The SDP and LP bounds for optimal spherical configurations using their distance distribution

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If unit spheres kiss the unit sphere $S$, then the set of kissing points is the arrangement on $S$ such that the angular distance between any two points is at least $60^\circ$. Thus, the kissing number is the maximal number of nonoverlapping spherical caps of radius $30^\circ$ on $S$. 

Packing by spherical caps
I. Area inequalities. **L. Fejes Tóth** (1943); for $d > 3$ **Coxeter** (1963) and **Böröczky** (1978)

II. Contact and distance graphs. **Schütte – van der Waerden** (1951); **Danzer** (1963); **Leech** (1956);...

III. LP bounds. **Delsarte et al** (1977); **Kabatiansky and Levenshtein** (1978); **Odlyzko & Sloane** (1979), ...

IV. SDP bounds. 3–point SDP: **Bachoc and Vallentin** (2008); $k$–point SDP: **M.** (2007, 2014); ...
Let $M$ be a metric space with distance function $d$. $M$ is said to be a **two-point homogeneous space** if for any two pairs $(p, q)$ and $(p', q')$ of points in $M$, satisfying the condition $d(p, q) = d(p', q')$, there is an isometry $F$ of $M$, such that $F(p) = p'$ and $F(q) = q'$.

Let $M$ be a compact connected two–point homogeneous spaces (Riemannian symmetric spaces of rank one). Then $M = S^n, \mathbb{RP}^n, \mathbb{CP}^n, \mathbb{QP}^n, \text{CayP}^2$ [Wang, 1952]
With any compact 2-point-homogeneous space $M$ are associated the zonal spherical functions $\Phi_k(t)$, $k = 0, 1, 2, \ldots$, and the distance function $\tau(x, y)$, where $x, y \in M$.

For all continuous compact $M$ and for all currently known finite cases: $\Phi_k(t)$ is a polynomial of degree $k$.

If $M = \text{Hamming space}$, then $\Phi_k(t)$ is the Krawtchouk polynomial $K_k(t, n)$.

If $M = \text{unit sphere } S^{n-1} \subset \mathbb{R}^n$, then the corresponding zonal spherical function $\Phi_k(t)$ is the Gegenbauer (or ultraspherical) polynomial $G_k^{(n)}(t)$. 
The main property for zonal spherical functions is called “positive-definite degenerate kernels” or p.d.k. This property first was discovered by Bochner (general spaces) and independently for spherical spaces by Schoenberg:

Let $M$ be a 2-point-homogeneous space. Then for any integer $k \geq 0$ and for any finite $C = \{x_i\} \subset M$ the matrix $(\Phi_k(\tau(x_i, x_j)))$ is positive semidefinite.
LP and SDP bounds for spherical codes

\[ N \leq \frac{f(1)}{f_0} \]

\[ N \leq \frac{f(1) + \hat{h}(n, T, f)}{f_0} \]

\[ N^2 \leq \frac{f(1, 1, 1) + 3(N - 1)B}{f_0} \]

\[ N^2 \leq \frac{f(1, 1, 1) + 3(N - 1)B + 3N\hat{h}(n, T, g)}{f_0} \]

\[ N^3 \leq \frac{f(1, 1, 1, 1, 1) + 4(N - 1)B_1 + 3(N - 1)B_2 + 6(N - 1)(N - 2)B_3}{f_0} \]
Uniqueness of the max kissing arrangement in 4 dim?

David de Laat, Nando M. Leijenhorst, Willem H. H. de Muinck Keizer: “Optimality and uniqueness of the $D_4$ root system”

arXiv:2404.18794

\[ N^3 \leq \frac{f(1,1,1,1,1,1) + 4(N-1)B_1 + 3(N-1)B_2 + 6(N-1)(N-2)B_3}{f_0} \]
Kissing numbers

The SDP and LP bounds for optimal spherical configurations using their distance distribution.
The only exact values of kissing numbers known:

<table>
<thead>
<tr>
<th>$n$</th>
<th>lattice</th>
<th>regular polytope</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k(1) = 2$</td>
<td>$A_1$</td>
<td></td>
</tr>
<tr>
<td>$k(2) = 6$</td>
<td>$A_2$</td>
<td>hexagon</td>
</tr>
<tr>
<td>$k(3) = 12$</td>
<td>$H_3$</td>
<td>icosahedron</td>
</tr>
<tr>
<td>$k(4) = 24$</td>
<td>?$D_4$</td>
<td>?24-cell</td>
</tr>
<tr>
<td>$k(8) = 240$</td>
<td>$E_8$</td>
<td></td>
</tr>
<tr>
<td>$k(24) = 196,560$</td>
<td>$\Lambda_{24}$</td>
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</tbody>
</table>
$n = 4$: There are 24 vectors with two zero components and two components equal to $\pm 1$; they all have length $\sqrt{2}$ and a minimum distance of $\sqrt{2}$. Properly rescaled (that is, multiplied by $\sqrt{2}$), they yield the centers for a kissing configuration of unit spheres and imply that $k(4) \geq 24$. The convex hull of the 24 points yields a famous 4-dimensional regular polytope, the “24-cell”, discovered in 1842 by Ludwig Schlafli. Its facets are 24 regular octahedra.
The four dimensional lattice packing $D_4$

The checkerboard lattice $D_n := \{(x_1, \ldots, x_n) \in \mathbb{Z}^n : x_1 + \ldots + x_n \text{ even}\}$

$D^*_4 = D_4$

The Voronoi cell of $D_4$ is the regular 24-cell

The density $\Delta_4 = \pi^2/16 = 0.6169...$

**The densest packing by unit spheres in four dimensions is conjectured to be the $D_4$**

The center density $= \Delta/B$:

$CD_4 = 0.12500$;

Cohn–Elkies bound $= 0.13126$;

de Laat – de Oliveira Filho – Vallentin $= 0.130587$
The 24–cell conjecture

Consider the Voronoi decomposition of any given packing $P$ of unit spheres in $\mathbb{R}^4$. The minimal volume of any cell in the resulting Voronoi decomposition of $P$ is at least as large as the volume of a regular 24–cell circumscribed to a unit sphere.
Theorem (Delsarte et al)

If

\[ f(t) = \sum_{k=0}^{d} c_k G_k^{(n)}(t) \]

is nonnegative combination of Gegenbauer polynomials, with \( c_k \geq 0 \) and \( c_0 > 0 \), and if \( f(t) \leq 0 \) holds for all \( t \in [-1, \frac{1}{2}] \), then the kissing number in \( n \) dimensions is bounded by

\[ k(n) \leq \frac{f(1)}{c_0} \]
G.A. Kabatiansky and V.I. Levenshtein (1978):

\[ 2^{0.2075n(1+o(1))} \leq k(n) \leq 2^{0.401n(1+o(1))} \]

In 1979: V. I. Levenshtein and independently A. Odlyzko and N.J.A. Sloane using Delsarte’s method have proved that \( k(8) = 240 \), and \( k(24) = 196560 \).

Odlyzko & Sloane: upper bounds on \( k(n) \) for \( n = 4, 5, 6, 7, \) and 8 are 25, 46, 82, 140, and 240, respectively.
Let \( f(x) = \sum f_k G_k^{(n)}(x), \ f_k \geq 0, \ f_0 > 0 \)
\( f(x) \leq 0 \) for all \( x \in [-1, 1/2] \setminus T \).

Then
\[
N \leq \frac{f(1) + \hat{h}(n, T, f)}{f_0}.
\]

\( n = 4; \ T = [-1, -0.6058], \ f_0 = 1, \ N < 24.865 \)
The kissing problem in four dimensions

\[ f_4(t) = 53.76t^9 - 107.52t^7 + 70.56t^5 + 16.38t^4 - 9.83t^3 - 4.12t^2 + 0.434t - 0.016 \]

**Lemma**

Let \( P = \{p_1, \ldots, p_m\} \) be unit vectors in \( \mathbb{R}^4 \) (i.e. points on the unit sphere \( S^3 \)). Then

\[
S(P) = \sum_{k, \ell} f_4(p_k \cdot p_\ell) \geq m^2.
\]

**Lemma**

Let \( P = \{p_1, \ldots, p_m\} \) be a kissing arrangement on the unit sphere \( S^3 \) (i.e. \( p_k \cdot p_\ell \leq \frac{1}{2} \)). Then

\[
S(P) = \sum_{k, \ell} f_4(p_k \cdot p_\ell) < 25m.
\]
The graph of $y = f_4(t)$
D := \{(x, y, z) : -1 \leq x, y, z \leq 1/2, 1 + 2xyz - x^2 - y^2 - z^2 \geq 0\}.

\text{BV}(n, f_0) := \{F : F(x, y, z) = \sum \langle F_k, S^n_k(x, y, z) \rangle, F_k \succeq 0, F_0 - f_0E_0 \succeq 0\}

Suppose
(1) \(F \in \text{BV}(n, f_0)\),
(2) \(F(x, x, 1) \leq B\) for all \(x \in [-1, 1/2]\),
(3) \(F(x, y, z) \leq 0\) for all \((x, y, z) \in D\),

Then
\[N^2 \leq \frac{F(1, 1, 1) + 3(N - 1)B}{f_0}\]
LP bound [Odlyzko & Sloane; Arestov & Babenko] = 25.558...

M. (2003): \( k(4) < 24.865 \)

C. Bachoc & F. Vallentin (2008): \( S_7(4) = 24.5797... \)


\[
\begin{align*}
S_{11}(4) &= 24.10550859... \\
S_{12}(4) &= 24.09098111... \\
S_{13}(4) &= 24.07519774... \\
S_{14}(4) &= 24.06628391...
\end{align*}
\]

F.C. Machado & F.M. de Oliveira Filho (2018)

\[
\begin{align*}
S_{15}(4) &= 24.062758... \\
S_{16}(4) &= 24.056903...
\end{align*}
\]
\( g_T(x) = g(x) \) for \( x \in T \) and \( g_T(x) = 0 \) otherwise.

**Definition**

For given \( n, f_0, T \subset [-1, 1], g : T \to \mathbb{R}, B \) and \( \theta \) denote by \( \mathcal{F}(n, f_0, T, g, B, \theta) \) the class of symmetric polynomials \( F(x, y, z) \) that satisfy the following properties:

1. \( F \in \text{BV}(n, f_0), \)
2. \( F(x, x, 1) \leq B + 6g_T(x) \) for all \( x \in [-1, \cos \theta], \)
3. \( F(x, y, z) \leq g_T(x) + g_T(y) + g_T(z) \) for all \( (x, y, z) \in D(\theta). \)

**Theorem (M., 2019)**

Let \( F \in \mathcal{F}(n, f_0, T, g, B, \theta). \) Then an \( (N, n, \theta) \) spherical code satisfies the following inequality

\[
N^2 \leq \frac{F(1, 1, 1) + 3(N - 1)B + 3N \hat{h}(n, \theta, T, g)}{f_0}.
\]
Let $C$ be an $(N, n, \theta)$ spherical code. The \textit{distance distribution} of $C$ is the system of numbers $\{A_t : -1 \leq t \leq 1\}$.

\[ A_t(u) := |\{v \in C : v \cdot u = t\}|, \quad A_t := \frac{1}{N} \sum_{u \in C} A_t(u). \]

$A_t = 0$ for $s := \cos \theta < t < 1$, $\sum_{-1 \leq t \leq s} A_t = N - 1$.

\[ A(T) := \sum_{t \in T : A_t > 0} A_t, \quad T \subset [-1, 1]. \]
SDP bounds for distance distribution

Theorem (M., 2019)

Let \( F \in \mathcal{F}(n, f_0, T, g, B, \theta) \). Suppose \( T \subset [-1, \cos \theta] \) and \( g(t) \leq -a < 0 \) for all \( t \in T \). Then for every \((N, n, \theta)\) spherical code \( C\) we have

\[
A(T) \leq \frac{2}{N} \lceil Q \rceil, \quad Q := \frac{F(1, 1, 1) + 3(N - 1)B - f_0N^2}{6a}.
\]

Theorem (M., 2019)

Let \( F \in \mathcal{F}(n, f_0, T, g, B, \theta) \). Let \( a > 0 \). Suppose \( T \subset [-1, \cos \theta] \) and \( g(t) \leq a \) for all \( t \in T \). Then for every \((N, n, \theta)\) spherical code \( C\) we have

\[
A(T) \geq \frac{2}{N} \lfloor R \rfloor, \quad R := \frac{f_0N^2 - F(1, 1, 1) - 3(N - 1)B}{6a}.
\]
Distance distribution of the 24–cell

Kissing arrangement in four dimensions:

\[ A(\{-1\}) = 1, \quad A(\{-1/2\}) = 8, \quad A(\{0\}) = 6, \quad A(\{1/2\}) = 8 \]

\[ A_t = 0 \quad \text{for all} \quad t \neq \{-1, -1/2, 0, 1/2, 1\} \]
Theorem (Dostert–Kolpakov–Moustrou–M.)

Let $C$ be a $(24, 4, \pi/3)$ – spherical code. Then

\[
A([-1, -0.45]) \leq 9; \quad A([-1, 0.35]) \leq 15,
\]

\[
A([-0.73, 0.35]) \leq 14, \quad A([-0.05, 0.5]) \leq 14,
\]

\[
A([-1, -0.73]) \geq 1, \quad A([0.35, 0.5]) \geq 8.
\]
Let $C$ be an $N$–element subset of the unit sphere $\mathbb{S}^{n-1} \subset \mathbb{R}^n$.

$$I(C) := \{ t = x \cdot y \mid x, y \in C \text{ & } x \neq y \}.$$ 

Let $T \subset [-1, 1)$. We say that $C$ is an $(N, n, T)$ spherical code if $I(C) \subset T$.

Let $g$ be a real function on $I(C)$. Define

$$E_g(C) := \sum_{(x, y) \in C^2, x \neq y} g(x \cdot y),$$

$$S_g(C) := \sum_{(x, y) \in C^2} g(x \cdot y) = E_g(C) + Ng(1).$$
Theorem

Let $C$ be an $(N, n, T)$ spherical code. Suppose $g : T \to \mathbb{R}$, $f : [-1, 1] \to \mathbb{R}$ and $f_0 \in \mathbb{R}$ are such that

1. $f(t) \leq g(t)$ for all $t \in T$.
2. $S_f(C) \geq f_0 N^2$.

Then

$$f_0 N^2 \leq Nf(1) + Eg(C)$$
\[ D_3(T) := \{(t, u, v) : t, u, v \in T \& 1 + 2tuv - t^2 - u^2 - v^2 \geq 0\} . \]

**Theorem**

Let \( C \) be an \((N, n, T)\) spherical code and \( F : [-1, 1]^3 \rightarrow \mathbb{R} \) be a symmetric function. Suppose \( f : T \rightarrow \mathbb{R} \) and \( g : T \rightarrow \mathbb{R} \), are such that

1. \( F(1, t, t) \leq f(t) \) for all \( t \in T \),
2. \( F(t, u, v) \leq g(t) + g(u) + g(v) \) for all \((t, u, v) \in D_3(T)\).

If

\[ S_F(C) := \sum_{(x, y, z) \in C^3} F(x \cdot y, x \cdot z, y \cdot z) \geq F_0 N^3, \]

where \( F_0 \in \mathbb{R} \), then

\[ F_0 N^3 \leq NF(1, 1, 1) + 3E_f(C) + (3N - 6)E_g(C). \]
Under the assumptions of Theorem let \( f(t) = B + 2g(t) - q(t) \) with \( q : [-1, 1] \rightarrow \mathbb{R} \). If \( q(C) \geq 0 \), then

\[
E_g(C) = \sum_{t \in T} A_t g(t) \geq r_g,
\]

\[
r_g = \frac{1}{3} (F_0 N^2 - F(1, 1, 1)) - q(1) - (N - 1)B.
\]

Let \( p \) be a Gegenbauer polynomial \( G_k^n \). Then \( S_p(C) \geq 0 \), i.e.

\[
E_p(C) = \sum_{t \in T} A_t p(t) \geq r_p, \quad r_p = -Np(1)
\]
Corollary

Let \( a_0, \ldots, a_d \geq 0, F_0, \ldots, F_d \geq 0, T \subset [-1, 1), g: T \to \mathbb{R}, M \in \mathbb{R} \), \( F(u, v, t) = \sum_{k} \left\langle F_k, S^n_k(u, v, t) \right\rangle \). If

\[
a_0 + \ldots + a_d + F(1, 1, 1) \leq M - 1, \tag{1}
\]

\[
\sum_{k=0}^d a_k G_k^n(u) + 3F(u, u, 1) \leq -1 + 6g(u) \text{ for } u \in T, \tag{2}
\]

\[
F(u, v, t) \leq g(u) + g(v) + g(t) \text{ for } (u, v, t) \in D_3(T). \tag{3}
\]

Then for every \((N, n, T)\) spherical code, we have

\[
\sum_{t \in T} A_t g(t) \geq \frac{N - M}{3N}
\]
The following polynomial gives a sharp lower bound in \([-1, -0.73]\), \(a = 1/50\) and \(M = 22.645212490128051\)

\[
p_1(x) = \sum_{k=0}^{22} c_k G_k^{(4)}(x),
\]

where \([c_0, \ldots, c_{22}] = [0.222, 0.8648, 1.8875, 3.1425, 4.5059, 5.7052, 6.5739, 6.9286, 6.7119, 6.0157, 4.9575, 3.7767, 2.6446, 1.6914, 0.9947, 0.5249, 0.2524, 0.1097, 0.0409, 0.0153, 0.0042, 0.001, 0.0002]\).

Let \(g_1 = kp_2\), where \(k = 100/p_1(-1)\). Then \(g_1(-1) = 100\). Let \(T = [-1, 0.5]\). The Corollary yields

\[
\sum_{t \in T} A_t g_1(t) \geq B_1(24) \approx 95 > -52.2431 = LP(24).
\]
Example: $gSDP$
Example

Since

\[ \sum_{t \in [-1, 0.5]} A_t g_1(t) \geq 95 \]

we have

\[ A([-1, -0.73]) \geq 1 \]
Polynomial $p_2$

\[ p_2(x) = \sum_{k=0}^{22} c_k G_k^{(4)}(x), \]

\[ [c_0, \ldots, c_{22}] = [-0.5438, -2.0024, -3.8887, -5.6414, -6.7025, -6.8508, -6.0698, -4.6566, -3.0047, -1.4686, 0.3704, 0.6521, 0.6486, 0.5104, 0.3361, 0.1911, 0.0963, 0.0411, 0.0157, 0.0056, 0.001, 0.0004]. \]

The SDP bound in the Corollary gives $M = M_2 := 22.5689$, $B_2(25) = 0.0324$ and $B_2(24) = 0.0199$. 
Theorem 1 (M., 2008) yields that

\[ k(4) \leq \frac{1}{c_0} \max\{ h_0, h_1, ..., h_\mu, \} \]

Let \( C \) be an \((25, 4, \pi/3)\) spherical code,

\[ R_2 := \sum_t A_t g_1(t) \]

Since \( g_2(t) \leq 0 \) for all \( t \in [-\sqrt{2}/2, 1/2] \), we have \( t_0 = -\sqrt{2}/2 \) and \( \mu = 4 \). Then we consider \( \mu = 0, 1, 2, 3, 4 \) to find the maximum of \( R_2 \).

This maximum is achieved at \( \mu = 2 \) and is 0.0266, i.e. \( R_2 < 0.0266 \). On the other side we have \( R_2 > B_2(25) = 0.0324 \), a contradiction.
Polynomial $g_3$

\[ c(0 : 17) = [3.2313 \ 34.6000 \ 97.5893 \ 137.3081 \ 119.9142 \ 74.1812 \ 36.5605 \ 15.0065 \ 4.2796 \ 0.0946 \ -0.7087 \ -0.4672 \ -0.1755 \ -0.0283 \ 0.0097 \ 0.0070 \ 0.0016 \ 0.0001] \]

\[
\sum_{t \in [-1,0.5]} A_t g_3(t) > R_3 = 7.93
\]
Polynomial $g_3$
Thank you