An algorithm for the construction of weighted degree lattice rules

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Outline

1. Introduction
2. Degree of exactness
3. Worst case error
4. CBC construction
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6. Conclusion
Approximate the \(d\)-dimensional integral

\[
I(\mathbf{f}) := \int_{[0,1]^d} \mathbf{f}(\mathbf{x}) \, d\mathbf{x}
\]

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

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

with “good” generating vector \(\mathbf{z} \in (\mathbb{Z}/n)^d\).

→ What kind of goodness?
Multivariate integration by lattice rules

Approximate the $d$-dimensional integral

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

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

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

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

→ 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
For $f$ with Fourier representation

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

we have

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

For $f$ with Fourier representation

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

we have

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

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

$$\{ h \in \mathbb{Z}^d : h \cdot z \equiv 0 \ (\text{mod } n) \} =: \Lambda^\perp.$$  

→ Denotes Fourier coefficients which contribute to error.

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Preliminaries

Weighted degree lattice rules

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Mark region of interest $A_d(m)$ in Fourier domain of “degree” $m$ (in $d$ dimensions).

Ask to integrate those Fourier terms exactly. I.e.

$$\Lambda^\perp \cap A_d(m) = \{0\}.$$ 

⇒ Rule of degree (at least) $m$.

Different regions $A_d(m)$ 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. → “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.)

Degrees of exactness

Different regions lead to different degrees of exactness:

- **Trigonometric degree**: crosspolytope (diamond shape)

\[
A_d(m) = \left\{ \mathbf{h} \in \mathbb{Z}^d : \sum_{j=1}^d |h_j| \leq m \right\}.
\]

- **Zaremba degree**: hyperbolic cross

\[
A_d(m) = \left\{ \mathbf{h} \in \mathbb{Z}^d : \prod_{j=1}^d \max(1, |h_j|) \leq m \right\}.
\]

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

- **Product degree**: hypercube

\[
A_d(m) = \left\{ \mathbf{h} \in \mathbb{Z}^d : \max_{1 \leq j \leq d} |h_j| \leq m \right\}.
\]
And their Fourier spectra in 2D

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

<table>
<thead>
<tr>
<th>Classical degrees</th>
</tr>
</thead>
<tbody>
<tr>
<td>Trigonometric degree</td>
</tr>
<tr>
<td>Zaremba degree</td>
</tr>
<tr>
<td>Product degree</td>
</tr>
</tbody>
</table>

For $d \to \infty$ these shapes grow exponentially...
Exponential growth

In fact:

- **Trigonometric degree** (Cools & Sloan, 1996)

\[
|A_d(m)| = \sum_{\ell=0}^{\min(d,m)} \binom{d}{\ell} \binom{m}{\ell} 2^\ell = O(m^d).
\]

- **Zaremba degree**

\[3^{d-1}(2m+1) \leq |A_d(m)| \leq (1+2\zeta(\tau))^d m^\tau \quad \text{for all} \quad \tau > 1.\]

- **Product degree**

\[|A_d(m)| = (2m + 1)^d.\]
And need exponential amount of nodes

When the set $A_d(m)$ is convex and centrally symmetric then the minimal number of points

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

to achieve degree $m$ with a rule of the form

$$\sum_{k=1}^{n} w_k f(t_k).$$

(Cools & Reztsov, 1997)
Assume some variables more important than others

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

- Importance of dimension $j$ modelled by weight $\beta_j$.
- Decaying sequence of positive weights
  \[ 1 = \beta_1 \geq \beta_2 \geq \cdots \geq 0. \]

- The set $A_d(m)$ intersects the $j$th 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:
  \[ \mathcal{A}_d(m) = \left\{ h \in \mathbb{Z}^d : \sum_{j=1}^{d} \frac{|h_j|}{\beta_j} \leq m \right\}. \]

- Weighted Zaremba degree:
  \[ \mathcal{A}_d(m) = \left\{ h \in \mathbb{Z}^d : \prod_{j=1}^{d} \max\left(1, \frac{|h_j|}{\beta_j}\right) \leq m \right\}. \]

- Weighted product degree:
  \[ \mathcal{A}_d(m) = \left\{ h \in \mathbb{Z}^d : \max_{1 \leq j \leq d} \frac{|h_j|}{\beta_j} \leq m \right\}. \]
Weighted degree of exactness

And their controlled sizes

- Weighted Zaremba degree:

\[ 2m + 1 \leq |A_d(m)| \leq m^\tau \prod_{j=1}^{d} \left( 1 + 2\zeta(\tau)\beta_j^\tau \right) \quad \text{for all} \quad \tau > 1. \]

- Weighted product degree:

\[ |A_d(m)| = \prod_{j=1}^{d} \left( 1 + 2\lfloor \beta_j m \rfloor \right) \leq \exp \left( 2m \sum_{j=1}^{d} \beta_j \right). \]

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

- Weighted trigonometric degree (see product degree).

→ These sets are bounded in size independently of \( d \) if

\[ \sum_{j=1}^{\infty} \beta_j < \infty. \]
Take $m = 5$, $\beta_1 = 1$, $\beta_2 = 0.6$ (and $d = 2$):
Classical Korobov space

Worst case error in Korobov space $E_\alpha$

Traditional setting for lattice rules:

- Absolutely convergent Fourier series representation

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

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

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

with

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

Worst case error in $E_\alpha$

Worst case error:

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

For rank-1 lattice rule in $E_\alpha$:

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

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

**Interpretation**

We had

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

So, the squared worst case error

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

is the error of a “worst case function” with Fourier expansion

\[
\xi(x) := \sum_{h \in \mathbb{Z}^d} \frac{\exp(2\pi i h \cdot x)}{r_\alpha(h, \gamma)}.
\]
A new worst case setting

Amend the Korobov space $E_\alpha$ to make new space $H$:

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

with

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

Reproducing kernel of $H$ is then

$$
K(x, y) = \sum_{h \in A_d(m)} \exp(2\pi i \ h \cdot (x-y)) + \sum_{h \notin A_d(m)} \frac{\exp 2\pi i \ h \cdot (x-y)}{r_\alpha(\gamma, h)}.
$$
The squared worst case error of a rank-1 lattice rule is now

\[ e_{n,d}^2(z) = \sum_{\substack{0 \neq h \in A_d(m) \\ h \cdot z \equiv 0 \pmod{n}}} 1 + \sum_{\substack{h \notin A_d(m) \\ h \cdot z \equiv 0 \pmod{n}}} \frac{1}{r_\alpha(\gamma, h)}. \]

When the rule has degree \( m \) this worst case error is the same as in the Korobov space \( E_\alpha \).
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.
  
  → Fast CBC construction (N. & Cools, 2006).
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

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

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

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

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

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

**On the number of points...**

The required $n$ is quite large:

$$n > 1 + \frac{c}{c - 1} \left| A_{s+1}(m) \right| - \left| A_s(m) \right| - 2 \left\lfloor \beta_{s+1} m \right\rfloor.$$  

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,

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

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

Add in result on the worst case error

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

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

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

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

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

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

A CBC algorithm

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

$$n > 1 + \frac{c}{c-1} \max_{1 \leq s \leq d-1} \frac{|A_{s+1}(m)| - |A_s(m)| - 2|\beta_{s+1}m|}{2}.$$  

1. Set $z_1 = 1$ and form the set $A_1(m)$.
2. For each $s = 1, \ldots, d-1$, with $z = (z_1, \ldots, z_s)$ fixed and $A_s(m)$ already formed, do the following:
   (a) Form the set $A_{s+1}(m)$ from $A_s(m)$.
   (b) Exclude $z_{s+1} \in \mathbb{Z}^*_n$ if $h_{s+1}z_{s+1} \equiv -h \cdot z \pmod{n}$ for any $(h, h_{s+1}) \in A_{s+1}(m) \setminus \{0\}$.
   (c) Find the $z_{s+1}$ from the remaining choices in $\mathbb{Z}^*_n$ that minimizes $e^2_{n,s+1}(z, z_{s+1})$.  

Weighted degree lattice rules

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Construction cost

If the conditions

\[ n > 1 + \frac{c}{c - 1} \frac{|A_{s+1}(m)| - |A_s(m)| - 2 \lfloor \beta_{s+1} m \rfloor}{2} \]

and

\[ \sum_{j=1}^{\infty} \beta_j < \infty \]

are fulfilled then the construction cost is

\[ O(|A_d(m)| + dn \log n) = O(dn \log n), \]

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

Tractability conditions

Suppose

\[ n > 1 + |A_d(m)| \]

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

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

From which

\[ n(\varepsilon, d) \leq \max \left( 1 + \frac{2}{\varepsilon 2\lambda} \prod_{j=1}^{d} \left( 1 + 2\zeta(\alpha \lambda) \gamma_j^\lambda \right), 1 + |A_d(m)| \right) \]

We have strong tractability when

\[ \sum_{j=1}^{\infty} \gamma_j^{1/\alpha} < \infty \quad \text{and} \quad \sum_{j=1}^{\infty} \beta_j < \infty. \]
Basic example for product degree $m = 3$ and $n = 4001$ where

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

| $s$ | $z_s$ | $|A_s(3)|$ | $e_{n,s}(z)$ | 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)  |

→ 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 \( \kappa \).
Modified algorithm

Results for modified algorithm

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

\[
\alpha = 2, \quad \gamma_j = 0.75^{j-1}, \quad \beta_j = 1.
\]

| \( s \) | \( z_s \) | \( m_s \) | \( |A_s(m_s)| \) | \( e_{n,s}(z) \) | 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.