A Belgian view on lattice rules

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Atomium – Brussels

built in 1958

height ≈ 103m

figure = 2€ coin
$5 \cdot 10^6$ in circulation

Body centered cubic lattice

Introduction

Given is an integral

$$I[f] := \int_\Omega w(\mathbf{x}) f(\mathbf{x})\, \mathrm{d}\mathbf{x}$$

where $\Omega \subseteq \mathbb{R}^s$ and $w(\mathbf{x}) \geq 0$, $\forall \mathbf{x} \in \mathbb{R}^s$.
Search an approximation for $I[f]$

$$I[f] \simeq Q[f] := \sum_{j=1}^{n} w_j f(\mathbf{y}^{(j)})$$

with $w_j \in \mathbb{R}$ and $\mathbf{y}^{(j)} \in \mathbb{R}^s$.
Webster:
quadrature: the process of finding a square equal in area to a given area.
cubature: the determination of cubic contents.
If $s = 1$ then Q is called a quadrature formula.
If $s \geq 2$ then Q is called a cubature formula.

$$Q[f] := \sum_{j=1}^{n} w_j f(\mathbf{y}^{(j)})$$

Cubature/quadrature formulas are basic integration rules
$\rightarrow$ choose points $\mathbf{y}^{(j)}$ and weights w_j independent of integrand f.

It is difficult (time consuming) to construct basic integration rules, but the result is usually hard coded in programs or tables.

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Restriction to unit cube: given is

$$I[f] = \int_0^1 \cdots \int_0^1 f(x_1, \ldots, x_s) \mathrm{d}x_1 \cdots \mathrm{d}x_s = \int_{[0,1)^s} f(\mathbf{x}) \mathrm{d}\mathbf{x}$$

Taxonomy: two major classes

1. polynomial based methods
   incl. methods exact for algebraic or trigonometric polynomials
2. number theoretic methods
   incl. Monte Carlo and quasi-Monte Carlo methods

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For example

Definition

An s-dimensional lattice rule is a cubature formula which can be expressed in the form

$$Q[f] = \frac{1}{d_1 d_2 \dots d_t} \sum_{j_1=1}^{d_1} \sum_{j_2=1}^{d_2} \dots \sum_{j_t=1}^{d_t} f\left(\left\{ \frac{j_1 \mathbf{z}_1}{d_1} + \frac{j_2 \mathbf{z}_2}{d_2} + \dots + \frac{j_t \mathbf{z}_t}{d_t} \right\}\right),$$

where $d_i \in \mathbb{N}_0$ and $\mathbf{z}_i \in \mathbb{Z}^s$ for all i.

Alternative formulation:

Definition

A multiple integration lattice Λ is a subset of $\mathbb{R}^s$ which is discrete and closed under addition and subtraction and which contains $\mathbb{Z}^s$ as a subset.

Definition

A lattice rule is a cubature formula where the n points are the points of a multiple integration lattice Λ that lie in $[0,1)^s$ and the weights are all equal to $1/n$.

$$n = n(Q) = \#\{\Lambda \cap [0,1)^s\} \ .$$

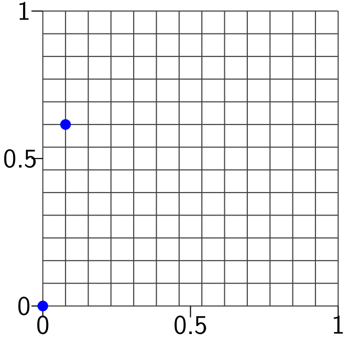
Example

The Fibonnaci lattice with $n = F_j$ and $\mathbf{z} = (1, F_{j-1})$

has points $\mathbf{x}^{(j)} = \left(\frac{j}{F_j}, \frac{jF_{j-1}}{F_j}\right)$

$$\Rightarrow \text{lattice rule } Q[f] = \frac{1}{n}\sum_{j=0}^{n-1} f\left(\left\{\frac{(j, jF_{j-1})}{n}\right\}\right)$$

Example: the lattice rule with $n = d_1 = F_7 = 13$ and $\mathbf{z}_1 = (1, 8)$



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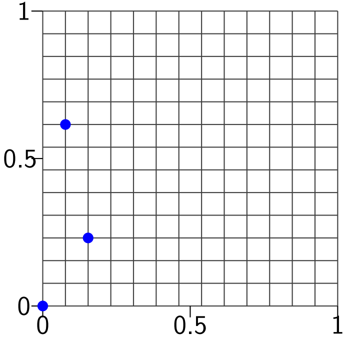

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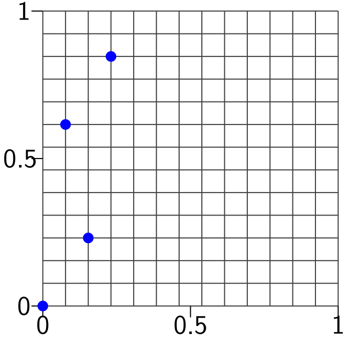

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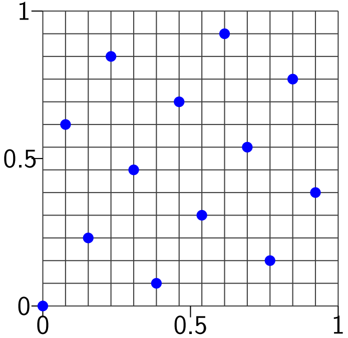

Polynomials

Let $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_s) \in \mathbb{Z}^s$ and $|\alpha| := \sum_{j=1}^{s} |\alpha_j|$.

algebraic polynomial

$$p(\mathbf{x}) = \sum a_\alpha \mathbf{x}^\alpha = \sum a_\alpha \prod_{j=1}^{s} x_j^{\alpha_j}, \quad \text{with } \alpha_j \geq 0$$

trigonometric polynomial

$$t(\mathbf{x}) = \sum a_\alpha e^{2\pi i \alpha \cdot \mathbf{x}} = \sum a_\alpha \prod_{j=1}^{s} e^{2\pi i x_j \alpha_j}$$

The degree of a polynomial $= \max_{a_\alpha \neq 0} |\alpha|$.

$\mathbb{P}_d^s$ = all algebraic polynomials in s variables of degree at most d.

$\mathbb{T}_d^s$ = all trigonometric polynomials in s variables of degree at most d.

Quality criteria?

Definition

A cubature formula Q for an integral I has algebraic (trigonometric) degree d if it is exact for all polynomials of algebraic (trigonometric) degree at most d.

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How many points are needed in a cubature formula to obtain a specified degree of precision?

The dimensions of the vector spaces of polynomials are:

$$\dim \mathbb{P}_d^s = \binom{s+d}{d}$$

$$\dim \mathbb{T}_d^s = \sum_{j=0}^{s} \binom{s}{j} \binom{d}{j} 2^j.$$

We will use the symbol $\mathbb{V}_d^s$ to refer to one of the vector spaces $\mathbb{P}_d^s$ or $\mathbb{T}_d^s$.

Theorem

If a cubature formula is exact for all polynomials of $\mathbb{V}_{2k}^s$*, then the number of points* $n \geq \dim \mathbb{V}_k^s$.

Algebraic degree: For $s = 2$ (Radon, 1948); general s (Stroud, 1960)
Trigonometric degree: (Mysovskikh, 1987)

J. Radon

A. Stroud

И.П. Мысовских

Theorem

If a cubature formula is exact for all polynomials of degree $d > 0$ and has only real points and weights, then it has at least $\dim \mathbb{V}_k^s$ positive weights, $k = \lfloor \frac{d}{2} \rfloor$.

Algebraic degree: (Mysovskikh, 1981)
Trigonometric degree: (C. 1997)
$\Rightarrow$ minimal formulas have only positive weights.

Corollary

If a cubature formula of trigonometric degree $2k$ has $n = \dim \mathbb{T}_k^s$ points, then all weights are equal.

This is a reason to restrict searches to

$$Q[f] = \frac{1}{n} \sum_{j=1}^{n} f(\mathbf{x}_j).$$

Improved bound for odd degrees

For algebraic degree, the improved lower bound for odd degrees takes into account the symmetry of the integration region.

E.g., centrally symmetric regions such as a cube
$\rightarrow$ (Möller, 1973)

H.M. Möller

Result for trigonometric degree is very similar.

Improved bound for odd degrees

$G_k :=$ span of trigonometric monomials of degree $\leq k$ with the same parity as k.

Theorem ((Noskov, 1985), (Mysovskikh, 1987))

The number of points n of a cubature formula for the integral over $[0,1)^s$ which is exact for all trigonometric polynomials of degree at most $d = 2k+1$ satisfies

$$n \geq 2 \dim G_k.$$

Definition

A cubature formula is called shift symmetric if it is invariant w.r.t. the group of transformations

$$\left\{ \mathbf{x} \mapsto \mathbf{x}, \mathbf{x} \mapsto \{\mathbf{x} + (\frac{1}{2}, \ldots, \frac{1}{2})\} \right\}$$

(*This is the 'central symmetry' for the trig. case.*)

Theorem (Beckers & C., 1993)

If a shift symmetric cubature formula of degree $2k+1$ *has* $n = 2 \dim G_k$ *points, then all weights are equal.*

Conjecture (C., 1997)

Any cubature formula that attains the lower bound is shift symmetric.

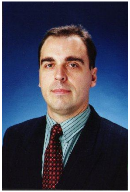
This became a Theorem (Osipov, 2001).

Known minimal formulas for trigonometric degree

- for all s
  - degree 1
  - degree 2 (Noskov, 1988)
  - degree 3 (Noskov, 1988)
- for $s = 2$
  - all even degrees (Noskov, 1988)
  - all odd degrees
    (Reztsov, 1990) (Beckers & C., 1993) (C. & Sloan, 1996)
- for $s = 3$
  - degree 5 (Frolov, 1977)

M. Beckers

M.B. Носков



A. Резцов

I.H. Sloan

All known minimal formulas of trigonometric degree are lattice rules, except...

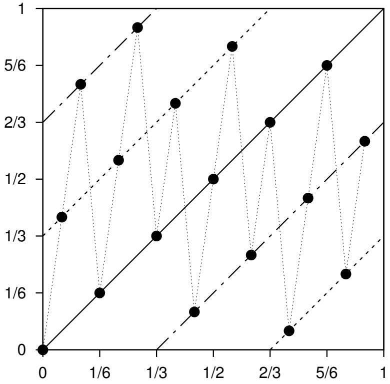
All known minimal formulas of trigonometric degree are lattice rules, except...

Theorem (C. & Sloan, 1996)

The following points

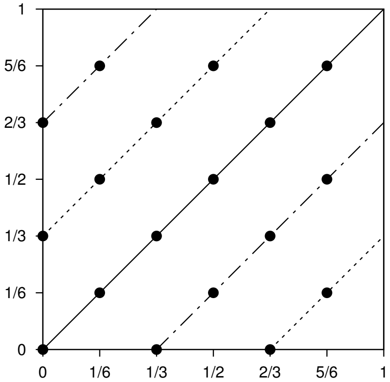
$$\left(C_p + \frac{j}{2(k+1)}, C_p + \frac{j+2p}{2(k+1)}\right) \quad \begin{array}{rcl} j & = & 0, \ldots, 2k+1 \\ p & = & 0, \ldots, k \end{array}$$

with $C_0 = 0$ *and* $C_1, \ldots, C_k$ *arbitrary are the points of a minimal cubature formula of trigonometric degree* $2k+1$.



$k = 2$, $n = 18$, $C_1 = \frac{1}{18}$, $C_2 = \frac{1}{9}$

$$Q[f] = \frac{1}{n} \sum_{j=0}^{n-1} f\left(\frac{j}{n}, \frac{j(2m+1)}{n}\right) \quad \text{with} \quad n = 2(m+1)^2$$



$k = 2$, $n = 18$, $C_1 = C_2 = 0$: body-centered cubic lattice

$$Q[f] = \frac{1}{2(m+1)^2} \sum_{k=0}^{2m+1} \sum_{j=0}^{m} f\left(\frac{2j+k}{2(m+1)}, \frac{k}{2(m+1)}\right) \quad \text{with} \quad n = 2(m+1)^2$$

Technology used to obtain these results: Reproducing kernels

The integral I defines an inner product $(\phi, \psi) = I[\overline{\phi} \cdot \psi]$.
Let $\mathbb{F}$ be a subspace of $\mathbb{T}^s$.
Choose $\phi_1(\mathbf{x}), \phi_2(\mathbf{x}), \ldots \in \mathbb{F}$ so that

- $\phi_i(\mathbf{x})$ is I-orthogonal to $\phi_j(\mathbf{x})$, $\forall j < i$, and
- $(\phi_i(\mathbf{x}), \phi_i(\mathbf{x})) = 1$.

For a given $k \in \mathbb{N}$ and $t := \dim(\mathbb{F} \cap \mathbb{T}^s_k)$ we define

$$K(\mathbf{x}, \mathbf{y}) := \sum_{j=1}^{t} \overline{\phi_j(\mathbf{x})} \cdot \phi_j(\mathbf{y})$$

$K(\mathbf{x}, \mathbf{y})$ is a polynomial in $2s$ variables of degree $\leq 2k$.

Definition

K is a reproducing kernel in the space $\mathbb{F} \cap \mathbb{T}_k^s$

$$\text{if } f \in \mathbb{F} \cap \mathbb{T}_k^s \text{ then } f(\mathbf{a}) = (f(\mathbf{x}), K(\mathbf{x}, \mathbf{a})) = \sum_{j=1}^{t} \phi_j(\mathbf{a}) \cdot I[f(\mathbf{x})\overline{\phi_j}(\mathbf{x})]$$

The trigonometric monomials form an orthonormal sequence.

$$K(\mathbf{x}, \mathbf{y}) = \sum_{\mathbf{k} \in \Lambda_d} e^{2\pi i \mathbf{k} \cdot (\mathbf{x} - \mathbf{y})}$$

$$\Lambda_d = \{\mathbf{k} \in \mathbb{Z}^s : 0 \leq \sum_{l=1}^{s} |k_l| \leq \lfloor \frac{d}{2} \rfloor\}$$

A simplifying aspect of the trigonometric case is that the reproducing kernel is a function of one variable:

$$K(\mathbf{x},\mathbf{y}) = \mathcal{K}(\mathbf{x}-\mathbf{y})$$

with

$$\mathcal{K}(\mathbf{x}') = \sum_{\mathbf{k}\in\Lambda_d} e^{2\pi i \mathbf{k}\cdot\mathbf{x}'}$$

For $s = 2$ it has the following simple form:
let $g(z) = \cos(\pi(2\lfloor \frac{d}{2} \rfloor + 1)z)\ \cos \pi z$, then

$$\mathcal{K}(\mathbf{x}') = \frac{g(x_1) - g(x_2)}{\sin(\pi(x_1+x_2))\sin(\pi(x_1-x_2))}.$$

On route to other quality criteria

Assume f can be expanded into
an absolutely convergent multiple Fourier series

$$f(\mathbf{x}) = \sum_{\mathbf{h} \in \mathbb{Z}^s} \hat{f}(\mathbf{h}) e^{2\pi i \mathbf{h} \cdot \mathbf{x}}$$

with

$$\hat{f}(\mathbf{h}) = \int_{[0,1)^s} f(\mathbf{x}) e^{-2\pi i \mathbf{h} \cdot \mathbf{x}} \, \mathrm{d}\mathbf{x}$$

Then

$$Q[f] - I[f] = \frac{1}{n}\sum_{j=1}^{n}\left(\sum_{\mathbf{h}\in\mathbb{Z}^s\setminus\{0\}} \hat{f}(\mathbf{h})e^{2\pi i \mathbf{h}\cdot\mathbf{x}_j}\right)$$
$$= \sum_{\mathbf{h}\in\mathbb{Z}^s\setminus\{0\}}\left(\hat{f}(\mathbf{h})\frac{1}{n}\sum_{j=1}^{n} e^{2\pi i \mathbf{h}\cdot\mathbf{x}_j}\right).$$

Observe that

$$\frac{1}{n}\sum_{j=1}^{n} e^{2\pi i \mathbf{h}\cdot\mathbf{x}_j} = \begin{cases} 1, & \mathbf{h}\cdot\mathbf{x}_j \in \mathbb{Z} \\ 0, & \mathbf{h}\cdot\mathbf{x}_j \notin \mathbb{Z} \end{cases}$$

A very important tool to investigate the error of a lattice rule is . . .

Definition

The dual of the multiple integration lattice Λ

$$\Lambda^{\perp} := \{\mathbf{h} \in \mathbb{Z}^s \ : \mathbf{h} \cdot \mathbf{x} \in \mathbb{Z}, \forall \mathbf{x} \in \Lambda\}.$$

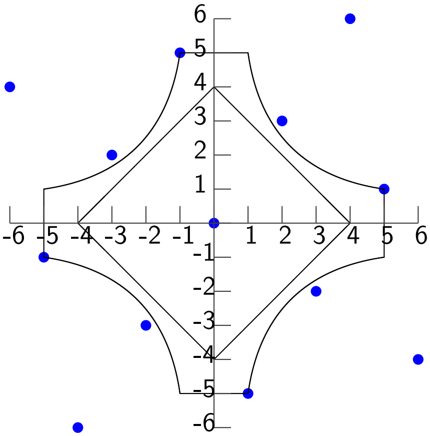
Theorem (Sloan & Kachoyan, 1987)

Let Λ be a multiple integration lattice.
Then the corresponding lattice rule Q has an error

$$Q[f] - I[f] = \sum_{\mathbf{h} \in \Lambda^{\perp} \setminus \{0\}} \hat{f}(\mathbf{h}).$$

Example

Dual lattice of Fibonnaci lattice



Construction criteria

For many years, only used in Russia...

Definition

The trigonometric degree is

$$d(Q) := \min_{\substack{\mathbf{h} \neq \mathbf{0} \\ \mathbf{h} \in \Lambda^\perp}} \left(\sum_{j=1}^{s} |h_j| \right) - 1 \,.$$

The enhanced degree $\delta := d + 1$.

Some names:
Mysovskikh (1985–1990), Reztsov (1990), Noskov (1985–1988), Temirgaliev (1991), Semenova (1996–1997), Osipov (2001–2010), Petrov (2004)

Construction criteria

Mainly used in the 'West'...

Definition

The Zaremba index or figure of merit is

$$\rho(Q) := \min_{\substack{\mathbf{h} \neq \mathbf{0} \\ \mathbf{h} \in \Lambda^\perp}} \left(\bar{h}_1 \bar{h}_2 \cdots \bar{h}_s\right) .$$

with

$$\bar{h}_j := \begin{cases} 1 & \text{if } h_j = 0 \\ |h_j| & \text{if } h_j \neq 0. \end{cases}$$

Some names:
Maisonneuve (1972), ..., Sloan & Joe (1994), Langtry (1996)

Where does this come from?

For $c > 0$ and fixed $\alpha > 1$,
let $E_s^\alpha(c)$ be the class of functions f
whose Fourier coefficients satisfy

$$|\hat{f}(\mathbf{h})| \le \frac{c}{(\overline{h}_1 \overline{h}_2 \cdots \overline{h}_s)^\alpha},$$

where $\overline{h} = \max(1, |h|)$.

Worst possible function in class $E_s^\alpha(1)$ is

$$f_\alpha := \sum_{\mathbf{h} \in \mathbb{Z}^s} \frac{1}{(\overline{h}_1 \overline{h}_2 \cdots \overline{h}_s)^\alpha} e^{2\pi i \mathbf{h} \cdot \mathbf{x}}$$

$P_\alpha(Q) :=$ the error of the lattice rule for f_α.

P_α is easy to compute for α an even integer
because f_α can be written as products of Bernoulli polynomials.

Theoretical convergence is

$$O\left((\log(n))^{\alpha s} n^{-\alpha}\right).$$

P_α introduced by (Korobov, 1959)

Obviously related to the figure of merit:

$$\frac{2}{\rho^\alpha} \leq P_\alpha.$$

Figure of merit used by (Maisonneuve, 1972)

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Other criteria:

- $R(\mathbf{z}, n)$ (Niederreiter, 1987)

$$P_\alpha(\mathbf{z}, n) < R(\mathbf{z}, n)^\alpha + \mathcal{O}(n^{-\alpha})$$

- Discrepancy

$$D_N = O\left(\frac{(\log N)^{s-1}}{\rho}\right)$$

H. Niederreiter

Yet another way to look at this

Assume f can be expanded into
an absolutely convergent multiple Fourier series

$$f(\mathbf{x}) = \sum_{\mathbf{h}\in\mathbb{Z}^s} \hat{f}(\mathbf{h}) e^{2\pi i \mathbf{h}\cdot\mathbf{x}} \quad \text{with} \quad \hat{f}(\mathbf{h}) = \int_{[0,1)^s} f(\mathbf{x}) e^{-2\pi i \mathbf{h}\cdot\mathbf{x}} \, \mathrm{d}\mathbf{x}$$

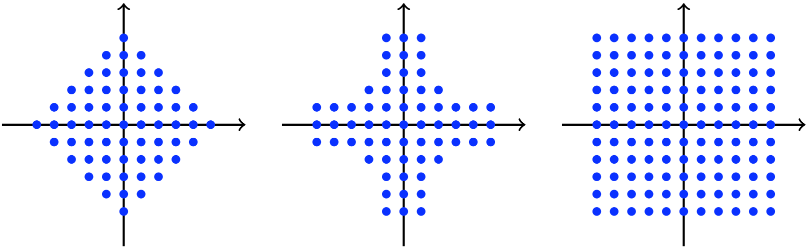
- Mark region of interest $\mathcal{A}_s(m)$ in Fourier domain of "degree" m.
- Ask to integrate those Fourier terms exactly, i.e.

$$\Lambda^\perp \cap \mathcal{A}_s(m) = \{\mathbf{0}\}.$$

- $\Rightarrow$ Rule of degree (at least) m.
- Different regions $\mathcal{A}_s(m)$ possible:
  - Trigonometric degree.
  - Zaremba cross degree.
  - Product trigonometric degree.
  - ...

Corresponding Fourier spectra

Take $m = 5$ (and $s = 2$):



Trigonometric degree | Zaremba degree | Product degree

For $s \to \infty$ these shapes grow exponentially.
Consequently the number of nodes grows exponentially.

Modern interpretation of P_α is the squared worst-case error in a RKHS with Korobov kernel with smoothness α.
In general, for a shift-invariant kernel K and rank-1 lattice points

$$e^2(\Lambda, K) = -\int_{[0,1)^s} K(\mathbf{x}, \mathbf{0}) \, \mathrm{d}\mathbf{x} + \frac{1}{n} \sum_{k=0}^{n-1} K\left(\left\{ \frac{k\mathbf{z}}{n} \right\}, \mathbf{0} \right)$$

see e.g. (Hickernell, 1998)

Typical form for a weighted space:

$$e_s^2(\mathbf{z}) = -1 + \frac{1}{n} \sum_{k=0}^{n-1} \prod_{j=1}^{s} \left[1 + \gamma_j \, \omega\left(\left\{ \frac{k z_j}{n} \right\} \right) \right]$$

This is a tensor product space: a product of 1-dimensional kernels

The weights γ_j, $\gamma_1 \geq \gamma_2 \geq \cdots \geq \gamma_s$, model anisotropicness of the integrand functions

Between the big braces we have the 1-dimensional kernel

Searches for lattice rules

Remember that

1. The cost to verify that a lattice rule has degree d is proportional to d^s, so only "moderate" dimensions are feasible.
2. The search space is huge.

$\Rightarrow$ Restrict the search space.

For example:

Definition

A rank-1 simple lattice is generated by one vector $\mathbf{z}$ and has the form

$$Q[f] := \frac{1}{n} \sum_{j=0}^{n-1} f\left(\left\{\frac{j\mathbf{z}}{n}\right\}\right)$$

$$P_n := \left\{ \left\{ \frac{j\mathbf{z}}{n} \right\} : j = 0, \ldots, n-1 \right\}, \quad \mathbf{z} \in U_n^s \,.$$

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- Restricting to rank-1 simple rules
  $\rightarrow$ only 1 vector, $s-1$ components, to be determined.
- Further restriction of the search space:
  consider only generator vectors of the form

$$\mathbf{z}(\ell) = (1, \ell, \ell^2 \mod n, ..., \ell^{s-1} \mod n), 1 \leq \ell < n$$

(Korobov, 1959)

Technology used: matrices

Any s-dimensional lattice Λ can be specified in terms of s linearly independent vectors $\{\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_s\}$.
$\rightarrow$ These vectors are known as generators of Λ.

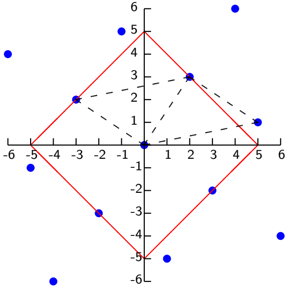
Associated with the generators is an $s \times s$ generator matrix A whose rows are $\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_s$.
All $\mathbf{h} \in \Lambda$ are of the form $\mathbf{h} = \sum_{i=1}^{s} \lambda_i \mathbf{a}_i = \boldsymbol{\lambda} A$ for some $\boldsymbol{\lambda} \in \mathbb{Z}^s$.

The dual lattice $\Lambda^\perp$ may be defined as having generator matrix $B = (A^{-1})^T$.

It can be shown that the number of points $n = |\det A|^{-1} = |\det B|$.

Recent searches for low dimensions: K-Optimal rules

Not restricted to rank-1 lattices.
Based on a property of the dual lattice:



Argument by (C. & Lyness, 2001):
It is reasonable to believe that the lattice Λ *of an optimal lattice rule will have* $\Lambda^{\perp}$ *with many elements on the boundary of* $\mathrm{conv} S(O_s, d+1)$ *(a scaled version of the unit octahedron).*

High computational cost, $\mathcal{O}(\delta^{s^2-1})$. $(\delta = d+1)$

- (C. & Lyness, *Math. Comp.*, 2001): 3D ($\delta \leq 30$, 4D ($\delta \leq 24$)
- (Lyness & Sørevik, *Math. Comp.*, 2006): 5D ($\delta \leq 12$)

High computational cost, $\mathcal{O}(\delta^{s^2-1})$. $(\delta = d+1)$

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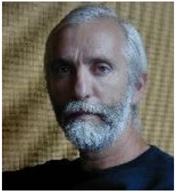
- (Lyness & Sørevik, *Math. Comp.*, 2006): 5D ($\delta \leq 12$)

Restricting the search to (skew-)circulant generator matrices, reduces the cost to $\mathcal{O}(\delta^{2s-2})$.

- (Lyness & Sørevik, *Math. Comp.*, 2004): 4D
- (C. & Govaert, *J. Complexity*, 2003): 5D, 6D

This also lead to closed expressions for arbitrary degrees.

J. Lyness



T. Sørevik

H. Govaert

Packing factor

Definition

The packing factor

$$\hat{\rho}(n) := \frac{\delta^s}{s!n}.$$

This is a measure of the efficiency of a rule.
It is convenient for making pictures because $0 \le \hat{\rho}(n) \le 1$.

Actually, $\hat{\rho}(n)$ is bounded above by
the density of the densest lattice packing
of the crosspolytope (octahedron) $\theta(O_s)$.
($\rightarrow$ link with "Geometry of numbers")

Known values:

- $\theta(O_1) = \theta(O_2) = 1$
- $\theta(O_3) = \frac{18}{19}$ (Minkowski, 1911) used by (Frolov, 1977)

This provides a (higher) lower bound for lattice rules for trigonometric degree:

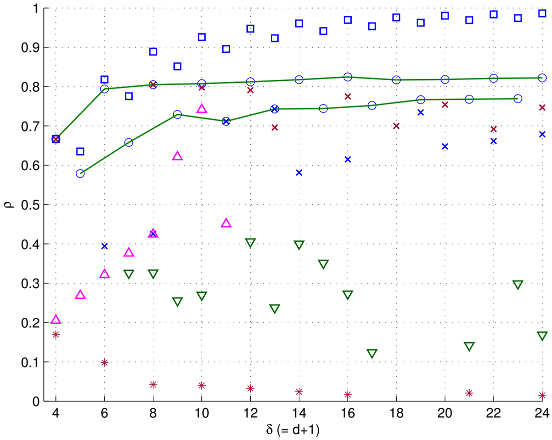
$$n \geq \frac{(d+1)^s}{s!\theta(O_s)}.$$

Lattice rules provide constructive lower bounds for $\theta(O_s)$. From a lattice rule with n points follows

$$\theta(O_s) \geq \frac{(d+1)^s}{s!n}.$$

The best known bounds for $\theta(O_4)$, $\theta(O_5)$ and $\theta(O_6)$ come from lattice rules
(C., *East Journal on Approximations*, 2006).

Results: 4D



○ refers to n_{KO}, □ refers to n_{ME}.
× refers to (Noskov & Semenova, 1996)+corrections
∗ refers to (C., Novak & Ritter, 1999)
× refers to (Temirgaliev, 1991), △ refers to Good lattices
▽ refers to Korobov rules (Maisonneuve, 1972)

K-optimal rules: conclusions

- The search for K-optimal lattice rules is expensive.
- The packing factor is related to the concept critical lattice (a global minimum)
  As a side effect it delivered the best known constructive lower bounds for $\theta(s)$, for $s = 4, 5, 6$.
- There are also local minima for the determinant of admissible lattices $\rightarrow$ extremal lattices
  The corresponding lattices can be used to bootstrap the construction of higher degree lattice rules (in no-time) and sequences.
- More recent: approach based on Golomb rules (Sørevik, MCQMC2012)

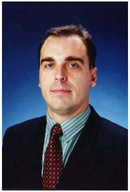
Recent searches for higher dimensions: Component-by-component construction

- Focus on rank-1 lattice rules $\Rightarrow$ find 1 vector $\mathbf{z}$.
- Idea: search $\mathbf{z}$ component by component

2000: I. Sloan & A. Reztsov (Tech. Report)
published Math. Comp. 2002
unweighted Korobov space, n prime

Note that Korobov (1959) presented a constructive proof using the CBC-principle.

I.H.Sloan



A. Reztsov

Some milestones of component-by-component

- 2000-2002: F. Kuo (PhD) with S. Joe
  weighted Korobov space, weighted Sobolev space
- MCQMC 2002: J. Dick & F. Kuo
  basically for weighted Korobov space, n a product of few primes, but partial search, faster and for millions of points
- MCQMC 2004, 2006: D. Nuyens & C.
  fast construction in $O(sn\log(n))$, basic case for n prime, but also possible for any composite n (and full search)

F. Kuo

S. Joe

J. Dick

D. Nuyens

The CBC algorithm in a shift-invariant RKHS

for $s = 1$ **to** s_{max} **do**

  for all z **in** U_n **do**

$$e_s^2(z) = -1 + \frac{1}{n}\sum_{k=0}^{n-1}\prod_{j=1}^{s}\left[1 + \gamma_j\,\omega\left(\left\{\frac{kz_j}{n}\right\}\right)\right]$$

  end for

$$z_s = \operatorname*{argmin}_{z\in U_n} e_s^2(z)$$

end for

Computational cost: $O(s_{\mathsf{max}} n^2)$

Rephrasing CBC: matrix-vector form

The inner loop can be formulated as a matrix-vector product with matrix

$$\mathbf{\Omega}_n := \left[\omega\left(\left\{\frac{kz}{n}\right\}\right)\right]_{\substack{z\in U_n\\ k\in\mathbb{Z}_n}} = \left[\omega\left(\frac{k\cdot z \bmod n}{n}\right)\right]_{\substack{z\in U_n\\ k\in\mathbb{Z}_n}}$$

This matrix has a lot of structure!

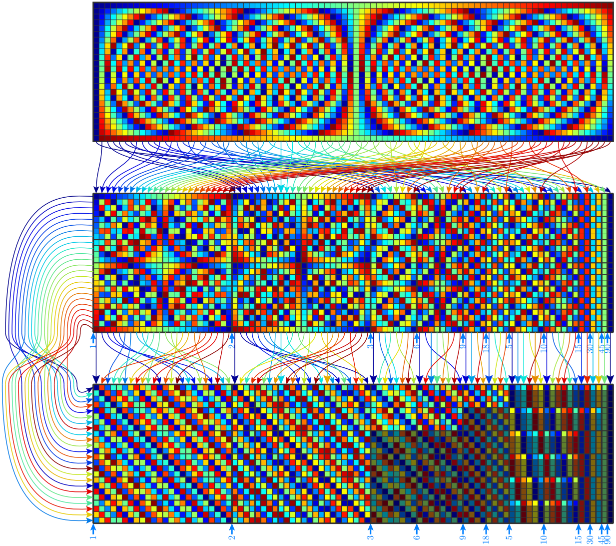
A matrix-vector multiplication can be done in $O(n\log n)$
(Nuyens & C. 2005, 2006)

$\Rightarrow$ Construction then takes $O(sn\log n)$ using $O(n)$ memory

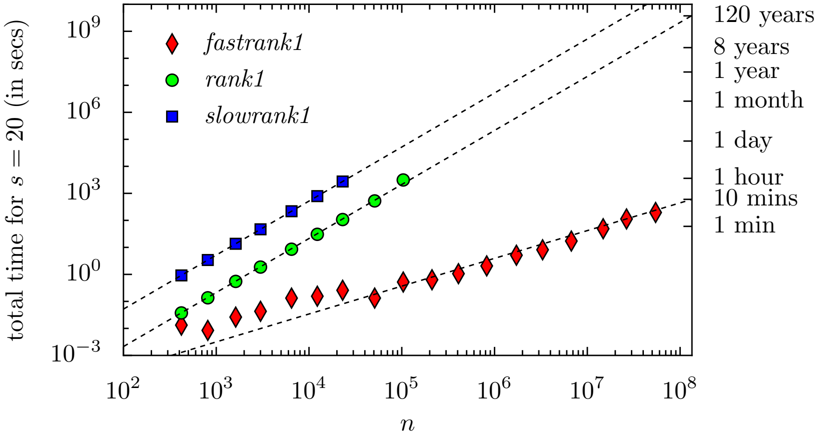
An example matrix Ω_n and its permutations

A nice view on $90 = 2 \times 3^2 \times 5$

The blocks of the last matrix are diagonizable by FFT's



Results in $O(sn\log(n))$



Timings anno 2004 for 20 dimensions
generated on a P4 2.4GHz ht, 2GB RAM

Combination of approaches

Inspired by “classical” approach and

Combination of approaches

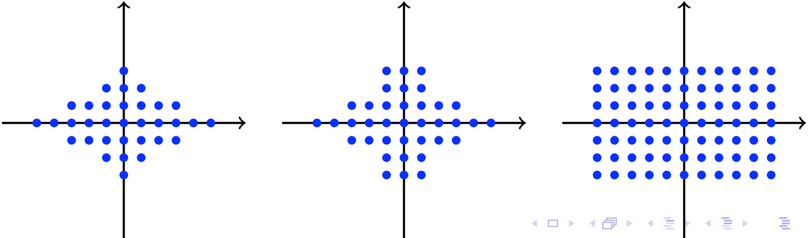
Inspired by "classical" approach and

H. Woźniakowski

I.H. Sloan

weighted spaces from QMC (Sloan & Woźniakowski, 1998),
$\rightarrow$ "weighted degree of exactness":

For example:



A new worst case setting

Amend the Korobov space E_α to make new space H with reproducing kernel

$$K(\boldsymbol{x}, \boldsymbol{y}) = \sum_{\boldsymbol{h} \in \mathcal{A}_s(m)} \exp(2\pi\mathrm{i}\, \boldsymbol{h} \cdot (\boldsymbol{x} - \boldsymbol{y})) + \sum_{\boldsymbol{h} \notin \mathcal{A}_s(m)} \frac{\exp 2\pi\mathrm{i}\, \boldsymbol{h} \cdot (\boldsymbol{x} - \boldsymbol{y})}{r_\alpha(\boldsymbol{\gamma}, \boldsymbol{h})}.$$

The squared worst case error of a rank-1 lattice rule is now

$$e^2_{n,s}(\boldsymbol{z}) = \sum_{\substack{\boldsymbol{0} \neq \boldsymbol{h} \in \mathcal{A}_s(m) \\ \boldsymbol{h} \cdot \boldsymbol{z} \equiv 0 \pmod n}} 1 + \sum_{\substack{\boldsymbol{h} \notin \mathcal{A}_s(m) \\ \boldsymbol{h} \cdot \boldsymbol{z} \equiv 0 \pmod n}} \frac{1}{r_\alpha(\boldsymbol{\gamma}, \boldsymbol{h})}.$$

$\rightarrow$ CBC-algorithm (C., Kuo & Nuyens, 2010)

Error estimation

In practice one wants more than 1 approximation.

Common approaches (for all types of cubature):

- randomization (randomly shifted rules) (Cranley & Patterson, 1976)

Error estimation

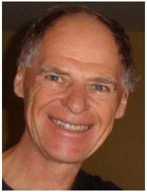
In practice one wants more than 1 approximation.

Common approaches (for all types of cubature):

- randomization (randomly shifted rules) (Cranley & Patterson, 1976)
- embedded sequences
    - copy rules, with intermediate lattice rules (Joe & Sloan, 1992) augmentation sequences (Li, Hill & Robinson, 2007)
    - embedded rank-1 rules
      (Hickernell, Hong, L'Ecuyer, Lemieux, *SISC* 2000)
      (C., Kuo, Nuyens, *SISC* 2006)
      (C. & Nuyens, *MCQMC2008*)

T. Patterson

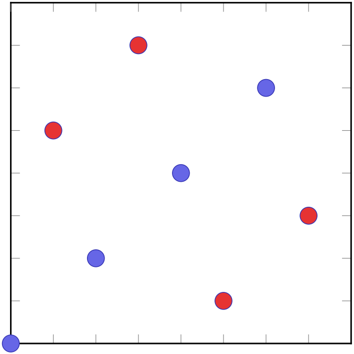
R. Hong



P. L'Ecuyer

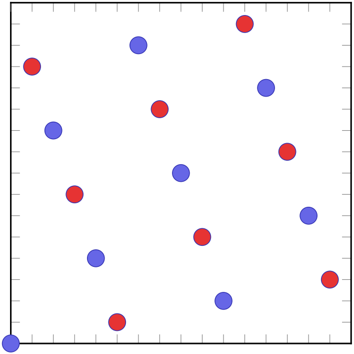
C. Lemieux

Example of embedded rank-1 rules



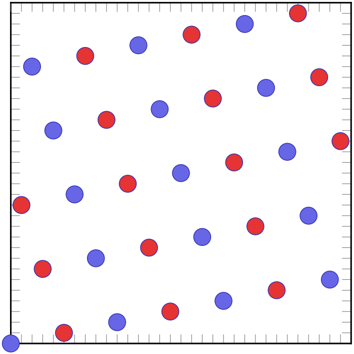
$n = 8$

Example of embedded rank-1 rules



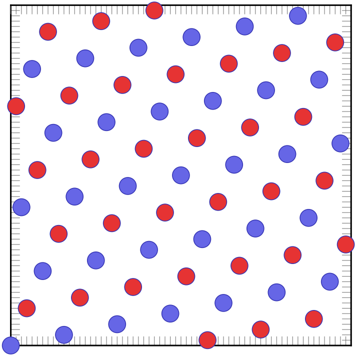
$n = 16$

Example of embedded rank-1 rules



$n = 32$

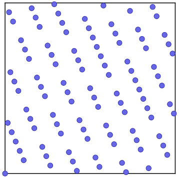
Example of embedded rank-1 rules



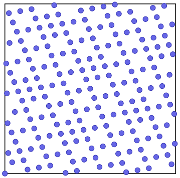
$n = 64$

This is not restricted to powers of 2

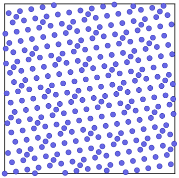
- The structure of the points using Gray code or radical inverse ordering is similar to that of a net. The unit cube gets filled with smaller lattices which consists of smaller lattices and so on.
- Starting from a good lattice sequence we can stop anywhere and have a good uniform distribution (Hickernell, Kritzer, Kuo, Nuyens, 2011)



$n = 100$



$n = 200$



$n = 300$

P. Kritzer

Is the Weyl sequence a relative?

- Simple rank-1 lattice:

$$\mathbf{x}^{(k)} = \left\{ \frac{k\,\mathbf{z}}{n} \right\}, \text{ for } k = 0, 1, 2, \ldots, n-1.$$

- Embedded rank-1 lattice: in order to stop at any time, you need a good ordering of the points:

$$\mathbf{x}^{(k)} = \left\{ \frac{\varphi(k)}{n}\,\mathbf{z} \right\}, \text{ for } k = 0, 1, 2, \ldots, n-1.$$

- If n is very large, this can be seen as an extensible cubature rule.
- Weyl sequence: Take $n \rightsquigarrow \infty$, then ℓ/n has an infinite digit expansion, i.e. think “irrational”.
  Now group on $\mathbf{z}/n$, and take each $z_j/n = \xi_j$ an irrational:

$$\mathbf{x}^{(k)} = \{k\,\boldsymbol{\xi}\}, \text{ for } k = 0, 1, 2, \ldots$$

  This could be interpreted as an infinite extensible “lattice”.

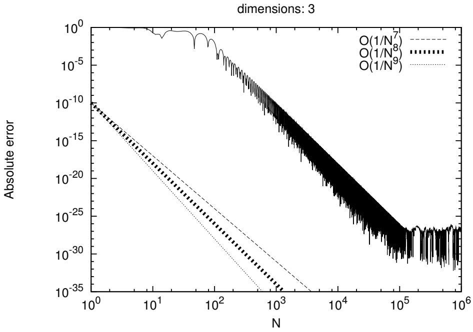
Weyl sequence for periodic functions

Introduce weights and achieve higher order of convergence for periodic functions.
(Niederreiter, 1973) (Sugihara & Murota, 1982)
(Vandewoestyne, C. & Warnock, 2007)

Example: 3D, $\mathcal{O}(n^{-8})$

M. Sugihara

B. Vandewoestyne



Final remarks

Construction:

- Searches for lattice rules using the "classical" criteria are doomed to fail for increasing dimensions.
- The CBC algorithm, relying on "worst-case-error" for "reproducing kernel Hilbert spaces" beats this curse of dimensionality. Rules can be constructed very fast even if n and s are large.

But work remains to be done, e.g.,

- for CBC, tuning of the function space using the weights,
- practical error estimates based on sequences.

Finally note that

- lattice rules are useful for low and high dimensions, and are not only for integrating periodic functions;
- all quality criteria have a reason to exist;
- the difference between lattice rules and "classical" low discrepancy sequences evaporates.
  Lattice rules with large n can be constructed easily and can be used as sequences.

Finally note that

- lattice rules are useful for low and high dimensions, and are not only for integrating periodic functions;
- all quality criteria have a reason to exist;
- the difference between lattice rules and "classical" low discrepancy sequences evaporates.
  Lattice rules with large n can be constructed easily and can be used as sequences.

Use a lattice rule anywhere & anytime!

This was a story about integration but the above suggestion also applies to you if you are involved in approximation.

The end.

Thank you!

The end.

Thank you!

A special “thank you” to those that put their picture on the web.
Don’t forget to update it!