Density estimation in uncertainty quantification using quasi-Monte Carlo with preintegration

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Wednesday 28. June, MCM 2023, Sorbonne University, Paris

Outline

1. PDE problem formulation
2. Computing distribution functions
3. Quasi-Monte Carlo methods for high-dimensional integration
4. Smoothing by preintegration
5. Approximating distributions using QMC with preintegration
6. Numerical results

PDE problem formulation

$$
\begin{aligned}
-\nabla\big(a(\boldsymbol{x},\boldsymbol{z})\nabla u(\boldsymbol{x},\boldsymbol{w},\boldsymbol{z})\big) &= f(\boldsymbol{x},\boldsymbol{w}) && \text{for } \boldsymbol{x}\in D\\
u(\boldsymbol{x},\boldsymbol{w},\boldsymbol{z}) &= 0 && \text{for } \boldsymbol{x}\in \partial D
\end{aligned}
$$

- $\boldsymbol{x} \in D \subset \mathbb{R}^d$, $d = 1, 2, 3$, is the *physical* variable,
- $\boldsymbol{w} = (w_0, w_1, \ldots, w_s)$ and $\boldsymbol{z} = (z_1, z_2, \ldots, s)$ are independent *stochastic parameters*, $w_i \sim \mathrm{N}(0,1)$ and $z_j \sim \mathrm{N}(0,1)$ i.i.d.,
- lognormal coefficient — for $a_j \in L^\infty(D)$ suff. smooth

$$
a(\boldsymbol{x},\boldsymbol{z}) = \exp\left(\sum_{j=1}^{s} z_j a_j(\boldsymbol{x})\right),
$$

- $f(\boldsymbol{x},\boldsymbol{w}) = \sum_{i=0}^{s} w_i f_i(\boldsymbol{x})$ with $f_i \in L^2(D)$, $f_0 > 0$ on $\overline{D}$

Goal: compute cdf of quantity of interest/functional $\mathcal{G}$ of the solution

$F(t) = \mathbb{P}[\mathcal{G}(u) \le t]$, for some $t \in \mathbb{R}$ also pdf $f = \dfrac{\mathrm{d}F}{\mathrm{d}t}$

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- write $\boldsymbol{y} = (y_0, y_1, \ldots, y_{2s}) = (w_0, w_1, \ldots, w_s, z_1, z_2, \ldots z_s)$

Goal: compute cdf of quantity of interest/functional $\mathcal{G}$ of the solution

$$
F(t) = \mathbb{P}[\mathcal{G}(u) \le t], \quad \text{for some } t \in \mathbb{R} \qquad \text{also pdf } f = \frac{\mathrm{d}F}{\mathrm{d}t}
$$

Formulate cdf as an expected value

Key idea: formulate the cdf at $t \in \mathbb{R}$ as an expected value/integral

$$\begin{aligned} F(t) &= \mathbb{E}\big[\mathrm{ind}(t - \mathcal{G}(u))\big] \\ &= \int_{\mathbb{R}^{2s+1}} \mathrm{ind}\big(t - \mathcal{G}(u(\cdot, \boldsymbol{y}))\big) \left(\prod_{j=0}^{2s} \rho(y_j) \right) \mathrm{d}\boldsymbol{y}, \end{aligned}$$

where $\mathrm{ind}(t) = 1$ if $t \geq 0$ and 0 otherwise, and $\rho(y) = \frac{1}{\sqrt{2\pi}} e^{-\frac{y^2}{2}}$.

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where $\mathrm{ind}(t) = 1$ if $t \geq 0$ and 0 otherwise, and $\rho(y) = \frac{1}{\sqrt{2\pi}} e^{-\frac{y^2}{2}}$.

Difficulties:

1. curse of dimensionality because s is large,
2. integrand $g(\boldsymbol{y}) = \mathrm{ind}(t - \mathcal{G}(u(\cdot, \boldsymbol{y})))$ is discontinuous, and
3. evaluating the QoI $\mathcal{G}(u)$ requires solving the PDE.

Strategy:

1. use quasi-Monte Carlo to tackle high-dimensional integral,
2. use preintegration to "smooth out" the discontinuity, and
3. approximate the PDE using finite elements.

Related work

- Conditional Monte Carlo/sampling:
  [L'Ecuyer, Perron 1994], [Fu, Hu 1998], [Glasserman, Staum 2001], [Holtz (PhD thesis) 2011], [Achtis, Cools, Nuyens 2013], [Asmussen 2018], [Bayer, Ben Hammouda, Tempone 2022] ...
- Preintegration theory:
  [Griebel, Kuo, Sloan 17], [Griewank, Kuo, Leövey, Sloan 2018]
- Density estimation using QMC with preintegration/conditioning:
  [L'Ecuyer, Puchhammer, Ben Abdellah 2022], [Gilbert, Kuo, Sloan 2022]
- QMC for approximating the *expected value* for lognormal PDEs:
  [Graham, Kuo, Nuyens, Scheichl, Sloan 2011], [Graham, Kuo, Nichols, Scheichl, Schwab, Sloan 2015], [Hermann, Schwab 2019]
  ...

Quasi-Monte Carlo methods on $\mathbb{R}^s$

N-point randomly shifted lattice rule:

$$\int_{\mathbb{R}^s} g(\boldsymbol{y}) \left(\prod_{j=1}^{s} \rho(y_j) \right) \mathrm{d}\boldsymbol{y} \approx Q_{s,N} g = \frac{1}{N} \sum_{k=0}^{N-1} g\left(\boldsymbol{\tau}_k\right).$$

- $\boldsymbol{\tau}_k = \boldsymbol{\Phi}^{-1}\left(\left\{ \frac{k \boldsymbol{z}_{\mathrm{gen}}}{N} + \boldsymbol{\Delta} \right\} \right)$,
- $\{\cdot\}$ is the fractional part,
- $\boldsymbol{\Phi}^{-1}$ is the inverse cdf of ρ,
- $\boldsymbol{z}_{\mathrm{gen}} \in \mathbb{N}^s$ is the *generating vector*,
- *random shift* $\boldsymbol{\Delta} \sim \mathrm{Uni}([0,1)^s)$.
- random shifting $\implies$ unbiased
- good vectors $\boldsymbol{z}_{\mathrm{gen}}$ constructed using *component-by-component* (CBC) algorithm

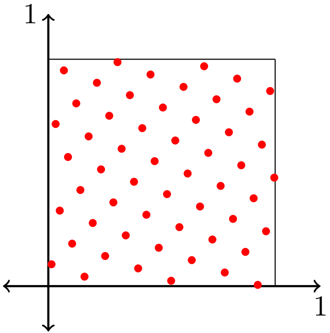

Figure: 2D lattice rule on $[0,1]^2$ with $N = 55$, $\boldsymbol{z}_{\mathrm{gen}} = (1, 34)$.

QMC error

Component-by-component error [Nichols & Kuo 2014]

For $g \in \mathcal{H}_s$, N prime and *good* $\boldsymbol{z}_{\mathrm{gen}}$

$$\sqrt{\mathbb{E}_{\boldsymbol{\Delta}}\left[\left|\int_{\mathbb{R}^s} g(\boldsymbol{y})\left(\prod_{j=1}^{s}\rho(y_j)\right)\mathrm{d}\boldsymbol{y} - Q_{d,N}g\right|^2\right]} \leq C_{\delta,\boldsymbol{\gamma}} N^{-1+\delta}\|g\|_{\mathcal{H}_s}, \quad \delta > 0.$$

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where $g \in \mathcal{H}_s =:$ s-*dimensional weighted Sobolev space* with:

- weights: $\boldsymbol{\gamma} := \{\gamma_{\mathfrak{u}} > 0 : \mathfrak{u} \subseteq \{1, \ldots, s\}\}$,
- weight function: $\psi : \mathbb{R} \to \mathbb{R}^+$,
- weighted norm

$$\|g\|_{\mathcal{H}_s}^2 = \sum_{\mathfrak{u}\subseteq\{1:s\}} \frac{1}{\gamma_{\mathfrak{u}}} \int_{\mathbb{R}^s} \left|\frac{\partial^{|\mathfrak{u}|}}{\partial \boldsymbol{y}_{\mathfrak{u}}} g(\boldsymbol{y})\right|^2 \left(\prod_{j\in\mathfrak{u}} \psi(y_j)\right)\left(\prod_{j\notin\mathfrak{u}} \rho(y_j)\right) \mathrm{d}\boldsymbol{y}$$

where $\{1 : s\} := \{1, \ldots, s\}$ and $\boldsymbol{y}_{\mathfrak{u}} = (y_j : j \in \mathfrak{u})$.

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$$\|g\|^2_{\mathcal{H}_s} = \sum_{\mathfrak{u}\subseteq\{1:s\}} \frac{1}{\gamma_{\mathfrak{u}}} \int_{\mathbb{R}^s} \left|\frac{\partial^{|\mathfrak{u}|}}{\partial \boldsymbol{y}_{\mathfrak{u}}} g(\boldsymbol{y})\right|^2 \left(\prod_{j\in\mathfrak{u}} \psi(y_j)\right)\left(\prod_{j\notin\mathfrak{u}} \rho(y_j)\right) \mathrm{d}\boldsymbol{y}$$

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Problem: $g = \mathrm{ind}(t - \mathcal{G}(u)) \notin \mathcal{H}_s$, even though $\mathcal{G}(u)$ is smooth!

Preintegration (a.k.a. conditional sampling)

Problem: $g = \mathrm{ind}(t - \mathcal{G}(u))$ is not smooth enough for QMC!

Solution: *preintegration*, i.e., smooth a simple discontinuity,

$g(\boldsymbol{y}, z) = \mathrm{ind}(t - \phi(\boldsymbol{y}, z))$, for a "sufficiently regular" $\phi : \mathbb{R}^{2s+1} \to \mathbb{R}$,

by integrating out a single (specifically chosen) dimension

$$\int_{\mathbb{R}^{2s+1}} g(\boldsymbol{y}) \left(\prod_{j=0}^{2s} \rho(y_j) \right) \mathrm{d}\boldsymbol{y}$$

$$= \int_{\mathbb{R}^{2s}} \Bigg[\underbrace{\int_{-\infty}^{\infty} g(y_0, \boldsymbol{y}_{1:2s}) \rho(y_0) \, \mathrm{d}y_0}_{=: P_0 g(\boldsymbol{y}_{1:2s})} \Bigg] \left(\prod_{j=1}^{2s} \rho(y_j) \right) \mathrm{d}\boldsymbol{y}_{1:2s}$$

$\boldsymbol{y}_{1:2s} := (y_1, y_2, \ldots, y_2 s)$.

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$\boldsymbol{y}_{1:2s} \coloneqq (y_1, y_2, \ldots, y_2 s)$.

[Griewank, Kuo, Leövey, Sloan 2018] showed that $P_0 g$ is as smooth as ϕ, but in one dimension less (under technical conditions)[1].

[1] See also [Griebel, Kuo, Sloan 2010], [Griebel, Kuo, Sloan 2013] and [Griebel, Kuo, Sloan 2017].

How to do preintegration in practice?

Assume

$$\frac{\partial}{\partial y_0}\phi(\boldsymbol{y}) > 0 \text{ for all } \boldsymbol{y} \in \mathbb{R}^{2s+1}, \quad \text{and} \quad \phi(\boldsymbol{y}) \to \infty \text{ as } y_0 \to \infty,$$

then the point of discontinuity in the y_0 direction is unique

$$\xi(\boldsymbol{y}_{1:2s}) = (\xi \in \mathbb{R} : \phi(\xi, \boldsymbol{y}_{1:2s}) = t).$$

Preintegration w.r.t. y_0 simplifies to

$$P_0 g(\boldsymbol{y}) = \int_{-\infty}^{\infty} \mathrm{ind}(t - \phi(\boldsymbol{y}))\rho(y_0)\, \mathrm{d}y_0 = \int_{-\infty}^{\xi(\boldsymbol{y}_{1:2s})} \rho(y_0)\, \mathrm{d}y_0 = \Phi(\xi(\boldsymbol{y}_{1:2s})).$$

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Numerical preintegration procedure: To evaluate $P_0 g(\boldsymbol{y}_{1:2s})$

1. Compute point of discontinuity $\xi(\boldsymbol{y}_{1:2s})$ (analytically/numerically)
2. Approximate the 1D integral $\displaystyle\int_{-\infty}^{\xi(\boldsymbol{y})} \rho(y_1)\, \mathrm{d}y_1$

Preintegration applied to QoI from PDE

$$\phi(\boldsymbol{y}) \;=\; \mathcal{G}(u(\cdot,\boldsymbol{y}))$$

where $\mathcal{G} \in H^{-1}(D)$ and $u(\boldsymbol{x},\boldsymbol{y})$ is PDE solution.
For our series RHS

$$u(\boldsymbol{x},\boldsymbol{y}) \;=\; \sum_{i=0}^{s} w_i u_i(\boldsymbol{x},\boldsymbol{z})$$

where

$$-\nabla\big(a(\boldsymbol{x},\boldsymbol{z})\nabla u_i(\boldsymbol{x},\boldsymbol{z})\big) = f_i(\boldsymbol{x}) \quad \text{for } i = 0,1,\ldots,s$$

Point of discontinuity is

$$\xi(\boldsymbol{y}_{1:2s}) \;=\; \frac{t - \sum_{i=1}^{s} w_i \mathcal{G}(u_i(\cdot,\boldsymbol{z}))}{\mathcal{G}(u_0(\cdot,\boldsymbol{z}))}$$

and the preintegration step simplifies to

$$P_0\big[\mathrm{ind}(t - \mathcal{G}(u)\big] \;=\; \Phi\left(\frac{t - \sum_{i=1}^{s} w_i \mathcal{G}(u_i(\cdot,\boldsymbol{z}))}{\mathcal{G}(u_0(\cdot,\boldsymbol{z}))}\right),$$

which is smooth if $\mathcal{G}(u_0(\cdot,\boldsymbol{z})) > 0$ for all $\boldsymbol{z}$.

Approximating cdf of QoI using QMC with preintegration

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After preintegration we apply QMC in the remaining $2s$ dimensions

$$F(t) \;\approx\; F_N(t) \;:=\; Q_{2s,N}\big(P_0\big[\mathrm{ind}(t-\mathcal{G}(u))\big]\big) \;=\; Q_{2s,N}(\Phi\circ\xi)$$

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Preintegration + QMC procedure for QoI

For each QMC lattice point $\boldsymbol{\tau}_k = (\tau_{k,1}, \tau_{k,2}, \ldots, \tau_{k,2s})$:

1. Solve PDEs for $u_0(\boldsymbol{\tau}_k)$ and $\widetilde{u}(\boldsymbol{\tau}_k) = \sum_{i=1}^{s} \tau_{k,i} u_i(\boldsymbol{\tau}_k)$

$$-\nabla\big(a(\boldsymbol{\tau}_k)\nabla u_0(\boldsymbol{\tau}_k)\big) = f_0 \quad \text{and} \quad -\nabla\big(a(\boldsymbol{\tau}_k)\nabla \widetilde{u}(\boldsymbol{\tau}_k)\big) = \sum_{i=1}^{s} \tau_{k,i} f_i$$

2. Compute point of discontinuity $\xi(\boldsymbol{\tau}_k) = \dfrac{t - \mathcal{G}\big(\sum_{i=1}^{s} \tau_{k,i} u_i(\boldsymbol{\tau}_k)\big)}{\mathcal{G}(u_0(\boldsymbol{\tau}_k))}$
3. Evaluate preintegrated function $P_0(\boldsymbol{\tau}_k) = \Phi(\xi(\boldsymbol{\tau}_k))$

Why are probabilities hard to compute using quadrature?

- white $= 0$, grey $= 1$ and blue is the line of discontinuity ξ.

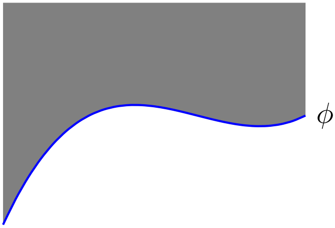

Figure: "Aerial view" of indicator function in 2D

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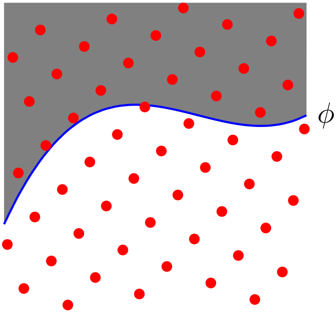
- QMC points are designed to be well-distributed on the *whole* domain, but here the important thing is to resolve the discontinuity.



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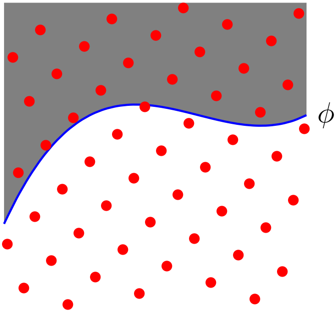
- Preintegration solves this problem by first computing ξ.



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Error of QMC with preintegration for cdf of QoI

Theorem (Gilbert, Kuo, Srikumar 2023+)

Let F be the cdf of the quantity of interest $\mathcal{G}(u)$, for some $\mathcal{G} \in H^{-1}(D)$, and suppose

1. *Monotone condition: $f_0 > 0$ on $\overline{D}$ and $\mathcal{G}(v) > 0$ for all $v > 0$,*
2. *QMC rule is constructed using CBC algorithm with N prime,*

Then the RMSE of the QMC with preintegration approximation, $F_N(t) = Q_{2s,N}(P_0(\mathrm{ind}(t - \mathcal{G}(u)))$, satisfies

$$\sqrt{\mathbb{E}\big[|F(t) - F_N(t)|^2\big]} \leq C \; N^{-1+\delta} \qquad , \qquad \text{for } \delta > 0,$$

where $C < \infty$ depends on δ, s, $\mathcal{G}$, $\{f_i\}$, and t.

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- Same rate as integrals/expected values!

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2. *QMC rule is constructed using CBC algorithm with N prime,*
3. *$u_h \approx u$ using piecewise linear FE with meshwidth $h > 0$.*

Then the RMSE of the QMC with preintegration & FE approximation, $F_{h,N}(t) = Q_{2s,N}(P_0(\mathrm{ind}(t - \mathcal{G}(u_h))))$, satisfies

$$\sqrt{\mathbb{E}\big[|F(t) - F_{h,N}(t)|^2\big]} \leq C(N^{-1+\delta} + h^2), \qquad \text{for } \delta > 0,$$

where $C < \infty$ depends on δ, s, $\mathcal{G}$, $\{f_i\}$, and t.

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Sketch proof for QMC error

- Verify $\mathcal{G}(u)$ satisfies the conditions for preintegration theory:
  (a) $\mathcal{G}(u)$ is suff. smooth, $\dfrac{\partial^\ell}{\partial y_0^\ell}\mathcal{G}(u) \in \mathcal{H}_{2s}$ for $\ell = 1, \ldots, 2s-1$, and
  (b) $\dfrac{\partial}{\partial y_0}\mathcal{G}(u(\cdot, \boldsymbol{y})) > 0$ for all $\boldsymbol{y} \in \mathbb{R}^{2s+1}$.
- Abi Srikumar has shown (a) using bounds from, e.g., [Graham, Kuo, Nichols, Scheichl, Schwab, Sloan 2015].
- $f_0 > 0 \implies \dfrac{\partial u}{\partial y_0} = u_0 > 0$ (by the Strong Maximum Principle)
  $\implies \dfrac{\partial \mathcal{G}(u)}{\partial y_0} = \mathcal{G}\left(\dfrac{\partial u}{\partial y_0}\right) > 0 \implies$ (b) (by condition on $\mathcal{G}$)
- Preintegration theory implies that $P_0[\mathrm{ind}(t - \mathcal{G}(u))] \in \mathcal{H}_{2s}$.
- CBC error bound in $\mathcal{H}_{2s}$ then gives the desired error bound.
  Explicit constant, which depends on $\boldsymbol{\gamma}$, δ, s, $\{\|a_j\|_{L^\infty}\}$, $\{f_i\}$.

Numerical results

$$
\begin{aligned}
-\nabla\big(a(\boldsymbol{x},\boldsymbol{w})\nabla u(\boldsymbol{x},\boldsymbol{w},z)\big) &= z f_0(\boldsymbol{x}) + f_1(\boldsymbol{x}), \qquad && \boldsymbol{x} \in D \\
u(\boldsymbol{x},\boldsymbol{w},z) &= 0, && \boldsymbol{x} \in \partial D
\end{aligned}
$$

- $D = (0,1)^2$ ($d = 2$)
- $a_j(x_1, x_2) = \dfrac{\alpha}{1 + (j\pi)^2} \sin(j\pi x_1) \sin((j+1)\pi x_2)$, with $\alpha > 0$
- $f_0(x_1, x_2) = \sin(\pi x_1) + \sin(\pi x_2)$ and $f_1 \equiv 1$
- QoI is point evaluation: $\mathcal{G}(v) = v(1/\sqrt(2), 1/\sqrt(2))$
- $s = 64$
- PDE solved using linear FEM

Approximations of cdf and pdf

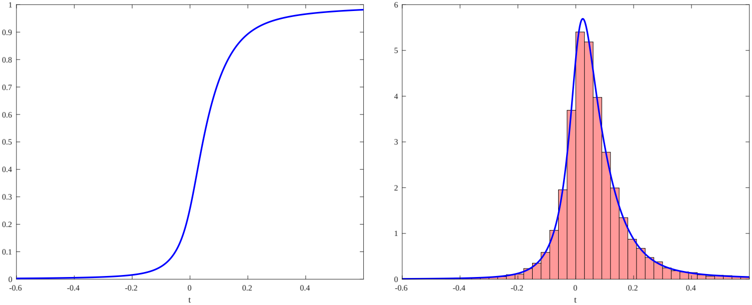

Figure: Plot of approximated cdf (left) and pdf (right) for $\alpha = 30$.

N convergence

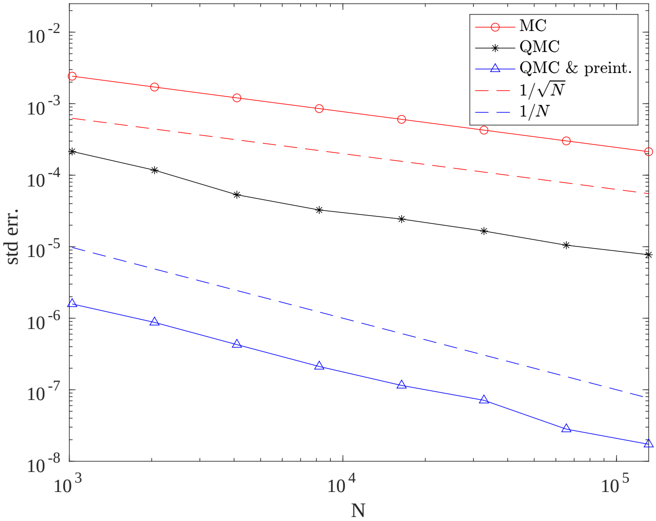

Figure: Convergence in N for MC, QMC and QMC after preintegration for $F(0)$, $\alpha = 30$. ($N_{\mathrm{MC}} = R \times N_{\mathrm{QMC}}$.)

Effect of α scaling

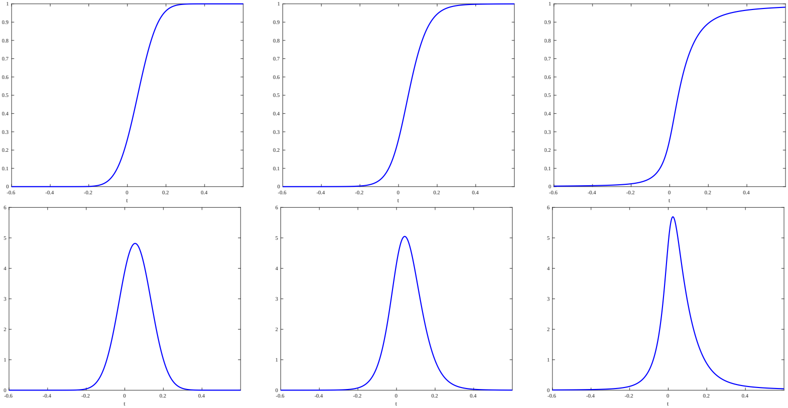

Figure: cdf (top) and pdf (bottom) for $\alpha = 1$ (left), 15 (middle) and 30 (right).

Conclusion

Summary

- Developed a QMC & preintegration algorithm to approximate cdf/pdf of QoI from lognormal PDE in UQ.
- Preintegration smooths the discontinuity from the indicator function and QMC methods tackle the curse of dimensionality.
- Error analysis gives $\mathcal{O}(N^{-1+\delta})$, which is observed in practice.

Extensions

- Approximate probability at multiple points $\{t_\ell\}$, then reconstruct the cdf, e.g., using polynomial interpolation, splines, etc.
- By formulating the density as an integral of a Dirac δ function, we can also approximate the pdf.
- $s = \infty$
- Other UQ problems?

Main references

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Thanks for listening!

Reconciling preintegration and QMC theories

QMC — weighted ANOVA space $\mathcal{W}_s$:

$$\|g\|_{\mathcal{W}_s}^2 = \sum_{\mathfrak{u}\subseteq\{1:d\}} \frac{1}{\gamma_{\mathfrak{u}}} \int_{\mathbb{R}^{|\mathfrak{u}|}} \left| \int_{\mathbb{R}^{d-|\mathfrak{u}|}} \frac{\partial^{|\mathfrak{u}|}}{\partial \boldsymbol{y}_{\mathfrak{u}}} g(\boldsymbol{y}) \boldsymbol{\rho}(\boldsymbol{y}_{\{1:d\}\setminus\mathfrak{u}}) \,\mathrm{d}\boldsymbol{y}_{\{1:d\}\setminus\mathfrak{u}} \right|^2 \boldsymbol{\psi}(\boldsymbol{y}_{\mathfrak{u}}) \,\mathrm{d}\boldsymbol{y}_{\mathfrak{u}}$$

Preintegration — Sobolev space of dominating mixed smoothness $\mathcal{H}_s$:

$$\|f\|_{\mathcal{H}_s}^2 = \sum_{\mathfrak{u}\subseteq\{1:d\}} \frac{1}{\gamma_{\mathfrak{u}}} \int_{\mathbb{R}^d} \left| \frac{\partial^{|\mathfrak{u}|}}{\partial \boldsymbol{y}_{\mathfrak{u}}} g(\boldsymbol{y}) \right|^2 \boldsymbol{\psi}(\boldsymbol{y}_{\mathfrak{u}}) \boldsymbol{\rho}(\boldsymbol{y}_{\{1:d\}\setminus\mathfrak{u}}) \,\mathrm{d}\boldsymbol{y}$$

Theorem (G., Kuo, Sloan 2022)

Suppose $\displaystyle\int_{-\infty}^{\infty} \frac{\Phi(t)(1-\Phi(t))}{\psi(t)}\,\mathrm{d}t < \infty.$

Then the spaces $\mathcal{W}_s$ and $\mathcal{H}_s$ are equivalent, with

$$\|g\|_{\mathcal{W}_s} \le \|g\|_{\mathcal{H}_s} \le C_{s,\boldsymbol{\gamma}} \|g\|_{\mathcal{W}_s},$$

where $C_{s,\boldsymbol{\gamma}} < \infty$ depends on s, $\boldsymbol{\gamma}$ and the reproducing kernel in $\mathcal{W}_s$.

Recap of assumptions

Assume $t \in \mathbb{R}$ is fixed.

For $s \geq 2$, let $\phi : \mathbb{R}^{2s+1} \to \mathbb{R}$ satisfy

1. $\frac{\partial}{\partial y_0}\phi(\boldsymbol{y}) > 0$ for all $\boldsymbol{y} \in \mathbb{R}^{2s+1}$;
2. for each $\boldsymbol{y} \in \mathbb{R}^{2s+1}$, $\phi(\boldsymbol{y}) \to \infty$ as $y_0 \to \infty$; and
3. $\phi \in \mathcal{H}_s^{\boldsymbol{\nu}} \cap C^{\boldsymbol{\nu}}(\mathbb{R}^d)$, where $\boldsymbol{\nu} = (s-1, 1, \ldots, 1) \in \mathbb{N}^s$,

Additionally, suppose that $\rho \in C^s(\mathbb{R})$.

For the equivalence and QMC theory assume that ψ and Φ (cdf of ρ) satisfy

$$\int_{-\infty}^{\infty} \frac{\Phi(t)(1-\Phi(t))}{\psi(t)}\,\mathrm{d}t < \infty.$$

Also, define

$$U \coloneqq \{\boldsymbol{y}_{1:2s} \in \mathbb{R}^{2s} : \phi(y_0, \boldsymbol{y}_{1:2s}) = t \text{ for some } y_0 \in \mathbb{R}\},$$

then define $\xi : U \to \mathbb{R}$ such that

$$\phi(\xi(\boldsymbol{y}_{1:2s}), \boldsymbol{y}_{1:2s}) = t.$$

(Both U and ξ depend on t)

technical conditions

Let $q \in \{0,1\}$ and for all $\boldsymbol{\eta} \in \{0,1\}^{2s}$ consider functions $h_{q,\boldsymbol{\eta}} : \overline{U} \to \mathbb{R}$ of the form

$$\begin{cases} h_{q,\boldsymbol{\eta}}(\boldsymbol{y}_{2:d}) \;:=\; \dfrac{(-1)^r \rho^{(\beta)}(\xi(\boldsymbol{y}_{2:d}))\, \prod_{\ell=1}^{r} \partial^{\boldsymbol{\alpha}_\ell} \phi(\xi(\boldsymbol{y}_{1:2s}), \boldsymbol{y}_{1:2s})}{[\partial^1 \phi(\xi(\boldsymbol{y}_{1:2s}), \boldsymbol{y}_{1:2s})]^{r+q}}, \\ \text{with } r \in \mathbb{N}_0,\ \boldsymbol{\alpha} = (\boldsymbol{\alpha}_\ell)_{\ell=1}^{r},\ \boldsymbol{\alpha}_\ell \in \mathbb{N}_0^{2s} \setminus \{\boldsymbol{e}_1, \boldsymbol{0}\},\ \beta \in \mathbb{N}_0 \text{ satisfying} \\ r \le 2|\boldsymbol{\eta}| + q - 1,\ \beta \boldsymbol{e}_0 + \displaystyle\sum_{\ell=1}^{r} \boldsymbol{\alpha}_\ell = (r + q - 1, \boldsymbol{\eta}). \end{cases}$$

We assume that all such functions $h_{q,\boldsymbol{\eta}}$ satisfy

$$\lim_{\boldsymbol{y}_{1:2s} \to \partial U} h_{q,\boldsymbol{\eta}}(\boldsymbol{y}_{1:2s}) \;=\; 0,$$

and there is a constant $B_{q,\boldsymbol{\eta}}$ such that

$$\int_U |h_{q,\boldsymbol{\eta}}(\boldsymbol{y}_{1:2s})|^2 \left(\prod_{\substack{j=1 \\ \eta_j \neq 0}}^{2s} \psi(y_j) \right) \left(\prod_{\substack{j=1 \\ \eta_j = 0}}^{2s} \rho(y_j) \right) \mathrm{d}\boldsymbol{y}_{1:2s} \;\le\; B_{q,\boldsymbol{\eta}} \;<\; \infty.$$