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

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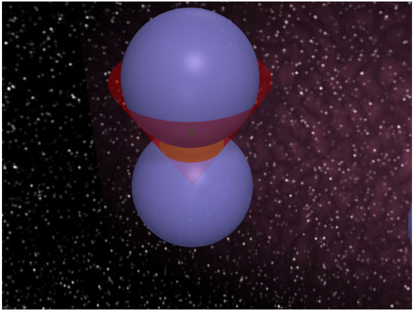
Packing by spherical caps

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°. Thus, the kissing number is the maximal number of nonoverlapping spherical caps of radius 30° on S.



Packing spheres by spherical caps: Methods

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); ...

Two-point-homogeneous space

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
$\mathbf{M} = \mathbf{S}^n, \mathbf{RP}^n, \mathbf{CP}^n, \mathbf{QP}^n, \mathbf{CayP}^2$ [Wang, 1952]

Zonal spherical functions

With any compact 2-point-homogeneous space $\mathbf{M}$ are associated the *zonal spherical functions* $\Phi_k(t)$, $k = 0, 1, 2, \ldots$, and the distance function $\tau(x, y)$, where $x, y \in \mathbf{M}$.
For all continuous compact $\mathbf{M}$ and for all currently known finite cases: $\Phi_k(t)$ *is a polynomial of degree* k.

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

If $M =$ unit sphere $\mathbf{S}^{n-1} \subset \mathbf{R}^n$, 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 $\mathbf{M}$ *be a 2-point-homogeneous space. Then for any integer* $k \geq 0$ *and for any finite* $C = \{x_i\} \subset M$ *the matrix* $\big(\Phi_k(\tau(x_i, x_j))\big)$ *is positive semidefinite.*

LP and SDP bounds for spherical codes

$$N \le \frac{f(1)}{f_0}$$

$$N \le \frac{f(1) + \hat{h}(n, T, f)}{f_0}$$

$$N^2 \le \frac{f(1,1,1) + 3(N-1)B}{f_0}$$

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

$$N^3 \le \frac{f(1,1,1,1,1,1) + 4(N-1)B_1 + 3(N-1)B_2 + 6(N-1)(N-2)B_3}{f_0}$$

Uniqueness of the max kissing arrangement in 4 dim?

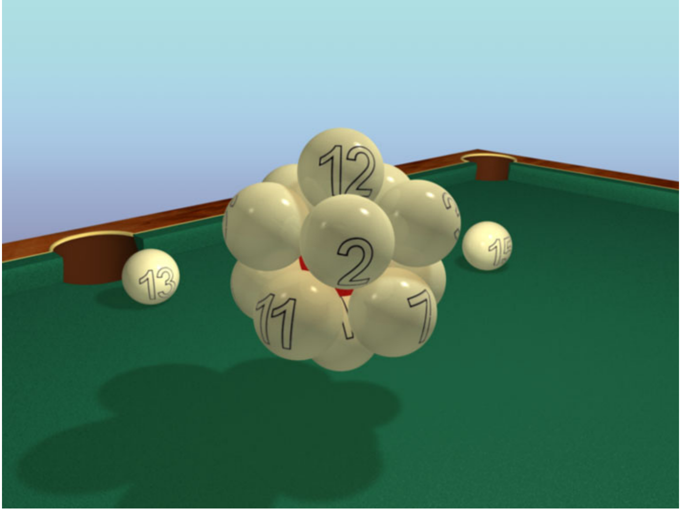
David de Laat, Nando M. Leijenhorst, Willem H. H. de Muinck Keizer:

"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



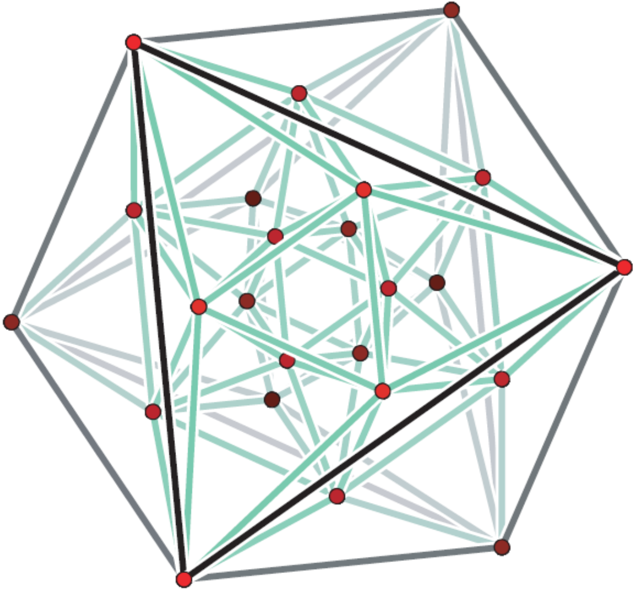
Status 2024: Kissing numbers

The only exact values of kissing numbers known:

n	lattice	regular polytope
$k(1) = 2$	A_1	
$k(2) = 6$	A_2	hexagon
$k(3) = 12$	H_3	icosahedron
$k(4) = 24$	$?D_4$	?24-cell
$k(8) = 240$	E_8	
$k(24) = 196{,}560$	Λ_{24}	

The 24–cell

$n = 4$: There are 24 vectors with two zero components and two components equal to ± 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 Schläfli. Its facets are 24 regular octahedra.



(Graphics: Michael Joswig/polymake [13])

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$=\Delta/B$:
$\mathrm{CD}_4 = 0.12500$;
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.

Delsarte's method

Ph. **Delsarte** (1972); **V. M. Sidelnikov** (1974)
Delsarte, **Goethals** and **Seidel** (1975, 1977)
G.A. Kabatiansky and **V.I. Levenshtein** (1978)

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*

$$k(n) \leq \frac{f(1)}{c_0}$$

K(8)=240; k(24)=196560

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.

The bound for kissing numbers (M., 2003, 2008)

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

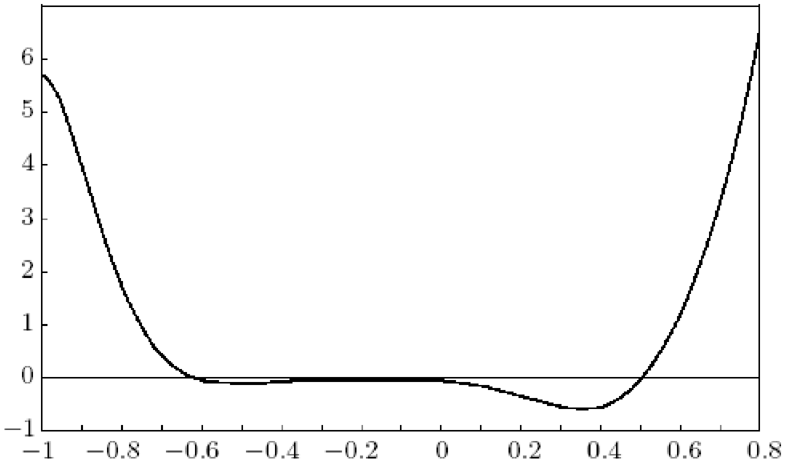
$$S(P) = \sum_{k,\ell} f_4(p_k \cdot p_\ell) \geq m^2.$$

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 $y = f_4(t)$



Bachoc–Vallentin SDP bound

$$D := \left\{(x,y,z) : -1 \le x,y,z \le 1/2,\ 1+2xyz-x^2-y^2-z^2 \ge 0\right\}.$$

$$\mathrm{BV(n,f_0)} := \{\mathrm{F} : \mathrm{F(x,y,z)} = \sum \langle \mathrm{F_k}, \mathrm{S^n_k(x,y,z)}\rangle,\ \mathrm{F_k} \succeq 0,\ \mathrm{F_0}-\mathrm{f_0}\mathrm{E_0} \succeq 0\}$$

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

$$N^2 \le \frac{F(1,1,1)+3(N-1)B}{f_0}$$

dim=4: uniqueness of the maximal kissing arrangement

LP bound [Odlyzko & Sloane; Arestov & Babenko] $= 25.558...$

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

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

H. D. Mittelmann & F. Vallentin (2010)
$S_{11}(4) = 24.10550859...$
$S_{12}(4) = 24.09098111...$
$S_{13}(4) = 24.07519774...$
$S_{14}(4) = 24.06628391...$

F.C. Machado & F.M. de Oliveira Filho (2018)
$S_{15}(4) = 24.062758...$
$S_{16}(4) = 24.056903...$

$g_T(x) = g(x)$ 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 θ 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. $F \in \mathrm{BV(n, f_0)}$,
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, θ) spherical code satisfies the following inequality

$$N^2 \leq \frac{F(1,1,1) + 3(N-1)\,B + 3N\,\hat{h}(n,\theta,T,g)}{f_0}.$$

Distance distribution

Let C be an (N, n, θ) spherical code. The *distance distribution* of C is the system of numbers $\{A_t : -1 \le t \le 1\}$.

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

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

$$A(T) := \sum_{t \in T : A_t > 0} A_t, \;\; T \subset [-1, 1].$$

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, θ) spherical code C we have

$$A(T) \leq \frac{2}{N} \lfloor Q \rfloor, \quad Q := \frac{F(1,1,1) + 3(N-1)B - f_0 N^2}{6a}.$$

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, θ) spherical code C we have

$$A(T) \geq \frac{2}{N} \lceil R \rceil, \quad R := \frac{f_0 N^2 - F(1,1,1) - 3(N-1)B}{6a}.$$

Distance distribution of the 24–cell

Kissing arrangement in four dimensions:

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

$$A_t = 0 \ \text{ for all } \ t \neq \{-1, \, -1/2, 0, \, 1/2, \, 1\}$$

SDP bounds on $(24, 4, \pi/3)$ – spherical code

Theorem (Dostert–Kolpakov–Moustrou–M.)

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

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

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

$$A([-1, -0.73]) \ge 1, \quad A([0.35, 0.5]) \ge 8$$

General bounds for spherical codes

Let C be an N–element subset of the unit sphere $\mathbb{S}^{n-1} \subset \mathbb{R}^n$.

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

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

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

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

General 2-point (Delsarte – Yudin) bound

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

$$f_0 N^2 \leq N f(1) + E_g(C)$$

General 3-point bound

$$D_3(T) := \left\{(t,u,v) : t,u,v \in T \,\&\, 1+2tuv-t^2-u^2-v^2 \geq 0\right\}.$$

Theorem

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

$$F_0 N^3 \leq NF(1,1,1) + 3E_f(C) + (3N-6)E_g(C).$$

General 3-point bound

Corollary

Under the assumptions of Theorem let $f(t) = B + 2g(t) - q(t)$ *with* $q : [-1, 1] \to \mathbb{R}$*. 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.

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

General 3-point bound: SDP program

Corollary

Let $a_0, \dots, a_d \geq 0$, $F_0, \dots, F_d \succeq 0$, $T \subset [-1,1)$, $g : T \to \mathbb{R}$, $M \in \mathbb{R}$, $F(u,v,t) = \sum_k \left\langle F_k, S_k^n(u,v,t) \right\rangle$. *If*

$$a_0 + \dots + a_d + F(1,1,1) \leq M - 1, \quad (1)$$

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

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

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

$$\sum_{t \in T} A_t g(t) \geq \frac{N - M}{3N}$$

Polynomial g_1

The following polynomial gives a sharp lower bound in $[-1, -0.73]$, a $=$ $1/50$ and M$=$ 22.645212490128051

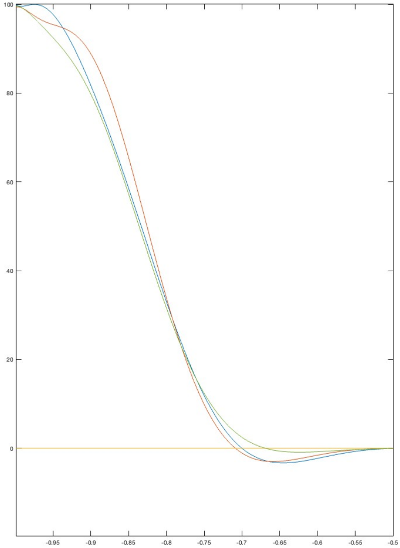
$$p_1(x) = \sum_{k=0}^{22} c_k G_k^{(4)}(x),$$

where $[c_0, ..., c_{22}] =$ [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 $g_1 = k\, p_2$, 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

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

$[c_0, ..., c_{22}]$= [-0.5438, -2.0024, -3.8887, -5.6414, -6.7025, -6.8508, -6.0698, -4.6566, -3.0047, -1.4686, -0.3226, 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 $B_2(24) = 0.0199$.

Short proof: $k(4) = 24$

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,

$$R_2 := \sum_t A_t g_1(t)$$

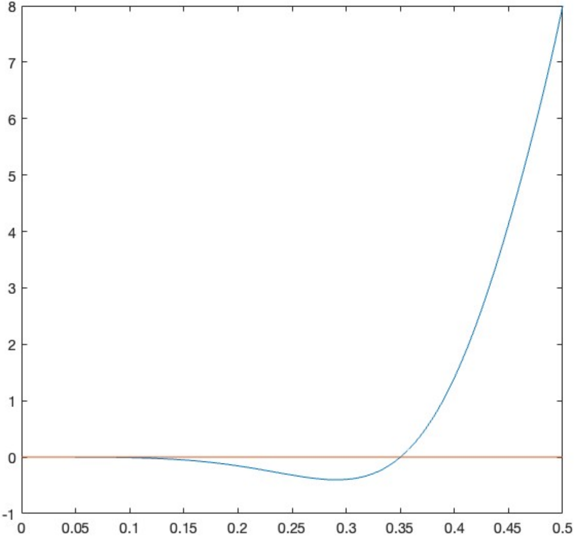
Since $g_2(t) \leq 0$ for all $t \in [-\sqrt{2}/2, 1/2]$, we have $t_0 = -\sqrt{2}/2$ and $\mu = 4$. Then we consider s $\mu = 0, 1, 2, 3, 4$ to find the maximum of R_2. This maximum is achieved at $\mu = 2$ and is 0.0266, i.e. $R_2 < 0.0266$. On the other side we have $R_2 > B_2(25) = 0.0324$, a contradiction.

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