An algorithm for the construction of weighted degree lattice rules

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Outline

Multivariate integration by lattice rules

Approximate the d-dimensional integral

$$I(f) := \int_{[0,1)^d} f(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x}$$

by an n-point (rank-1) lattice rule

$$Q(f; \boldsymbol{z}, n) := \frac{1}{n} \sum_{k=0}^{n-1} f\left(\left\{ \frac{\boldsymbol{z} k}{n} \right\} \right)$$

with “good” generating vector $\boldsymbol{z} \in (\mathbb{Z}_n^\times)^d$.

→ What kind of goodness?

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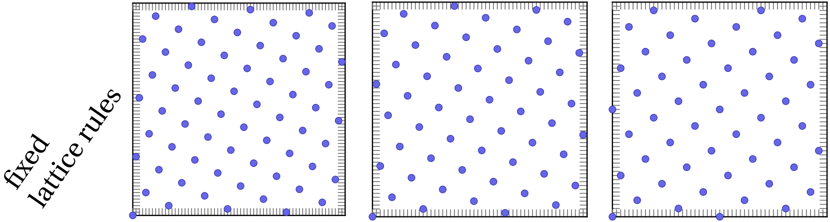
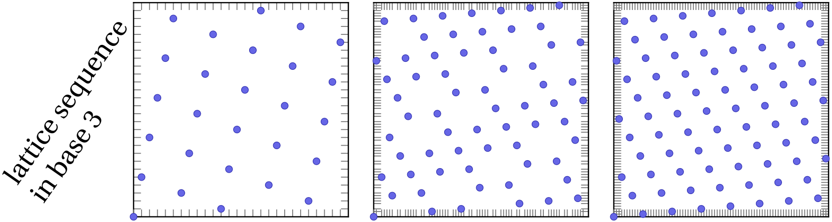
→ What kind of goodness?

→ Combine degree of exactness *and* worst case error.

Imagery of good lattice rules and sequences



(a) rank-1 rule (b) Fibonacci lattice (c) rank-2 copy rule



(d) 3^3 seq points (e) 64 seq points (f) 3^4 seq points

Error of integration

For f with Fourier representation

$$f(\boldsymbol{x}) = \sum_{\boldsymbol{h} \in \mathbb{Z}^d} \hat{f}(\boldsymbol{h}) \, \exp(2\pi \mathrm{i} \, \boldsymbol{h} \cdot \boldsymbol{x})$$

we have

$$Q(f; \boldsymbol{z}, n) - I(f) = \sum_{\boldsymbol{h} \in \mathbb{Z}^d} \hat{f}(\boldsymbol{h}) \, \frac{1}{n} \sum_{k=0}^{n-1} \exp(2\pi \mathrm{i} \, \boldsymbol{h} \cdot \boldsymbol{z} k / n) - \hat{f}(\boldsymbol{0})$$

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$$f(\boldsymbol{x}) = \sum_{\boldsymbol{h} \in \mathbb{Z}^d} \hat{f}(\boldsymbol{h}) \exp(2\pi \mathrm{i}\, \boldsymbol{h} \cdot \boldsymbol{x})$$

we have

$$Q(f; \boldsymbol{z}, n) - I(f) = \sum_{\substack{\boldsymbol{0} \neq \boldsymbol{h} \in \mathbb{Z}^d \\ \boldsymbol{h} \cdot \boldsymbol{z} \equiv 0 \pmod{n}}} \hat{f}(\boldsymbol{h}).$$

The error is given as a sum over the dual lattice:

$$\{\boldsymbol{h} \in \mathbb{Z}^d : \boldsymbol{h} \cdot \boldsymbol{z} \equiv 0 \pmod{n}\} =: \Lambda^\perp.$$

$\rightarrow$ Denotes Fourier coefficients which contribute to error.

Degree of exactness

- Mark region of interest $\mathcal{A}_d(m)$ in Fourier domain of "degree" m (in d dimensions).
- Ask to integrate those Fourier terms exactly. I.e.

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

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

Aim: create construction algorithm for relatively high d.

The result

We show:

- Need extra weights to control exponential growth in number of dimensions. No surprise.
  $\rightarrow$ "Weighted degree of exactness"
- Standard CBC construction delivers rules with "reasonable" degree of exactness.
- New algorithm delivers quite good degrees of exactness. (Comparison for classical trigonometric degree.)

Results published in R. Cools, F. Y. Kuo and D. Nuyens, *Constructing lattice rules based on weighted degree of exactness and worst case error*, Computing (2010) 87:63–89.

Degrees of exactness

Different regions lead to different degrees of exactness:

- Trigonometric degree: crosspolytope (diamond shape)

$$\mathcal{A}_d(m) = \left\{ \boldsymbol{h} \in \mathbb{Z}^d : \sum_{j=1}^{d} |h_j| \le m \right\}.$$

- Zaremba degree: hyperbolic cross

$$\mathcal{A}_d(m) = \left\{ \boldsymbol{h} \in \mathbb{Z}^d : \prod_{j=1}^{d} \max(1, |h_j|) \le m \right\}.$$

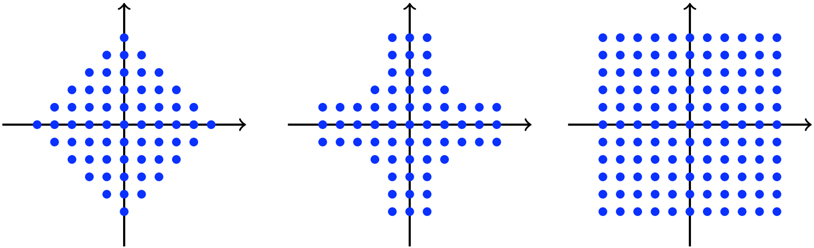
  Note: classical Zaremba index $\rho = m + 1$.

- Product degree: hypercube

$$\mathcal{A}_d(m) = \left\{ \boldsymbol{h} \in \mathbb{Z}^d : \max_{1 \le j \le d} |h_j| \le m \right\}.$$

And their Fourier spectra in 2D

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



Trigonometric degree Zaremba degree Product degree

For $d \to \infty$ these shapes grow exponentially…

Exponential growth

In fact:

- Trigonometric degree (Cools & Sloan, 1996)

$$|\mathcal{A}_d(m)| = \sum_{\ell=0}^{\min(d,m)} \binom{d}{\ell}\binom{m}{\ell} 2^\ell = O(m^d).$$

- Zaremba degree

$$3^{d-1}(2m+1) \le |\mathcal{A}_d(m)| \le (1+2\zeta(\tau))^d \, m^\tau \quad \text{for all} \quad \tau > 1.$$

- Product degree

$$|\mathcal{A}_d(m)| = (2m+1)^d.$$

And need exponential amount of nodes

When the set $\mathcal{A}_d(m)$ is convex and centrally symmetric then minimal number of points

$$n_{\min} \geq \left| \mathcal{A}_d \left(\left\lfloor \frac{m}{2} \right\rfloor \right) \right| = O(m^d),$$

to achieve degree m with a rule of the form

$$\sum_{k=1}^{n} w_k f(\boldsymbol{t}_k).$$

(Cools & Reztsov, 1997)

Assume some variables more important than others

Inspired by classical theory of product rules and weighted spaces from QMC (Sloan & Woźniakwoski, 1998), introduce a "weighted degree of exactness":

- Importance of dimension j modelled by weight β_j.
- Decaying sequence of positive weights

$$1 = \beta_1 \geq \beta_2 \geq \cdots \geq 0.$$

- The set $\mathcal{A}_d(m)$ intersects the jth axis at $\lfloor \beta_j m \rfloor$.

Note: For rank-1 lattice rules with n prime the one-dimensional (projected) degrees are always $n-1$.

Weighted degrees

- Weighted trigonometric degree:

$$\mathcal{A}_d(m) = \left\{ \boldsymbol{h} \in \mathbb{Z}^d : \sum_{j=1}^{d} \frac{|h_j|}{\beta_j} \le m \right\}.$$

- Weighted Zaremba degree:

$$\mathcal{A}_d(m) = \left\{ \boldsymbol{h} \in \mathbb{Z}^d : \prod_{j=1}^{d} \max\left(1, \frac{|h_j|}{\beta_j}\right) \le m \right\}.$$

- Weighted product degree:

$$\mathcal{A}_d(m) = \left\{ \boldsymbol{h} \in \mathbb{Z}^d : \max_{1 \le j \le d} \frac{|h_j|}{\beta_j} \le m \right\}.$$

And their controlled sizes

- Weighted Zaremba degree:

$$2m+1 \;\le\; |\mathcal{A}_d(m)| \;\le\; m^\tau \prod_{j=1}^{d} \left(1 + 2\zeta(\tau)\beta_j^\tau\right) \quad \text{for all} \quad \tau > 1.$$

- Weighted product degree:

$$|\mathcal{A}_d(m)| \;=\; \prod_{j=1}^{d} \left(1 + 2\lfloor \beta_j m \rfloor\right) \;\le\; \exp\left(2m \sum_{j=1}^{d} \beta_j\right).$$

(Similar proof as in (Kuo, Sloan & Woźniakowksi, 2006).)

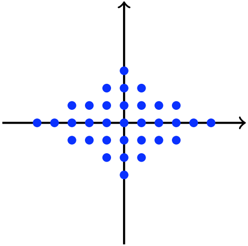
- Weighted trigonometric degree (see product degree).

→ These sets are bounded in size independently of d if

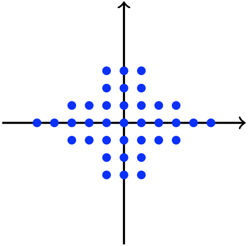
$$\sum_{j=1}^{\infty} \beta_j < \infty.$$

And their 2D Fourier spectra

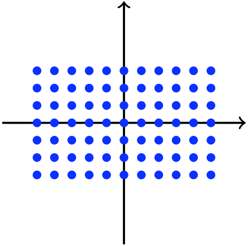
Take $m = 5$, $\beta_1 = 1$, $\beta_2 = 0.6$ (and $d = 2$):



Trigonometric degree



Zaremba degree



Product degree

Worst case error in Korobov space E_α

Traditional setting for lattice rules:

- Absolutely convergent Fourier series representation

$$f(\boldsymbol{x}) = \sum_{\boldsymbol{h} \in \mathbb{Z}^d} \hat{f}(\boldsymbol{h}) \exp(2\pi \mathrm{i}\, \boldsymbol{h} \cdot \boldsymbol{x}).$$

- Then $f \in E_\alpha$, for an $\alpha > 1$, if

$$\|f\|_{E_\alpha}^2 := \sum_{\boldsymbol{h} \in \mathbb{Z}^d} r_\alpha(\boldsymbol{h}, \boldsymbol{\gamma})\, |\hat{f}(\boldsymbol{h})|^2 < \infty$$

with

$$r_\alpha(\boldsymbol{h}, \boldsymbol{\gamma}) := \prod_{j=1}^{d} r_\alpha(h_j, \gamma_j), \quad r_\alpha(h_j, \gamma_j) := \begin{cases} 1, & \text{if } h_j = 0, \\ \dfrac{|h_j|^\alpha}{\gamma_j}, & \text{otherwise.} \end{cases}$$

Worst case error in E_α

Worst case error:

$$e(Q;H) := \sup_{\substack{f \in H \\ \|f\|_H \le 1}} |I(f) - Q(f)|.$$

For rank-1 lattice rule in E_α:

$$e^2(\boldsymbol{z}, n; E_\alpha) = -1 + \frac{1}{n} \sum_{k=0}^{n-1} \prod_{j=1}^{d} \left(1 + \gamma_j \sum_{0 \neq h \in \mathbb{Z}} \frac{\exp(2\pi \mathrm{i}\, h z_j k/n)}{|h|^\alpha} \right)$$

$$= \sum_{\substack{\boldsymbol{0} \neq \boldsymbol{h} \in \mathbb{Z}^d \\ \boldsymbol{h} \cdot \boldsymbol{z} \equiv 0 \pmod{n}}} \frac{1}{r_\alpha(\boldsymbol{h}, \boldsymbol{\gamma})}.$$

Interpretation

We had

$$Q(f; \boldsymbol{z}, n) - I(f) = \sum_{\substack{\boldsymbol{0} \neq \boldsymbol{h} \in \mathbb{Z}^d \\ \boldsymbol{h} \cdot \boldsymbol{z} \equiv 0 \pmod{n}}} \hat{f}(\boldsymbol{h}).$$

So, the squared worst case error

$$e^2(\boldsymbol{z}, n; E_\alpha) = \sum_{\substack{\boldsymbol{0} \neq \boldsymbol{h} \in \mathbb{Z}^d \\ \boldsymbol{h} \cdot \boldsymbol{z} \equiv 0 \pmod{n}}} \frac{1}{r_\alpha(\boldsymbol{h}, \boldsymbol{\gamma})}$$

is the error of a "worst case function" with Fourier expansion

$$\xi(\boldsymbol{x}) := \sum_{\boldsymbol{h} \in \mathbb{Z}^d} \frac{\exp(2\pi \mathrm{i}\, \boldsymbol{h} \cdot \boldsymbol{x})}{r_\alpha(\boldsymbol{h}, \gamma)}.$$

A new worst case setting

Amend the Korobov space E_α to make new space H:

$$\|f\|_H := \left(\sum_{\boldsymbol{h} \in \mathcal{A}_d(m)} |\hat{f}(\boldsymbol{h})|^2 + \sum_{\boldsymbol{h} \notin \mathcal{A}_d(m)} |\hat{f}(\boldsymbol{h})|^2 \, r_\alpha(\boldsymbol{\gamma}, \boldsymbol{h}) \right)^{1/2},$$

with

$$1 \geq \gamma_1 \geq \gamma_2 \geq \cdots > 0.$$

Reproducing kernel of H is then

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

Worst case error

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

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

When the rule has degree m this worst case error is the same as in the Korobov space E_α.

Towards an algorithm

We now want an algorithm which:

- Is component-by-component (extensibility in d), (Sloan, Joe, Kuo, Dick, ...).
- Achieves a prescribed (weighted) degree m.
- Has near optimal worst case error in our function space.
- Is strongly tractable with respect to increasing dimensions (given conditions on the weights).
- Has acceptable construction cost.
  $\rightarrow$ Fast CBC concstruction (N. & Cools, 2006).

Component-by-component construction

Theorem (Inductive step for degree of exactness: $s \to s+1$)

Let $c > 1$ be fixed, m be given, and suppose that $n > m$ is a prime number satisfying

$$n \; > \; 1 + \frac{c}{c-1} \frac{|\mathcal{A}_{s+1}(m)| - |\mathcal{A}_s(m)| - 2\lfloor \beta_{s+1} m \rfloor}{2}.$$

If $\boldsymbol{z} \in {\mathbb{Z}_n^*}^s$ satisfies

$$\boldsymbol{h} \cdot \boldsymbol{z} \not\equiv 0 \pmod{n} \qquad \forall\, \boldsymbol{h} \in \mathcal{A}_s(m) \setminus \{\boldsymbol{0}\},$$

then there are "more than $\frac{1}{c}(n-1)$" choices of z_{s+1} such that

$$(\boldsymbol{h}, h_{s+1}) \cdot (\boldsymbol{z}, z_{s+1}) \not\equiv 0 \pmod{n} \quad \forall\, (\boldsymbol{h}, h_{s+1}) \in \mathcal{A}_{s+1}(m) \setminus \{\boldsymbol{0}\}.$$

On the number of points…

The required n is quite large:

$$n > 1 + \frac{c}{c-1} \frac{|\mathcal{A}_{s+1}(m)| - |\mathcal{A}_s(m)| - 2\lfloor \beta_{s+1} m \rfloor}{2}.$$

For unweighted product degree the lower bound is

$$n_{\min} \gtrsim (m+1)^{s+1}$$

while the condition above (for $c = 2$) says

$$n > 1 + 2m((2m+1)^s - 1).$$

This is due to a very conservative estimate in the proof where we exclude "bad choices" for z_{s+1}: every bad choice is excluded at least twice by point-symmetry,

$$\boldsymbol{h} \cdot \boldsymbol{z} \equiv -h_{s+1} z_{s+1} \pmod{n} \quad \equiv \quad -\boldsymbol{h} \cdot \boldsymbol{z} \equiv h_{s+1} z_{s+1} \pmod{n},$$

but the same z_{s+1} may be excluded many times more.

Add in result on the worst case error

Theorem (Combined inductive step: $s \to s+1$)

Let $c > 1$ and $n > m$ be a prime number large enough (previous condition). Suppose that $\boldsymbol{z} \in {\mathbb{Z}_n^*}^s$ has weighted degree m, and

$$e_{n,s}^2(\boldsymbol{z}) \leq \left(\frac{c}{n-1} \prod_{j=1}^{s} \left(1 + 2\zeta(\alpha\lambda)\gamma_j^\lambda\right) \right)^{1/\lambda} \text{ for all } \lambda \in (1/\alpha, 1].$$

Then there is "at least one" z_{s+1} such that we have weighted degree m in $s+1$ dimensions, and

$$e_{n,s+1}^2(\boldsymbol{z}, z_{s+1}) \leq \left(\frac{c}{n-1} \prod_{j=1}^{s+1} \left(1 + 2\zeta(\alpha\lambda)\gamma_j^\lambda\right) \right)^{1/\lambda}.$$

Proof uses idea from (Dick, Pillichshammer & Waterhouse, 2008).

A CBC algorithm

Let $c > 1$ and $n > m$ be a prime number satisfying

$$n > 1 + \frac{c}{c-1} \max_{1 \le s \le d-1} \frac{|\mathcal{A}_{s+1}(m)| - |\mathcal{A}_s(m)| - 2\lfloor \beta_{s+1} m \rfloor}{2}.$$

1. Set $z_1 = 1$ and form the set $\mathcal{A}_1(m)$.
2. For each $s = 1, \ldots, d-1$, with $\boldsymbol{z} = (z_1, \ldots, z_s)$ fixed and $\mathcal{A}_s(m)$ already formed, do the following:
   (a) Form the set $\mathcal{A}_{s+1}(m)$ from $\mathcal{A}_s(m)$.
   (b) Exclude $z_{s+1} \in \mathbb{Z}_n^*$ if $h_{s+1} z_{s+1} \equiv -\boldsymbol{h} \cdot \boldsymbol{z} \pmod{n}$ for any $(\boldsymbol{h}, h_{s+1}) \in \mathcal{A}_{s+1}(m) \setminus \{\boldsymbol{0}\}$.
   (c) Find the z_{s+1} from the remaining choices in $\mathbb{Z}_n^*$ that minimizes $e^2_{n,s+1}(\boldsymbol{z}, z_{s+1})$.

Construction cost

If the conditions

$$n > 1 + \frac{c}{c-1} \frac{|\mathcal{A}_{s+1}(m)| - |\mathcal{A}_s(m)| - 2\lfloor \beta_{s+1} m \rfloor}{2}.$$

and

$$\sum_{j=1}^{\infty} \beta_j < \infty$$

are fulfilled then the construction cost is

$$O(|\mathcal{A}_d(m)| + dn \log n) = O(dn \log n),$$

using a modified fast component-by-component algorithm based on (N. & Cools, 2006).

Tractability conditions

Suppose

$$n > 1 + |\mathcal{A}_d(m)|$$

then to have $e_{n,d}(\boldsymbol{z}) \leq \varepsilon$ it is sufficient to take

$$n \;\geq\; 1 + \frac{c}{\varepsilon^{2\lambda}} \prod_{j=1}^{d} \left(1 + 2\zeta(\alpha\lambda)\gamma_j^{\lambda}\right) \quad \text{for all } \lambda \in (1/\alpha, 1].$$

From which

$$n(\varepsilon, d) \;\leq\; \max\left(1 + \frac{2}{\varepsilon^{2\lambda}} \prod_{j=1}^{d} \left(1 + 2\zeta(\alpha\lambda)\gamma_j^{\lambda}\right) \;,\; 1 + |\mathcal{A}_d(m)|\right)$$

We have strong tractability when

$$\sum_{j=1}^{\infty} \gamma_j^{1/\alpha} < \infty \qquad \text{and} \qquad \sum_{j=1}^{\infty} \beta_j < \infty.$$

Numerical results

Basic example for product degree $m = 3$ and $n = 4001$ where

$$\alpha = 2, \qquad \gamma_j = 0.75^{j-1}, \qquad \beta_j = \gamma_j^{1/\alpha} = (0.866025\ldots)^{j-1}.$$

s	z_s	$\lvert\mathcal{A}_s(3)\rvert$	$e_{n,s}(\boldsymbol{z})$	drop	
1	1	7	4.53e-04		
2	1478	35	3.30e-03	10	(12)
3	563	175	1.66e-02	60	(68)
4	1844	525	4.88e-02	174	(174)
5	827	1575	1.07e-01	524	(524)
6	1318	4725	1.79e-01	1574	(1574)
7	586	14175	2.63e-01	3324	(4724)
8	121	42525	3.53e-01	3982	(14174)
9	1339	42525	4.26e-01	0	(0)

$\rightarrow$ Almost always same choice as classical CBC.

A modified algorithm

The basic algorithm fixes the degree m throughout the entire CBC construction. Therefore:

- We might not get the highest degree possible.
- The claimed degree might be much lower than the actual degree.

Modification: dynamically change degree m in each step, decreasing the degree when the number of bad choices is above a preset threshold κ.

Results for modified algorithm

Example for trigonometric degree for $n = 4001$ and $\kappa = 4000 - 2$ where

$$\alpha = 2, \qquad \gamma_j = 0.75^{j-1}, \qquad \beta_j = 1.$$

s	z_s	m_s	$\|\mathcal{A}_s(m_s)\|$	$e_{n,s}(\boldsymbol{z})$	drop	
1	1	4000	8001	4.53e-04		
2	899	88	15665	3.77e-03	3990	(7656)
3	525	25	22151	1.98e-02	3996	(10400)
4	538	14	29961	7.45e-02	3998	(12922)
5	1717	9	22363	1.18e-01	3862	(8352)
6	919	8	40081	1.94e-01	3996	(13496)
7	1610	6	19825	2.72e-01	3438	(5412)
8	635	6	40081	3.54e-01	3910	(10122)
9	64	6	75517	4.28e-01	3996	(17712)
10	1518	5	36365	4.94e-01	3716	(6996)
11	24	5	56695	5.50e-01	3894	(10160)

Comparison for trigonometric degree

This new algorithm can quickly construct rules in tens of dimensions for the unweighted trigonometric degree.

How does it compare?

- Comparing to (Cools & Lyness, 2001) in three and four dimensions and (Cools & Govaert, 2003) in five and six dimensions we do slightly worse.
- Comparing to higher dimensional results as in (Cools, Novak & Ritter, 1999) we do much better.

Conclusion

- Introduced a concept of weighted degree.
- Derived component-by-component algorithm which achieves
  - a prescribed weighted degree; *and*
  - optimal worst case error.
- Adjustable to other degrees of exactness.

R. Cools, F. Y. Kuo and D. Nuyens, *Constructing lattice rules based on weighted degree of exactness and worst case error*, Computing (2010) 87:63–89.