What’s new in high-dimensional integration? – designing for applications

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The theme

- High dimensional problems are important, but hard.
- Some interesting problems can now be tackled successfully.
- What’s new? What’s new is that we now know how to **design** high dimensional integration rules that are good for particular problems.

These are **Quasi-Monte Carlo** (or **QMC**) rules

High-dimensional integration

Consider

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Where might integrals with hundreds of dimensions occur?

- finance
- statistics
- flow through a porous medium
- other stochastic pde – e.g. climate change done properly

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To design a good integration rule we need to be guided by **applications**.

PDE with random coefficients

PDE with random coefficients are now attracting great interest.

Example: flow through a porous medium

Darcy's law is $$\vec{q}(\mathbf{x}) \;=\; -a(\mathbf{x})\nabla p(\mathbf{x}),$$

where

$p(\mathbf{x})$ is pressure of the fluid

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$a(\mathbf{x})$ is “permeability” of the medium

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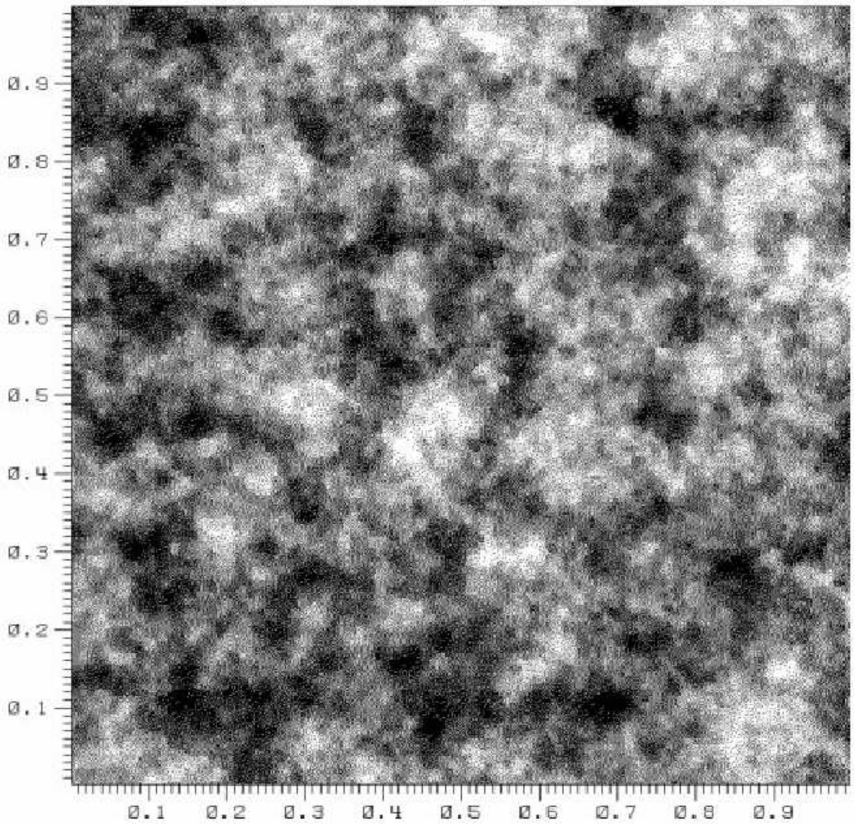
Incompressibility: $\nabla \cdot \vec{q} = 0$

Together these give a second order elliptic PDE:

$$\nabla \cdot (\boldsymbol{a}(\mathbf{x})\nabla \boldsymbol{p}(\mathbf{x})) = 0$$

Modelling the permeability

Describing in all the microscopic pores and channels in a real material is commonly considered much too hard. So it is common engineering practice to model the permeability as a random field:



A model problem – the “uniform” case

$$-\boldsymbol{\nabla}\cdot\left(a(\mathrm{x},\mathrm{y})\,\boldsymbol{\nabla} u(\mathrm{x},\mathrm{y})\right) \;=\; f(\mathrm{x}) \quad \text{in} \quad D\,,$$

$$u(\mathrm{x},\mathrm{y}) \;=\; 0 \quad \text{on} \quad \partial D, \qquad \mathrm{y}\in U := [0,1]^{\mathbb{N}},$$

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where $y_1, y_2, \ldots$ are independent random variables uniformly distributed on $[0,1]$; with $\overline{a}, \psi_j$ such that $\sum_j \|\psi_j\|_\infty < \infty$, and

$$a_{\max} \geq a(\mathrm{x},\mathrm{y}) \geq a_{\min} > 0,$$

making the PDE **strongly elliptic** for every y.

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In practice truncate the sum after s terms.

Example

Take $d = 1$,

$$a(x, \mathrm{y}) \;=\; \overline{a} + \sum_{j=1}^{\infty} (y_j - \tfrac{1}{2})\, \psi_j(x), \qquad x \in [0, \pi], \quad \mathrm{y} \in U\ ,$$

and

$$\psi_j(x) := \frac{\sin(jx)}{j^\alpha}, \qquad \text{for some } \alpha > 1.$$

The bigger is α, the smoother the field $a(\cdot, \mathrm{y})$.

The lognormal case

In the lognormal case

$$\boldsymbol{a}(\mathrm{x},\mathrm{y}) = \overline{a}(\mathrm{x}) + \mathbf{exp}\left(\sum_{j=1}^{\infty} \boldsymbol{y_j} \sqrt{\mu_j}\xi_j(\mathrm{x})\right), \qquad \mathrm{x} \in D,$$

- $\boldsymbol{y_j}$ are i.i.d. standard normal random numbers
- $\boldsymbol{\mu_j}, \boldsymbol{\xi_j}$ are the eigenvalues and normalized eigenfunctions of the covariance operator for the Gaussian random field in the exponent

What might we want to compute?

- The mean pressure at a particular point or over a particular small region
- The effective permeability
- The mean “breakthrough time”
- . . .

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All are expected values – and expected values are integrals.

If there are many random variables, then the expected values are high-dimensional integrals.

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$$I[F] := \int_{[0,1]^{\mathbb{N}}} F(\mathbf{y})\,\mathrm{d}\mathbf{y}$$

$$:= \lim_{s\to\infty} \int_{[0,1]^s} F(y_1, \ldots, y_s, \tfrac{1}{2}, \tfrac{1}{2}, \ldots)\,\mathrm{d}y_1 \ldots \mathrm{d}y_s.$$

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Note that replacing $y_{s+1}, y_{s+2}, \ldots$ by $\frac{1}{2}$ is equivalent to replacing $a(\mathbf{x},\mathbf{y})$ by

$a_s(\mathbf{x},\mathbf{y}) \;:=\; \overline{a} + \sum_{j=1}^{s}(y_j - \frac{1}{2})\,\psi_j(\mathbf{x}).$

Many approaches:

- polynomial chaos,
- generalized polynomial chaos,
- stochastic Galerkin,
- stochastic collocation
- Monte Carlo
- multilevel Monte Carlo
- Quasi-Monte Carlo (QMC)
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All methods face serious challenges when the effective dimensionality is high. And when all else fails, people turn to Monte Carlo methods. QMC aims to beat Monte Carlo.

Many contributors:

Norbert Wiener, "The Homogeneous Chaos", 1938

Babuska/Nobile/Tempone, Babuska/Tempone/Zouraris, Barth/Schwab/Zollinger,

Charrier, Charrier/Scheichl/Teckentrup, Cliffe, Giles/Scheichl/Teckentrup, Cliffe,

Graham/Scheichl/Stals, Cohen/ Chkifa/Schwab, Cohen/De Vore/Schwab,

Graham/Scheichl/Ullmann, Hansen/Schwab, Harbrecht/Peters/Siebenmorgen,

Hoang/Schwab, Karniadakis/ Xiu, Kunoth/Schwab, Nobile/Tempone/Webster,

Schwab/Todor, Schillings/Schwab, Teckentrup/Scheichl/Giles/Ullmann, Webster

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And for QMC applied to PDE with random coefficients:

Graham/Kuo/Nuyens/Scheichl/Sloan 2011 (lognormal case, no error analysis, circulant embedding), Kuo/Schwab/Sloan (uniform case with error analysis), Kuo/Schwab/Sloan (multi-level for the uniform case), Schwab (uniform case, general operator equations), Le Gia (uniform case for sphere), Graham/Kuo/Nichols/Scheichl/Schwab/Sloan (lognormal case, analysis and numerics), Graham/Kuo/Scheichl/Schwab/Sloan/Ullmann), (multi-level lognormal case), Harbrecht/Peters/Siebenmorgen

Monte Carlo (MC)

$$Q^{\mathrm{MC}}_{N,s}(F) := \frac{1}{N}\sum_{k=1}^{N} F(\mathbf{t}_k),$$

with $\mathbf{t}_1,\ldots,\mathbf{t}_N$ chosen **randomly** and independently from a uniform distribution on $[0,1]^s$.

Quasi-Monte Carlo

For QMC we take

$$I_s(F) \approx Q_{N,s}(F) := \frac{1}{N} \sum_{k=1}^{N} F(\mathrm{t}_k) \ ,$$

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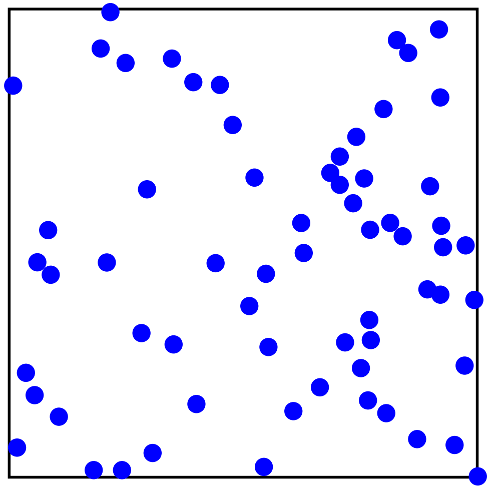
How to choose $\mathbf{t}_1, \ldots, \mathbf{t}_N$?

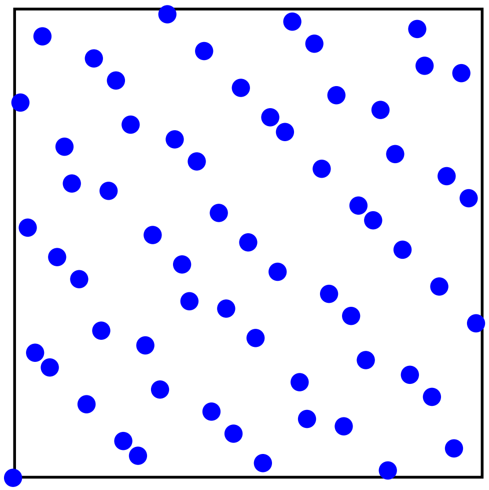
MC and QMC points for 2 dimensions

$$I_s(F) \approx \frac{1}{N}\sum_{k=1}^{N} F(\mathbf{t}_k), \quad \mathbf{t}_k \in [0,1]^s$$

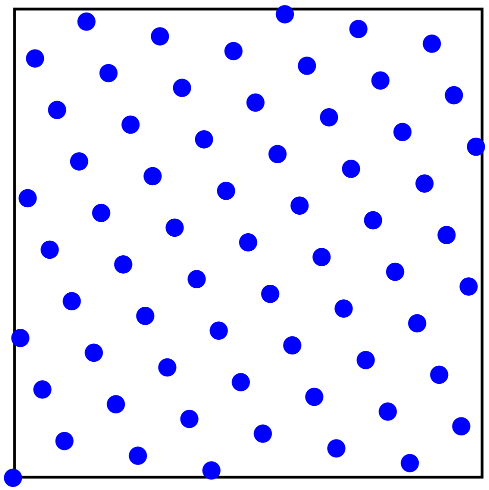
The points:



Monte Carlo method
with 64 “random” points



First 64 points of
2D Sobol′ sequence



A lattice rule
with 64 points

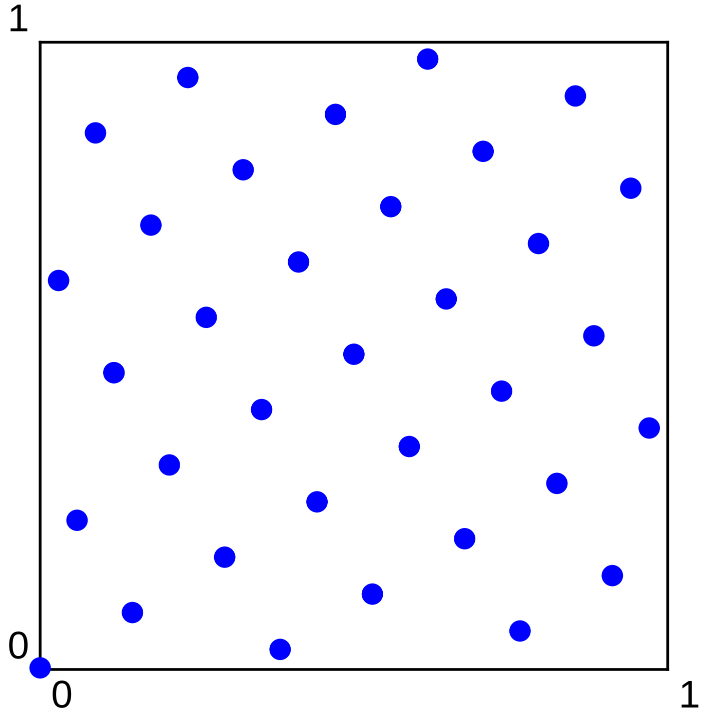
We consider only the simplest kind of lattice rule, given by

$$Q_{N,s}(\mathbf{z};F) = \frac{1}{N}\sum_{k=0}^{N-1} F\left(\left\{k\frac{\mathbf{z}}{N}\right\}\right),$$

where $\mathbf{z} \in \{1,\ldots,N-1\}^s$, and the braces mean that each component of the s-vector in the braces is to be replaced by its fractional part.

Example of lattice rule

$$N = 34, \mathbf{z} = (1, 21)$$



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- Fast convergence (or at at least better than the MC rate $O(N^{-1/2})$);
- And integration errors that are independent of s.

If we are to use a lattice rule **how to choose $\mathbf{z}$?**

Recall: the lattice rule for the integral over $[0,1]^s$ is

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Can we **construct** a good $\mathbf{z}$? Yes, it's possible!

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And choose z to minimise the "**worst-case error**" in H.

Worst-case error

Definition: The **worst case error** in the space H of a QMC rule $Q_{N,s}(P;\cdot)$ using the point set $P = \{\mathbf{t}_0, \mathbf{t}_1, \cdots, \mathbf{t}_{N-1}\}$ is

$$\boxed{e_{N,s}(P;H) := \sup_{\|F\|_H \le 1} |I_s(F) - Q_{N,s}(P;F)|},$$

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The following Hilbert space of functions has the big advantage that **the worst case error is computable**.

A good choice of H

A good choice for the norm squared of $\boldsymbol{F}$ in $\boldsymbol{H}$ is

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

where

$$(\mathbf{y}_{\mathfrak{u}}; \tfrac{\mathbf{1}}{\mathbf{2}})_j = \begin{cases} \boldsymbol{y}_{\boldsymbol{j}} \text{ if } \boldsymbol{j} \in \mathfrak{u}, \\ \frac{1}{2} \text{ if } j \notin \mathfrak{u}. \end{cases}$$

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The norm squared is the SUM OVER ALL SUBSETS $\mathfrak{u}$ OF $\{1,\ldots,s\}$.

For example, for $\mathfrak{u} = \{1,3\}$ the corresponding term is

$$\frac{1}{\gamma_{\{1,3\}}} \int_0^1 \int_0^1 \left| \frac{\partial^2 F}{\partial y_1 \partial y_3}(y_1, \tfrac{1}{2}, y_3, \tfrac{1}{2}, \tfrac{1}{2}, \ldots)\right|^2 \mathbf{d}y_1\mathbf{d}y_3$$

Weights

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

The norm squared is the SUM OVER ALL SUBSETS $\mathfrak{u}$ OF $\{1, \ldots, s\}$.

The term for subset $\mathfrak{u}$ is divided by the **weight** $\gamma_{\mathfrak{u}}$. So there are 2^s weights!

The weight $\gamma_{\mathfrak{u}}$ is a positive number that measures the importance of the subset $\mathfrak{u}$. A small weight forces the corresponding derivative to be small.

We denote by $H = H_{s,\boldsymbol{\gamma}}$ the space with weights $\{\gamma_{\mathfrak{u}}\}$.

What's so good about this H?

It's a reproducing kernel Hilbert space with a very simple kernel:

$$K(\mathbf{y},\mathbf{y}') = \sum_{\mathfrak{u}\subseteq\{1,\ldots,s\}} \gamma_{\mathfrak{u}} \prod_{j\in\mathfrak{u}} \eta(y_j, y_j') \quad , \quad \text{with}$$

$$\eta(y,y') = \begin{cases} \min(y,y') - \frac{1}{2} & \text{if } y, y' > \frac{1}{2}, \\ \frac{1}{2} - \max(y,y') & \text{if } y, y' < \frac{1}{2}, \\ 0 & \text{otherwise.} \end{cases}$$

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$K(\mathbf{y},\cdot) \in H$, and

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The great thing about a RKHS with kernel is that there is a simple formula for the worst-case error:

The worst case error in a RKHS

For the QMC rule with points $P = \{\mathbf{t}_0, \ldots, \mathbf{t}_{N-1}\}$ the squared WCE is:

$$\begin{aligned} e^2_{N,s}(P;H) &= \int_{[0,1]^s} \int_{[0,1]^s} K(\mathbf{y}, \mathbf{y}')\, d\mathbf{y}\, d\mathbf{y}' \\ &\quad - \frac{2}{N} \sum_{i=0}^{N-1} \int_{[0,1]^s} K(\mathbf{t}_i, \mathbf{y})\, d\mathbf{y} + \frac{1}{N^2} \sum_{i=0}^{N-1} \sum_{k=0}^{N-1} K(\mathbf{t}_i, \mathbf{t}_k), \end{aligned}$$

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$$\begin{aligned} e^2_{N,s}(P;H) &= \int_{[0,1]^s} \int_{[0,1]^s} K(\mathbf{y}, \mathbf{y}')\, \mathrm{d}\mathbf{y}\, \mathrm{d}\mathbf{y}' \\ &\quad - \frac{2}{N} \sum_{i=0}^{N-1} \int_{[0,1]^s} K(\mathbf{t}_i, \mathbf{y})\, \mathrm{d}\mathbf{y} + \frac{1}{N^2} \sum_{i=0}^{N-1} \sum_{k=0}^{N-1} K(\mathbf{t}_i, \mathbf{t}_k), \end{aligned}$$

Thus in a RKHS with a known kernel the WCE can be **computed**

except for the little fact that 2^s terms are needed for each $K(\mathbf{y}, \mathbf{y}')$! .

The case of product weights

Originally we considered only **product weights** (IHS and H Wozniakowski, 98),

$$\gamma_{\mathfrak{u}} = \prod_{j\in\mathfrak{u}} \alpha_j .$$

In this case the WCE is easily computed:

$$\left(\frac{1}{N} \sum_{k=0}^{N-1} \prod_{j=1}^{s} \left(1 + \alpha_j \left[B_2\left(\left\{\frac{kz_j}{N}\right\}\right) + \frac{1}{12} \right]\right) - \prod_{j=1}^{s} \left(1 + \frac{\alpha_j}{12}\right) \right)^{1/2},$$

where $B_2(x) := x^2 - x + 1/6$.

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where $B_2(x) := x^2 - x + 1/6$.

Actually, this is the worst case error in an appropriate root mean square sense for a **randomly shifted** lattice rule.

How to minimise the worst case error?

- Since $\mathbf{z}$ is an integer vector of length s, with values between 1 and $N-1$, in principle we could evaluate the WCE for all possible values of $\mathbf{z}$.

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- Since $\mathbf{z}$ is an integer vector of length s, with values between 1 and $N-1$, in principle we could evaluate the WCE for all possible values of $\mathbf{z}$.

- But that would be exponentially costly.

- Fortunately, we can provably get close to the best WCE by the **component-by-component (CBC) algorithm**:

CBC

The CBC algorithm: Korobov, IHS, Reztsov, Kuo, Joe

With CBC, a good generator $\mathbf{z} = (z_1, \ldots, z_s)$ is constructed one component at a time:

- choose $z_1 = 1$
- choose z_2 to minimise WCE for $s = 2$, then
- choose z_3 to minimise WCE for $s = 3$, then
- $\ldots$

so that at each step there are only (at most) $N - 1$ choices.

A naive implementation costs $O(s^2 N^2)$ operations.

Fast CBC

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The Nuyens and Cools implementation allows the CBC algorithm for product weights to be run with s in the thousands, N in the millions.

Now to fix the weights. This is what's new!

Recall the worst case error for integration over $[0,1]^s$:

$$e_{N,s,\boldsymbol{\gamma}}(\mathbf{t}_1,\ldots,\mathbf{t}_N) := \sup_{\|F\|_{s,\boldsymbol{\gamma}}\le 1} |I_s(F) - Q_{s,N}(F)| \,.$$

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Given F, we can use the resulting error bound:

$$\boxed{|I_s(F) - Q_{s,N}(F)| \le e_{N,s,\boldsymbol{\gamma}}(\mathbf{t}_1,\ldots,\mathbf{t}_N) \ \times\ \|F\|_{s,\boldsymbol{\gamma}}}$$

and choose weights that minimize the right-hand side

or some upper bound on the right-hand side.

Skipping details, for the PDE problem

$$\text{Error} \;\leq \frac{\boldsymbol{C}}{\boldsymbol{N}^{(1/2\boldsymbol{\lambda})}} \left(\sum_{0<|\mathfrak{u}|<\infty} \boldsymbol{\gamma}_{\mathfrak{u}}{}^{\boldsymbol{\lambda}} \boldsymbol{A}_{\mathfrak{u}} \right)^{1/2\boldsymbol{\lambda}} \times \left(\sum_{|\mathfrak{u}|<\infty} \frac{\boldsymbol{B}_{\mathfrak{u}}}{\boldsymbol{\gamma}_{\mathfrak{u}}} \right)^{1/2},$$

for all $\boldsymbol{\lambda} \in (\frac{1}{2}, 1]$, where $\boldsymbol{A}_{\mathfrak{u}} = \ldots$ and $\boldsymbol{B}_{\mathfrak{u}} = \ldots$.

We cannot take $\boldsymbol{\lambda} = \frac{1}{2}$ because $\boldsymbol{A}_{\mathfrak{u}} \to \infty$ as $\boldsymbol{\lambda} \to \frac{1}{2}+$.

Skipping details, for the PDE problem

$$\text{Error} \;\le\; \frac{C}{N^{(1/2\lambda)}} \left(\sum_{0<|\mathfrak{u}|<\infty} {\gamma_{\mathfrak{u}}}^{\lambda} A_{\mathfrak{u}} \right)^{1/2\lambda} \times \left(\sum_{|\mathfrak{u}|<\infty} \frac{B_{\mathfrak{u}}}{\gamma_{\mathfrak{u}}} \right)^{1/2},$$

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We cannot take $\lambda = \frac{1}{2}$ because $A_{\mathfrak{u}} \to \infty$ as $\lambda \to \frac{1}{2}+$.

Minimising the product yields:

$$\gamma_{\mathfrak{u}} = \left(\frac{B_{\mathfrak{u}}}{A_{\mathfrak{u}}} \right)^{1/(1+\lambda)} = (|\mathfrak{u}|!)^{\frac{2}{1+\lambda}} \prod_{j\in\mathfrak{u}} \alpha_j, \quad \alpha_j = \ldots$$

The $\gamma_{\mathfrak{u}}$ are “POD” (for product and order dependent) weights.

For the PDE application assuming exact PDE solution

Convergence theorem. (Kuo/Schwab/IHS 2012) If $\mathbf{z}$ is chosen by CBC, using the minimising weights, then with $F(\mathrm{y}) = G(u(\mathrm{y}))$,

$$\text{Cubature error for approximating } F \le \frac{C_\delta}{N^{1-\delta}}. \quad \text{for all } \delta > 0.$$

And generalizations ....

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And generalizations ....

The error is independent of s provided $\sum_{j=1}^{\infty} \|\psi_j\|_{\infty}^{2/3} < \infty$

Thus the convergence is **provably** faster than the Monte Carlo rate $N^{-1/2}$ – **and the CURSE OF DIMENSIONALITY has disappeared!**

What else is new?

- Similar analysis of the **lognormal** case.
- Analysis of a **multilevel** method for both uniform and lognormal cases:

[Kuo, Schwab, Sloan (to appear)]

$$I(G(u)) \approx Q_*^L(G(u)) = \sum_{\ell=0}^{L} Q_{s_\ell,n_\ell}\left(G(u_{h_\ell}^{s_\ell} - u_{h_{\ell-1}}^{s_{\ell-1}})\right)$$

$$\mathrm{cost} = \mathcal{O}\left(\sum_{\ell=0}^{L} s_\ell n_\ell {h_\ell}^{-d}\right)$$

What's newer still?

We know how to construct **higher order** QMC rules, with e.g. O(N^{-2}), and even how to apply them the above PDE problem.

(Dick, Kuo, Le Gia, Nuyens and Schwab 2015 for the uniform case)

[The best convergence rate achievable with a lattice rule is (close to) O(N^{-1}).]

Lattice rules are now replaced by **interlaced polynomial lattice rules**, and POD weights by **SPOD** weights (standing for "smoothness-driven product and order-dependent weights")

Now randomisation is not needed, and the rate of convergence is better: the theoretical convergence rate is $O(N^{-1/p})$, instead of $O(N^{-1/p+1/2})$ for lattice rules with $\frac{2}{3} < p \leq 1.$

But higher order QMC is still very new, and there are few calculations.

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Summarising the PDE+QMC story

- we truncate the ∞-dimensional problem at a high enough s;
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- using those good weights, we compute good a lattice parameter $\mathbf{z}$ by the fast CBC algorithm;
- using the corresponding lattice points $\mathbf{y}_k, k = 1, \ldots, N$ we compute the field $a(\mathbf{x}, \mathbf{y}_k)$, then find the approximate solution of the PDE and compute the quantity of interest (QOI), and then average the QOI over all N realisations;

Summarising the PDE+QMC story

- we truncate the ∞-dimensional problem at a high enough s;
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- using those good weights, we compute good a lattice parameter $\mathbf{z}$ by the fast CBC algorithm;
- using the corresponding lattice points $\mathbf{y}_k, k = 1, \ldots, N$ we compute the field $a(\mathbf{x}, \mathbf{y}_k)$, then find the approximate solution of the PDE and compute the quantity of interest (QOI), and then average the QOI over all N realisations;
- and so obtain rigorously and constructively **a convergence rate better than MC, and an error bound independent of s.**

But some cautions

- The constants may be very large.
- The numerical evidence is so far not completely convincing. We always do better than MC, but often no better than with an off-the-shelf QMC rule.
- For other high-dimensional applications the present theory cannot be applied at all (option pricing), or is way in the future (weather and climate).

Nevertheless, high-dimensional problems will not go away, and we are perhaps making some progress.

In the world of high dimensions, we live in interesting times!

Some reading

- I H Sloan, *What's new in high dimensional integration? – designing quasi-Monte Carlo for applications*, Proceedings of ICIAM 2015, Beijing, China, Higher Education Press, 2015. pp. 365–386.
- J. Dick, F.Y. Kuo, & I.H. Sloan, *Numerical integration in high dimensions – the Quasi Monte Carlo way*, Acta Numerica 2013.
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