# Quasi-Monte Carlo methods for optimal control problems subject to parabolic PDE constraints under uncertainty

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# Part I: Quasi-Monte Carlo methods

# High-dimensional numerical integration

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

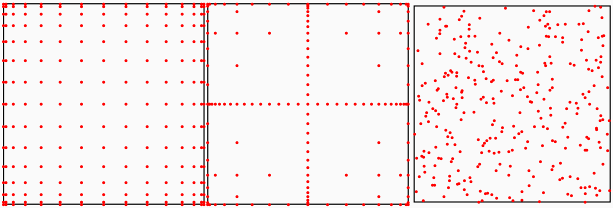


**Figure 1:** Tensor product grid, sparse grid, Monte Carlo nodes (not QMC rules)

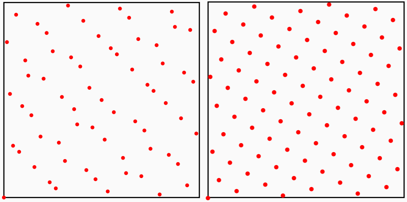


**Figure 2:** Sobol′ points, lattice rule (examples of QMC rules)

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

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

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

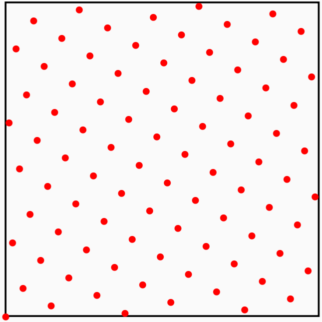
*Rank-1 lattice rules*

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

have the points

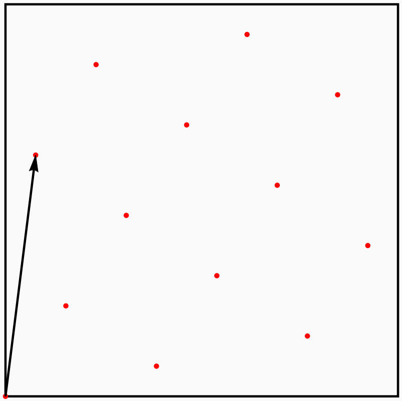
$$\boldsymbol{t}_i = \mathrm{mod}\left(\frac{i\boldsymbol{z}}{n}, 1\right), \quad i \in \{1, \ldots, n\},$$

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 $\boldsymbol{z}$.*



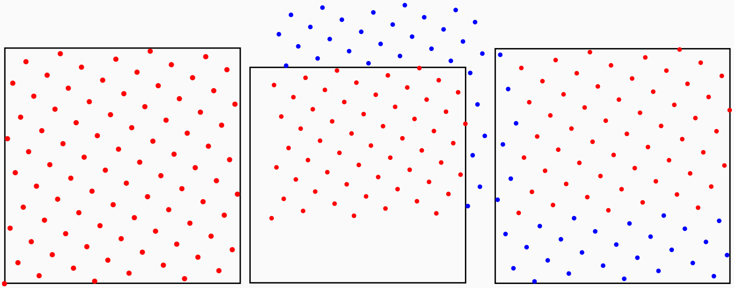
# Randomly shifted lattice rules

Shifted rank-1 lattice rules have points

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

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

*Use a number of random shifts for error estimation.*



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

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

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

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):

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

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

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

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

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

and (squared) worst case error

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

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 $z_1 = 1$ (this is a freebie since $P(1) = P(z)$ for all $z \in \mathbb{N}$);
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 $P(z_1, z_2, z_3)$

   $\vdots$

Notes:

- The CBC algorithm is a *greedy algorithm*: in general, it will not find the generating vector $\boldsymbol{z}$ that minimizes $P(\boldsymbol{z})$. However, it can be shown that the generating vector obtained by the CBC algorithm satisfies an error bound (more on this later).
- For generic $\boldsymbol{\gamma} = (\gamma_{\mathfrak{u}})_{\mathfrak{u} \subseteq \{1:s\}}$, evaluating $P(\boldsymbol{z}) = P(\boldsymbol{\gamma}, \boldsymbol{z})$ takes $\mathcal{O}(2^s)$ operations. For an efficient implementation, it is desirable that the weights $\boldsymbol{\gamma}$ can be characterized by an expression that does not contain too many degrees of freedom.

# CBC with POD weights

Suppose that we have QMC weights in *product and order dependent* (POD) form

$$\gamma_{\mathfrak{u}} := \Gamma_{|\mathfrak{u}|} \prod_{j \in \mathfrak{u}} \gamma_j, \quad \varnothing \neq \mathfrak{u} \subseteq \{1:s\},$$

for some positive scalars $(\Gamma_k)_{k \geq 1}$ and $(\gamma_j)_{j=1}^s$.

In this case, it turns out that the error criterion

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

can be written in the dimensionally recursive form

$$P(z_1, \ldots, z_s) = P(z_1, \ldots, z_{s-1}) + \frac{1}{n} \sum_{k=0}^{n-1} \sum_{\ell=1}^{s} p_{s,\ell}(k),$$

where $p_{s,\ell}(k) = p_{s-1,\ell}(k) + \frac{\Gamma_\ell}{\Gamma_{\ell-1}} \gamma_s \omega\left(\left\{\frac{kz_s}{n}\right\}\right) p_{s-1,\ell-1}(k)$ together with $p_{s,0}(k) = 1$ for all $k$.

For simplicity, let $n$ be prime. We note that the CBC algorithm can be implemented using the recurrence on the previous page, i.e.,

$$P(z_1,\ldots,z_d)=P(z_1,\ldots,z_{d-1})+\frac{1}{n}\sum_{k=0}^{n-1}\sum_{\ell=1}^{d}p_{d,\ell}(k),$$

where $p_{d,\ell}(k)=p_{d-1,\ell}(k)+\frac{\Gamma_\ell}{\Gamma_{\ell-1}}\gamma_d\omega\big(\big\{\frac{kz_d}{n}\big\}\big)p_{d-1,\ell-1}(k)$ together with $p_{d,0}(k)=1$ for all $k$, as follows:

1. Define the matrix $\Omega_n=\big[\omega\big(\big\{\frac{kz}{n}\big\}\big)\big]_{\substack{z\in\{1,\ldots,n-1\}\\ k\in\{0,\ldots,n-1\}}}$ and initialize vectors $\boldsymbol{p}_{0,\ell}=1_n$ for $\ell=1,\ldots,s$.

**for** $d=1,\ldots,s$**, do**

2. Pick the value of $z_d\in\{1,\ldots,n-1\}$ corresponding to the smallest entry in the matrix-vector product

$$\Omega_n\boldsymbol{x},\quad\text{with}\quad \boldsymbol{x}:=\sum_{\ell=1}^{d}\frac{\Gamma_\ell}{\Gamma_{\ell-1}}\gamma_d\boldsymbol{p}_{d-1,\ell-1}.$$

3. Update $\boldsymbol{p}_{d,\ell}:=\boldsymbol{p}_{d-1,\ell}+\Omega_n(z_d).*\left(\frac{\Gamma_\ell}{\Gamma_{\ell-1}}\gamma_d\boldsymbol{p}_{d-1,\ell-1}\right)$.

**end for**

# What makes fast CBC fast?

Note that the matrix-vector product $\Omega_n \boldsymbol{x}$ in the CBC loop costs $\mathcal{O}(n^2)$ operations. However, it was shown by Kuo, Nuyens, and Cools (2006) that the blocks of $\Omega_n$ can be permuted into circulant form $\rightarrow$ the matrix-vector product can be implemented in $\mathcal{O}(n \log n)$ operations using FFT.

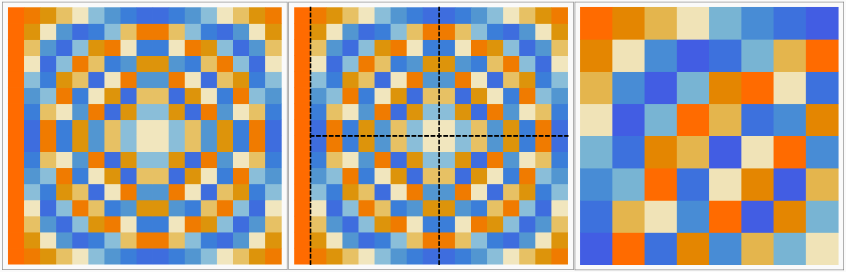


**Figure 3:** Example with $\Omega_{17}$. Note that the first column is a constant and can be left out (the components of $\Omega_n \boldsymbol{x}$ are shifted by a constant $\rightarrow$ the smallest component stays invariant). Noting the obvious symmetries in the remaining four blocks, we can focus on the top left block.

When $n$ is prime, it is possible to use the so-called Rader transformation to permute the block matrices into circulant form. (The permutation matrices can be easily generated by computing the "generator", i.e., primitive root modulo $n$.)

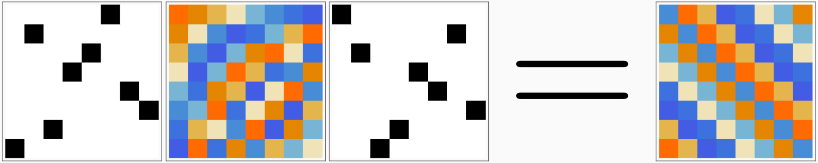


**Figure 4:** The original block matrix is multiplied from both sides by Rader permutation matrices (the black elements indicate the value 1 and white elements indicate the value 0) to obtain a circulant matrix.

# Example with $n = 1009$

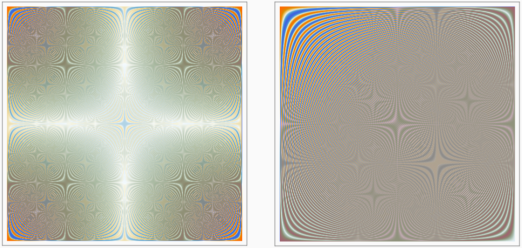


**Figure 5:** LHS: Original $\Omega_{1009}$. RHS: top left block of $\Omega_{1009}$ (sans first column).

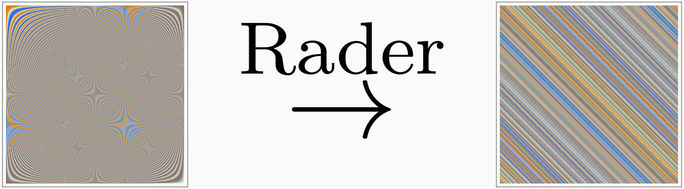



**Figure 6:** Rader transformation turns the top left block matrix circulant.

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.
- CBC works for any (composite) number $n \geq 2$, but the implementation is more involved when $n$ is not prime.

Application of QMC theory:

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

- Estimate the norm (critical step)
- Choose the weights
- Weights as input to the CBC construction

# Part II: Optimal control problems subject to parabolic PDE constraints 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

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

- Suppose $a^{\boldsymbol{y}}$ *uncertain*, $\boldsymbol{y}$ random parameter. Optimal control problem $\min_z J(z)$,

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

subject to

$$\partial_t u - \nabla \cdot (a^{\boldsymbol{y}} \nabla u) = z \quad \text{in } D \times (0, T)$$
$$+ \text{ initial-boundary values at } t = 0 \text{ and on } \partial D$$

- How do we handle uncertainty in $a^{\boldsymbol{y}}(\boldsymbol{x})$, parameterized by $\boldsymbol{y} \in U$?
- $\mathcal{R}$ risk measure
  - Expected value risk measure: $\mathcal{R}(\cdot) = \int_U \cdot \,\mathrm{d}\boldsymbol{y}$ (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

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

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

- $u^{\boldsymbol{y}}$ 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

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

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

# Discretization of the problem (expected value 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 (expected value risk measure)** A randomly shifted lattice rule can be constructed using the fast CBC algorithm using POD weights such that

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

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

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

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

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

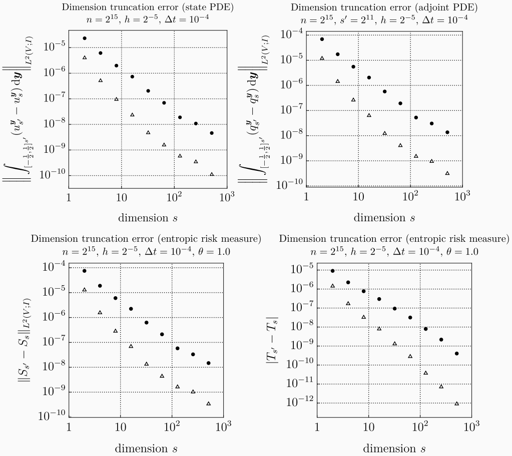
where $(k_j,\ell_j)_{j\geq 1}$ are ordered s.t. $(\|\psi_j\|_{L^\infty(D)})_{j\geq 1}$ is non-increasing.

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

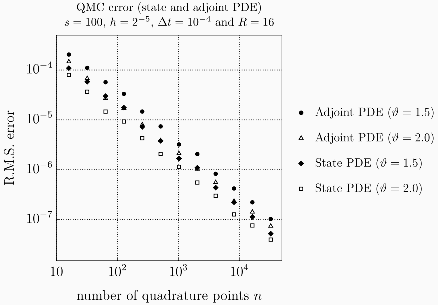
We use $s = 2^{11}$ as the reference solution.

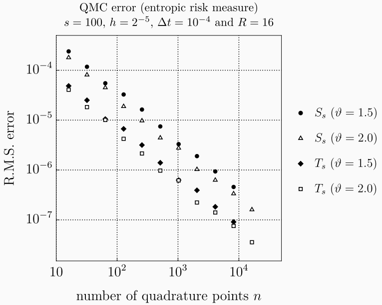


# Numerical experiments

## QMC error

We use $R = 16$ random shifts $\Delta$ 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 $\min_{z\in L^2(D\times(0,T))} J(z)$,

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

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

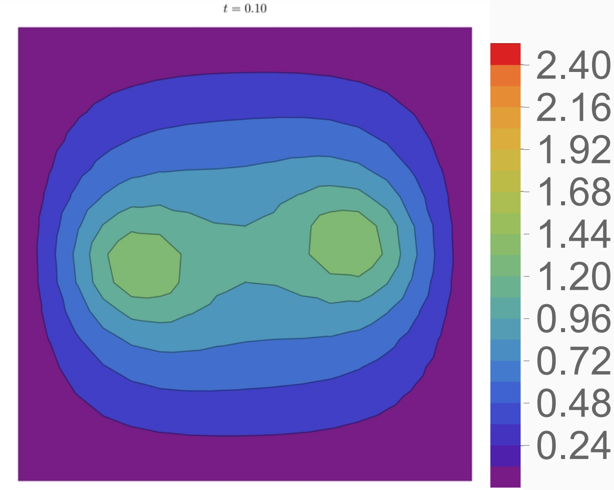



**Figure 7:** The reconstructed optimal control $z^*$ (without box constraints).

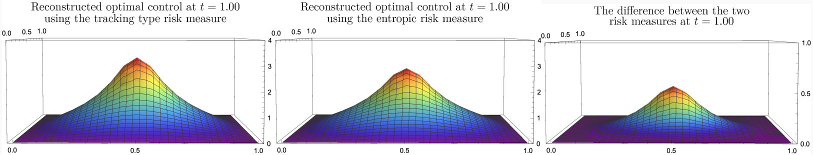



**Figure 8:** Left: the reconstructed optimal control using the tracking type risk measure at time $t = 1.00$. Middle: the reconstructed optimal control using the entropic risk measure at time $t = 1.00$. Right: The difference between the two reconstructed optimal controls.

# Conclusions

- We applied QMC to an optimal control problem with time-dependent PDE constraints under uncertainty. The QMC discretization preserves convexity, unlike sparse grids (which have negative weights).
- QMC approximations of high-dimensional integrals converge faster than MC.

References:


Guth, K., Kuo, Schillings, and Sloan. *Parabolic PDE-constrained optimal control under uncertainty with entropic risk measure using quasi-Monte Carlo integration*. Preprint 2022. arXiv:2208.02767

Guth, K., Kuo, Schillings, and Sloan. *A quasi-Monte Carlo method for optimal control under uncertainty*. SIAM/ASA Journal on Uncertainty Quantification **9**(2), 354–383, 2021.