High-Accuracy Semidefinite Programming Bounds for Kissing Numbers

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CONTENTS

The kissing number in n-dimensional Euclidean space is the maximal number of nonoverlapping unit spheres that simultaneously can touch a central unit sphere. Bachoc and Vallentin developed a method to find upper bounds for the kissing number based on semidefinite programming. This paper is a report on high-accuracy calculations of these upper bounds for $n \leq 24$. The bound for $n = 16$ implies a conjecture of Conway and Sloane: there is no 16-dimensional periodic sphere packing with average theta series $1 + 7680q^3 + 4320q^4 + 276480q^5 + 61440q^6 + \cdots$.

1. INTRODUCTION

In geometry, the *kissing number* in n-dimensional Euclidean space is the maximal number of nonoverlapping unit spheres that simultaneously can touch a central unit sphere. The kissing number is known only in dimensions $n = 1, 2, 3, 4, 8, 24$, and there have been many attempts to find good lower and upper bounds. We refer to [Casselman 04] for the history of this problem and to [Pfender and Ziegler 04, Elkies 00, Conway and Sloane 99] for more background information on sphere-packing problems.

In [Bachoc and Vallentin 08] a method is developed (Section 2 recalls it) to find upper bounds for the kissing number based on semidefinite programming. Table 1, the main contribution of this paper, gives the values—the first ten significant digits—of these upper bounds for all dimensions $3, \ldots, 24$. In all cases they are the best known upper bounds. Dimension 5 is the first dimension in which the kissing number is not known.

With our computation we could limit the range of possible values from $\{40, \ldots, 45\}$ to $\{40, \ldots, 44\}$. In Section 4 we show that the high-accuracy computations for the upper bounds in dimension 4 lead to a question about a possible approach to proving the uniqueness of the kissing configuration in four dimensions.

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Although acquiring the data for the table is a purely computational task, we think that providing this table is valuable for several reasons: The kissing number is an important constant in geometry and results can depend on good upper bounds for it. For instance, in Section 5 we show that there is no periodic point set in dimension 16 with average theta series

$$1 + 7680q^3 + 4320q^4 + 276480q^5 + 61440q^6 + \cdots .$$

This proves a conjecture from [Conway and Sloane 99, p. 190]. Furthermore, the actual computation of the table was very challenging. Results are given in [Bachoc and Vallentin 08] for dimensions $3, \ldots, 10$. However, the authors report on numerical difficulties that prevented them from extending their results. Now using new, more sophisticated, high-accuracy software and faster computers and more computation time, we were able to overcome some of the numerical difficulties. Section 3 contains details about the computations.

2. NOTATION

In this section we set up the notation that is needed for our computation. For more information we refer to [Bachoc and Vallentin 08]. For natural numbers d and $n \geq 3$ let $s_d(n)$ be the optimal value of the following minimization problem:

$$\text{Minimize} \qquad 1 + \sum_{k=1}^{d} a_k + b_{11} + \langle F_0, S_0^n(1,1,1)\rangle$$

subject to the following conditions:

$$a_1, \ldots, a_d \in \mathbb{R}, \quad a_1, \ldots, a_d \geq 0,$$
$$b_{11}, b_{12}, b_{22} \in \mathbb{R}, \quad \left(\begin{smallmatrix} b_{11} & b_{12} \\ b_{12} & b_{22}\end{smallmatrix}\right) \text{ is positive semidefinite},$$
$$F_k \in \mathbb{R}^{(d+1-k)\times(d+1-k)}, \quad F_k \text{ is positive semidefinite}, \quad k = 0, \ldots, d,$$
$$q, q_1 \in \mathbb{R}[u], \quad \deg(p + pq_1) \leq d, \quad p, p_1 \text{ sums of squares},$$
$$r, r_1, \ldots, r_4 \in \mathbb{R}[u,v,t], \quad \deg\left(r + \sum_{i=1}^{4} p_i r_i\right) \leq d, \quad r, r_1, \ldots, r_4 \text{ sums of squares},$$
$$1 + \sum_{k=1}^{d} a_k P_k^n(u) + 2b_{12} + b_{22} + 3\sum_{k=0}^{d}\langle F_k, S_k^n(u,u,1)\rangle + q(u) + p(u)q_1(u) = 0,$$
$$b_{22} + \sum_{k=0}^{d}\langle F_k, S_k^n(u,v,t)\rangle + r(u,v,t) + \sum_{i=1}^{4} p_i(u,v,t) r_i(u,v,t) = 0.$$

Here P_k^n is the normalized Jacobi polynomial of degree k with $P_k^n(1) = 1$ and parameters $((n-3)/2, (n-3)/2)$. In general, *Jacobi polynomials* with parameters (α, β) are orthogonal polynomials for the measure $(1-u)^\alpha(1+u)^\beta\, du$ on the interval $[-1,1]$. Before we can define the matrices S_k^n, we first define the entry (i,j) with $i, j \geq 0$ of the (infinite) matrix Y_k^n containing polynomials in the variables u, v, w by

$$\left(Y_k^n\right)_{i,j}(u,v,t) = u^i v^j \left((1-u^2)(1-v^2)\right)^{k/2} P_k^{n-1} \times \left(\frac{t - uv}{\sqrt{(1-u^2)(1-v^2)}}\right).$$

Then we get S_k^n by symmetrization: $S_k^n = \frac{1}{6}\sum_\sigma \sigma Y_k^n$, where σ runs through all permutations of the variables u, v, t, which acts on the matrix coefficients in the obvious way. The polynomials $p, p_1, \ldots, p_4$ are given by

$$p(u) = -(u+1)(u+1/2),$$
$$p_1(u,v,t) = p(u), \quad p_2(u,v,t) = p(v), \quad p_3(u,v,t) = p(t),$$
$$p_4(u,v,t) = 1 + 2uvt - u^2 - v^2 - t^2.$$

By $\langle A, B\rangle$ we denote the inner product between symmetric matrices trace(AB).

In [Bachoc and Vallentin 08] it is shown that this minimization problem is a semidefinite program and that every upper bound on $s_d(n)$ provides an upper bound for the kissing number in dimension n. Clearly, the numbers $s_d(n)$ form a monotonic decreasing sequence in d.

3. BOUNDS FOR KISSING NUMBERS

Finding the solution of the semidefinite program defined in Section 2 is a computational challenge. It turns out that the major obstacle is numerical instability and not the problem size. When d is fixed, the size of the input matrices stays constant with n; when n is fixed, it grows rather moderately with d.

There are several software packages available for solving semidefinite programs. Many existing packages are compared in [Mittelmann 03]. For our purpose, first-order gradient-based methods such as `SDPLR` are far too inaccurate, and second-order primal-dual interior-point methods are more suitable. Here increasingly ill-conditioned linear systems have to be solved even if the underlying problem is well conditioned. This happens in the final phase of the algorithm when one approaches an optimal solution. Our problems are not well conditioned, and even the most robust solver, `SeDuMi`, which

n	Best Lower Bound Known	Best Upper Bound Previously Known	SDP Bound
3	12	$\underline{12}$ [Schütte and van der Waerden 53]	$s_{11}(3) = 12.42167009\dots$, $s_{12}(3) = 12.40203212\dots$ $s_{13}(3) = 12.39266509\dots$, $s_{14}(3) = 12.38180947\dots$
4	24	$\underline{24}$ [Musin 08]	$s_{11}(4) = 24.10550859\dots$, $s_{12}(4) = 24.09098111\dots$ $s_{13}(4) = 24.07519774\dots$, $s_{14}(4) = 24.06628391\dots$
5	40	45 [Bachoc and Vallentin 08]	$s_{11}(5) = 45.06107293\dots$, $s_{12}(5) = 45.02353644\dots$ $s_{13}(5) = 45.00650838\dots$, $s_{14}(5) = \underline{44}.99899685\dots$
6	72	$\underline{78}$ [Bachoc and Vallentin 08]	$s_{11}(6) = 78.58344077\dots$, $s_{12}(6) = 78.35518719\dots$ $s_{13}(6) = 78.29404232\dots$, $s_{14}(6) = 78.24061272\dots$
7	126	135 [Bachoc and Vallentin 08]	$s_{11}(7) = \underline{134}.8824614\dots$, $s_{12}(7) = 134.7319671\dots$ $s_{13}(7) = 134.5730609\dots$, $s_{14}(7) = 134.4488169\dots$
8	240	$\underline{240}$ [Odlyzko 79] [Levenshtein 79]	$s_{11}(8) = 240.0000000\dots$
9	306	366 [Bachoc and Vallentin 08]	$s_{11}(9) = 365.3229274\dots$, $s_{12}(9) = \underline{364}.7282746\dots$ $s_{13}(9) = 364.3980087\dots$, $s_{14}(9) = 364.0919287\dots$
10	500	567 [Bachoc and Vallentin 08]	$s_{11}(10) = 558.1442813\dots$, $s_{12}(10) = 556.2840736\dots$ $s_{13}(10) = 555.2399024\dots$, $s_{14}(10) = \underline{554}.5075418\dots$
11	582	915 [Odlyzko 79]	$s_{11}(11) = 878.6158044\dots$, $s_{12}(11) = 873.3790094\dots$ $s_{13}(11) = 871.9718533\dots$, $s_{14}(11) = \underline{870}.8831157\dots$
12	840	1416 [Odlyzko 79]	$s_{11}(12) = 1364.683810\dots$, $s_{12}(12) = 1362.200297\dots$ $s_{13}(12) = 1359.283834\dots$, $s_{14}(12) = \underline{1357}.889300\dots$
13	1154	2233 [Odlyzko 79]	$s_{11}(13) = 2089.116331\dots$, $s_{12}(13) = 2080.631518\dots$ $s_{13}(13) = 2073.074796\dots$, $s_{14}(13) = \underline{2069}.587585\dots$
14	1606	3492 [Odlyzko 79]	$s_{11}(14) = 3224.950751\dots$, $s_{12}(14) = 3202.448902\dots$ $s_{13}(14) = 3189.127644\dots$, $s_{14}(14) = \underline{3183}.133169\dots$
15	2564	5431 [Odlyzko 79]	$s_{11}(15) = 4949.650431\dots$, $s_{12}(15) = 4893.479446\dots$ $s_{13}(15) = 4876.037229\dots$, $s_{14}(15) = \underline{4866}.245659\dots$
16	4320	8312 [Pfender 07]	$s_{11}(16) = 7515.952644\dots$, $s_{12}(16) = 7432.720718\dots$ $s_{13}(16) = 7374.093742\dots$, $s_{14}(16) = \underline{7355}.809036\dots$
17	5346	12210 [Pfender 07]	$s_{11}(17) = 11568.41674\dots$, $s_{12}(17) = 11333.84265\dots$ $s_{13}(17) = 11128.26227\dots$, $s_{14}(17) = \underline{11072}.37543\dots$
18	7398	17877 [Odlyzko 79]	$s_{11}(18) = 17473.48016\dots$, $s_{12}(18) = 17034.32488\dots$ $s_{13}(18) = 16686.28908\dots$, $s_{14}(18) = \underline{16572}.26478\dots$
19	10668	25900 [Boyvalenkov 94]	$s_{11}(19) = 26397.34794\dots$, $s_{12}(19) = 25636.98958\dots$ $s_{13}(19) = 25029.87432\dots$, $s_{14}(19) = \underline{24812}.30254\dots$
20	17400	37974 [Odlyzko 79]	$s_{11}(20) = 39045.32761\dots$, $s_{12}(20) = 37844.10380\dots$ $s_{13}(20) = 37067.18966\dots$, $s_{14}(20) = \underline{36764}.40138\dots$
21	27720	56851 [Boyvalenkov 94]	$s_{11}(21) = 58087.03857\dots$, $s_{12}(21) = 56079.21685\dots$ $s_{13}(21) = 55170.03449\dots$, $s_{14}(21) = \underline{54584}.76757\dots$
22	49896	86537 [Odlyzko 79]	$s_{11}(22) = 87209.06261\dots$, $s_{12}(22) = 84922.09101\dots$ $s_{13}(22) = 84117.92103\dots$, $s_{14}(22) = \underline{82340}.08003\dots$
23	93150	128095 [Boyvalenkov 94]	$s_{11}(23) = 128360.7969\dots$, $s_{12}(23) = 127323.7095\dots$ $s_{13}(23) = 125978.7655\dots$, $s_{14}(23) = \underline{124416}.9796\dots$
24	196560	$\underline{196560}$ [Odlyzko 79] [Levenshtein 79]	$s_{11}(24) = 196560.0000\dots$

TABLE 1. New upper bounds for the kissing number (best known values are underlined).

uses partial quadruple arithmetic in the final phase, does not produce reliable results for $d > 10$.

We thus had to fall back on the implementation `SDPA-GMP` [Fujisawa et al. 08], which is much slower but much more accurate than other software packages because it uses the GNU Multiple Precision Arithmetic Library. We worked with 200 to 300 binary digits and relative stopping criteria of 10^{-30}. The ten significant digits listed in the table are thus guaranteed to be correct. One problem was convergence. Even with the control parameter settings recommended by the authors of SDPA-GMP for "slow but stable" computations, the algorithm failed to converge in several instances. However, we found parameter choices that worked for all cases: We varied the parameter lambdaStar between 100 and 10,000 depending on the case, while the other parameters could be chosen at or near the values recommended for "slow but stable" performance.

The computations were done on Intel Core 2 platforms with one and two Quad processors. The computation time varied between five and ten weeks per case for $d = 12$. An accuracy of 128 bits in SDPA-GMP did yield sufficient accuracy but did not yield a reduction in computing time.

After the computations for the cases $d = 11$ and $d = 12$ were finished, new 128-bit versions (quadruple precision) of SDPA and CSDP became available, partly with our assistance. These new versions do not rely on the GNU Multiple Precision Arithmetic Library. So the computation times for the cases $d = 13$ and $d = 14$ were reasonable: from one week to two and a half weeks.

4. QUESTION ABOUT THE OPTIMALITY OF THE D_4 ROOT SYSTEM

Looking at the values $s_d(4)$ in Table 1, one is led to the following question:

Question 4.1. Is $\lim_{d\to\infty} s_d(4) = 24$?

If the answer to this question is yes (which at the moment appears unlikely because we computed $s_{15}(4) = 23.06274835\ldots$), then it would have two noteworthy consequences about optimality properties of the root system D_4.

The root system D_4 defines (up to orthogonal transformations) a point configuration on the unit sphere $S^3 = \{x \in \mathbb{R}^4 : x \cdot x = 1\}$ consisting of 24 points; it is the same point configuration as the one coming from the vertices of the regular 24 cell. This point configuration has the property that the spherical distance of every two distinct points is at least $\arccos \frac{1}{2}$. Hence, these points can be the maximal 24 touching points of unit spheres kissing the central unit sphere S^3.

If $\lim_{d\to\infty} s_d(4) = 24$, then this would prove that the root system D_4 is the unique optimal point configuration of cardinality 24. Here optimality means that one cannot distribute 24 points on S^3 in such a way that the minimal spherical distance between two distinct points exceeds $\arccos \frac{1}{2}$. Thus, the root system D_4 would be characterized by its kissing property. This is generally believed to be true, but so far, no proof has been given.

Another consequence would be that there is no universally optimal point configuration of 24 points in S^3 as conjectured in [Cohn et al. 07]. Universally optimal point configurations minimize every absolutely monotonic potential function. The conjecture will follow if the answer to our question is yes: every universally optimal point configuration is automatically optimal, and it is shown in [Cohn et al. 07] that the root system D_4 is not universally optimal.

5. NONEXISTENCE OF A SPHERE PACKING

Our new upper bound of 7355 for the kissing number in dimension 16 implies that there is no periodic point set in dimension 16 whose average theta series equals

$$1 + 7680q^3 + 4320q^4 + 276480q^5 + 61440q^6 + \cdots. \quad (5\text{–}1)$$

This settles a conjecture from [Conway and Sloane 99, p. 190]. In this section we explain this result. We refer to [Conway and Sloane 99, Elkies 00, Bowert 04] for more information.

An n-dimensional *periodic point set* Λ is a finite union of translates of an n-dimensional lattice, i.e., one can write Λ as $\Lambda = (A\mathbb{Z}^n + v_1) \cup \cdots \cup (A\mathbb{Z}^n + v_N)$, with $v_1, \ldots, v_N \in \mathbb{R}^n$, and $A : \mathbb{R}^n \to \mathbb{R}^n$ is a linear isomorphism. The *average theta series* of Λ is

$$\Theta_\Lambda(z) = \frac{1}{N}\sum_{i=1}^{N}\sum_{j=1}^{N}\sum_{v\in\mathbb{Z}^n} q^{\|Av - v_i + v_j\|^2}, \text{ with } q = e^{\pi i z}.$$

This is a holomorphic function defined on the complex upper half-plane. A holomorphic function f that is defined on the complex upper half-plane is meromorphic for $z \to i\infty$ and satisfies the transformation laws

$$f\left(-\frac{1}{z}\right) = z^8 f(z),$$
$$f(z+2) = f(z) \quad \text{for all } z \in \mathbb{C} \text{ with } \Im z > 0,$$

is called a *modular form* of weight 8 for the Hecke group $G(2)$. The expression (5–1) defines the unique modular form of weight 8 for the Hecke group $G(2)$ that begins $1 + 0q^1 + 0q^2$. It is also called an *extremal modular form*; see [Scharlau and Schulze-Pillot 99].

If there were a 16-dimensional periodic point set whose average theta series coincided with (5–1), then this periodic point set would define the sphere centers of a sphere packing with extraordinarily high density (see [Conway and Sloane 99, p. 190]). At the same time, the existence of such a periodic point set would show that the kissing number in dimension 16 was at least 7680. This is not the case.

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