More about cubature formulas and densest lattice packings

Ronald Cools

Report TW 331, October 2001

Katholieke Universiteit Leuven
Department of Computer Science
Celestijnenlaan 200A – B-3001 Heverlee (Belgium)

More about cubature formulas and densest lattice packings

Ronald Cools

Report TW 331, October 2001

Department of Computer Science, K.U.Leuven

Abstract

In this short note we improve the lower bounds of the density of the densest lattice packing for a crosspolytope in 4 and 5 dimensions. In the course of the calculations we are able to correct some errors in the literature.

Keywords : lattices; packings; cubature; crosspolytope.

More about cubature formulas and densest lattice packings

Ronald Cools

Dept. of Computer Science, Katholieke Universiteit Leuven, Celestijnenlaan 200A, B-3001 Heverlee, Belgium

Abstract

In this short note we improve the lower bounds of the density of the densest lattice packing for a crosspolytope in 4 and 5 dimensions. In the course of the calculations we are able to correct some errors in the literature.

Key words: Lattices; Packings; Cubature; Crosspolytope.

1 Introduction

The search for the density of a densest lattice packing of a convex body is still very active. A practical algorithm to compute the packing density for an arbitrary polytope in $\mathbb{R}^3$ was only recently published [1]. For higher dimensions very little is known. In 1995, Klyuchnikov and Reztsov [5] used results on numerical integration lattices to obtain a lower bound for the density of densest lattice packing of a crosspolytope in 4 and 5 dimensions. Already in 1977, Frolov [4] pointed our attention to the relation between the density of the densest lattice packing of a octahedron and the minimal number of points of a lattice rule for numerical integration. He considered only lattice rules in 3 dimensions and exploited a result of Minkowski [7]. A recent result of Cools and Lyness [2] improves the lower bound of Klyuchnikov and Reztsov for the 4-dimensional case. Their result for 5 dimensions was based on an erroneous lattice rule published by Noskov [8]. The errors in [8] will be corrected and the results in [5] will be improved in this note.

In Section 2 we will briefly introduce some concepts and notations. Section 3 is devoted to the 4-dimensional case and Section 4 is devoted to the 5-dimensional case. In the Appendix we describe how one can compute the trigonometric degree of a lattice rule and we give a short Fortran program for this.

2 Underlying Theory

An s-dimensional cubature formula (or rule) $Q[f]$ for $[0,1)^s$ is a weighted sum of function values

$$Q[f] := \sum_{j=1}^{N(Q)} w_j f(\mathbf{x}_j),$$

which approximates in some way the integral

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

We consider cubature rules of trigonometric degree d. Such a rule integrates correctly all s-dimensional trigonometric polynomials of degree d. Specifically, it integrates $\exp(2\pi i \mathbf{h} \cdot \mathbf{x})$ correctly for all $\mathbf{h} := (h_1, h_2, \ldots, h_s) \in \mathbb{Z}^s$ that satisfy $|\mathbf{h}| := \sum_{k=1}^{s} |h_k| \leq d$. For more information on cubature formulas of trigonometric degree, we refer to [3] and its references.

In this theory it is conventional to refer to $\mathbb{Z}^s$ as the s-dimensional *unit lattice* denoted by Λ_0^s. An *integration lattice* Λ is a discrete subset of $\mathbb{R}^s$ that is closed under addition and subtraction and that contains Λ_0^s. An integration lattice is thus a special kind of lattice that is suitable for numerical integration.

The *lattice rule* $Q(\Lambda)$ is a cubature formula whose abscissas lie on the intersection of an integration lattice Λ and $[0,1)^s$. It can always be written in a form

$$Q[f] = \frac{1}{d_1 d_2 \ldots d_t} \sum_{j_1=1}^{d_1} \sum_{j_2=1}^{d_2} \cdots \sum_{j_t=1}^{d_t} f(\{\sum j_i \mathbf{z}_i / d_i\}), \tag{1}$$

with $t \leq s$ where, as is conventional, $\mathbf{y} = \{\mathbf{x}\}$ is defined as the vector obtained from the fractional parts of each component of $\mathbf{x}$. For more about lattice rules we refer to [9] and its references.

We now return to general lattices and define a lattice packing. Let Ω be a centrally symmetric bounded convex subset of $\mathbb{R}^s$ and let $\tau > 0$. Denote by $\tau\Omega(\cdot - a)$ the shifted set

$$\tau\Omega(\cdot - a) := \left\{ x \in \mathbb{R}^s : \frac{x-a}{\tau} \in \Omega \right\}. \tag{2}$$

For an arbitrary lattice $\Lambda \subset \mathbb{R}^s$, consider those $\tau > 0$ such that the shifted sets satisfy the condition

$$\forall x, y \in \Lambda, x \neq y \ : \ \mathrm{mes}(\tau\Omega(\cdot - x) \cap \tau\Omega(\cdot - y)) = 0. \tag{3}$$

The collection of Ω, τ and Λ given by (2) and (3) is called a *lattice packing of* Ω and will be denoted by $P := P(\Omega, \tau, \Lambda)$.

Denote by $V(\Lambda)$ the volume of the unit cell of the lattice Λ. Let $P_s(\Omega)$ be the set of all lattice packings $P(\Omega, \tau, \Lambda)$ with every possible $\tau > 0$ and lattices $\Lambda \subset \mathbb{R}^s$. The quantity

$$\theta_s(\Omega) := \sup \left\{ \frac{\mathrm{mes}(\tau\Omega)}{V(\Lambda)} : P(\Omega, \tau, \Lambda) \in P_s(\Omega) \right\}$$

is called *the density of the densest lattice packing of* Ω .

We are now ready to combine what is known about lattice rules for numerical integration and lattice packings. Frolov [4] already used the connection between lattice rules and the density of the densest lattice packing for an octahedron. Consider the s-dimensional octahedron (crosspolytope)

$$O_s = \{x \in \mathbb{R}^n : \sum_{j=1}^{s} |x_i| \leq 1\}$$

with $\mathrm{mes}(O_s) = 2^s/s!$. One can show (worked out in detail in [5]) that the number of points N of a lattice rule of trigonometric degree τ satisfies

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

From this follows that every lattice rule provides a constructive lower bound for $\theta(O_s)$:

$$\theta(O_s) \geq \frac{(\tau+1)^s}{Ns!}. \tag{4}$$

This is particularly interesting because for $s \geq 4$, $\theta(O_s)$ is not known. The right-hand side of (4) is a quality measure for a lattice rule. In [2] it is called the rho-index $\rho(Q)$ of the lattice rule Q.

3 The 4-dimensional case

At the time of writing of [5] the best lower bound for $\theta(O_4)$ known to us was $128/159 = 0.80504...$ Cools and Lyness [2] obtained the following lattice rule of trigonometric degree 15:

$$\frac{1}{3312}\sum_{j_1=1}^{1656}\sum_{j_2=1}^{2} f\left(\left\{\frac{j_1}{1656}, \frac{919j_1}{1656}, \frac{1161j_1}{1656}, \frac{1431j_1}{1656} + \frac{j_2}{2}\right\}\right).$$

From this result follows $\theta(O_4) \geq \frac{512}{621} = 0.82447....$

4 The 5-dimensional case

The results of Klyuchnikov and Reztsov [5] are based on the lattice rule

$$\frac{1}{2686}\sum_{j=0}^{2685} f\left(\left\{\frac{j}{2686}, \frac{11j}{2686}, \frac{61j}{2686}, \frac{443j}{2686}, \frac{722j}{2686}\right\}\right). \tag{5}$$

These authors followed Noskov [8] in believing that this lattice rule has trigonometric degree 10. In fact this is wrong. It is straightforward to verify that it is only of degree 9. The effect of this is that the result in [5] has no justification.

In the Appendix we give a straightforward Fortran program that computes the trigonometric degree of any lattice rule given in the form (1).

The bound for $\theta(O_5)$ that corresponds to the lattice rule (5) is

$$\theta(O_5) \geq 0.31025...$$

which is lower than the 0.49965 mentioned in [5].

This rule can be modified into a rule of degree 10 if one uses $d_1 = 3036$ (instead of 2686) in (5). The corresponding bound is

$$\theta(O_5) \geq 0.442...$$

Actually another error appeared in [8]. In that paper the following lattice rule is presented to have degree 12:

$$\frac{1}{6522}\sum_{j=0}^{6521} f\left(\left\{\frac{j}{6522}, \frac{13j}{6522}, \frac{85j}{6522}, \frac{488j}{6522}, \frac{1726}{6522}\right\}\right). \tag{6}$$

In fact, this rule only has degree 10. This rule can be modified into a rule of degree 12 if one uses $d_1 = 7859$ (instead of 6522) in (6). The corresponding bound is

$$\theta(O_5) \geq 0.3937...$$

The highest lower bound for $\theta(O_5)$ we know at the moment comes from the following lattice rule of degree 9:

$$\frac{1}{1306} \sum_{j=0}^{1305} f\left(\left\{\frac{j}{1306}, \frac{41j}{1306}, \frac{51j}{1306}, \frac{321j}{1306}, \frac{389j}{1306}\right\}\right). \qquad (7)$$

The corresponding bound is

$$\theta(O_5) \geq \frac{1250}{1959} = 0.63808...$$

This improves the highest accepted (but incorrectly calculated) lower bound significantly. The lattice rule (7) is not yet accepted to be published elsewhere. The fact that a rule of degree 9 with 1306 points exists, was first established in the GRISK project [10]. There the method described in [2] for 3 and 4 dimensions, is applied to 5 dimensions, which is significantly more time consuming.

Acknowledgements

James Lyness [6] first drew my attention to the incorrect results in [8] in 1998 and provided the correct degrees.

A Computing the trigonometric degree of a lattice rule

A lattice rule has trigonometric degree d if it integrates $\exp(2\pi i\mathbf{h}\cdot\mathbf{x})$ correctly for all $\mathbf{h} := (h_1, h_2, \ldots, h_s) \in \mathbb{Z}^s$ that satisfy $|\mathbf{h}| := \sum_{k=1}^{s} |h_k| \leq d$. This means that

$$\begin{cases} Q[1] & = I[1] & = 1 \\ Q[\exp(2\pi i\mathbf{h}\cdot\mathbf{x})] & = I[\exp(2\pi i\mathbf{h}\cdot\mathbf{x})] & = 0 \ \forall\mathbf{h} : 0 < |\mathbf{h}| \leq d. \end{cases}$$

The first equation above is trivially satisfied. The second equation can be rewritten as

$$\begin{aligned} 0 &= Q[\exp(2\pi i\mathbf{h}\cdot\mathbf{x})] \\ &= \frac{1}{d_1 d_2 \ldots d_t} \sum_{j_1=1}^{d_1} \sum_{j_2=1}^{d_2} \cdots \sum_{j_t=1}^{d_t} \exp(2\pi i\mathbf{h}\cdot(\{\sum j_i\mathbf{z}_i/d_i\})) \\ &= \frac{1}{d_1 d_2 \ldots d_t} \sum_{j_1=1}^{d_1} \sum_{j_2=1}^{d_2} \cdots \sum_{j_t=1}^{d_t} \exp(\frac{2\pi i j_1}{d_1}\mathbf{h}\cdot\mathbf{z}_1) \cdots \exp(\frac{2\pi i j_t}{d_t}\mathbf{h}\cdot\mathbf{z}_t) \end{aligned}$$

$$\iff 0 = \sum_{j_1=1}^{d_1} \exp(2\pi i j_1\mathbf{h}\cdot\mathbf{z}_1/d_1) \ldots \sum_{j_t=1}^{d_t} \exp(2\pi i j_t\mathbf{h}\cdot\mathbf{z}_t/d_t).$$

Consequently, the lattice rule has degree d if

$$\forall\mathbf{h} : 0 < |\mathbf{h}| \leq d, \exists k : \sum_{j_k=1}^{d_k} \exp(2\pi i j_k\mathbf{h}\cdot\mathbf{z}_k/d_k) = 0$$

or equivalently

$$\forall\mathbf{h} : 0 < |\mathbf{h}| \leq d, \exists k : \mathbf{h}\cdot\mathbf{z}_k \bmod d_k \neq 0.$$

The Fortran 90 program below checks this condition for increasing values of d until it fails.

```
      program trigdegree
!
! Verify a given rank t rule for s dimensions.
! The rule must be entered in D-Z form.
!
      implicit none
      integer, dimension(:), allocatable :: alfa, tmp, d
      integer, dimension(:,:), allocatable :: a
      integer :: i, j, s, t, sfac, trydeg

      print *,'Give dimension.'
      read *,s
      print *,'Give rank.'
      read *,t
      allocate(a(s,t),alfa(s),tmp(t),d(t))

      print *,'Give d(j), j=1..rank.'
      read *,(d(i),i=1,t)
      print *,'Give generators (rows of Z).'
      read *,((a(i,j),i=1,s),j=1,t)

      trydeg = 1
      alfa(1) = -trydeg
      alfa(2:s) = 0
out:  do
         do j=1,t
            tmp(j) = dot_product(a(:,j),alfa)
         end do
         if ( all(mod(tmp,d) == 0) ) then
            print *,'Lattice rule has degree ',trydeg-1
            sfac = product( (/ (i,i=1,s) /) )
            print *,'rho-index = ',(real(trydeg)**s)/(sfac*product(d))
            stop
         endif
         do i = s-1,1,-1
            if (trydeg - sum(abs(alfa(1:i-1))) > alfa(i) ) then
               alfa(i) = alfa(i) + 1
               alfa(i+1) = -trydeg + sum(abs(alfa(1:i)))
               alfa(i+2:s) = 0
               cycle out
            end if
          end do
          trydeg = trydeg + 1
          alfa(1) = -trydeg
          alfa(2:s) = 0
      end do out
      end program trigdegree
```

References

[1] U. Betke and M. Henk. Densest lattice packings of 3-polytopes. *Computational Geometry*, 16:157–186, 2000.

[2] R. Cools and J.N. Lyness. Three- and four-dimensional K-optimal lattice rules of moderate trigonometric degree. *Math. Comp.*, 70(236):1549–1567, 2001. (Electronically published on May 14, 2001.)

[3] R. Cools and I.H. Sloan. Minimal cubature formulae of trigonometric degree. *Math. Comp.*, 65(216):1583–1600, 1996.

[4] K.K. Frolov. On the connection between quadrature formulas and sublattices of the lattice of integral vectors. *Dokl. Akad. Nauk SSSR*, 232:40–43, 1977. (Russian) Soviet Math. Dokl. 18: 37–41, 1977 (English).

[5] B.V. Klyuchnikov and A.V. Reztsov. A relation between cubature formulas and densest lattice packings. *East Journal on Approximations*, 1(4):557–570, 1995.

[6] J.N. Lyness. Private Communication, 1998.

[7] H. Minkowski. *Gesammelte Abhandlungen.* Chelsea Publishing Company, New York, Reprinted (originally published, in 2 volumes, Leipzig, 1911) edition, 1967.

[8] M.V. Noskov. Cubature formulae for the approximate integration of periodic functions. *Metody Vychisl.*, 14:15–23, 1985. (Russian).

[9] I.H. Sloan and S. Joe. *Lattice Methods for Multiple Integration.* Oxford University Press, 1994.

[10] T. Sørevik and J. F. Myklebust. GRISK: An internet based search for K-optimal lattice rules. In *Proceedings of PARA2000*, volume 1947 of *Lecture Notes in Computer Science*, pages 196–205. Springer Verlag, 2001. See the webpage of this project at `http://www.ii.uib.no/grisk/`.