Quasi-Monte Carlo for optimal control and optimal experimental design problems governed by PDEs

Vesa Kaarnioja (FU Berlin)
With special thanks to collaborators: Philipp Guth (RICAM), Tapio Helin (LUT), Frances Kuo (UNSW Sydney), Claudia Schillings (FU Berlin), Ian Sloan (UNSW Sydney), Philipp Wacker (University of Canterbury)

Table of contents

Part I: Quasi-Monte Carlo methods

Part II: Optimal control problems under uncertainty

Part III: Toward Bayesian optimal experimental design

Part I: Quasi-Monte Carlo methods

Lattice rules

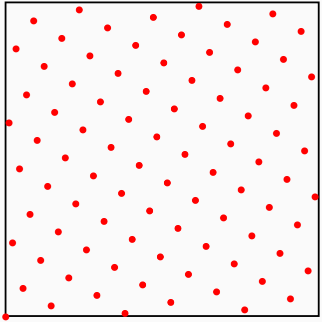
Rank-1 lattice rules

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

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 $\boldsymbol{z}$.

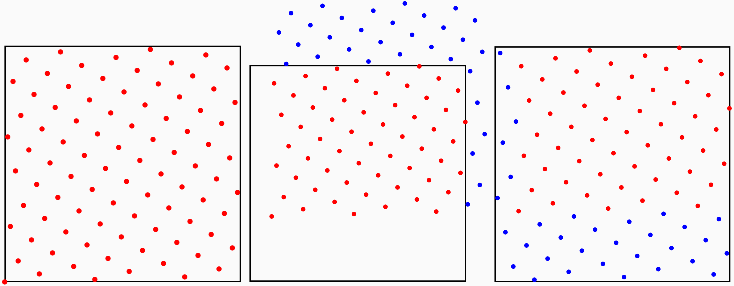
Randomly shifted lattice rules

Shifted rank-1 lattice rules have points

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

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

Use a number of random shifts for error estimation.



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

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

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

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):

$$|I_s(f) - Q^{\boldsymbol{\Delta}}_{s,n}(f)| \le e^{\boldsymbol{\Delta}}_{s,n,\boldsymbol{\gamma}}(\boldsymbol{z}) \|f\|_{\boldsymbol{\gamma}}.$$

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

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

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

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

and (squared) worst case error

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

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 weights have certain structure (e.g., POD weights).

Theorem (CBC error bound)
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*

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

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

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

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: Optimal control problems under uncertainty

Optimal control

- Goal:
  - steer u toward target g

$$\min_u \left(\frac{\alpha_1}{2} \int_0^T \|u(\cdot,t) - g(\cdot,t)\|^2 \, \mathrm{d}t + \frac{\alpha_2}{2} \|u(\cdot,T) - g(\cdot,T)\|^2 \right)$$

  - control u through the source z via the PDE

$$\partial_t u - \nabla \cdot (a \nabla u) = z \quad \text{in } D \times (0,T)$$

- Resulting optimal control problem $\min_z J(z)$, where

$$J(z) = \mathcal{R}\left(\frac{\alpha_1}{2} \int_0^T \|u(\cdot,t) - g(\cdot,t)\|^2 \, \mathrm{d}t + \frac{\alpha_2}{2} \|u(\cdot,T) - g(\cdot,T)\|^2 \right) + \frac{\alpha_3}{2} \int_0^T \|z(\cdot,t)\|^2 \, \mathrm{d}t$$

  subject to

$$\partial_t u - \nabla \cdot (a \nabla u) = z \quad \text{in } D \times (0,T)$$

$$+ \text{ initial-boundary values at } t = 0 \text{ and on } \partial D$$

- How do we handle uncertainty in $a^{\boldsymbol{y}}(\boldsymbol{x})$, parameterized by $\boldsymbol{y} \in U$?
- $\mathcal{R}$ risk measure
  - Robust optimization: $\mathcal{R}(\cdot) = \int_U \cdot \, \mathrm{d}\boldsymbol{y}$ (risk neutral)
  - Entropic risk measure: $\mathcal{R}(\cdot) = \frac{1}{\theta} \ln \left(\int_U \exp(\theta \, \cdot) \, \mathrm{d}\boldsymbol{y} \right)$ (risk averse)

Optimal control problems

[Borzì, Schulz, Schillings, Winckel (2010); Ali, Ullmann, Hinze (2017)]

- **Mean-based control**: replace a by $\int_U a^{\boldsymbol{y}} \, \mathrm{d}\boldsymbol{y}$
- **Pathwise control**: for several $\boldsymbol{y}$, find

$$z^*(\boldsymbol{y}) = \arg\min \left(\frac{\alpha_1}{2} \int_0^T \|u^{\boldsymbol{y}}(\cdot, t) - g(\cdot, t)\|^2 \, \mathrm{d}t + \frac{\alpha_2}{2} \|u^{\boldsymbol{y}}(\cdot, T) - g(\cdot, T)\|^2 \right)$$

$$+ \frac{\alpha_3}{2} \int_0^T \|z(\cdot, t)\|^2 \, \mathrm{d}t$$

  and compute the statistics of $z^*(\boldsymbol{y})$, e.g., $\mathbb{E}[z^*(\cdot)]$
- **Stochastic control**:

$$J(z) = \mathcal{R}\left(\frac{\alpha_1}{2} \int_0^T \|u^{\boldsymbol{y}}(\cdot, t) - g(\cdot, t)\|^2 \, \mathrm{d}t + \frac{\alpha_2}{2} \|u^{\boldsymbol{y}}(\cdot, T) - g(\cdot, T)\|^2 + \frac{\alpha_3}{2} \int_0^T \|z^{\boldsymbol{y}}(\cdot, t)\|^2 \, \mathrm{d}t \right)$$

  [Kouri et al. (2013); Kunoth, Schwab (2013); Ali, Ullmann, Hinze (2017); Chen, Ghattas (2018)]
- **Deterministic control**:

$$J(z) = \mathcal{R}\left(\frac{\alpha_1}{2} \int_0^T \|u^{\boldsymbol{y}}(\cdot, t) - g(\cdot, t)\|^2 \, \mathrm{d}t + \frac{\alpha_2}{2} \|u^{\boldsymbol{y}}(\cdot, T) - g(\cdot, T)\|^2 \right) + \frac{\alpha_3}{2} \int_0^T \|z(\cdot, t)\|^2 \, \mathrm{d}t$$

  • Taylor approximations [Chen, Villa, Ghattas (2019)], Sparse grids [Kouri (2014); Kouri Surowiec (2016)], Multilevel Monte Carlo [Van Barel, Vandewalle (2019)]

Problem formulation

- Optimal control problem $\min_{z\in\mathcal{Z}} J(z)$, where

$$J(z) = \mathcal{R}\left(\frac{\alpha_1}{2}\int_0^T \|u^{\boldsymbol{y}}(\cdot,t)-g(\cdot,t)\|^2\,\mathrm{d}t + \frac{\alpha_2}{2}\|u^{\boldsymbol{y}}(\cdot,T)-g(\cdot,T)\|^2\right) + \frac{\alpha_3}{2}\int_0^T \|z(\cdot,t)\|^2\,\mathrm{d}t$$

subject to

$$\begin{aligned} \partial_t u^{\boldsymbol{y}}(\boldsymbol{x},t) - \nabla\cdot(a^{\boldsymbol{y}}(\boldsymbol{x})\nabla u^{\boldsymbol{y}}(\boldsymbol{x},t)) &= z(\boldsymbol{x},t) && \boldsymbol{x}\in D,\ t\in(0,T),\ \boldsymbol{y}\in U,\\ u^{\boldsymbol{y}}(\boldsymbol{x},t) &= 0 && \boldsymbol{x}\in\partial D,\ t\in(0,T),\ \boldsymbol{y}\in U,\\ u^{\boldsymbol{y}}(\boldsymbol{x},0) &= u_0(\boldsymbol{x}) && \boldsymbol{x}\in D,\ \boldsymbol{y}\in U, \end{aligned}$$

- Look for optimal control z in feasible set $\mathcal{Z}$, where we consider

$$\mathcal{Z} := L^2(D\times(0,T)) \qquad \text{(unconstrained)}$$

$$\mathcal{Z} := \{z\in L^2(D\times(0,T)) \mid z_{\min}(\boldsymbol{x},t)\le z(\boldsymbol{x},t)\le z_{\max}(\boldsymbol{x},t)\ a.e.\} \qquad \text{(constrained)}$$

- "**Uniform**" or "**affine**" model:

$$a^{\boldsymbol{y}}(\boldsymbol{x}) = \bar{a}(\boldsymbol{x}) + \sum_{j=1}^{\infty} y_j\psi_j(\boldsymbol{x}), \quad \boldsymbol{x}\in D,\ \boldsymbol{y}\in U := [-\tfrac{1}{2},\tfrac{1}{2}]^{\mathbb{N}}$$

with assumptions

  - $0 < a_{\min} \le a^{\boldsymbol{y}}(\boldsymbol{x}) \le a_{\max} < \infty$
  - $\sum_{j=1}^{\infty}\|\psi_j\|_{L^\infty}^p < \infty$ for some $p\in(0,1)$
  - $\|\psi_1\|_{L^\infty} \ge \|\psi_2\|_{L^\infty} \ge \cdots$

Reduced formulation (robust optimization)

- Optimal control problem $\min_{z \in \mathcal{Z}} J(z)$, with

$$J(z) = \mathcal{R}\Bigg(\underbrace{\frac{\alpha_1}{2}\int_0^T \|u^{\boldsymbol{y}}(\cdot,t) - g(\cdot,t)\|^2\,\mathrm{d}t + \frac{\alpha_2}{2}\|u^{\boldsymbol{y}}(\cdot,T) - g(\cdot,T)\|^2}_{=:\Phi(\boldsymbol{y})}\Bigg) + \frac{\alpha_3}{2}\int_0^T \|z(\cdot,t)\|^2\,\mathrm{d}t$$

- $u^{\boldsymbol{y}}$ is the "state" corresponding to the control z
- $\mathcal{Z}$ is the feasible set, which is bounded, closed, convex, nonempty
- **Theorem**: *There exists a unique optimal solution* z^*.
- The Fréchet derivative of J is given by

$$J'(z) = \mathcal{R}(q) + \alpha_3 z \qquad \text{(linear risk measure } \mathcal{R}\text{)}$$

$$J'(z) = \frac{1}{\int_U \exp(\theta\Phi(\boldsymbol{y}))\,\mathrm{d}\boldsymbol{y}} \int_U \exp(\theta\Phi(\boldsymbol{y}))q^{\boldsymbol{y}}\,\mathrm{d}\boldsymbol{y} + \alpha_3 z \qquad \text{(entropic risk measure)}$$

where q is the adjoint state.

Theorem: Let $\mathcal{R}$ be the expected value or the entropic risk measure. A control $z = z^*$ is the unique minimizer of the problem if and only if it satisfies the KKT system

$$\begin{cases} \partial_t u^{\boldsymbol{y}}(\boldsymbol{x},t) - \nabla\cdot(a^{\boldsymbol{y}}(\boldsymbol{x})\nabla u^{\boldsymbol{y}}(\boldsymbol{x},t)) = z(\boldsymbol{x}) & \boldsymbol{x}\in D,\ t\in(0,T), \\ u^{\boldsymbol{y}}(\boldsymbol{x},t) = 0 & \boldsymbol{x}\in\partial D,\ t\in(0,T), \\ u^{\boldsymbol{y}}(\boldsymbol{x},0) = u_0(\boldsymbol{x}) & \boldsymbol{x}\in D, \\ -\partial_t q^{\boldsymbol{y}}(\boldsymbol{x},t) - \nabla\cdot(a^{\boldsymbol{y}}(\boldsymbol{x})\nabla q^{\boldsymbol{y}}(\boldsymbol{x},t)) & \\ \qquad\qquad = \alpha_1(u^{\boldsymbol{y}}(\boldsymbol{x},t) - g(\boldsymbol{x},t)) & \boldsymbol{x}\in D,\ t\in(0,T), \\ q^{\boldsymbol{y}}(\boldsymbol{x},t) = 0 & \boldsymbol{x}\in\partial D,\ t\in(0,T), \\ q^{\boldsymbol{y}}(\boldsymbol{x},T) = \alpha_2(u^{\boldsymbol{y}}(\boldsymbol{x},T) - g(\boldsymbol{x},T)) & \boldsymbol{x}\in D, \\ J'(z^*) - \mu_a + \mu_b = 0 & \boldsymbol{x}\in D,\ t\in(0,T), \\ z_{\min}(\boldsymbol{x},t) \le z(\boldsymbol{x},t) \le z_{\max}(\boldsymbol{x},t) & \boldsymbol{x}\in D,\ t\in(0,T) \\ \mu_a(\boldsymbol{x},t)\ge 0,\ \mu_b(\boldsymbol{x},t)\ge 0 & \boldsymbol{x}\in D,\ t\in(0,T) \\ (z(\boldsymbol{x},t) - z_{\min}(\boldsymbol{x},t))\mu_a(\boldsymbol{x},t) & \\ \qquad\qquad = (z_{\max}(\boldsymbol{x},t) - z(\boldsymbol{x},t))\mu_b(\boldsymbol{x},t) = 0 & \boldsymbol{x}\in D,\ t\in(0,T), \end{cases}$$

for all $\boldsymbol{y}\in U$. Can be solved, e.g., using projected gradient descent.

Discretization of the problem (robust risk measure $\mathcal{R} = \int_U \cdot \, \mathrm{d}\boldsymbol{y}$)

- Optimal control problem:

$$J(z) = \int_U \left(\frac{\alpha_1}{2} \int_0^T \|u^{\boldsymbol{y}}(\cdot,t) - g(\cdot,t)\|^2 \, \mathrm{d}t + \frac{\alpha_2}{2} \|u^{\boldsymbol{y}}(\cdot,T) - g(\cdot,T)\|^2 \right) \mathrm{d}\boldsymbol{y} + \frac{\alpha_3}{2} \int_0^T \|z(\cdot,t)\|^2 \, \mathrm{d}t$$

$$J'(z) = \int_U q^{\boldsymbol{y}} \, \mathrm{d}\boldsymbol{y} + \alpha_3 z$$

- Discretized problem:
  - Dimension truncation to s terms
  - Quasi-Monte Carlo quadrature with n points

$$J_{s,n}(z) = \frac{1}{n} \sum_{i=1}^{n} \left(\frac{\alpha_1}{2} \int_0^T \|u_s^{\boldsymbol{y}^{(i)}}(\cdot,t) - g(\cdot,t)\|^2 \, \mathrm{d}t + \frac{\alpha_2}{2} \|u_s^{\boldsymbol{y}^{(i)}}(\cdot,T) - g(\cdot,T)\|^2 \right) + \frac{\alpha_3}{2} \int_0^T \|z(\cdot,t)\|^2 \, \mathrm{d}t$$

$$J'_{s,n}(z) = \frac{1}{n} \sum_{i=1}^{n} q_s^{\boldsymbol{y}^{(i)}} + \alpha_3 z$$

  - Positive (equal) weights of QMC preserve convexity of the problem

Discretization of the problem (entropic risk measure)

- Optimal control problem:

$$J(z) = \frac{1}{\theta} \ln \left(\int_U \exp(\theta \Phi(\boldsymbol{y})) q^{\boldsymbol{y}} \, \mathrm{d}\boldsymbol{y} \right) + \frac{\alpha_3}{2} \int_0^T \|z(\cdot,t)\|^2 \, \mathrm{d}t$$

$$J'(z) = \frac{\int_U \exp(\theta \Phi(\boldsymbol{y})) q^{\boldsymbol{y}} \, \mathrm{d}\boldsymbol{y}}{\int_U \exp(\theta \Phi(\boldsymbol{y})) \, \mathrm{d}\boldsymbol{y}} + \alpha_3 z$$

$$\Phi(\boldsymbol{y}) = \frac{\alpha_1}{2} \int_0^T \|u^{\boldsymbol{y}}(\cdot,t) - g(\cdot,t)\|^2 \, \mathrm{d}t + \frac{\alpha_2}{2} \|u^{\boldsymbol{y}}(\cdot,T) - g(\cdot,T)\|^2$$

- Discretized problem:
  - Dimension truncation to s terms
  - Quasi-Monte Carlo quadrature with n points

$$J_{s,n}(z) = \frac{1}{\theta} \ln \left(\frac{1}{n} \sum_{i=1}^{n} \exp(\theta \Phi_s(\boldsymbol{y}^{(i)})) {q_s}^{\boldsymbol{y}^{(i)}} \right) + \frac{\alpha_3}{2} \int_0^T \|z(\cdot,t)\|^2 \, \mathrm{d}t$$

$$J'_{s,n}(z) = \frac{\sum_{i=1}^{n} \exp(\theta \Phi_s(\boldsymbol{y}^{(i)}) {q_s}^{\boldsymbol{y}^{(i)}})}{\sum_{i=1}^{n} \exp(\theta \Phi_s(\boldsymbol{y}^{(i)}))} + \alpha_3 z$$

Error analysis

- **Theorem (robust risk measure)** A randomly shifted lattice rule can be constructed using the fast CBC algorithm using POD weights such that

$$\sqrt{\mathbb{E}_{\boldsymbol{\Delta}}\|z^* - z^*_{s,n}\|^2_{L^2(D\times(0,T))}} = \mathcal{O}(s^{-2/p+1} + n^{-\min\{1/p-1/2,1-\delta\}}),$$

where the implied coefficient is independent of s.

- **Theorem (entropic risk measure)** A randomly shifted lattice rule can be constructed using the fast CBC algorithm using POD weights such that

$$\sqrt{\mathbb{E}_{\boldsymbol{\Delta}}\|z^* - z^*_{s,n}\|^2_{L^2(D\times(0,T))}} = \mathcal{O}(s^{-2/p+1} + n^{-\min\{1/p-1/2,1-\delta\}}),$$

where the implied coefficient is independent of s.

Numerical experiments

Consider the coupled PDE system

$$\begin{cases} \partial_t u^{\boldsymbol{y}}(\boldsymbol{x},t) - \nabla\cdot(a^{\boldsymbol{y}}(\boldsymbol{x})\nabla u^{\boldsymbol{y}}(\boldsymbol{x},t)) = z(\boldsymbol{x}) & \boldsymbol{x}\in D\,, t\in(0,T)\,, \\ u^{\boldsymbol{y}}(\boldsymbol{x},t) = 0 & \boldsymbol{x}\in\partial D\,, t\in(0,T)\,, \\ u^{\boldsymbol{y}}(\boldsymbol{x},0) = u_0(\boldsymbol{x}) & \boldsymbol{x}\in D\,, \\ -\partial_t q^{\boldsymbol{y}}(\boldsymbol{x},t) - \nabla\cdot(a^{\boldsymbol{y}}(\boldsymbol{x})\nabla q^{\boldsymbol{y}}(\boldsymbol{x},t)) & \\ \qquad\qquad = \alpha_1(u^{\boldsymbol{y}}(\boldsymbol{x},t) - g(\boldsymbol{x})) & \boldsymbol{x}\in D\,, t\in(0,T), \\ q^{\boldsymbol{y}}(\boldsymbol{x},t) = 0 & \boldsymbol{x}\in\partial D\,, t\in(0,T) \\ q^{\boldsymbol{y}}(\boldsymbol{x},T) = \alpha_2(u^{\boldsymbol{y}}(\boldsymbol{x},T) - g(\boldsymbol{x})) & \boldsymbol{x}\in D\,, t\in(0,T), \end{cases}$$

for $\boldsymbol{y}\in[-\frac{1}{2},\frac{1}{2}]^s$ in $D=(0,1)^2$, equipped with

$$a(\boldsymbol{x},\boldsymbol{y}) = 1 + c\sum_{j=1}^{\infty} y_j \underbrace{\frac{1}{(k_j^2+\ell_j^2)^{\vartheta}}\sin(k_j\pi x_1)\sin(\ell_j\pi x_2)}_{=\psi_j}\,,$$

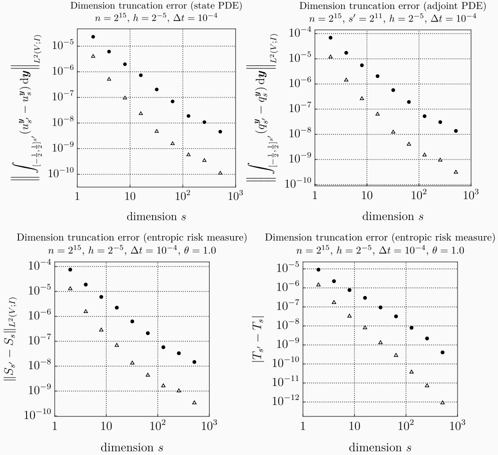
where $(k_j,\ell_j)_{j\geq 1}$ are ordered s.t. $(\|\psi_j\|_{L^\infty(D)})_{j\geq 1}$ is non-increasing.

Weyl asymptotics: $\|\psi_j\|_{L^\infty(D)}\sim j^{-\vartheta}$ as $j\to\infty$. We fix $z(\boldsymbol{x}) = x_2$.

Numerical experiments

Dimension truncation error

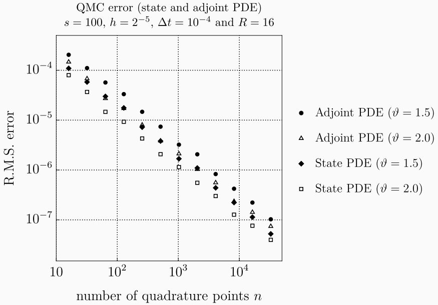
We use $s = 2^{11}$ as the reference solution.

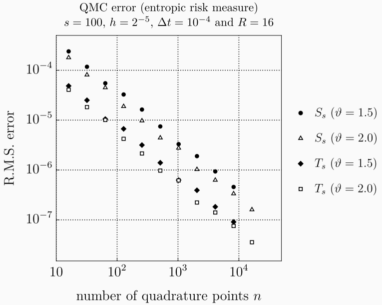


Numerical experiments

QMC error

We use $R = 16$ random shifts $\boldsymbol{\Delta}$ drawn from $U([0,1]^s)$.





LHS: QMC errors corresponding to $\int_{[-\frac{1}{2},\frac{1}{2}]^{100}} u^{\boldsymbol{y}}\,\mathrm{d}\boldsymbol{y}$ (state PDE) and $\int_{[-\frac{1}{2},\frac{1}{2}]^{100}} q^{\boldsymbol{y}}\,\mathrm{d}\boldsymbol{y}$ (adjoint PDE).

RHS: QMC errors corresponding to $S_{100} = \int_{[-\frac{1}{2},\frac{1}{2}]^{100}} \exp(\Phi_s(\boldsymbol{y}))q^{\boldsymbol{y}}\,\mathrm{d}\boldsymbol{y}$ and $T_{100} = \int_{[-\frac{1}{2},\frac{1}{2}]^{100}} \exp(\Phi_s(\boldsymbol{y}))\,\mathrm{d}\boldsymbol{y}$

Numerical experiments

Optimal control problem – unconstrained gradient descent $\min_{z\in L^2(D\times(0,T))} J(z)$,

$$J(z,u)=\mathcal{R}_{\boldsymbol{y}}\left(\frac{\alpha_1}{2}\int_0^T\|u^{\boldsymbol{y}}(\cdot,t)-g\|^2_{L^2(D\times(0,T))}\,\mathrm{d}t+\frac{\alpha_2}{2}\|u^{\boldsymbol{y}}(\cdot,T)-g(\cdot,T)\|^2_{L^2(D)}\right)+\frac{\alpha_3}{2}\|z\|^2_{L^2(D\times(0,T))}$$

We fix $\vartheta=1.2$, $h=2^{-4}$, $\Delta t=10^{-2}$, $n=2^{10}$, $s=100$, $T=1.0$, $u_0(\boldsymbol{x})=\sin(2\pi x_1)\sin(2\pi x_2)$, $\alpha_1=1$, $\alpha_2=\alpha_3=10^{-4}$, and $\theta=10^5$. As the diffusion coefficient, we take

$$a(\boldsymbol{x},\boldsymbol{y})=100+55\sum_{j=1}^{100}y_j j^{-1.2}\sin(j\pi x_1)\sin(j\pi x_2).$$

As the target, we choose

$$g(\boldsymbol{x},t):=\chi_{\|\boldsymbol{x}-(c_1(t),c_2(t))\|_\infty\le\frac{1}{10}}(\boldsymbol{x})g_1(\boldsymbol{x},t)+\chi_{\|\boldsymbol{x}+(c_1(t),c_2(t))-(1,1)\|_\infty\le\frac{1}{10}}(\boldsymbol{x})g_2(\boldsymbol{x},t),$$

where $g_1(\boldsymbol{x},t):=(4\sqrt{10})^4(x_1-c_1(t)-\frac{1}{10})(x_2-c_2(t)-\frac{1}{10})(x_1-c_1(t)+\frac{1}{10})(x_2-c_2(t)+\frac{1}{10})$,
$g_2(\boldsymbol{x},t):=(4\sqrt{10})^4(x_1+c_1(t)-\frac{11}{10})(x_2+c_2(t)-\frac{11}{10})(x_1+c_1(t)-\frac{9}{10})(x_2+c_2(t)-\frac{9}{10})$,
$c_1(t):=\frac{1}{2}+\frac{1}{4}(1-t^{10})\cos(4\pi t^2)$, and $c_2(t):=\frac{1}{2}+\frac{1}{4}(1-t^{10})\sin(4\pi t^2)$.

Unconstrained optimization

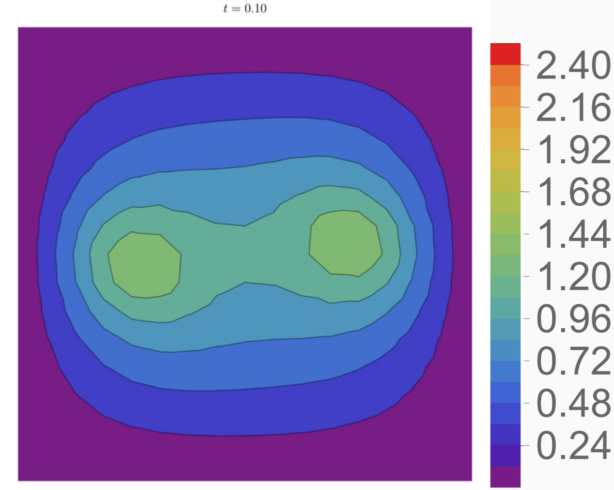


Figure 3: The reconstructed optimal control z^* (without box constraints).

Reference

P. A. Guth, K., F. Y. Kuo, C. Schillings, I. H. Sloan. Parabolic PDE-constrained optimal control under uncertainty with entropic risk measure using quasi-Monte Carlo integration. Preprint 2022, arXiv:2208.02767 [math.NA].

Part III: Toward Bayesian optimal experimental design

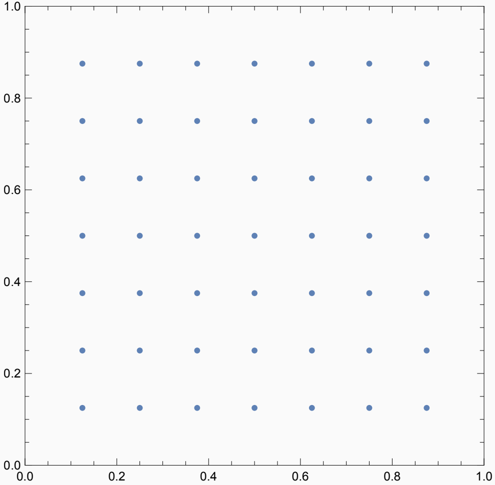
Let $G\colon \Theta \times \Xi \to \mathbb{R}^k$ be a forward mapping depending on a true parameter $\boldsymbol{\theta} \in \Theta$ and a design parameter $\boldsymbol{\xi} \in \Xi$.

Measurement model:

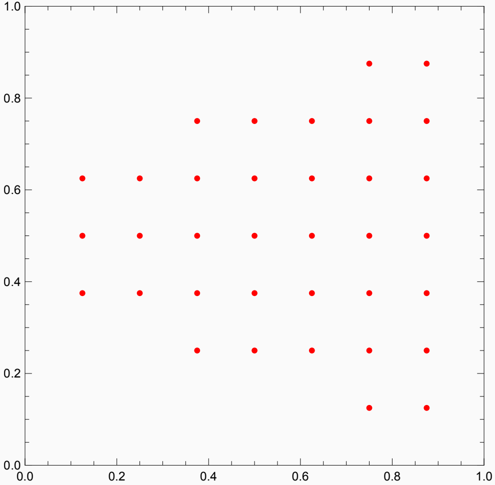
$$\boldsymbol{y} = G(\boldsymbol{\theta}, \boldsymbol{\xi}) + \boldsymbol{\eta},$$

where $\boldsymbol{y} \in \mathbb{R}^k$ 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 $\boldsymbol{\theta}$, which we model as a random variable endowed with prior distribution $\pi(\boldsymbol{\theta})$.



1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0


1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0

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

$$D_{\mathrm{KL}}(\pi(\cdot|\boldsymbol{y},\boldsymbol{\xi})\|\pi(\cdot)) := \int_{\Theta} \log\left(\frac{\pi(\boldsymbol{\theta}|\boldsymbol{y},\boldsymbol{\xi})}{\pi(\boldsymbol{\theta})}\right)\pi(\boldsymbol{\theta}|\boldsymbol{y},\boldsymbol{\xi})\,\mathrm{d}\boldsymbol{\theta}. \tag{2}$$

A Bayesian optimal design $\boldsymbol{\xi}^*$ maximizing the expected utility (2) over the design space Ξ with respect to the data $\boldsymbol{y}$ and model parameters $\boldsymbol{\theta}$ is given by

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

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

The posterior is given by Bayes' theorem

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

which means that the expected utility can be written as

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

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)

Why QMC might work

Assume, e.g., the following:

- The forward model $\boldsymbol{y} = G(\boldsymbol{\theta}, \boldsymbol{\xi}) + \boldsymbol{\eta}$ satisfies

$$|\partial_{\boldsymbol{\theta}}^{\boldsymbol{\nu}} G_j(\boldsymbol{\theta}, \boldsymbol{\xi})| \leq C_0 |\boldsymbol{\nu}|! \boldsymbol{b}^{\boldsymbol{\nu}}, \quad j \in \{1, \dots, k\},$$

  where $\boldsymbol{b} := (b_j)_{j \geq 1} \in \ell^p$ for some $p \in (0,1)$ and $C_0 > 0$ is independent of $\boldsymbol{\xi}$.
- $\Theta = [-\frac{1}{2}, \frac{1}{2}]^s$ and $\pi(\boldsymbol{\theta}) = 1$ for $\boldsymbol{\theta} \in \Theta$ and 0 otherwise.
- We have the likelihood

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

Under these conditions, it is easy to see that

$$\mathrm{EIG} = \int_Y \int_\Theta \log\left(\frac{\pi(\boldsymbol{y}|\boldsymbol{\theta}, \boldsymbol{\xi})}{\pi(\boldsymbol{y}|\boldsymbol{\xi})}\right) \pi(\boldsymbol{y}|\boldsymbol{\theta}, \boldsymbol{\xi}) \pi(\boldsymbol{\theta}) \, \mathrm{d}\boldsymbol{\theta} \, \mathrm{d}\boldsymbol{y}$$

$$= \log C - 1 - \int_Y \log\left(\int_\Theta C \mathrm{e}^{-\frac{1}{2}\|\boldsymbol{y} - G(\boldsymbol{\theta}, \boldsymbol{\xi})\|_{\Gamma^{-1}}^2} \, \mathrm{d}\boldsymbol{\theta}\right) \int_\Theta C \mathrm{e}^{-\frac{1}{2}\|\boldsymbol{y} - G(\boldsymbol{\theta}, \boldsymbol{\xi})\|_{\Gamma^{-1}}^2} \, \mathrm{d}\boldsymbol{\theta} \, \mathrm{d}\boldsymbol{y}.$$

Consider

$$\int_Y \log\left(\int_\Theta C\mathrm{e}^{-\frac{1}{2}\|\boldsymbol{y}-G(\boldsymbol{\theta},\boldsymbol{\xi})\|^2_{\Gamma^{-1}}}\,\mathrm{d}\boldsymbol{\theta}\right)\int_\Theta C\mathrm{e}^{-\frac{1}{2}\|\boldsymbol{y}-G(\boldsymbol{\theta},\boldsymbol{\xi})\|^2_{\Gamma^{-1}}}\,\mathrm{d}\boldsymbol{\theta}\,\mathrm{d}\boldsymbol{y} \tag{3}$$

Observations:

- Parametric regularity of the integrand

$$\int_\Theta C\mathrm{e}^{-\frac{1}{2}\|\boldsymbol{y}-G(\boldsymbol{\theta},\boldsymbol{\xi})\|^2_{\Gamma^{-1}}}\,\mathrm{d}\boldsymbol{\theta}$$

  well-understood (as long as the parametric regularity of G can be quantified); straightforward modification of Herrmann–Keller–Schwab (2021).
- If we replace $\int_\Theta C\mathrm{e}^{-\frac{1}{2}\|\boldsymbol{y}-G(\boldsymbol{\theta},\boldsymbol{\xi})\|^2_{\Gamma^{-1}}}\,\mathrm{d}\boldsymbol{\theta}$ by a QMC approximation

$$\int_\Theta C\mathrm{e}^{-\frac{1}{2}\|\boldsymbol{y}-G(\boldsymbol{\theta},\boldsymbol{\xi})\|^2_{\Gamma^{-1}}}\,\mathrm{d}\boldsymbol{\theta} \approx \frac{C}{n}\sum_{i=1}^n \mathrm{e}^{-\frac{1}{2}\|\boldsymbol{y}-G(\boldsymbol{\theta}_i,\boldsymbol{\xi})\|^2_{\Gamma^{-1}}}$$

  then (3) can be approximated by

$$\int_Y \log\left(\frac{C}{n}\sum_{i=1}^n \mathrm{e}^{-\frac{1}{2}\|\boldsymbol{y}-G(\boldsymbol{\theta}_i,\boldsymbol{\xi})\|^2_{\Gamma^{-1}}}\right)\frac{C}{n}\sum_{i=1}^n \mathrm{e}^{-\frac{1}{2}\|\boldsymbol{y}-G(\boldsymbol{\theta}_i,\boldsymbol{\xi})\|^2_{\Gamma^{-1}}}\,\mathrm{d}\boldsymbol{y}.$$

Lemma
Under the previous conditions, we have the a priori *bound for the higher-order derivatives*

$$\partial_{\boldsymbol{y}}^{\boldsymbol{\nu}} \log\left(C\frac{1}{n}\sum_{j=1}^{n} \mathrm{e}^{-\frac{1}{2}\|\boldsymbol{y}-G(\boldsymbol{\theta}_j,\boldsymbol{\xi})\|_{\Gamma^{-1}}^2}\right)$$
$$\leq 1.1^{k|\boldsymbol{\nu}|}k^{|\boldsymbol{\nu}|}\mu_{\min}^{-|\boldsymbol{\nu}|/2}\sum_{\lambda=1}^{|\boldsymbol{\nu}|}(\lambda-1)!\left(\sum_{j=1}^{n} \mathrm{e}^{-\frac{1}{2}\|\boldsymbol{y}-G(\boldsymbol{\theta}_j,\boldsymbol{\xi})\|_{\Gamma^{-1}}^2}\right)^{-\lambda} S(|\boldsymbol{\nu}|,\lambda)$$

for all $\boldsymbol{y} \in \mathbb{R}^k =: Y$ *and* $\boldsymbol{\nu} \in \mathbb{N}_0^k$*. Here* $\mu_{\min}$ *is a lower bound for the largest eigenvalue of* Γ *and* $S(n,k)$ *denotes the* Stirling number of the second kind*.*

Numerical example

Let $D = (0,1)^2$ and consider the parametric PDE

$$\begin{cases} -\nabla \cdot (a(\boldsymbol{x},\boldsymbol{\theta})\nabla u(\boldsymbol{x},\boldsymbol{\theta})) = x_1, & \boldsymbol{x} \in D,\ \boldsymbol{\theta} \in \Theta, \\ u(\boldsymbol{x},\boldsymbol{\theta}) = 0, & \boldsymbol{x} \in \partial D,\ \boldsymbol{\theta} \in \Theta \end{cases}$$

equipped with an uncertain diffusion coefficient

$$a(\boldsymbol{x},\boldsymbol{\theta}) = 1 + \sum_{j=1}^{s} j^{-2}\theta_j \sin(j\pi x_1)\sin(j\pi x_2), \quad \boldsymbol{x} \in D,\ \boldsymbol{\theta} \in \Theta.$$

Experiment 1: QMC convergence of the inner integral

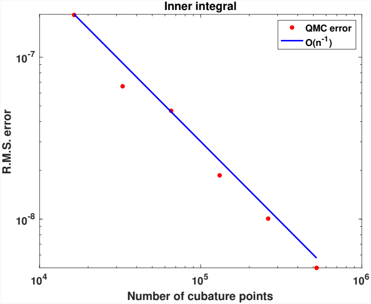
First we consider the QMC convergence of the "inner integral"

$$\int_{\Theta} C e^{-\frac{1}{2}\|\boldsymbol{y}-G(\boldsymbol{\theta},\boldsymbol{\xi})\|^2_{\Gamma^{-1}}}\,\mathrm{d}\boldsymbol{\theta}.$$

Set $\boldsymbol{\xi} := \left(\frac{5}{8}, \frac{7}{8}\right)$, $\Gamma := 0.2^2 I$, and with $k = 1$ consider

$$G(\boldsymbol{\xi},\boldsymbol{\theta}) = u(\boldsymbol{\xi},\boldsymbol{\theta}).$$

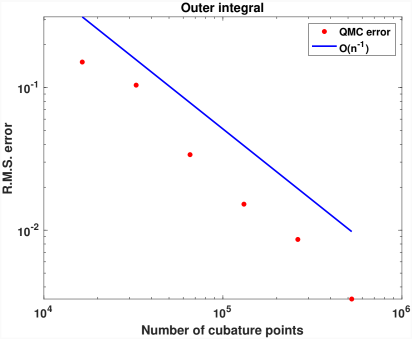
Finally, we use $\boldsymbol{y} = y = 0.396586$, and $s = 100$. We use an off-the-shelf cubature rule to compute QMC approximations of this integral.



Experiment 2: QMC convergence of the outer integral

$$\int_Y \log\left(\frac{C}{n}\sum_{i=1}^{n} \mathrm{e}^{-\frac{1}{2}\|\boldsymbol{y}-G(\boldsymbol{\theta}_i,\boldsymbol{\xi})\|^2_{\Gamma^{-1}}}\right)\frac{C}{n}\sum_{i=1}^{n} \mathrm{e}^{-\frac{1}{2}\|\boldsymbol{y}-G(\boldsymbol{\theta}_i,\boldsymbol{\xi})\|^2_{\Gamma^{-1}}}\,\mathrm{d}\boldsymbol{y}.$$

Fix QMC discretization of the inner integral ($n = 32$). Also, take $Y = [-1/2, 1/2]^{10}$ and fix design ξ s.t. the observation operator corresponds to $k = 10$ point evaluations within the computational domain.



- Use Laplace approximation for the integral over the data?
- In addition to discrete optimal design problems, continuous design problems? Consider the input current as a (continuous) design variable for EIT?