



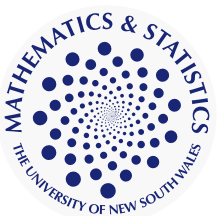
Liberating the Dimension

Quasi Monte Carlo Methods
for High Dimensional Integration

Frances Kuo

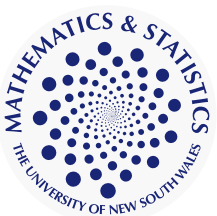
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Outline

- Motivating example – a flow through a porous medium
- Quasi-Monte Carlo (**QMC**) methods
- Component-by-component (**CBC**) construction
- Application of QMC to PDEs with random coefficients
 - uniform, lognormal
 - single level, multi-level
 - first order, higher order
- Other applications
 - maximum likelihood estimation
 - option pricing



Motivating example

Uncertainty in groundwater flow

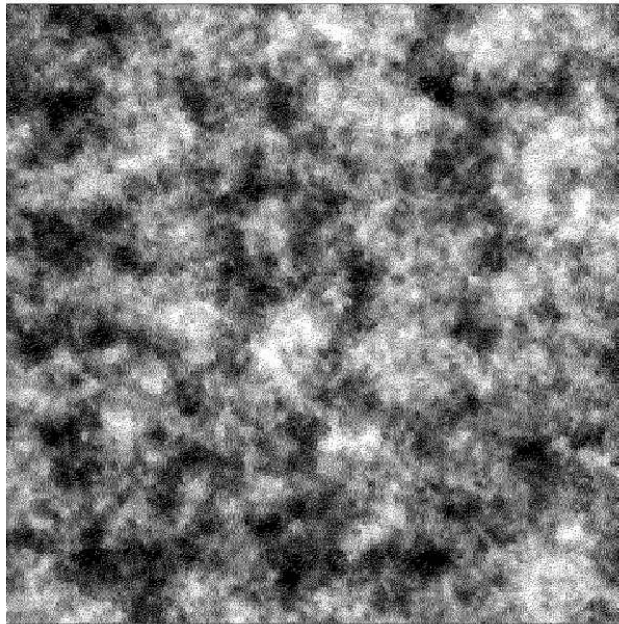
eg. risk analysis of radwaste disposal or CO₂ sequestration

Darcy's law

mass conservation law

$$\begin{aligned} q + a \vec{\nabla} p &= f \\ \nabla \cdot q &= 0 \end{aligned} \quad \text{in } D \subset \mathbb{R}^d, \quad d = 1, 2, 3$$

together with boundary conditions



[Cliffe, *et. al.* (2000)]

Uncertainty in $a(\mathbf{x}, \omega)$ leads to uncertainty in $q(\mathbf{x}, \omega)$ and $p(\mathbf{x}, \omega)$

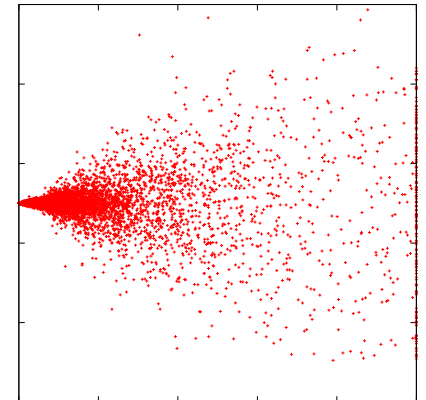
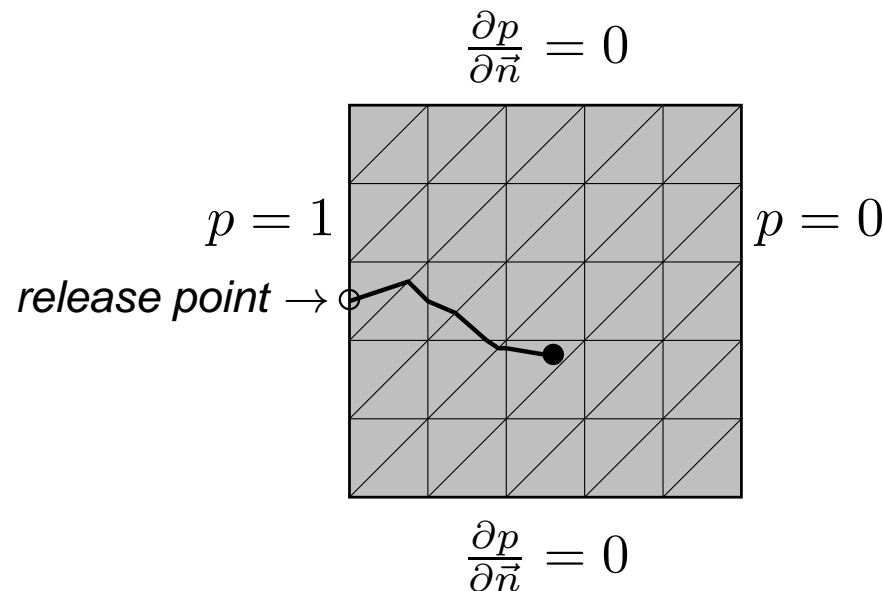
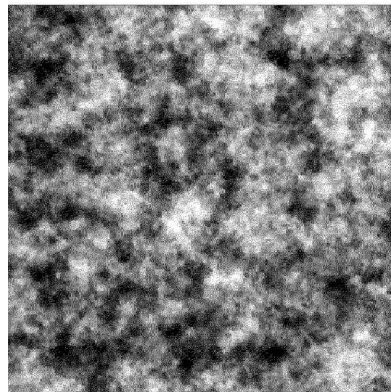
Expected values of quantities of interest

To compute the expected value of some quantity of interest:

1. Generate a number of realizations of the random field
(Some approximation may be required)
2. For each realization, solve the PDE using e.g. FEM / FVM / mFEM
3. Take the average of all solutions from different realizations

This describes **Monte Carlo simulation**.

Example: particle dispersion



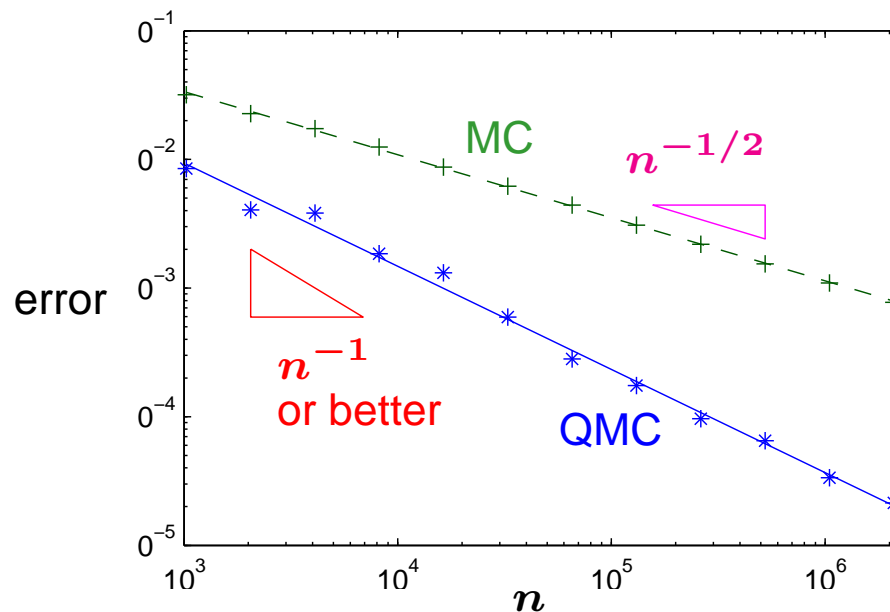
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NOTE: **expected value** = (high dimensional) **integral**



→ use **quasi-Monte Carlo methods**

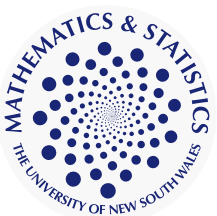
s = stochastic dimension

Curse of dimensionality

s = the number of variables = the dimension

How large is s in practical applications?

- Collateralized Mortgage Obligations (CMO)
30 years \times 12 monthly repayment calculations = 360 dimensions
- Daily counts of asthma patients seeking hospital treatments
5 years \times 365 days = 1825 dimensions
- Macquarie Bank ALPS series (a.k.a. CEO)
5 years \times 250 trading days \times 80 stocks = one million dimensions
- Porous flow with permeability modeled as a random field
501 by 501 mesh with circulant embedding = one million dimensions
Karhunen-Loève expansion of covariance function = ∞ dimensions



MC v.s. QMC in the unit cube

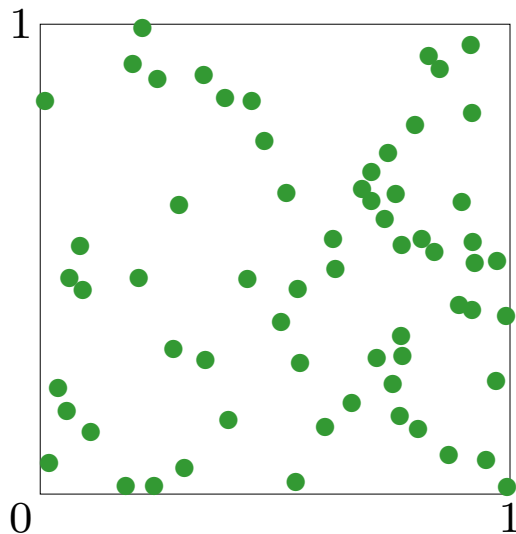
$$\int_{[0,1]^s} F(\mathbf{y}) \, d\mathbf{y} \approx \frac{1}{n} \sum_{i=1}^n F(\mathbf{t}_i)$$

Monte Carlo method

\mathbf{t}_i random uniform

$n^{-1/2}$ convergence

order of variables irrelevant



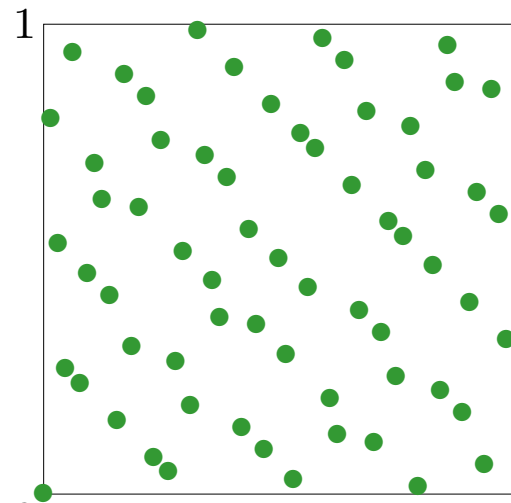
64 random points

Quasi-Monte Carlo methods

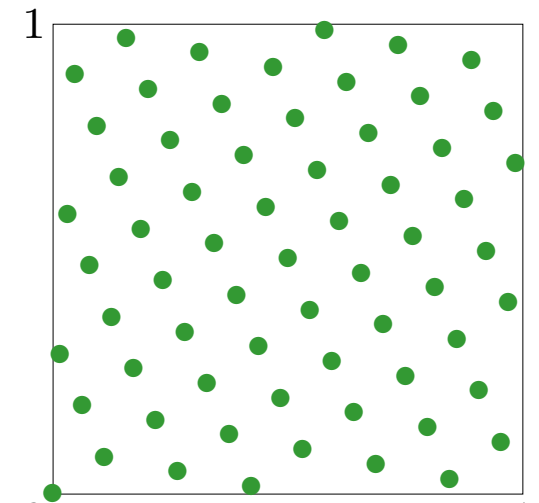
\mathbf{t}_i deterministic

close to n^{-1} convergence or better

more effective for earlier variables and lower-order projections
order of variables very important



First 64 points of a
2D Sobol' sequence



A lattice rule with 64 points

use *randomized* QMC methods for error estimation

QMC

Two main families of QMC methods:

- **(t,m,s)-nets** and **(t,s)-sequences**
- **lattice rules**

Niederreiter book (1992)

Sloan and Joe book (1994)

Important developments:

- **component-by-component (CBC) construction**
- **higher order digital nets**

Dick and Pillichshammer book (2010)

Dick, Kuo, Sloan Acta Numerica (2013)

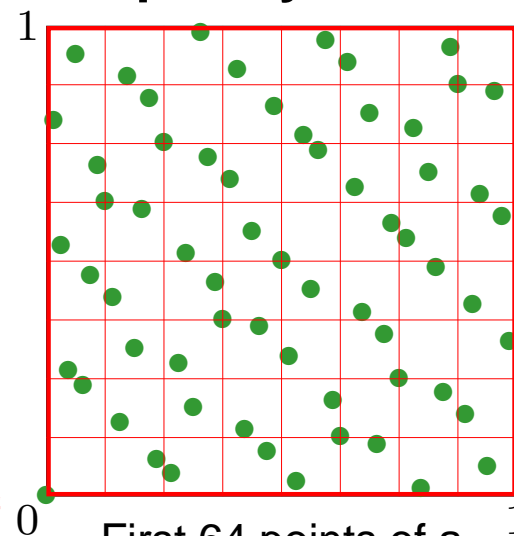
Contribute to:

- **Information-Based Complexity**
- **Tractability**

Traub, Wasilkowski, Woźniakowski book (1988)

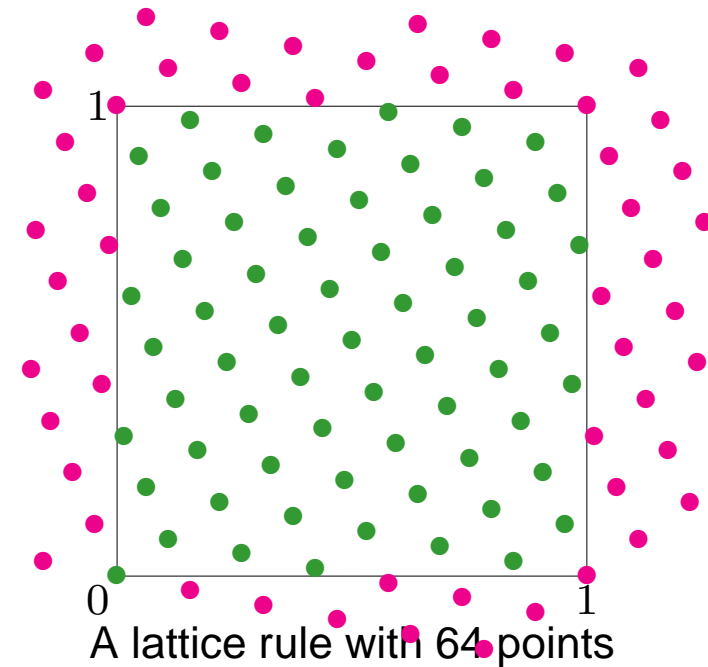
Novak and Woźniakowski books (2008, 2010, 2012)

A group under addition modulo \mathbb{Z} and includes the integer points

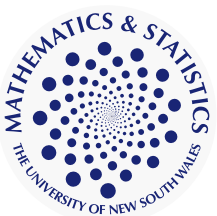


Having the right number of points in various sub-cubes

First 64 points of a 2D Sobol' sequence (0,6,2)-net



A lattice rule with 64 points



Lattice rules

Rank-1 lattice rules have points

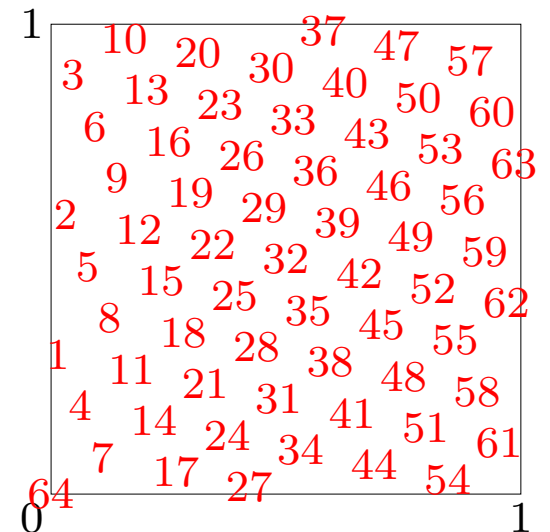
$$\mathbf{t}_i = \text{frac} \left(\frac{i}{n} \mathbf{z} \right), \quad i = 1, 2, \dots, n$$

$\mathbf{z} \in \mathbb{Z}^s$ – the **generating vector**, with all components *coprime* to n

$\text{frac}(\cdot)$ – means to take the fractional part of all components

~ quality determined by the choice of \mathbf{z} ~

$$n = 64 \quad \mathbf{z} = (1, 19) \quad \mathbf{t}_i = \text{frac} \left(\frac{i}{64} (1, 19) \right)$$



A lattice rule with 64 points

Component-by-component construction

- Want to find \mathbf{z} with (shift-averaged) “*worst case error*” as small possible.
~ Exhaustive search is practically impossible - too many choices! ~
- **CBC algorithm** [Sloan, K., Joe (2002);...]
 1. Set $z_1 = 1$.
 2. With z_1 fixed, choose z_2 to minimize the worst case error in 2D.
 3. With z_1, z_2 fixed, choose z_3 to minimize the worst case error in 3D.
 4. etc.
- Cost of algorithm is only $\mathcal{O}(n \log n s)$ using FFTs. [Nuyens, Cools (2005)]
- Optimal rate of convergence $\mathcal{O}(n^{-1+\delta})$ in “weighted Sobolev space”, with the implied constant independent of s under an appropriate condition on the weights. [K. (2003); Dick (2004)]
~ Averaging argument: there is always one choice as good as average! ~
- Extensible/embedded variants. [Cools, K., Nuyens (2006);
Dick, Pillichshammer, Waterhouse (2007)]

<http://www.maths.unsw.edu.au/~fkuo/lattice/>

<http://www.maths.unsw.edu.au/~fkuo/sobol/>

Application of QMC theory

Worst case error bound

$$\left| \int_{[0,1]^s} F(\mathbf{y}) \, d\mathbf{y} - \frac{1}{n} \sum_{i=1}^n F(\mathbf{t}_i) \right| \leq e_{\gamma}^{\text{wor}}(\mathbf{t}_1, \dots, \mathbf{t}_n) \|F\|_{\gamma}$$

Weighted Sobolev space

[Sloan & Woźniakowski, 1998]

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

2^s subsets \nearrow γ_u "weights" \uparrow "anchor" at 0 (also "unanchored")

Mixed first derivatives are square integrable

Small weight γ_u means that F depends weakly on the variables \mathbf{y}_u

Choose weights to minimize the error bound

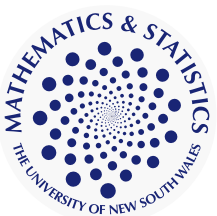
$$\underbrace{\left(\frac{2}{n} \sum_{u \subseteq \{1:s\}} \gamma_u^{\lambda} a_u \right)^{1/(2\lambda)}}_{\text{bound on worst case error (CBC)}} \underbrace{\left(\sum_{u \subseteq \{1:s\}} \frac{b_u}{\gamma_u} \right)^{1/2}}_{\text{bound on norm}} \Rightarrow \gamma_u = \left(\frac{b_u}{a_u} \right)^{1/(1+\lambda)}$$

Construct points (CBC) to minimize the worst case error

PDEs with random coefficients

Many important results using various methods by

- 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
- Kunothe, Schwab
- Nobile, Tempone, Webster
- Schwab, Todor
- Schillings, Schwab
- Teckentrup, Scheichl, Giles, Ullmann
-



See also http://people.maths.ox.ac.uk/~gilesm/mlmc_community.html

Application of QMC to PDEs with random coefficients

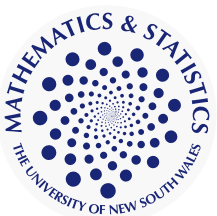
- Graham, K., Nuyens, Scheichl, Sloan (J. Comput. Physics, 2011)
 - Application of QMC to the **lognormal** case, no error analysis
 - Use **circulant embedding** to avoid truncation of KL expansion

- ✓ ● K., Schwab, Sloan (SIAM J. Numer. Anal., 2012)
 - Application of QMC to the **uniform** case [cf. Cohen, De Vore, Schwab, 2010]
 - **First complete error analysis: how to choose “weights”**

- ✓ ● K., Schwab, Sloan (J. FoCM, to appear) [cf. Heinrich 1998; Giles 2008]
 - A **multi-level** version of the analysis for the **uniform** case

- Schwab (Proceedings of MCQMC 2012)
 - Application of QMC to the **uniform** case for **affine** operator equations

- Le Gia (Proceedings of MCQMC 2012)
 - Application of QMC to the **uniform** case for PDE over the **sphere**

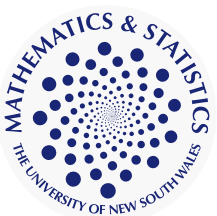


Application of QMC to PDEs with random coefficients

- ✓ ● Dick, K., Le Gia, Nuyens, Schwab (SIAM J. Numer. Anal., 2014)
 - Application of **higher order QMC** to the **uniform** case
- ✓ ● Dick, K., Le Gia, Schwab (submitted)
 - A **multi-level** version of the **higher order** analysis for the **uniform** case
- Dick, Le Gia, Schwab (submitted)
 - **Holomorphic extension** of the **higher order** analysis for the **uniform** case
- ✓ ● Graham, K., Nichols, Scheichl, Schwab, Sloan (Numer. Math., 2014)
 - Application of QMC to the **lognormal** case, full analysis and numerics
- Graham, K., Scheichl, Schwab, Sloan, Ullmann (in progress)
 - A **multi-level** version of the analysis for the **lognormal** case



Also QMC works by Harbrecht, Peters, Siebenmorgen



The uniform case

[K., Schwab, Sloan (2012)]

$$-\nabla \cdot (a(\mathbf{x}, \mathbf{y}) \nabla u(\mathbf{x}, \mathbf{y})) = f(\mathbf{x}) \text{ in } D, \quad u(\mathbf{x}, \mathbf{y}) = 0 \text{ on } \partial D$$

$$a(\mathbf{x}, \mathbf{y}) = \bar{a}(\mathbf{x}) + \sum_{j=1}^{\infty} y_j \psi_j(\mathbf{x}), \quad \mathbf{y} \in \left(-\frac{1}{2}, \frac{1}{2}\right)^{\infty}$$

Assumptions:

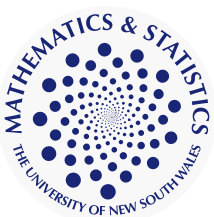
- There exists a_{\min} and a_{\max} such that $0 < a_{\min} \leq a(\mathbf{x}, \mathbf{y}) \leq a_{\max}$
- There exists $p_0 \in (0, 1]$ such that $\sum_{j=1}^{\infty} \|\psi_j\|_{L^{\infty}(D)}^{p_0} < \infty$
- ...

Goal: for $F(\mathbf{y}) = G(u(\cdot, \mathbf{y}))$ a linear functional of u , we want to approximate

$$\int_{\left(-\frac{1}{2}, \frac{1}{2}\right)^{\infty}} F(\mathbf{y}) \, d\mathbf{y} = \lim_{s \rightarrow \infty} \int_{\left(-\frac{1}{2}, \frac{1}{2}\right)^s} F(y_1, \dots, y_s, \mathbf{0}, \mathbf{0}, \dots) \, dy_1 \cdots dy_s$$

Our strategy:

- Truncate the infinite sum to s terms (truncation error)
- Solve the PDE using FEM (discretization error)
- Approximate the integral using QMC (quadrature error)



Error analysis – a sum of three terms

$$I(G(u)) \approx Q_{s,n}(G(u_h^s)) \\ = \frac{1}{n} \sum_{i=1}^n G(u_h^s(\cdot, \mathbf{t}_i))$$

- $\sum_{j=1}^{\infty} \|\psi_j\|_{L^\infty(D)}^{p_0} < \infty$
- $f \in H^{-1+t}(D)$
- $G \in H^{-1+t'}(D)$

- **Truncation error** = $\mathcal{O}(s^{-2(1/p_0-1)})$ use “integration”
- **Discretization error** = $\mathcal{O}(h^{t+t'})$ Aubin-Nitsche duality trick
- **Quadrature error** = $\mathcal{O}(n^{-\min(1/p_0-1/2, 1-\delta)})$ constant independent of s

- Differentiate the PDE w.r.t. \mathbf{y}

[Cohen, De Vore, Schwab, 2010]

$$\|\partial_{\mathbf{y}}^{\boldsymbol{\nu}} u(\cdot, \mathbf{y})\|_{H_0^1(D)} \leq C |\boldsymbol{\nu}|! \prod_{j \geq 1} \|\psi_j\|_{L^\infty(D)}^{\nu_j}$$

- Weighted Sobolev space with square-integrable mixed first derivatives
- Fast CBC construction of **randomly shifted lattice rules**
- Minimize error bound: get **POD weights** (product and order dependent)

$$\gamma_{\mathbf{u}} = (c^{|\mathbf{u}|} |\mathbf{u}|! \prod_{j \in \mathbf{u}} \|\psi_j\|_{L^\infty(D)})^b$$

Multi-level version

[K., Schwab, Sloan (to appear)]

$$\begin{aligned}
 I(G(u)) &\approx Q_*^L(G(u)) \\
 &= \sum_{\ell=0}^L Q_{s_\ell, n_\ell} \left(G(u_{h_\ell}^{s_\ell} - u_{h_{\ell-1}}^{s_{\ell-1}}) \right) \quad \text{cost} = \mathcal{O} \left(\sum_{\ell=0}^L s_\ell n_\ell h_\ell^{-d} \right)
 \end{aligned}$$

Key estimate (challenge):

$$\|G(u_{h_\ell}^{s_\ell} - u_{h_{\ell-1}}^{s_{\ell-1}})\|_\gamma \leq \|G(u_{h_\ell}^{s_\ell} - u_{h_{\ell-1}}^{s_\ell})\|_\gamma + \|G(u_{h_{\ell-1}}^{s_\ell} - u_{h_{\ell-1}}^{s_{\ell-1}})\|_\gamma$$

RMS error with randomly shifted lattice rules:

$$h_L^{t+t'} + s_L^{-2(1/p_0-1)} + \sum_{\ell=0}^L n_\ell^{-\min(1/p_1-1/2, 1-\delta)} \left(h_{\ell-1}^{t+t'} + s_{\ell-1}^{-(1/p_0-1/p_1)} \right)$$

New Assumption: there exists $p_1 \in [p_0, 1]$ s.t.

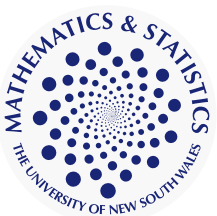
$$\sum_{j=1}^{\infty} \|\psi_j\|_{W^{1,\infty}(D)}^{p_1} < \infty$$

- differentiate PDE w.r.t. \mathbf{y}
- need stronger regularity w.r.t. \mathbf{x}
- use duality argument

- Constants are independent of truncation dimension s_L
- Minimize some error bound \Rightarrow get different POD weights
- Lagrange multipliers \Rightarrow choose s_ℓ, n_ℓ, h_ℓ

Higher order QMC rules

- Classical polynomial lattice rule [Niederreiter, 1992]
 - $n = b^m$ points with prime b
 - An irreducible polynomial with degree m
 - A generating vector of s polynomials with degree $< m$
- Interlaced polynomial lattice rule [Goda and Dick, 2012]
 - Interlacing factor α
 - An irreducible polynomial with degree m
 - A generating vector of αs polynomials with degree $< m$
 - Digit interlacing function $\mathcal{D}_\alpha : [0, 1)^\alpha \rightarrow [0, 1)$
 $(0.x_{11}x_{12}x_{13}\cdots)_b, (0.x_{21}x_{22}x_{23}\cdots)_b, \dots, (0.x_{\alpha 1}x_{\alpha 2}x_{\alpha 3}\cdots)_b$
becomes $(0.x_{11}x_{21}\cdots x_{\alpha 1}x_{12}x_{22}\cdots x_{\alpha 2}x_{13}x_{23}\cdots x_{\alpha 3}\cdots)_b$



Non-Hilbert, fast CBC, SPOD weights

$$\|F\|_{q,r} =$$

[Dick, K., Le Gia, Nuyens, Schwab (2014)]

$$\left[\sum_{u \subseteq \{1:s\}} \left(\frac{1}{\gamma_u^q} \sum_{v \subseteq u} \sum_{\tau_{u \setminus v} \in \{1:\alpha\}^{|u \setminus v|}} \int_{[0,1]^{|v|}} \left| \int_{[0,1]^{s-|v|}} (\partial_{\mathbf{y}}^{(\alpha_v, \tau_{u \setminus v}, \mathbf{0})} F)(\mathbf{y}) d\mathbf{y}_{\{1:s\} \setminus v} \right|^q d\mathbf{y}_v \right)^{r/q} \right]^{1/r}$$

- Combine L^q norm for functions and ℓ^r norm for vectors
- Recover Hilbert space setting with $q = r = 2$
- Obtain worst case error bound for digital nets
- Take $r = \infty$ and any q . Choose γ_u to make $\|F\|_{q,\infty} \leq c$.
- Get **SPOD weights** (smoothness-driven product and order dependent)

$$\gamma_u = \sum_{\nu_u \in \{1:\alpha\}^{|u|}} |\nu_u|! \prod_{j \in u} \left(c \|\psi_j\|_{L^\infty(D)}^{\nu_j} \right)$$

- Fast (using FFT) CBC construction with SPOD weights
 - Work with s blocks of α dimensions
 - Cost $\mathcal{O}(\alpha s n \log n + \alpha^2 s^2 n)$ operations

Higher order multi-level analysis

First order single level [K., Schwab, Sloan (2012)]

$$s^{-2(1/p_0-1)} + h^{t+t'} + n^{-\min(1/p_0-1/2, 1-\delta)}$$

First order multi-level [K., Schwab, Sloan (to appear)]

$$s_L^{-2(1/p_0-1)} + h_L^{t+t'} + \sum_{\ell=0}^L n_\ell^{-\min(1/p_1-1/2, 1-\delta)} \left(s_{\ell-1}^{-(1/p_0-1/p_1)} + h_{\ell-1}^{t+t'} \right)$$

Higher order single level [Dick, K., Le Gia, Nuyens, Schwab (2014)]

$$s^{-2(1/p_0-1)} + h^{t+t'} + n^{-1/p_0}$$

Higher order multi-level [Dick, K., Le Gia, Schwab (submitted)]

$$s_L^{-2(1/p_0-1)} + h_L^{t+t'} + \sum_{\ell=0}^L n_\ell^{-1/p_t} \left(s_{\ell-1}^{-(1/p_0-1/p_t)} + h_{\ell-1}^{t+t'} \right)$$

- New assumption: there exists $p_t \in [p_0, 1]$ s.t. $\sum_{j=1}^{\infty} \|\psi_j\|_{\mathcal{X}_t}^{p_t} < \infty$
- In many examples $p_t = p_0 / (1 - tp_0)$
- Interlacing factor $\alpha = \lfloor 1/p_t \rfloor + 1 \geq 2$

QMC theory for integration over \mathbb{R}^s

Change of variables

$$\int_{\mathbb{R}^s} q(\mathbf{z}) \rho(\mathbf{z}) \, d\mathbf{z} = \int_{\mathbb{R}^s} F(\mathbf{y}) \prod_{j=1}^s \phi(y_j) \, d\mathbf{y} = \int_{[0,1]^s} F(\Phi^{-1}(\mathbf{w})) \, d\mathbf{w}$$

ϕ - any pdf, Φ - cdf, Φ^{-1} - icdf

$F \circ \Phi^{-1}$ rarely belongs to weighted Sobolev space

Norm with weight function [Wasilkowski & Woźniakowski (2000)]

$$\|F\|_{\gamma}^2 = \sum_{\mathbf{u} \subseteq \{1:s\}} \frac{1}{\gamma_{\mathbf{u}}} \int_{\mathbb{R}^{|\mathbf{u}|}} \left| \frac{\partial^{|\mathbf{u}|} F}{\partial \mathbf{y}_{\mathbf{u}}}(\mathbf{y}_{\mathbf{u}}; \mathbf{0}) \right|^2 \prod_{j=1}^s \psi^2(y_j) \, d\mathbf{y}_{\mathbf{u}}$$

weight function

Nichols & K. (2014) cf. [K., Sloan, Wasilkowski, Waterhouse (2010)]

- Also **unanchored** variant, coordinate dependent ψ_j
- Randomly shifted lattice rules CBC error bound for general weights $\gamma_{\mathbf{u}}$
- Convergence rate depends on the relationship between ϕ and ψ
- Fast CBC for POD weights $\gamma_{\mathbf{u}} = \Gamma_{|\mathbf{u}|} \prod_{j \in \mathbf{u}} \gamma_j$

Important for applications: ϕ and ψ and $\gamma_{\mathbf{u}}$ are up to us to choose (tune)

Application: the lognormal case

Elliptic PDE with lognormal random coefficient

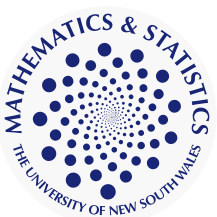
$$-\nabla \cdot (a(\mathbf{x}, \mathbf{y}) \nabla u(\mathbf{x}, \mathbf{y})) = f(\mathbf{x}), \quad \mathbf{x} \in D \subseteq \mathbb{R}^d, d = 1, 2, 3$$

$$a(\mathbf{x}, \mathbf{y}) = \exp \left(\sum_{j=1}^{\infty} \sqrt{\mu_j} \xi_j(\mathbf{x}) y_j \right), \quad y_j \sim \text{i.i.d. normal}$$

$$\int_{\mathbb{R}^{\infty}} G(u(\cdot, \mathbf{y})) \prod_{j=1}^{\infty} \phi_{\text{nor}}(y_j) d\mathbf{y} = \int_{[0,1]^{\infty}} G(u(\cdot, \Phi_{\text{nor}}^{-1}(\mathbf{x}))) d\mathbf{x}$$

Graham, K., Nichols, Scheichl, Schwab, Sloan (2014)

- Differentiate PDE to obtain bound on the norm
- Choose $\phi \equiv \phi_{\text{nor}}$
- Choose $\psi_j(y_j) = \exp(-\alpha_j y_j)$, $\alpha_j > 0$
- Choose POD weights $\gamma_u = \Gamma_{|u|} \prod_{j \in u} \gamma_j$

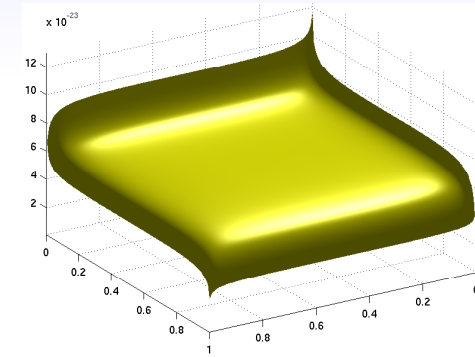


Application: maximum likelihood

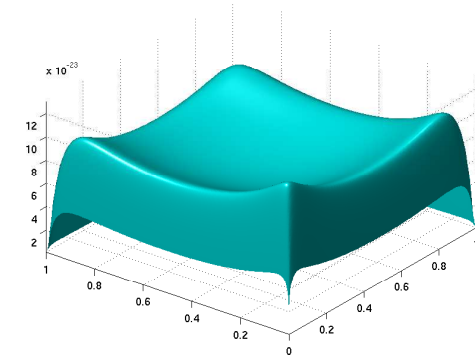
Generalized linear mixed model

[K., Dunsmuir, Sloan, Wand, Womersley (2008)]

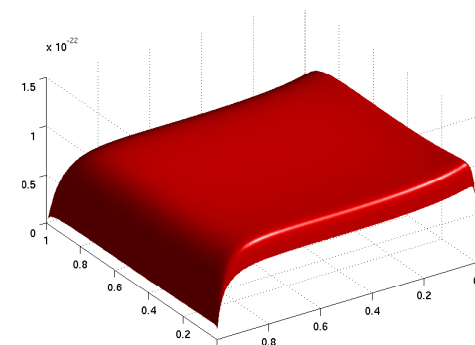
$$\int_{\mathbb{R}^s} \left(\prod_{j=1}^s \frac{\exp(\tau_j(\beta + z_j) - e^{\beta+z_j})}{\tau_j!} \right) \frac{\exp(-\frac{1}{2}\mathbf{z}^T \Sigma^{-1} \mathbf{z})}{\sqrt{(2\pi)^s \det(\Sigma)}} d\mathbf{z}$$



ϕ normal (good)



ϕ logistic (better)



ϕ Student-t (best)

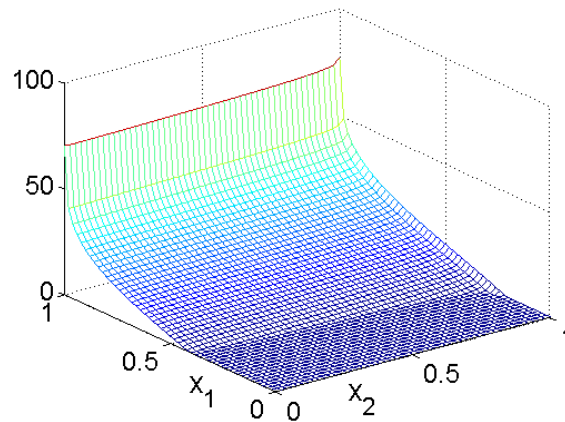
Sinescu, K., Sloan (2013)

- Differentiate integrand to obtain bound on the norm
- Choose $\phi \equiv \phi_{\text{nor}}$ or ϕ_{logit} or ϕ_{stud}
- Choose $\psi \equiv \mathbf{1}$
- Choose POD weights $\gamma_u = \Gamma_{|u|} \prod_{j \in u} \gamma_j$

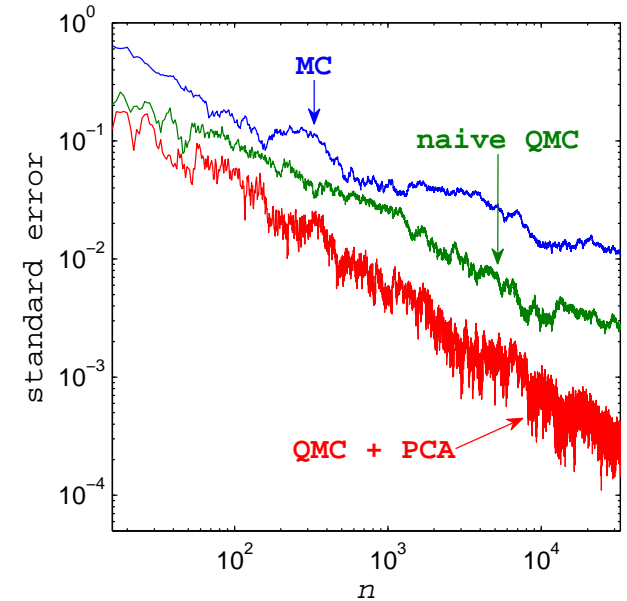
Application: option pricing

Black-Scholes model

$$\int_{\mathbb{R}^s} \max\left(\frac{1}{s} \sum_{j=1}^s S_j(\mathbf{z}) - K, 0\right) \frac{\exp(-\frac{1}{2} \mathbf{z}^T \Sigma^{-1} \mathbf{z})}{\sqrt{(2\pi)^s \det(\Sigma)}} d\mathbf{z}$$



$$S_j(\mathbf{z}) = \exp(\dots \sum a_j z_j)$$



Griebel, K., Sloan (2010, 2013, 2014)

- ANOVA decomposition: $g = \sum_{\mathbf{u} \subseteq \{1:s\}} g_{\mathbf{u}}$ in $[0, 1]^s$ or $f = \sum_{\mathbf{u}} f_{\mathbf{u}}$ in \mathbb{R}^s
- RW/BB: all $g_{\mathbf{u}}$ with $|\mathbf{u}| \leq \frac{s+1}{2}$ belong to Sobolev space; PCA: similar
- RW/BB: all $f_{\mathbf{u}}$ with $\mathbf{u} \neq \{1 : s\}$ are smooth; PCA: similar
- ANOVA decomposition for ∞ -variate function f : all terms are smooth
- Remains to see how to apply the theory of Nichols & K. (2014)