymbol{y})\|_{H_0^1(D_{ref})} \leq C_1 \, C_2^{|\boldsymbol{\nu}|} (|\boldsymbol{\nu}|!)^{\beta} \boldsymbol{b}^{\boldsymbol{\nu}},$$

where

$$C_1 = 1 + \left(\frac{\sigma_{\max}}{\sigma_{\min}}\right)^d \frac{\sigma_{\max}^2 C_{D_{\mathrm{ref}}} |D_{\mathrm{ref}}|^{1/2} C_{\boldsymbol{V}}}{2^{\beta}}$$

$$C_2 = ((d^2)!)^{\beta} 2^{\beta(d^2+1)+1}$$
$$\times \max\left\{\left(\frac{\sigma_{\max}^d}{\sigma_{\min}^{d+2}((d^2)!)^{\beta}}, 2\left(\frac{2^{\beta} C_{\boldsymbol{V}}}{\sigma_{\min}}\right)^3, \frac{C_1 - 1}{\sigma_{\max}^2((d^2)!)^{\beta}}, \frac{(2^{\beta} C_{\boldsymbol{V}})^2}{\sigma_{\min}} \max\{1, \|\boldsymbol{\rho}\|_{\ell^{1/\beta}}\right\}\right\}$$

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

This fits into our theoretical framework!

As the reconstruction of the unknown domain, we consider

$$\hat{\boldsymbol{V}}(\boldsymbol{x}) = \frac{\int_U \boldsymbol{V}(\boldsymbol{x}, \boldsymbol{y}) \mathrm{e}^{-\frac{1}{2}\|\boldsymbol{\delta} - G(\boldsymbol{y})\|_{\Gamma^{-1}}^2} \, \mathrm{d}\boldsymbol{y}}{\int_U \mathrm{e}^{-\frac{1}{2}\|\boldsymbol{\delta} - G(\boldsymbol{y})\|_{\Gamma^{-1}}^2} \, \mathrm{d}\boldsymbol{y}}.$$

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

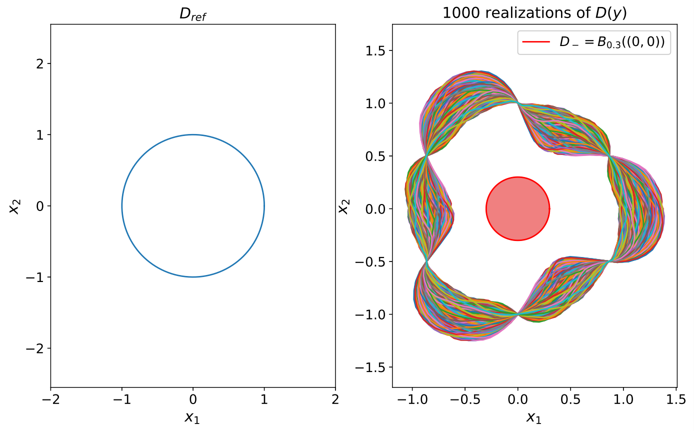
Thus the reference domain in this case is the unit disk, and the uncertain boundary is the curve defined by the radial transformation $r = 1 + \sum_{j=1}^{s} j^{-2.1} \sin(3j\,\theta + \pi)\mathrm{e}^{-(\frac{1}{2}+y_j)^{-1}}$ for each realization of $\boldsymbol{y}$.

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

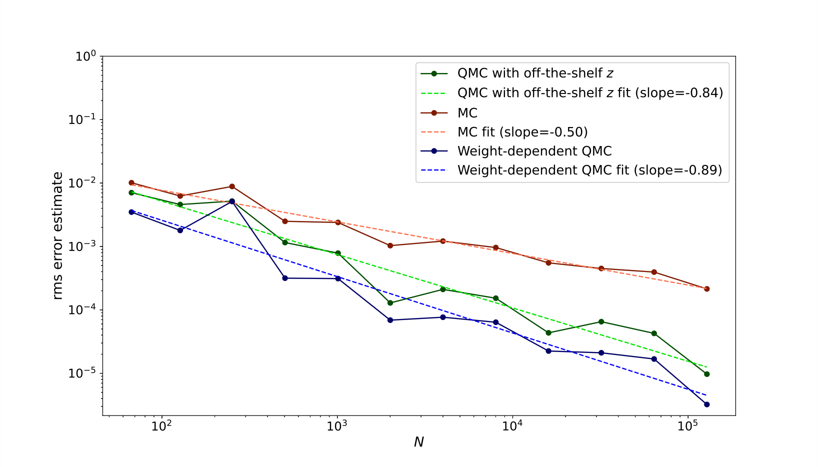
To assess the convergence behavior, we first consider the observation operator

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

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.



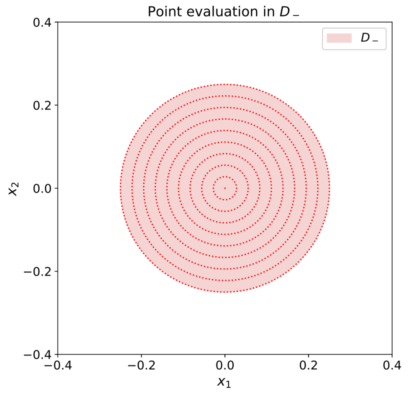
QMC convergence of $\hat{V}$



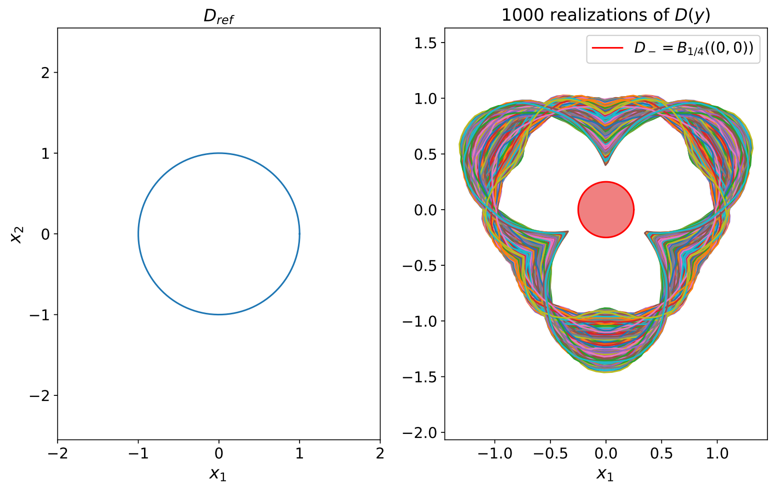
Next, we consider reconstructing the domain shape based on measurements. Here, we consider the observation operator

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

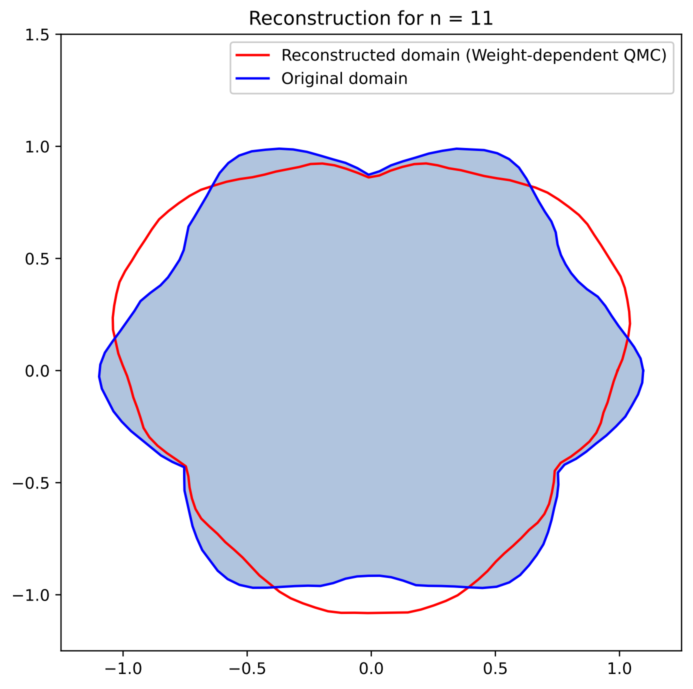
where the PDE solution is sampled over a point set with $k = 996$ belonging to D_- (below). The observations were generated using a finer FE mesh ($h = 2^{-6}$) and contaminated with 5% relative Gaussian noise.

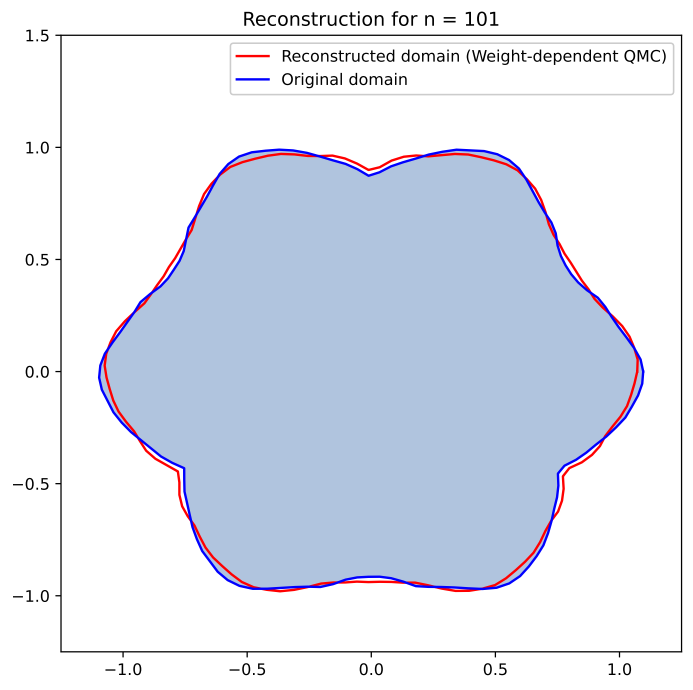


First, we generate the ground truth domain as a realization of the random field with $s = 200$ terms. Then we compute the reconstruction using $s = 20$ terms.

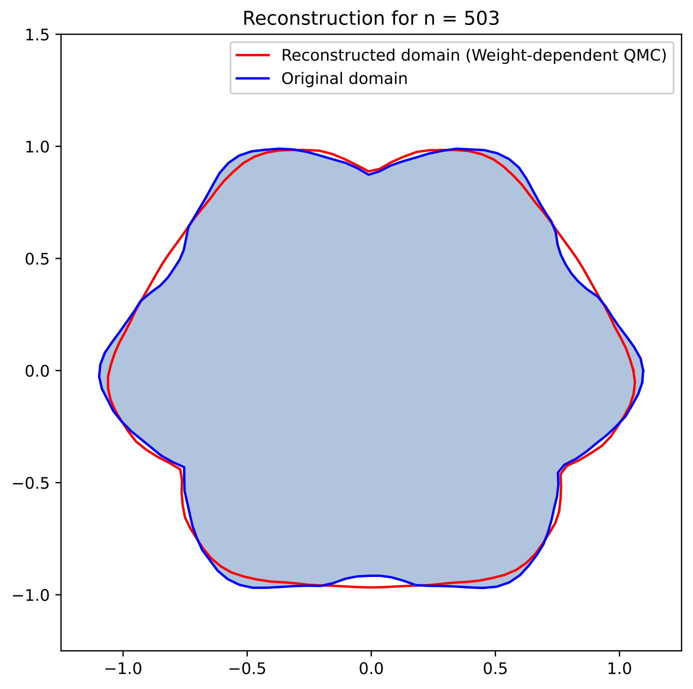


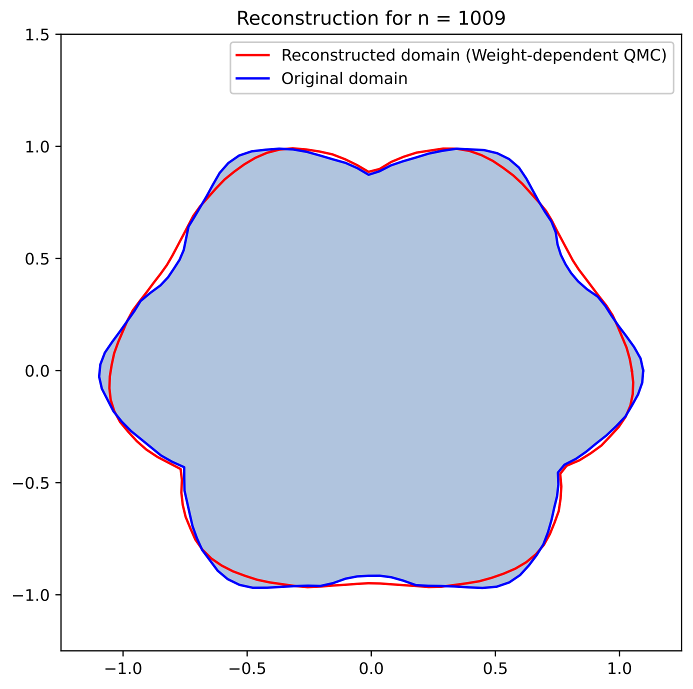
$$a(\boldsymbol{x}, \boldsymbol{y}) := 1 + 1.2 \sum_{j=1}^{s} j^{-2.1} \sin(3j \operatorname{atan2}(x_1, x_2) - \pi/2) \mathrm{e}^{-(\frac{1}{2}+y_j)^{-1}}$$

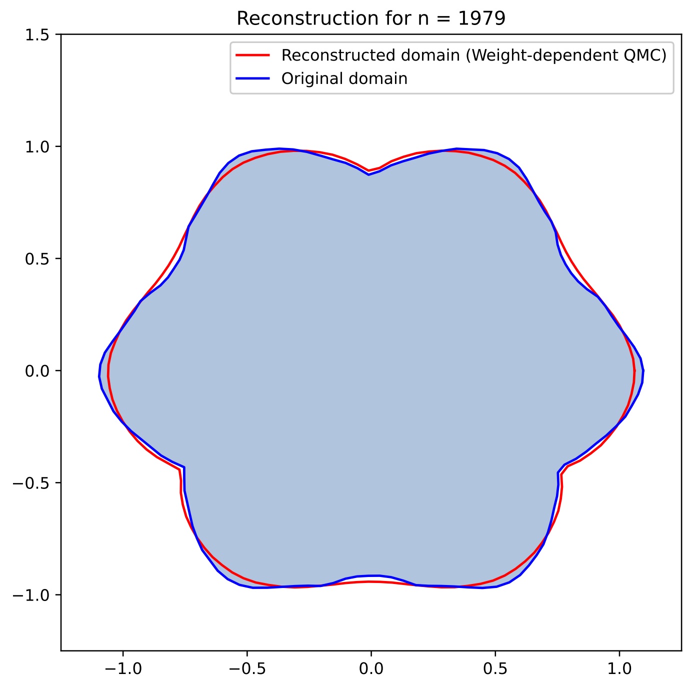

Reconstruction for n = 11
Reconstructed domain (Weight-dependent QMC)
Original domain
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.0
−0.5
0.0
0.5
1.0



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

Application 3: Bayesian optimal experimental design

Let $G \colon U \times \Xi \to \mathbb{R}^k$ be a forward mapping depending on a true parameter $\boldsymbol{y} \in U$ and a design parameter $\boldsymbol{\xi} \in \Xi$.

Measurement model:

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

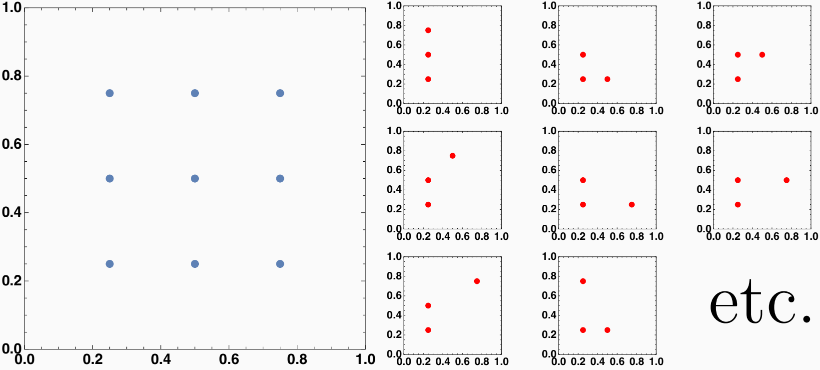
where $\boldsymbol{\delta} \in \mathbb{R}^k$ is the measurement data and $\boldsymbol{\eta} \in \mathbb{R}^k$ is Gaussian noise such that $\boldsymbol{\eta} \sim \mathcal{N}(0, \Gamma)$ with positive definite covariance matrix $\Gamma \in \mathbb{R}^{k \times k}$.

Goal in Bayesian optimal experimental design: Recover the design parameter $\boldsymbol{\xi}$ for the Bayesian inference of $\boldsymbol{y}$, which we model as a random variable endowed with prior distribution $\pi(\boldsymbol{y})$.

Example

Suppose we have 9 slots and 3 sensors. Before carrying out the experiment, which 3 slots do we expect to be the most informative for the recovery of the unknown parameter?

$\to \binom{9}{3} = 84$ possible configurations



Left: 9 slots. Right: We have 84 possible ways to place 3 sensors into 9 slots.

How to rank the 84 different possibilities from most informative to least informative?

A measure of the information gain for a given design $\boldsymbol{\xi}$ and data $\boldsymbol{\delta}$ is given by the Kullback–Leibler divergence

$$D_{\mathrm{KL}}(\pi(\cdot|\boldsymbol{\delta},\boldsymbol{\xi})\|\pi(\cdot)) := \int_{U} \log\left(\frac{\pi(\boldsymbol{y}|\boldsymbol{\delta},\boldsymbol{\xi})}{\pi(\boldsymbol{y})}\right)\pi(\boldsymbol{y}|\boldsymbol{\delta},\boldsymbol{\xi})\,\mathrm{d}\boldsymbol{y}. \tag{4}$$

We wish to maximize the expected utility (4) over the design space Ξ with respect to the data $\boldsymbol{\delta}$ and model parameters $\boldsymbol{y}$:

$$\max_{\boldsymbol{\xi}\in\Xi} \underbrace{\int_{Y}\int_{U} \log\left(\frac{\pi(\boldsymbol{y}|\boldsymbol{\delta},\boldsymbol{\xi})}{\pi(\boldsymbol{y})}\right)\pi(\boldsymbol{y}|\boldsymbol{\delta},\boldsymbol{\xi})\pi(\boldsymbol{\delta}|\boldsymbol{\xi})\,\mathrm{d}\boldsymbol{y}\,\mathrm{d}\boldsymbol{\delta}}_{=:\mathrm{EIG}},$$

where $\pi(\boldsymbol{y}|\boldsymbol{\delta},\boldsymbol{\xi})$ corresponds to the posterior distribution of the parameter $\boldsymbol{y}$ and $\pi(\boldsymbol{\delta}|\boldsymbol{\xi}) = \int_{U}\pi(\boldsymbol{\delta}|\boldsymbol{y},\boldsymbol{\xi})\pi(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y}$ is the marginal distribution of the data $\boldsymbol{\delta}$.

The posterior is given by Bayes' theorem

$$\pi(\boldsymbol{y}|\boldsymbol{\delta},\boldsymbol{\xi}) = \frac{\pi(\boldsymbol{\delta}|\boldsymbol{y},\boldsymbol{\xi})\pi(\boldsymbol{y})}{\pi(\boldsymbol{\delta}|\boldsymbol{\xi})},$$

which means that the expected utility can be written as

$$\begin{aligned}\mathrm{EIG} &= \int_Y \int_U \log\left(\frac{\pi(\boldsymbol{y}|\boldsymbol{\delta},\boldsymbol{\xi})}{\pi(\boldsymbol{y})}\right)\pi(\boldsymbol{y}|\boldsymbol{\delta},\boldsymbol{\xi})\,\mathrm{d}\boldsymbol{y}\,\pi(\boldsymbol{\delta}|\boldsymbol{\xi})\mathrm{d}\boldsymbol{\delta} \\ &= \int_U \left[\int_Y \log\left(\frac{\pi(\boldsymbol{\delta}|\boldsymbol{y},\boldsymbol{\xi})}{\pi(\boldsymbol{\delta}|\boldsymbol{\xi})}\right)\pi(\boldsymbol{\delta}|\boldsymbol{y},\boldsymbol{\xi})\mathrm{d}\boldsymbol{\delta}\right]\pi(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y}.\end{aligned}$$

Approaches taken in the literature:

- Double-loop Monte Carlo (Beck, Mansour, Espath, Long, Tempone)
- MCLA (Beck, Mansour, Espath, Long, Tempone)
- DLMCIS (Beck, Mansour, Espath, Long, Tempone)

If $\boldsymbol{y} \perp \boldsymbol{\eta}$, then the likelihood is given by

$$\pi(\boldsymbol{\delta}|\boldsymbol{y},\boldsymbol{\xi}) = C\mathrm{e}^{-\frac{1}{2}\|\boldsymbol{\delta}-G(\boldsymbol{y},\boldsymbol{\xi})\|^2_{\Gamma^{-1}}}, \quad C = \frac{1}{(2\pi)^{k/2}\sqrt{\det\Gamma}}.$$

Under these conditions, it is easy to see that

$$\begin{aligned}\mathrm{EIG} &= \int_Y \int_U \log\left(\frac{\pi(\boldsymbol{\delta}|\boldsymbol{y},\boldsymbol{\xi})}{\pi(\boldsymbol{\delta}|\boldsymbol{\xi})}\right)\pi(\boldsymbol{\delta}|\boldsymbol{y},\boldsymbol{\xi})\pi(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y}\,\mathrm{d}\boldsymbol{\delta}\\ &= \log C - 1 - \int_Y \log\left(\int_U C\mathrm{e}^{-\frac{1}{2}\|\boldsymbol{\delta}-G(\boldsymbol{y},\boldsymbol{\xi})\|^2_{\Gamma^{-1}}}\,\mathrm{d}\boldsymbol{y}\right)\int_U C\mathrm{e}^{-\frac{1}{2}\|\boldsymbol{\delta}-G(\boldsymbol{y},\boldsymbol{\xi})\|^2_{\Gamma^{-1}}}\,\mathrm{d}\boldsymbol{y}\,\mathrm{d}\boldsymbol{\delta}.\end{aligned}$$

Observations:

- The **inner integral** can be approximated independently of the dimension s using QMC exactly as before.
- In general, the data dimension k affects the QMC cubature error bound of the **outer integral**.
- How to efficiently approximate the nested integrals?

$$\int_Y \log\left(\int_U C\mathrm{e}^{-\frac{1}{2}\|\boldsymbol{\delta}-G(\boldsymbol{y},\boldsymbol{\xi})\|_{\Gamma^{-1}}^2}\,\mathrm{d}\boldsymbol{y}\right)\int_U C\mathrm{e}^{-\frac{1}{2}\|\boldsymbol{\delta}-G(\boldsymbol{y},\boldsymbol{\xi})\|_{\Gamma^{-1}}^2}\,\mathrm{d}\boldsymbol{y}\,\mathrm{d}\boldsymbol{\delta}$$

QMC weights for the **inner integral**:

$$\gamma_{\mathfrak{u}} = \left((|\mathfrak{u}|!)^{\beta}\prod_{j\in\mathfrak{u}}\frac{\rho_j}{\sqrt{2\zeta(2\lambda)/(2\pi^2)^{\lambda}}}\right)^{\frac{2}{1+\lambda}}, \quad \lambda = \begin{cases}\frac{p}{2-p} & \text{if } p\in(2/3,1),\\ \frac{1}{2-2\delta} & \text{if } p\in(0,2/3],\end{cases}$$

with $\rho_j := \frac{2C_0}{\sqrt{\mu_{\min}}}b_j$, $j\in\{1,\dots,s\}$, and $\delta>0$ arbitrary, yields the QMC convergence rate

$$\mathcal{O}(\varphi(n)^{\max\{-1/p+1/2,-1+\delta\}})$$

independently of the dimension s with $\varphi(n)$ denoting the Euler totient function.

For simplicity, assume that the data is in $Y = [-K, K]$.

$$\int_{[-K,K]^k} \log\left(\int_U C\mathrm{e}^{-\frac{1}{2}\|\boldsymbol{\delta}-G(\boldsymbol{y},\boldsymbol{\xi})\|^2_{\Gamma^{-1}}}\,\mathrm{d}\boldsymbol{y}\right)\int_U C\mathrm{e}^{-\frac{1}{2}\|\boldsymbol{\delta}-G(\boldsymbol{y},\boldsymbol{\xi})\|^2_{\Gamma^{-1}}}\,\mathrm{d}\boldsymbol{y}\,\mathrm{d}\boldsymbol{\delta}$$

QMC weights for the **outer integral**:

$$\widetilde{\gamma}_{\mathfrak{u}} = \left((|\mathfrak{u}|!)^{\beta}\prod_{j\in\mathfrak{u}}\frac{k\mu_{\min}^{-1/2}\mathrm{e}^{\frac{1}{2\sigma^2}(kK^2+2\sqrt{k}KC+C^2)}}{\log(2)\sqrt{2\zeta(2\widetilde{\lambda})/(2\pi^2)^{\widetilde{\lambda}}}}\right)^{\frac{2}{1+\widetilde{\lambda}}}, \quad \widetilde{\lambda} = \frac{1}{2-2\widetilde{\delta}},$$

with $\widetilde{\delta} > 0$ arbitrary, yields the QMC convergence rate

$$\mathcal{O}(\varphi(n)^{-1+\widetilde{\delta}})$$

with $\varphi(n)$ denoting the Euler totient function. Note that the implied coefficient depends on k.

The nested integral

Goal of computation:

$$\mathcal{I}(f) = \int_Y g\bigg(\int_U f(\boldsymbol{y},\boldsymbol{\delta},\boldsymbol{\xi})\,\mathrm{d}\boldsymbol{y}\bigg)\,\mathrm{d}\boldsymbol{\delta},$$

where $g(x) := x\log x$, $Y = [-K,K]^k$, and $f(\boldsymbol{y},\boldsymbol{\delta},\boldsymbol{\xi}) := C\mathrm{e}^{-\frac{1}{2}\|\boldsymbol{\delta}-G(\boldsymbol{y},\boldsymbol{\xi})\|^2_{\Gamma^{-1}}}$.

Define a hierarchy of QMC cubature operators for the **outer integral**, i.e.,

$$I^{(1)}F := \int_Y F(\boldsymbol{\delta})\,\mathrm{d}\boldsymbol{\delta} \approx 2^{-\ell}\sum_{k=1}^{2^\ell} F(\boldsymbol{\delta}_k^{(\ell)}) =: Q_\ell^{(1)}F,\ \ell = \ell_0^{(1)}, \ell_0^{(1)}+1, \ell_0^{(1)}+2, \ldots,$$

for a given function $F \in \widetilde{H}_{k,\widetilde{\gamma}}$, and likewise for the **inner integral**

$$I^{(2)}F := \int_U F(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y} \approx 2^{-\ell}\sum_{k=1}^{2^\ell} F(\boldsymbol{y}_k^{(\ell)}) =: Q_\ell^{(2)}F,\ \ell = \ell_0^{(2)}, \ell_0^{(2)}+1, \ell_0^{(2)}+2, \ldots,$$

for a given function $F \in H_{s,\boldsymbol{\gamma}}$.

Why full tensor product cubature is a bad idea

Approximating the integral

$$\mathcal{I}(f) = \int_Y g\bigg(\int_U f(\boldsymbol{y},\boldsymbol{\delta},\boldsymbol{\xi})\,\mathrm{d}\boldsymbol{y}\bigg)\,\mathrm{d}\boldsymbol{\delta},$$

by

$$\mathcal{I}(f) \approx Q_\ell^{(1)} g(Q_\ell^{(2)} f) \tag{5}$$

is inefficient. A hand-wavy argument would be as follows:

- Suppose that we have the approximation rates (recall $n = 2^\ell$)

$$|I^{(1)}F - Q_\ell^{(1)}F| \asymp n^{-\alpha} \quad \text{and} \quad |I^{(2)}F - Q_\ell^{(2)}F| \asymp n^{-\alpha}.$$

- Evaluating (5) takes $N = n^2$ function calls, but the cubature accuracy will not be better than $\mathcal{O}(n^{-\alpha}) = \mathcal{O}(N^{-\alpha/2})$
  $\rightarrow$ the convergence rate is effectively halved! ("Curse of dimensionality")

Sparse tensor product cubature in the vein of Gilch, Griebel, Oettershagen (2022)

Define the difference cubature operator corresponding to the **outer integral**

$$\Delta_\ell^{(1)} F := \begin{cases} Q_\ell^{(1)} F - Q_{\ell-1}^{(1)} F & \text{if } \ell \geq 1, \\ Q_0^{(1)} F & \text{if } \ell = 0, \end{cases}$$

as well as the generalized difference cubature operators corresponding to the **inner integral**

$$\Delta_\ell^{(2)} F := \begin{cases} g(Q_\ell^{(2)} F) - g(Q_{\ell-1}^{(2)} F) & \text{if } \ell \geq 1, \\ g(Q_0^{(2)} F) & \text{if } \ell = 0. \end{cases}$$

Generalized sparse grid cubature operator:

$$\mathcal{Q}_{L,\varsigma}(f) := \sum_{\varsigma \ell_1 + \frac{\ell_2}{\varsigma} \leq L} \Delta_{\ell_1}^{(1)} \Delta_{\ell_2}^{(2)}(f) = \sum_{\ell_1=0}^{L/\varsigma} \Delta_{\ell_1}^{(1)} g(Q_{\varsigma L - \varsigma^2 \ell_1}^{(2)} f).$$

Sparse tensor product cubature

$$\mathcal{Q}_{L,\varsigma}(f) := \sum_{\varsigma\ell_1 + \frac{\ell_2}{\varsigma} \leq L} \Delta^{(1)}_{\ell_1}\Delta^{(2)}_{\ell_2}(f) = \sum_{\ell_1=0}^{L/\varsigma} \Delta^{(1)}_{\ell_1} g(Q^{(2)}_{\varsigma L - \varsigma^2 \ell_1} f).$$

Sparse grid error: Our **inner** and **outer** QMC cubatures have essentially linear convergence rates, i.e.,

$$|I^{(1)}f - Q^{(1)}_\ell f| \lesssim 2^{-(1-\delta)\ell} \quad \text{and} \quad |I^{(2)}f - Q^{(2)}_\ell f| \lesssim 2^{-(1-\delta)\ell}.$$

For an isotropic ($\varsigma = 1$) sparse tensor product cubature operator, we obtain

$$\|\mathcal{I}(f) - \mathcal{Q}_{L,\varsigma}(f)\|_{\boldsymbol{\Delta}} \lesssim 2^{-(1-\delta)L}(L+1)$$

under some additional technical assumptions.

Numerical experiment

Let $D = (0,1)^2$. We consider the elliptic PDE

$$\begin{cases} -\nabla \cdot (a(\boldsymbol{x},\boldsymbol{y})\nabla u(\boldsymbol{x},\boldsymbol{y})) = 10x_1, & \boldsymbol{x} \in D,\ \boldsymbol{y} \in [-1/2,1/2]^{100}, \\ u(\cdot,\boldsymbol{y})|_{\partial D} = 0, & \boldsymbol{y} \in [-1/2,1/2]^{100}, \end{cases}$$

equipped with the parametric diffusion coefficient

$$a(\boldsymbol{x},\boldsymbol{y}) = 1 + 0.1\sum_{j=1}^{100} j^{-2} y_j \sin(\pi j x_1)\sin(\pi j x_2), \boldsymbol{y} \in [-1/2,1/2]^{100}.$$

Numerical experiment

The goal is to find a design $\boldsymbol{\xi}^*$ from the set

$$\Xi = \{(\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3) \in \Upsilon^3 \mid \boldsymbol{x}_i \neq \boldsymbol{x}_j \text{ for } i \neq j\},$$

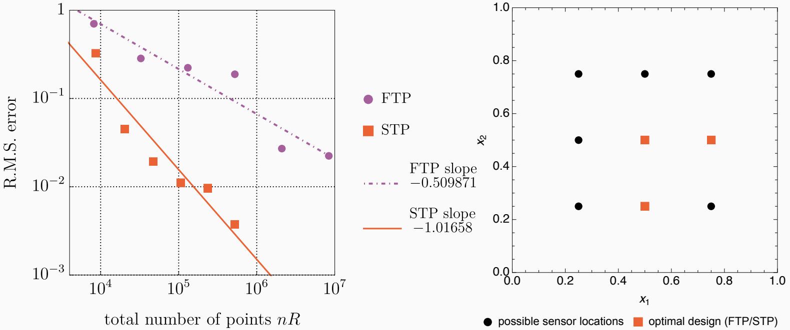
where

$$\begin{aligned}\Upsilon =& \{(0.25, 0.25), (0.25, 0.50), (0.25, 0.75),\\ &(0.50, 0.25), (0.50, 0.50), (0.50, 0.75),\\ &(0.75, 0.25), (0.75, 0.50), (0.75, 0.75)\},\end{aligned}$$

maximizing the expected information gain subject to the observation operator

$$G(\boldsymbol{y}, \boldsymbol{\xi}) = (u(\boldsymbol{x}, \boldsymbol{y}))_{\boldsymbol{x} \in \boldsymbol{\xi}}, \quad \boldsymbol{y} \in [-1/2, 1/2]^{100},\ \boldsymbol{\xi} \in \Xi.$$

Numerical experiment



Left: R.M.S. errors for the full tensor product (FTP) and sparse tensor product (STP) cubatures of the nested integral subject to affine and uniform parameterization of the input random field with $R = 8$ random shifts.
Right: the optimal design corresponding to the cubature rule with the largest number of points.

Conclusions

- Modeling the uncertain inputs 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 the uncertain input than those covered by affine and uniform models.
- This approach could be extended to simultaneous recovery of the domain shape and diffusion coefficient a.
- QMC for DOE: sparse approach can recover almost the optimal rate. Future work: optimizing electrode positions, input current patterns or the measurement geometry for Bayesian inversion?

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Thank you for your attention!