New upper bounds for the density of translative packings of superspheres

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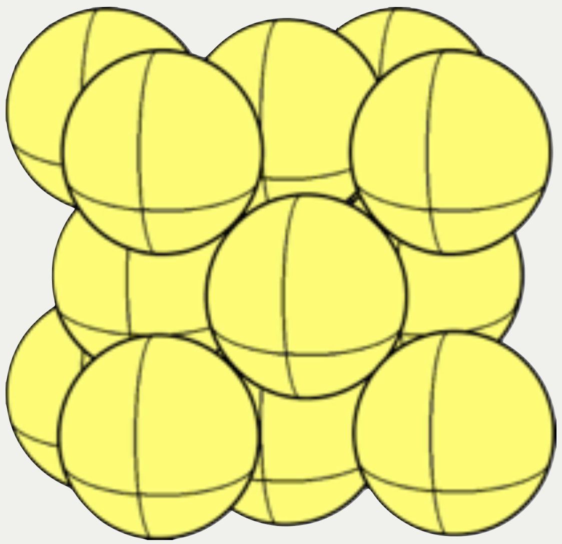
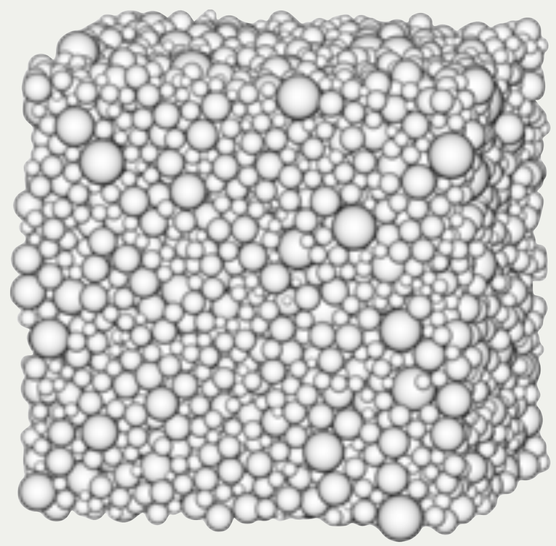
1. Overview

Densest packings



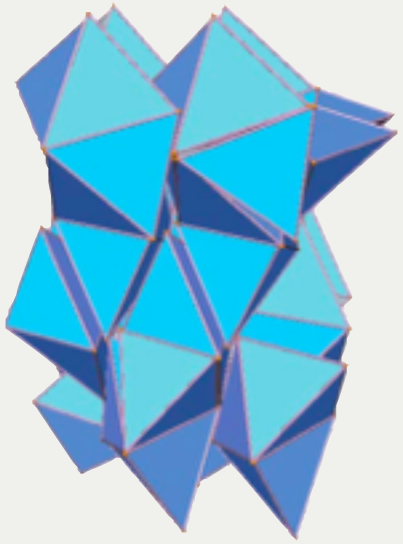
equal spheres

different spheres



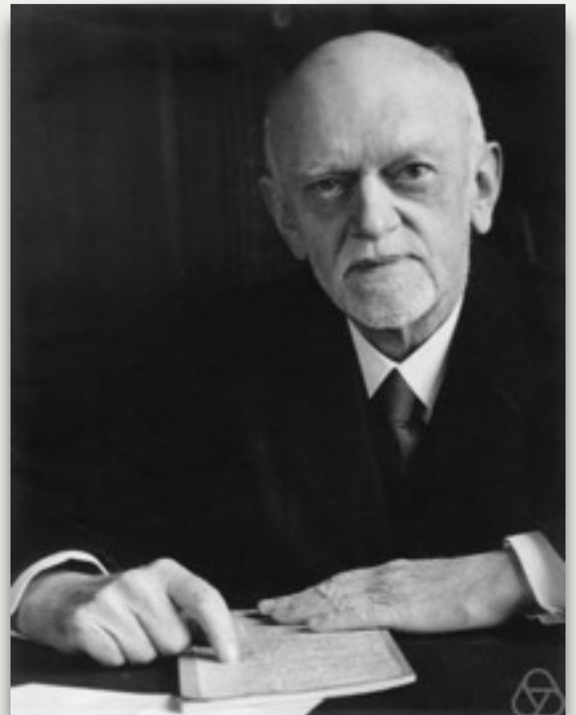
M&Ms

tetrahedra



superballs

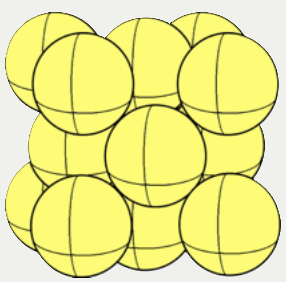
Rich history



Hilbert's 18th problem

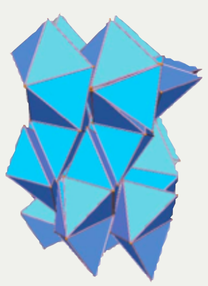
Arrange most densely equal solids of a given form, e.g. spheres, regular tetrahedra

Extremely difficult



$n = 3$: solved by Hales (1998, 2014)

$n > 3$: open

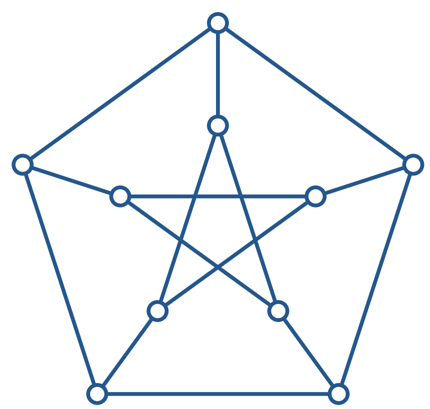


wide open, maximum density between 0.85 and $1 - 10^{-26}$

$\leadsto$ Mathematical tools for proving upper bounds are needed

Extending combinatorial optimization

finite	→	compact	→	locally compact

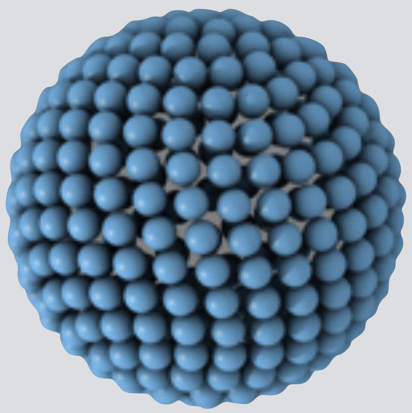


$G = (V, E)$ finite graph

INDEPENDENT SET

pos. semidef. $\mathbb{R}^{V \times V}$

combinatorics

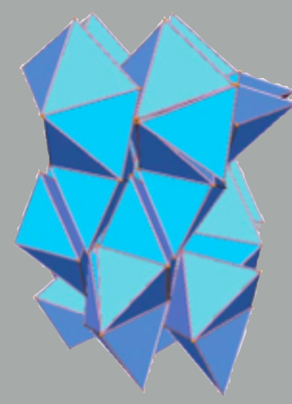


$V = S^{n-1} = O(n)/O(n-1)$

packing

pos. kernel
$\mathcal{C}(S^{n-1} \times S^{n-1})$

geometry



$V = \mathbb{R}^n \rtimes O(n)$

packing

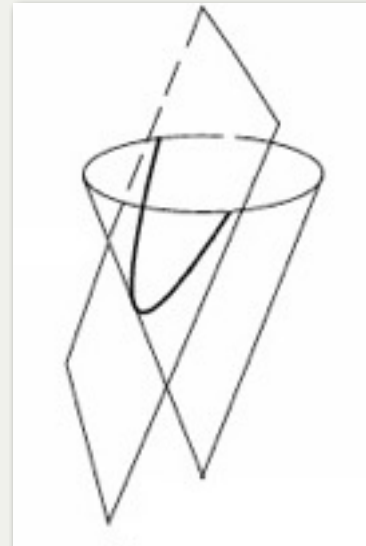
pos. type
$f \in L^1(\mathbb{R}^n \rtimes O(n))$

geometry

→ computational challenge

Method: Using harmonic analysis

semidefinite programming



extend

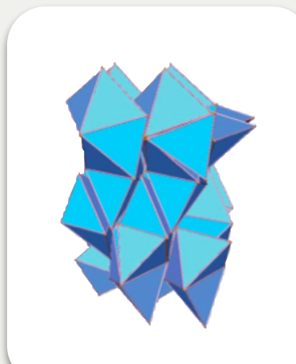
∞-dim. SDP

use

harmonic analysis

solve / approx.

difficult geometric problems



efficient parametrization of
cone of positive type functions

$$f(x) = \int_{\widehat{G}} \mathrm{trace}(\pi(x)\hat{f}(\pi))\, d\nu(\pi)$$

$\hat{f}(\pi) : H_\pi \to H_\pi$
positive trace class operator
optimization variable

2. Modelling

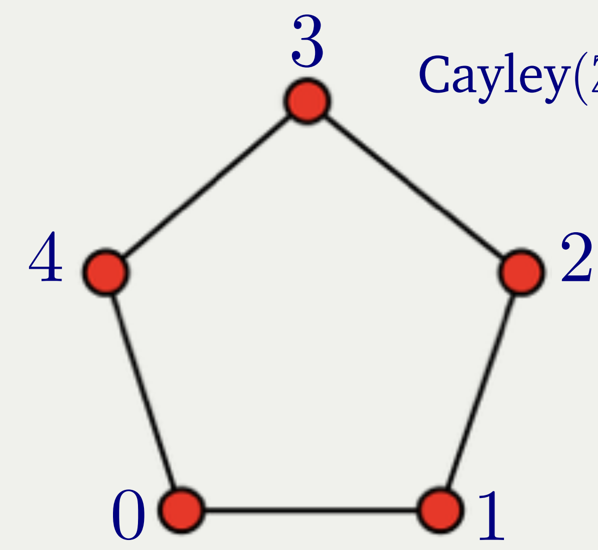
Independent sets in Cayley graphs

$\text{Cayley}(G, \Sigma)$ $\quad x \sim y \iff xy^{-1} \in \Sigma$

group $\quad \Sigma \subseteq G, \Sigma = \Sigma^{-1}$

undirected graph on G

may contain loops



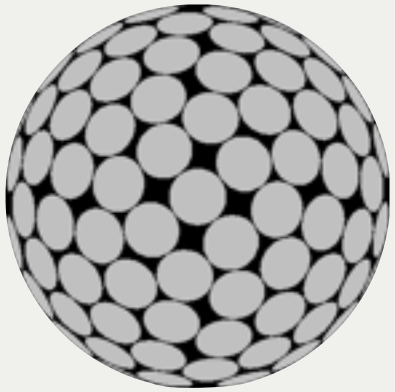
$\text{Cayley}(\mathbb{Z}/5\mathbb{Z}, \{1, 4\})$

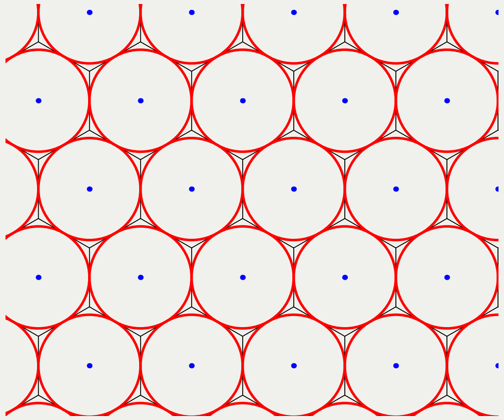
$I \subseteq G$ independent: $\forall x, y \in I, x \neq y, x \not\sim y$

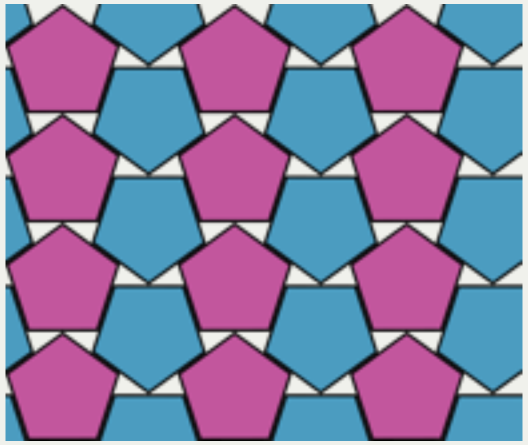
find indep. sets in $\text{Cayley}(G, \Sigma)$ which are as “large” as possible

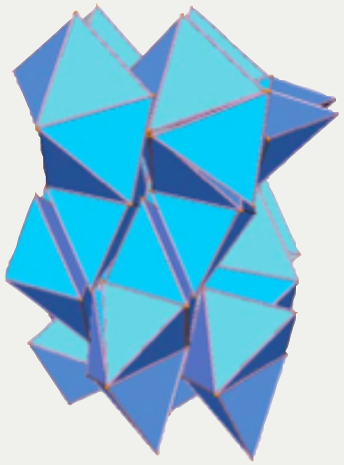
Examples

G	Σ
$\mathbb{F}_2^n$ *finite*	$\{x : \|x\|_H < d\}$, $\|\cdot\|_H$ Hamming distance *error correcting codes*
$\mathrm{SO}(n)$ *compact*	$\{A : AC(\alpha)^\circ \cap C(\alpha)^\circ \neq \emptyset\}$, $C(\alpha) \subseteq S^{n-1}$ spherical cap *spherical codes*
$\mathrm{SO}(n) \ltimes \mathbb{R}^n$ *locally compact*	$\{(A, x) : \mathcal{K}^\circ \cap x + A\mathcal{K}^\circ \neq \emptyset\}$, $\mathcal{K} \subseteq \mathbb{R}^n$ convex body *body packing*





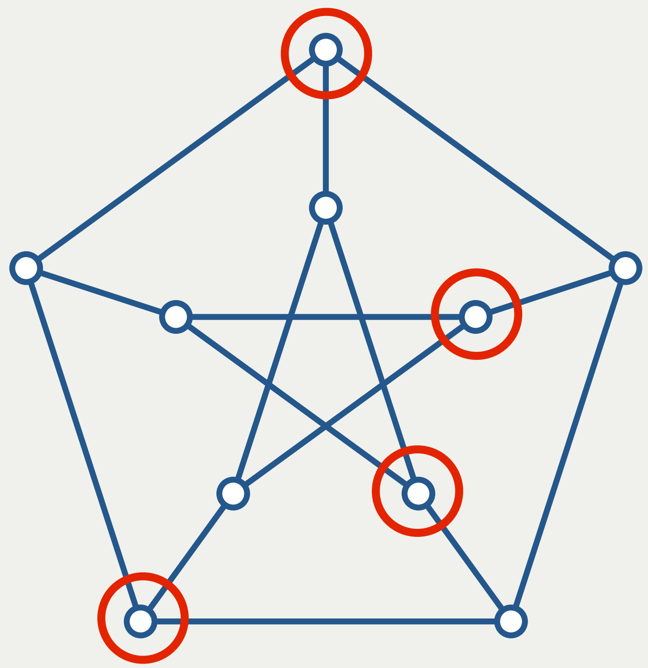




Complete SDP proof system

polynomial optimization formulation

$$\alpha(G) = \max \sum_{v \in V} x_v^2$$
$$x_v \geq 0$$
$$x_v^2 - x_v = 0 \text{ for } v \in V$$
$$x_u x_v = 0 \text{ if } u \sim v$$



$\rightsquigarrow$ apply Lasserre's hierarchy for polynomial optimization

t-th step of Lasserre's hierarchy

$$\text{las}_t(G) = \max\left\{ \sum_{x \in V} y_{\{x\}} : y \in \mathbb{R}^{I_{2t}}_{\geq 0},\ y_\emptyset = 1,\ M_t(y) \succeq 0 \right\},$$

I_{2t} = independent sets with $\leq 2t$ elements

moment matrix $\quad (M_t(y))_{J,J'} = \begin{cases} y_{J \cup J'} & \text{if } J \cup J' \in I_{2t}, \\ 0 & \text{otherwise.} \end{cases}$

	$\emptyset$	1	2	3	12	13	23
$\emptyset$	$y_\emptyset$	y_1	y_2	y_3	y_{12}	y_{13}	y_{23}
1	y_1	y_1	y_{12}	y_{13}	y_{12}	y_{13}	y_{123}
2	y_2	y_{12}	y_2	y_{23}	y_{12}	y_{123}	y_{23}
3	y_3	y_{13}	y_{23}	y_3	y_{123}	y_{13}	y_{23}
12	y_{12}	y_{12}	y_{12}	y_{123}	y_{12}	y_{123}	y_{123}
13	y_{13}	y_{13}	y_{123}	y_{13}	y_{123}	y_{13}	y_{123}
23	y_{23}	y_{123}	y_{23}	y_{23}	y_{123}	y_{123}	y_{23}

Properties of Lasserre's hierarchy

- $\star$ the t-th step $\text{las}_t(G)$ is a semidefinite program
- $\star$ SDP proof system is complete:

$$\vartheta'(G) = \text{las}_1(G) \geq \text{las}_2(G) \geq \ldots \geq \text{las}_{\alpha(G)}(G) = \alpha(G)$$

  every intermediate step gives rigorous upper bound

- $\star$ $\text{las}_t(G)$ is a $2t$-bound: makes use of $2t$-point correlation functions
- $\star$ can be generalized to infinite graphs

Complete SDP proof system for infinite graphs

need topological assumptions

Graph $G = (V, E)$ is a *topological packing graph* if

- V is a Hausdorff topological space
- every finite clique is contained in a clique which is open

$$\text{las}_t(G) = \max\left\{\sum_{x\in V} y_{\{x\}} : y \in \mathbb{R}^{I_{2t}}_{\geq 0},\ y_\emptyset = 1,\ M_t(y) \succeq 0\right\},$$

↓

$$\text{las}_t(G) = \sup\left\{\lambda(I_{=1}) : \lambda \in \mathcal{M}(I_{2t})_{\geq 0},\ \lambda(\{\emptyset\}) = 1,\ A_t^*\lambda \in \mathcal{M}(I_t \times I_t)_{\succeq 0}\right\}.$$

Borel measure

⇝ SDP proof system complete if G compact top. packing graph

3. Explicit Computations

Rough guide to the literature

Packing problem	**2-point bound**	**3-point bound**	**4-point bound**
Binary codes	Delsarte 1973	Schrijver 2005	Gijswijt, Mittelmann, Schrijver 2011
Spherical codes	Delsarte, Goethals, Seidel 1977	Bachoc, Vallentin 2008	
Sphere packings	Cohn, Elkies 2003		
Congruent copies of a convex body	Oliveira, Vallentin 2013		

2-point bounds

$$\mathrm{las}_1(\mathrm{Cayley}(G,\Sigma)) = \vartheta'(\mathrm{Cayley}(G,\Sigma))$$

$$= \inf \quad f(e)$$

$f : G \to \mathbb{R}$ positive type

$\int_G f(x)\, d\mu(x) = 1$

$f(x) \leq 0$ for $x \notin \Sigma$

$\forall x_1, \ldots, x_N \in G : \left(f(x_i x_j^{-1})\right)_{1 \leq i,j \leq N}$ is pos. semidefinite

parametrize cone of positive type functions
& use conic optimization

Harmonic analysis

$\inf \quad f(e)$

$f : G \to \mathbb{R}$ positive type

$\int_G f(x)\, d\mu(x) = 1$

$f(x) \leq 0$ for $x \notin \Sigma$

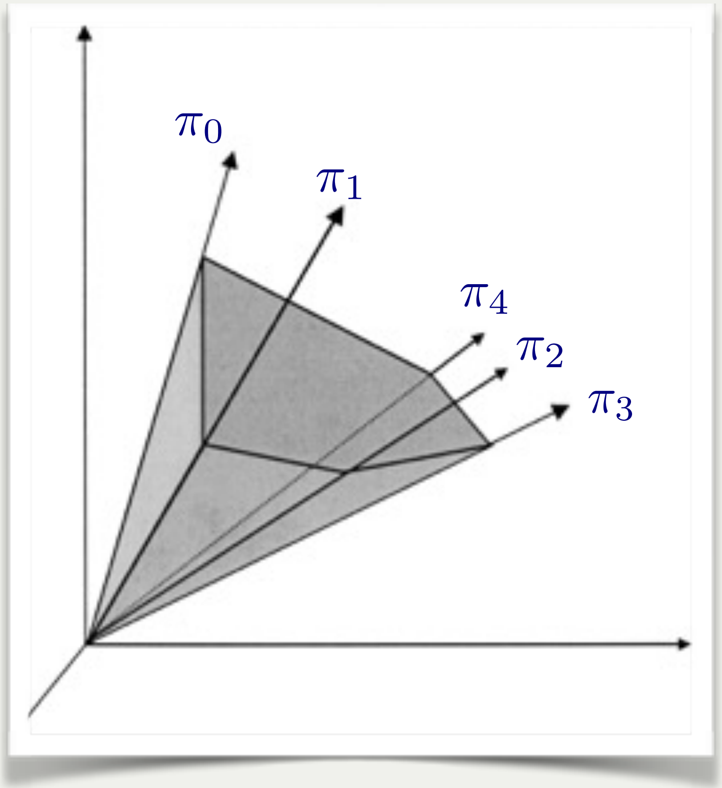
parametrize cone of positive type functions
& use conic optimization

construction of positive type functions

$\pi : G \to U(H_\pi)$ unitary representation, $h \in H_\pi$

then $f(x) = (\pi(x)h, h)$ is positive type

- Gelfand-Raikov 1942:
  - all positive type functions are of this form
  - extreme rays of cone of pos. type functions come from irreducible rep.



Fourier inversion formula (Segal-Mautner, 1950)

f is pos. type $\iff$

optimization variable

$$f(x) = \int_{\widehat{G}} \operatorname{trace}(\pi(x)\hat{f}(\pi))\, d\nu(\pi)$$

explicit formula needed

for positive, trace-class operators $\widehat{f}(\pi) : H_\pi \to H_\pi$

$\widehat{G} = \{\text{irred. unitary rep. of } G\}/\sim$

$\nu =$ Plancherel measure on $\widehat{G}$

$\hat{f}(\pi) = \int_G f(x)\pi(x^{-1})\, d\mu(x)$ Fourier transform

2-point bounds for translative packings in Euclidean space

Theorem. (Cohn-Elkies (2003))
Suppose continuous $f \in L^1(\mathbb{R}^n)$ satisfies

(i) f is of positive type, i.e. $\widehat{f}(u) \geq 0$ for every $u \in \mathbb{R}^n$,

(ii) $\widehat{f}(0) = 1$,

(iii) $f(x) \leq 0$ whenever $\mathcal{K}^\circ \cap (x + \mathcal{K}^\circ) = \emptyset$,

Then the density of any translative packing of $\mathcal{K}$ in $\mathbb{R}^n$ is $\leq f(0)\,\mathrm{vol}\,\mathcal{K}$.

$\widehat{f}(u) = \int_{\mathbb{R}^n} f(x) e^{-2\pi i x \cdot u} dx$ Fourier transform of f

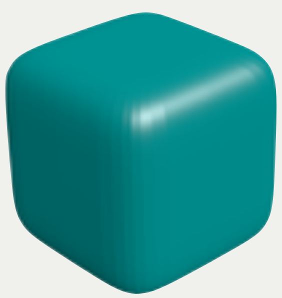
4. Results

Superspheres

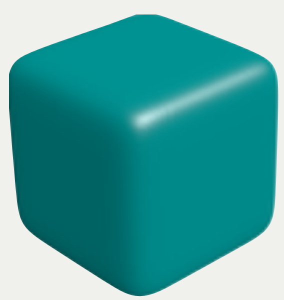
$$B_3^p = \{(x, y, z) \in \mathbb{R}^3 : |x|^p + |y|^p + |z|^p \leq 1\}.$$

$p = 2$

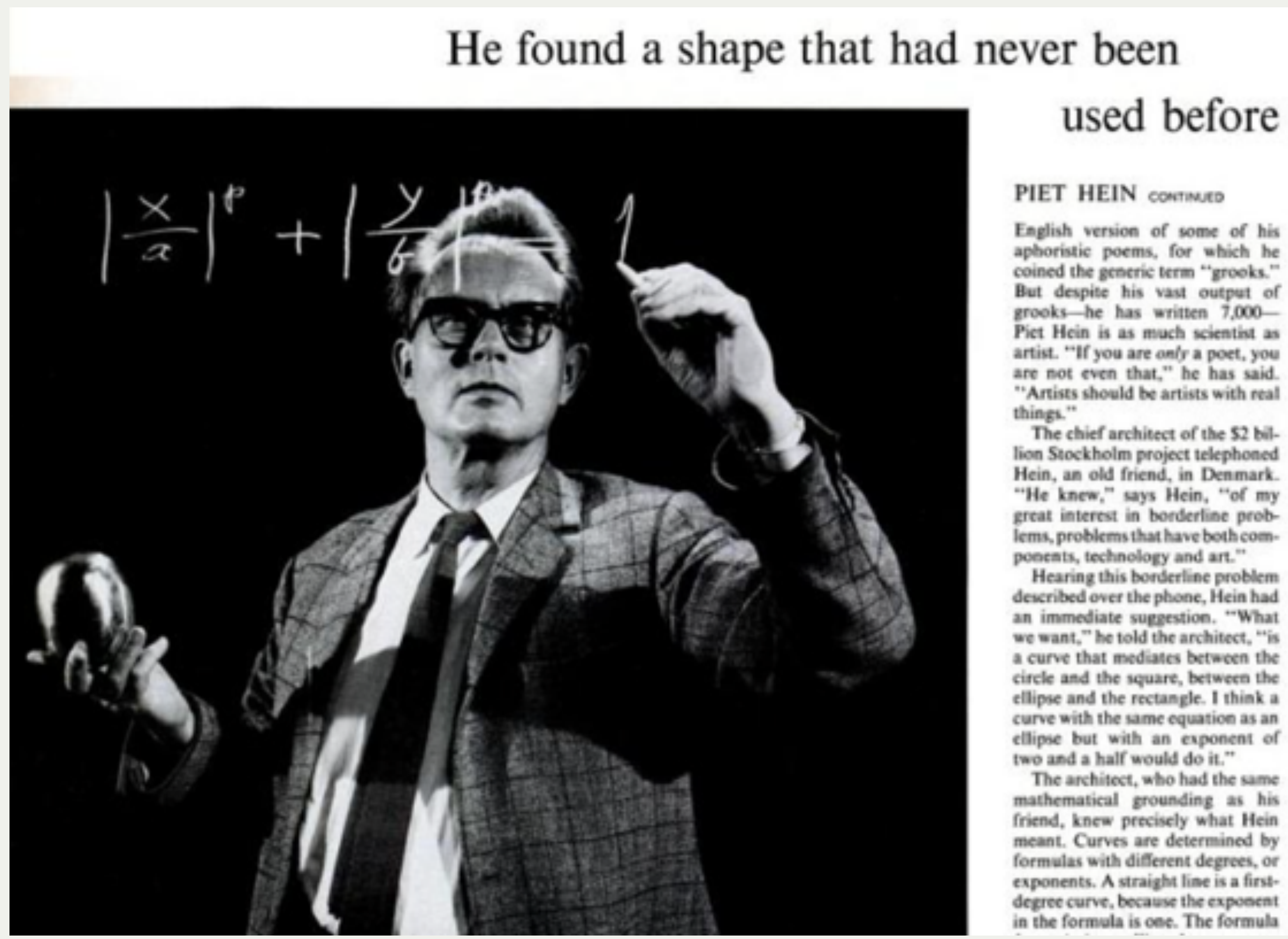
$p = 4$



$p = 6$



$p = 8$



He found a shape that had never been used before

PIET HEIN CONTINUED

English version of some of his aphoristic poems, for which he coined the generic term "grooks." But despite his vast output of grooks—he has written 7,000—Piet Hein is as much scientist as artist. "If you are *only* a poet, you are not even that," he has said. "Artists should be artists with real things."

The chief architect of the $2 billion Stockholm project telephoned Hein, an old friend, in Denmark. "He knew," says Hein, "of my great interest in borderline problems, problems that have both components, technology and art."

Hearing this borderline problem described over the phone, Hein had an immediate suggestion. "What we want," he told the architect, "is a curve that mediates between the circle and the square, between the ellipse and the rectangle. I think a curve with the same equation as an ellipse but with an exponent of two and a half would do it."

The architect, who had the same mathematical grounding as his friend, knew precisely what Hein meant. Curves are determined by formulas with different degrees, or exponents. A straight line is a first-degree curve, because the exponent in the formula is one. The formula

Life Magazine 1966

Piet Hein (1905–1996): inventor of the superellipse

Infinite dimensional linear program

$$\delta^t(\mathcal{K}) \leq \inf \quad \begin{array}{l} f(0) \\ f \in L^1(\mathbb{R}^n) \\ \widehat{f}(0) \geq \text{vol}\, \mathcal{K} \\ \widehat{f}(u) \geq 0 \text{ for all } u \in \mathbb{R}^n \setminus \{0\} \\ f(x) \leq 0 \text{ for all } x \notin \mathcal{K}^\circ - \mathcal{K}^\circ \end{array}$$

approximate by semi-infinite linear program

optimize over polynomials $p \in \mathbb{R}[u_1, \ldots, u_n]_{\leq 2d}$
and set $\widehat{f}(u) = p(u)e^{-\pi\|u\|^2}$

$$\delta^t(\mathcal{K}) \leq \inf \quad \begin{array}{l} \int_{\mathbb{R}^n} p(u)e^{-\pi\|u\|^2}\, du \\ p \in \mathbb{R}[u]_{\leq 2d} \\ p(0) \geq \text{vol}\, \mathcal{K} \\ p(u) \geq 0 \text{ for all } u \in \mathbb{R}^n \setminus \{0\} \\ \int_{\mathbb{R}^n} p(u)e^{-\pi\|u\|^2} e^{2\pi i u\cdot x}\, du \leq 0 \text{ for all } x \notin \mathcal{K}^\circ - \mathcal{K}^\circ \end{array}$$

Technical "details": Solving the optimization problem

$$\delta^t(\mathcal{K}) \leq \inf \quad \begin{array}{l} \int_{\mathbb{R}^n} p(u) e^{-\pi\|u\|^2}\, du \\ p \in \mathbb{R}[u]_{\leq 2d} \\ p(0) \geq \text{vol}\, \mathcal{K} \\ p(u) \geq 0 \text{ for all } u \in \mathbb{R}^n \setminus \{0\} \\ \int_{\mathbb{R}^n} p(u) e^{-\pi\|u\|^2} e^{2\pi i u \cdot x}\, du \leq 0 \text{ for all } x \notin \mathcal{K}^\circ - \mathcal{K}^\circ \end{array}$$

— checking that p is globally nonnegative: NP-hard

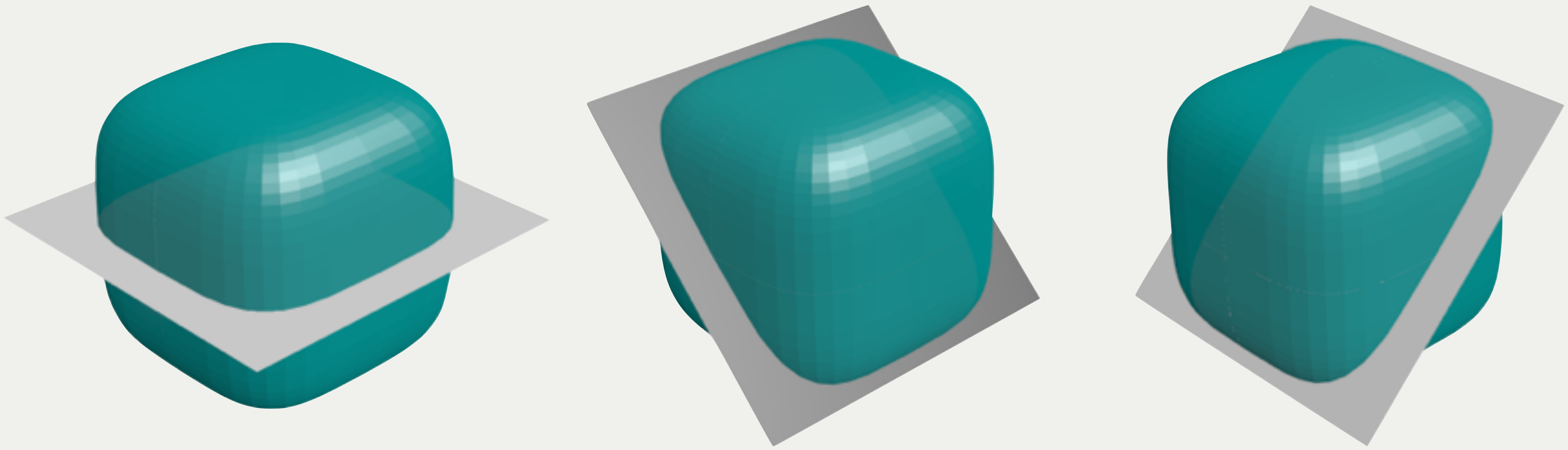
— semidefinite relaxation: p is a sum of squares (SOS), $p = p_1^2 + \cdots + p_m^2$

— p with $\deg p = 2d$ is SOS $\Longleftrightarrow \exists Q \in \mathcal{S}_{\succeq 0}^{\binom{n+d}{d}} : p(u) = [u]_d^{\mathsf{T}} Q [u]_d$

— if $n = 3$, $d = 15$, then $Q \in \mathcal{S}_{\succeq 0}^{816}$; too big for high precision SDP solvers

— idea: can assume that p is invariant under symmetry group of $\mathcal{K}-\mathcal{K}$

Finite reflection group



$$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

reflection group B_3, 48 elements

Chevalley-Shephard-Todd-Serre theory

finite reflection group: $G \subseteq \mathsf{GL}(\mathbb{C}^n)$

invariant ring: $\mathbb{C}[x]^G = \{p \in \mathbb{C}[x] : p(g^{-1}x) = p(x) \text{ for all } g \in G\}$

generated by basic invariants: $\mathbb{C}[x]^G = \mathbb{C}[\theta_1, \ldots, \theta_n]$

$\theta_1 = x^2 + y^2 + z^2,\ \theta_2 = x^4 + y^4 + z^4,\ \theta_3 = x^6 + y^6 + z^6$

coinvariant algebra: $\mathbb{C}[x]_G = \mathbb{C}[x]/I, \quad \text{where} \quad I = (\theta_1, \ldots, \theta_n)$

$$\mathbb{C}[x] = \mathbb{C}[x]^G \otimes \mathbb{C}[x]_G$$

has dimension $|G|$ and is isomorphic to regular representation of G

$\mathbb{C}[x]_G$ has basis φ^π_{ij} with

$$g\varphi^\pi_{ij} = (\pi(g)_j)^{\mathsf{T}} \begin{pmatrix} \varphi^\pi_{i1} \\ \vdots \\ \varphi^\pi_{id_\pi} \end{pmatrix},\ i = 1, \ldots, d_\pi,$$

$$\varphi^\pi_{ij}, \quad \text{with} \quad \pi \in \widehat{G},\ 1 \le i, j \le d_\pi$$

Invariant SOS polynomials

Theorem. (Gatermann, Parrilo (2004), DGOV (2015))

The cone of SOS polynomials which are G-invariant equals

$$\left\{ p \in \mathbb{R}[x] : p = \sum_{\pi \in \widehat{G}} \langle P^\pi, Q^\pi \rangle, P^\pi \text{ is Hermitian SOS matrix polynomial in } \theta_i \right\}.$$

where $\langle A, B \rangle = \mathrm{Tr}(B^* A)$

$P^\pi = (L^\pi)^* L^\pi$ with matrix L^π having entries in $\mathbb{C}[x]^G$

$$[Q^\pi]_{kl} = \sum_{i=1}^{d_\pi} \varphi^\pi_{ki} \overline{\varphi^\pi_{li}}.$$

advantages:

— substantial size reduction: one semdefinite matrix for every $\pi \in \widehat{G}$

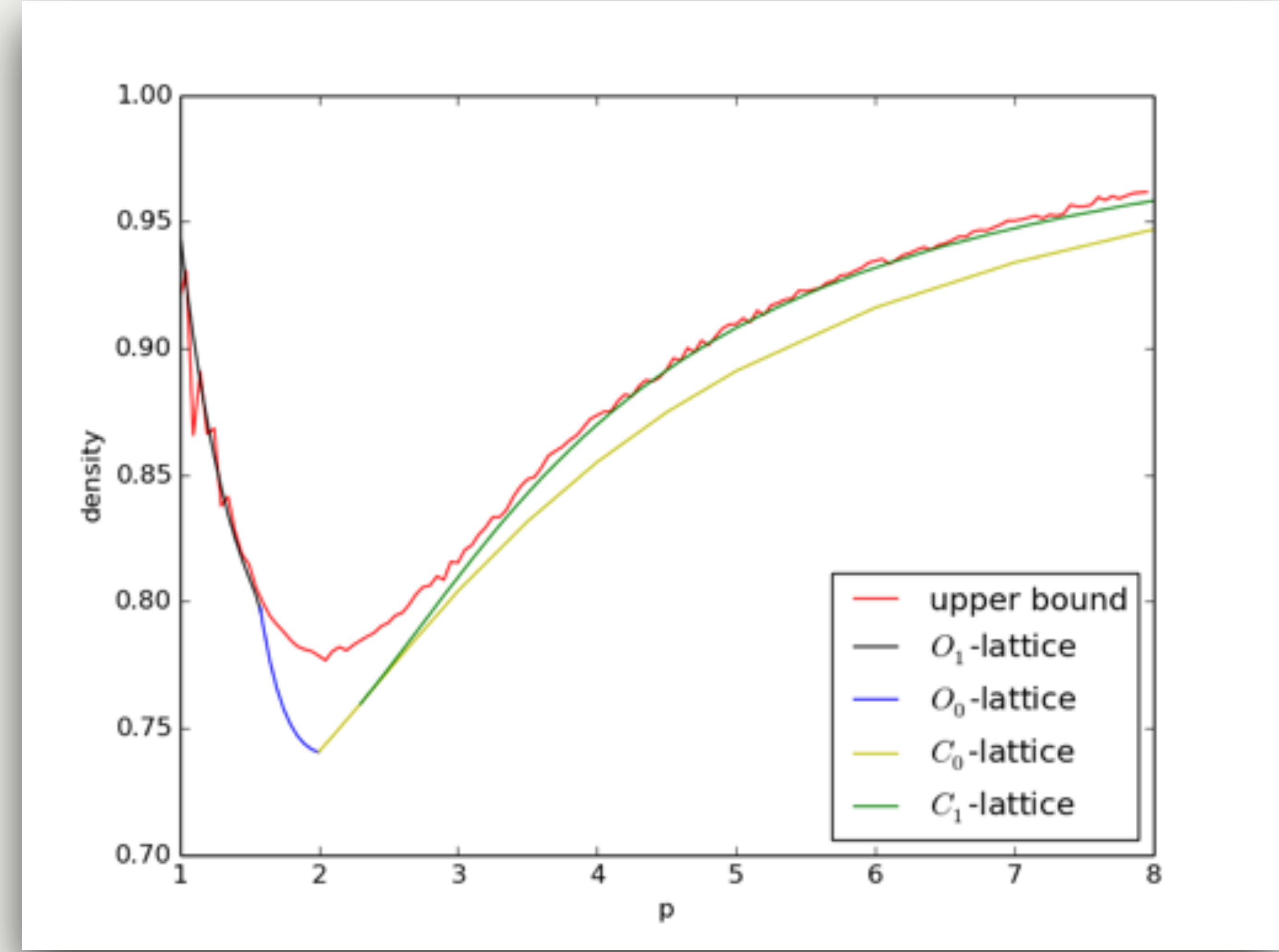
— only computation of matrix Q^π needed (independent of degree)

$n = 3, d = 15$: 10 matrices $(31, 23, 11, 7, 27, 39, 34, 50, 50, 70)$ vs. 876

Q^π matrices

A_{1g}	1
A_{1u}	$\theta_1^3 - 3\theta_1\theta_2 + 2\theta_3$
A_{2g}	$-\theta_1^6 + 9\theta_1^4\theta_2 - 8\theta_1^3\theta_3 - 21\theta_1^2\theta_2^2 + 36\theta_1\theta_2\theta_3 + 3\theta_2^3 - 18\theta_3^2$
A_{2u}	$-\theta_1^9 + 12\theta_1^7\theta_2 - 10\theta_1^6\theta_3 - 48\theta_1^5\theta_2^2 + 78\theta_1^4\theta_2\theta_3 + 66\theta_1^3\theta_2^3 - 34\theta_1^3\theta_3^2 - 150\theta_1^2\theta_2^2\theta_3$
	$-9\theta_1\theta_2^4 + 126\theta_1\theta_2\theta_3^2 + 6\theta_2^3\theta_3 - 36\theta_3^3$
E_g	$-2\theta_1^5 + 12\theta_1^3\theta_2 - 4\theta_1^2\theta_3 - 18\theta_1\theta_2^2 + 12\theta_2\theta_3$
	$-2\theta_1^4\theta_2 + 6\theta_1^3\theta_3 + 6\theta_1^2\theta_2^2 - 22\theta_1\theta_2\theta_3 + 12\theta_3^2$
	$\theta_1^7 - 9\theta_1^5\theta_2 + 10\theta_1^4\theta_3 + 19\theta_1^3\theta_2^2 - 36\theta_1^2\theta_2\theta_3 - 3\theta_1\theta_2^3 + 16\theta_1\theta_3^2 + 2\theta_2^2\theta_3$
E_u	$-2\theta_1^2 + 6\theta_2$
	$-2\theta_1\theta_2 + 6\theta_3$
	$\theta_1^4 - 6\theta_1^2\theta_2 + 8\theta_1\theta_3 + \theta_2^2$
T_{1g}	$12\theta_1\theta_3 - 12\theta_2^2$
	$2\theta_1^5 - 12\theta_1^3\theta_2 + 16\theta_1^2\theta_3 + 6\theta_1\theta_2^2 - 12\theta_2\theta_3$
	$2\theta_1^6 - 12\theta_1^4\theta_2 + 10\theta_1^3\theta_3 + 12\theta_1^2\theta_2^2 - 6\theta_1\theta_2\theta_3 - 6\theta_2^3$
	$2\theta_1^6 - 10\theta_1^4\theta_2 + 10\theta_1^3\theta_3 + 10\theta_1\theta_2\theta_3 - 12\theta_3^2$
	$\theta_1^7 - 3\theta_1^5\theta_2 + 2\theta_1^4\theta_3 - 9\theta_1^3\theta_2^2 + 24\theta_1^2\theta_2\theta_3 + 3\theta_1\theta_2^3 - 12\theta_1\theta_3^2 - 6\theta_2^2\theta_3$
	$4\theta_1^6\theta_2 - 3\theta_1^5\theta_3 - 21\theta_1^4\theta_2^2 + 32\theta_1^3\theta_2\theta_3 + 12\theta_1^2\theta_2^3 - 12\theta_1^2\theta_3^2 - 9\theta_1\theta_2^2\theta_3 - 3\theta_2^4$
T_{1u}	$-12\theta_1^3 + 48\theta_1\theta_2 - 36\theta_3$
	$-6\theta_1^4 + 24\theta_1^2\theta_2 - 12\theta_1\theta_3 - 6\theta_2^2$
	$-6\theta_1^3\theta_2 + 6\theta_1^2\theta_3 + 18\theta_1\theta_2^2 - 18\theta_2\theta_3$
	$-2\theta_1^5 + 6\theta_1^3\theta_2 + 2\theta_1^2\theta_3 - 6\theta_2\theta_3$
	$\theta_1^6 - 9\theta_1^4\theta_2 + 8\theta_1^3\theta_3 + 15\theta_1^2\theta_2^2 - 12\theta_1\theta_2\theta_3 - 3\theta_2^3$
	$\theta_1^7 - 6\theta_1^5\theta_2 + 5\theta_1^4\theta_3 + 3\theta_1^3\theta_2^2 + 6\theta_1\theta_2^3 - 9\theta_2^2\theta_3$
T_{2g}	$3\theta_1^2 - 3\theta_2$
	$6\theta_1\theta_2 - 6\theta_3$
	$-\theta_1^4 + 6\theta_1^2\theta_2 - 2\theta_1\theta_3 - 3\theta_2^2$
	$-2\theta_1^4 + 12\theta_1^2\theta_2 - 10\theta_1\theta_3$
	$-\theta_1^5 + 4\theta_1^3\theta_2 - 2\theta_1^2\theta_3 + 3\theta_1\theta_2^2 - 4\theta_2\theta_3$
	$-2\theta_1^4\theta_2 + \theta_1^3\theta_3 + 9\theta_1^2\theta_2^2 - 7\theta_1\theta_2\theta_3 - 3\theta_2^3 + 2\theta_3^2$
T_{2u}	$6\theta_1$
	$6\theta_2$
	$6\theta_3$
	$6\theta_3$
	$\theta_1^4 - 6\theta_1^2\theta_2 + 8\theta_1\theta_3 + 3\theta_2^2$
	$\theta_1^5 - 5\theta_1^3\theta_2 + 5\theta_1^2\theta_3 + 5\theta_2\theta_3$

Translative packings of superspheres



lower bounds by
Jiao, Stillinger, Torquato (2009)

p	1	2 (CE, 2003)	4	6	8
lower bound	$0.9473\ldots$	$0.7404\ldots$	$0.8698\ldots$	$0.9318\ldots$	$0.9582\ldots$
upper bound	$0.9699\ldots$	$0.7797\ldots$	$0.8740\ldots$	$0.9338\ldots$	$0.9619\ldots$

Rigorous computer proofs

— proof by exhibiting a certificate

— aim: find solution and check feasibility rigorously

— high precision SDP solver (`SDPA-GMP`)

— important: choosing well-conditioned polynomial basis

— post processing (rational approximation)

— interval arithmetic (`MPFI`)

5. References

References

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Tetrahedra packing with translates

M. Dostert, C. Guzmán, F.M. de Oliveira Filho, F. Vallentin, *New upper bounds for the density of translative packings of superspheres and tetrahedra*, in preparation