Higher order QMC integration for Bayesian estimations

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Outline

An example

- Consider

$$-\nabla \cdot (u(\boldsymbol{x};\boldsymbol{y})\nabla q(\boldsymbol{x};\boldsymbol{y})) = F(\boldsymbol{x}) \text{ in } D \subset \mathbb{R}^d$$
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- We are interested in the inverse problem of finding u from δ where

$$\delta_j = \mathcal{G}_j(q) + \eta_j, \qquad j = 1, \ldots, K.$$

Here $\mathcal{G}_j$ is a continuous linear functional and η_j is a noise.

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  Here $\mathcal{G}_j$ is a continuous linear functional and η_j is a noise.
- Problem: The unknown u is a function (infinite dimensional) whereas the data $\eta \in \mathbb{R}^K$ is finite dimensional.

General setup

Let

- the uncertainty $u \in X$, e.g. $X = L^\infty(D)$, be parametrized by

$$u(\boldsymbol{x}; \boldsymbol{y}) = u_0(\boldsymbol{x}) + \sum_{j \geq 1} y_j \psi_j(\boldsymbol{x}), \quad y_j \in [-1/2, 1/2].$$

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- the forward response map $G : X \times \mathcal{X}' \to \mathcal{X}$

$$q = G(u; F)$$

be given, e.g. G is the solution operator of the above elliptic PDE.

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- Goal: to compute a Bayesian estimate of QoI ϕ, given measurements of the observations.

Bayesian Estimation

Theorem 1

Assume that the potential $\Phi_\Gamma(u;\delta) = \frac{1}{2}\|\delta - \mathcal{G}(u)\|_\Gamma^2$ *is, for fixed data* $\delta \in \mathbb{R}^K$, π_0 *measurable and that, for* $\mathbb{Q}_0$*-a.e. data* $\delta \in \mathbb{R}^K$ *there holds*

$$Z := \int_U \exp\left(-\Phi_\Gamma(u;\delta)\right) \pi_0(\mathrm{d}u) > 0 \,.$$

Then the conditional distribution of $u|\delta$ *(u given* δ*) exists and is denoted by* π^δ*. It is absolutely continuous with respect to* π_0 *and there holds*

$$\frac{d\pi^\delta}{d\pi_0}(u) = \frac{1}{Z}\exp\left(-\Phi_\Gamma(u;\delta)\right) \,. \tag{1.1}$$

With the QoI ϕ we associate parametric map

$$\begin{aligned}\Psi(\boldsymbol{y}) &= \Theta(\boldsymbol{y})\phi(q(u)) \\ &= \exp\big(-\Phi_\Gamma(u;\delta)\big)\phi(q(u))\,.\end{aligned} \tag{2.1}$$

Then the Bayesian estimate of the QoI ϕ, given noisy data δ, takes the form

$$\mathbb{E}^{\boldsymbol{\pi}^\delta}[\phi] = Z'/Z, \qquad Z' := \int_U \Psi(\boldsymbol{y})\,\boldsymbol{\pi}_0(\mathrm{d}\boldsymbol{y})\,. \tag{2.2}$$

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- The solution $q = G(u)$ is approximated by q_h via a Galerkin method
- The high dimensional integrals Z, Z' are approximated by higher order QMC method

Higher order QMC method

We approximate the s-dimensional integral

$$I_s(F) := \int_{[0,1]^s} F(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y} \tag{3.1}$$

by an N-point QMC method, i.e., an equal-weight quadrature rule of the form

$$Q_{N,s}(F) := \frac{1}{N}\sum_{n=0}^{N-1} F(\boldsymbol{y}_n)\,, \tag{3.2}$$

Digital net

Definition 1 (Digital net)

Let b be prime and $\alpha, s, m \in \mathbb{N}$. Let $C_1, \dots, C_s$ be $\alpha m \times m$ matrices over $\mathbb{Z}_b$; these are known as the generating matrices. For each integer $0 \le n < b^m$, let $n = \xi_0 + \xi_1 b + \cdots + \xi_{m-1} b^{m-1}$ be the b-adic expansion of n. For each $1 \le j \le s$ we compute

$$(\zeta_1, \zeta_2, \dots, \zeta_{\alpha m})^\top = C_j (\xi_0, \xi_1, \dots, \xi_{m-1})^\top ,$$

set

$$y_j^{(n)} = \frac{\zeta_1}{b} + \frac{\zeta_2}{b^2} + \cdots + \frac{\zeta_{\alpha m}}{b^{\alpha m}}$$

and set $\boldsymbol{y}_n = (y_1^{(n)}, y_2^{(n)}, \dots, y_s^{(n)})$.
Then, the resulting point set $S = \{\boldsymbol{y}_n\}_{n=0}^{b^m-1} \subset [0,1]^s$ is called a digital net.

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- Given $s \geq 1$, select s polynomials $q_1(x), \ldots, q_s(x)$ from the set $G_{b,m}$ and write collectively
$$\boldsymbol{q} \,=\, \boldsymbol{q}(x) \,=\, (q_1(x), \ldots, q_s(x)) \in G_{b,m}^s\,; \qquad (3.4)$$

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- For each integer $0 \leq n < b^m$, let $n = \xi_0 + \xi_1 b + \cdots + \xi_{m-1} b^{m-1}$ be the b-adic expansion of n, and we associate with n the polynomial
$$n(x) = \sum_{r=0}^{m-1} \xi_r \, x^r \in \mathbb{Z}_b[x] .$$

Polynomial lattice rule

- Denote by v_m the map from $\mathbb{Z}_b((x^{-1}))$ to the interval $[0,1)$ defined for any integer w by

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- The QMC point set $S_{P,b,m,s}(\boldsymbol{q})$ of a (classical) polynomial lattice rule comprises the points

$$\boldsymbol{y}_n = \left(v_m\left(\frac{n(x)q_1(x)}{P(x)}\right), \ldots, v_m\left(\frac{n(x)q_s(x)}{P(x)}\right)\right) \in [0, 1)^s,$$
$$n = 0, \ldots, b^m - 1.$$

Interlaced polynomial lattice rules

- A *digit interlacing function* with interlacing factor $\alpha \in \mathbb{N}$ is given by

$$\begin{array}{rcl} \mathscr{D}_\alpha : [0,1)^\alpha & \to & [0,1) \\ (x_1, \ldots, x_\alpha) & \mapsto & \sum_{a=1}^{\infty} \sum_{j=1}^{\alpha} \xi_{j,a} b^{-j-(a-1)\alpha} \end{array}, \tag{3.5}$$

where $x_j = \xi_{j,1} b^{-1} + \xi_{j,2} b^{-2} + \cdots$ for $1 \le j \le \alpha$.

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  where $x_j = \xi_{j,1} b^{-1} + \xi_{j,2} b^{-2} + \cdots$ for $1 \le j \le \alpha$.
- For vectors, set

$$\begin{array}{rcl} \mathscr{D}_\alpha : [0,1)^{\alpha s} & \to & [0,1)^s \\ (x_1, \ldots, x_{\alpha s}) & \mapsto & (\mathscr{D}_\alpha(x_1, \ldots, x_\alpha), \ldots, \mathscr{D}_\alpha(x_{(s-1)\alpha+1}, \ldots, x_{s\alpha})) \,. \end{array} \tag{3.6}$$

Proposition 1

Let $s \geq 1$ and $N = b^m$ for $m \geq 1$ be integers and b be prime. Let $\boldsymbol{\beta} = (\beta_j)_{j\geq 1}$ be a sequence of positive numbers. Assume that

$$\exists\, 0 < p \leq 1 : \quad \sum_{j=1}^{\infty} \beta_j^p < \infty \,. \tag{3.7}$$

Define, for $0 < p < 1$ as in (3.7),

$$\alpha \;:=\; \lfloor 1/p \rfloor + 1 \,. \tag{3.8}$$

Consider $F(\boldsymbol{y})$ whose mixed partial derivatives of order α satisfy $\forall\, \boldsymbol{y} \in U\ \forall \boldsymbol{s} \in \mathbb{N}$

$$\forall\, \boldsymbol{\nu} \in \{0, 1, \ldots, \alpha\}^s : \quad |(\partial_{\boldsymbol{y}}^{\boldsymbol{\nu}} F)(\boldsymbol{y})| \le c(F) \boldsymbol{\nu}_E! \prod_{j \in E} \beta_j^{\nu_j} \times |\boldsymbol{\nu}_{E^c}|! \prod_{j \in E^c} \beta_j^{\nu_j} \tag{3.9}$$

for some fixed integer $J \in \mathbb{N}$ where $E = \{1, 2, \ldots, J\}$ and $E^c = \mathbb{N} \setminus E$, and where $c(g) > 0$ is independent of $\boldsymbol{y}$, s and of $\boldsymbol{\nu}$. Then, for every $N \in \mathbb{N}$, one can construct an interlaced polynomial lattice rule of order α with N points such that there holds the error bound

$$\forall s, N \in \mathbb{N} : \quad |I_s(F) - Q_{N,s}(F)| \le C_{\alpha,\boldsymbol{\beta},b,p} N^{-1/p} , \tag{3.10}$$

where $C_{\alpha,\boldsymbol{\beta},b,p} < \infty$ is a constant independent of s and N.

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- Parametric regularity of solutions: $\exists \boldsymbol{\beta} \in \ell^1(\mathbb{N})$,

$$\forall \boldsymbol{y} \in U : \|(\partial_{\boldsymbol{y}}^{\boldsymbol{\nu}} q)(\boldsymbol{y})\|_{\mathcal{X}} \leq C_0 |\boldsymbol{\nu}|! \boldsymbol{\beta}^{\boldsymbol{\nu}} \|f\|_{\mathcal{Y}'}, \quad \forall \boldsymbol{\nu} \in \mathbb{N}^{\mathbb{N}}, |\boldsymbol{\nu}| < \infty.$$

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$$\forall v \in \mathcal{X}_t : \inf_{v^h \in \mathcal{X}^h} \|v - v^h\|_{\mathcal{X}} \le C_t h^t \|v\|_{\mathcal{X}_t},$$

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- The sparsity condition imposed on the KL expansion of u

$$\{\|\psi_j\|_X\}_{j \ge 1} \in \ell^p(\mathbb{N})$$

Theorem 2

The QMC-Petrov Galerkin approximation of the Bayesian estimate $\mathbb{E}^{\pi^\delta}[\phi]$ in (2.2) obtained as $Z'_{N,s,h}/Z_{N,s}$ with QMC-PG approximations $Z'_{N,s,h}$ and $Z_{N,s}$ of the integrals Z' and Z in (2.2), the error bound

$$\left|\mathbb{E}^{\pi^\delta}[\phi] - Z'_{N,s,h}/Z_{N,s}\right| \leq C(\Gamma, p)\left(h^t + s^{-(1/p-1)} + N^{-1/p}\right) .$$

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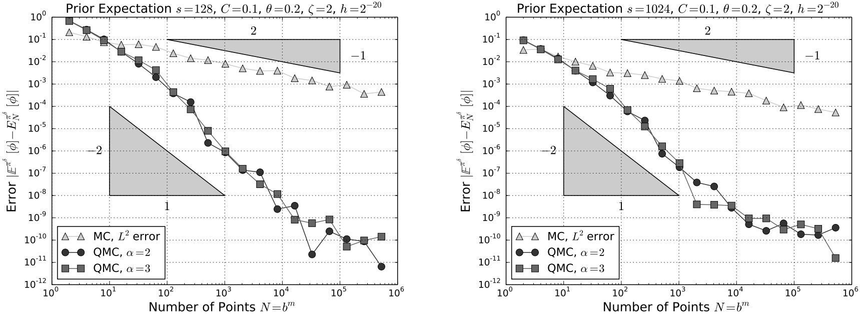
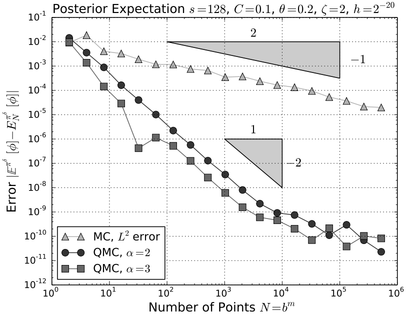
- QoI: parametric solution $q(x, \boldsymbol{y})$ evaluated at $x = \bar{x} = 0.25$.



(a) $s = 128$ **(b)** $s = 1024$

Figure: Convergence of the error of the prior mean approximation vs. the number of samples $N = b^m$ for $s = 128, 1024$, $\zeta = 2$, $\alpha = 2, 3$, $h = 2^{-20}$.

Observation operator: evaluation of the solution $q(, \boldsymbol{y})$ at $\boldsymbol{x}_{obs} = (0.2, 0.5, 0.7)$.



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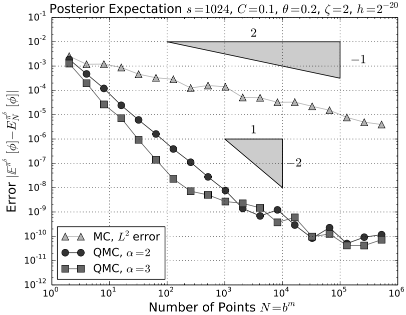

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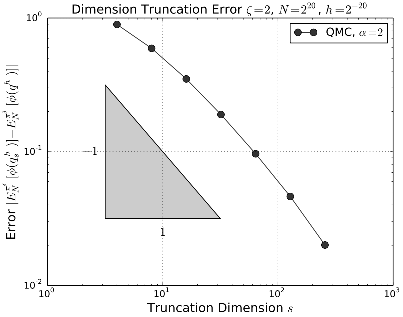
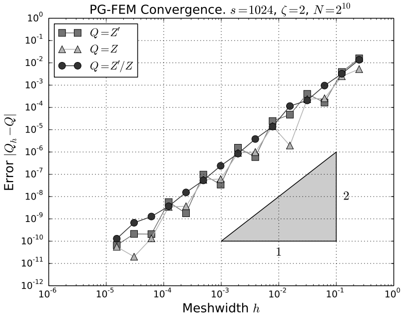


(a) Dimension truncation error



(b) FEM error, KL basis

Figure: Dimension truncation and FEM errors. Reference solutions were obtained using $s = 1024$ dimensions for (a) and $h = 2^{-20}$ for (b).

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- Future work: A multi-level QMC approach for Bayesian estimates

References

- J.Dick, F.Y.Kuo, Q.T.Le Gia, D. Nuyens, Ch. Schwab: Higher order QMC Galerkin discretization for parametric operator equations, SINUM, 2014.

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THANK YOU FOR YOUR ATTENTION

Infinite-Dim Parametric Operator Equations

Let $f \in \mathcal{Y}'$ be given, for every $\boldsymbol{y} \in U$, find

$$q(\boldsymbol{y}) \in \mathcal{X} : A(\boldsymbol{y})q(\boldsymbol{y}) = f$$

Assume that for every $\boldsymbol{y} \in U$, there is a sequence $\{A_j\}$

$$A(\boldsymbol{y}) = A_0 + \sum_{j \geq 1} y_j A_j \tag{5.1}$$

In the previous example, we can define $A_0 = -\nabla \cdot (u\nabla)$ and $A_j = -\nabla \cdot (\psi_j \nabla)$

We associate with the operator A_j the bilinear forms $\mathfrak{a}_j(\cdot,\cdot) : \mathcal{X} \times \mathcal{Y} \to \mathbb{R}$ via

$$\forall v \in \mathcal{X},\ w \in \mathcal{Y} : \quad \mathfrak{a}_j(v, w) \ = \ {}_{\mathcal{Y}}\langle w, A_j v\rangle_{\mathcal{Y}'} \ , \quad j = 0, 1, 2, \ldots \ .$$

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1. *The nominal operator* $A_0 \in \mathcal{L}(\mathcal{X}, \mathcal{Y}')$ *is boundedly invertible, i.e., there exists* $\mu_0 > 0$ *such that*

$$\inf_{0\neq v\in\mathcal{X}} \sup_{0\neq w\in\mathcal{Y}} \frac{\mathfrak{a}_0(v,w)}{\|v\|_{\mathcal{X}}\|w\|_{\mathcal{Y}}} \geq \mu_0 \ , \quad \inf_{0\neq w\in\mathcal{Y}} \sup_{0\neq v\in\mathcal{X}} \frac{\mathfrak{a}_0(v,w)}{\|v\|_{\mathcal{X}}\|w\|_{\mathcal{Y}}} \geq \mu_0 \ . \tag{5.2}$$

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$$\inf_{0\neq v\in\mathcal{X}} \sup_{0\neq w\in\mathcal{Y}} \frac{\mathfrak{a}_0(v,w)}{\|v\|_{\mathcal{X}}\|w\|_{\mathcal{Y}}} \geq \mu_0 \,, \quad \inf_{0\neq w\in\mathcal{Y}} \sup_{0\neq v\in\mathcal{X}} \frac{\mathfrak{a}_0(v,w)}{\|v\|_{\mathcal{X}}\|w\|_{\mathcal{Y}}} \geq \mu_0 \,. \tag{5.2}$$

2. *The fluctuation operators $\{A_j\}_{j\geq 1}$ are small with respect to A_0: there exists a constant $0 < \kappa < 2$ s.t. for μ_0 as in (5.2) and some $s \geq 1$ we have*

$$\sum_{j\geq s+1} \beta_j \leq \kappa < 2 \,, \quad \textit{where} \quad \beta_j := \|A_0^{-1}A_j\|_{\mathcal{L}(\mathcal{X},\mathcal{Y}')} \,, \quad j = 1, 2, \ldots \,. \tag{5.3}$$

Go back...