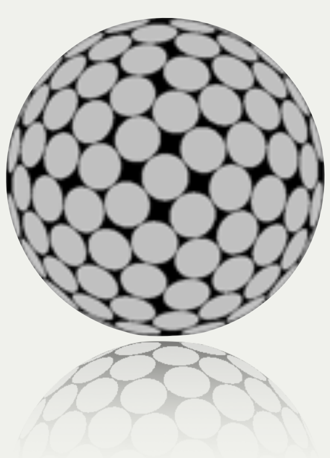
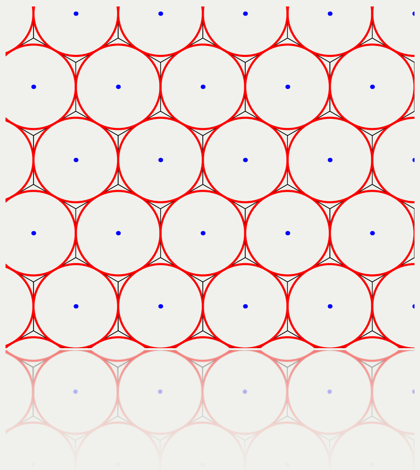
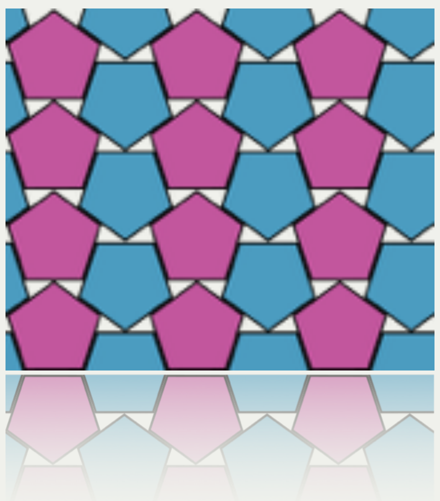
Spectral bounds and SDP hierarchies for geometric packing problems

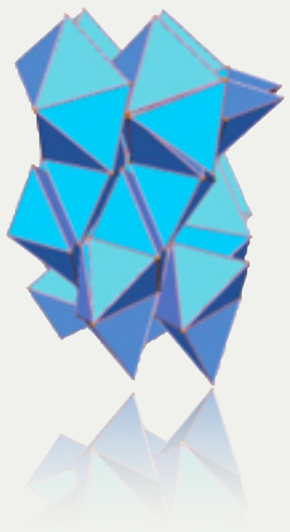
Frank Vallentin (Universität zu Köln)

September 24, 2014









Workshop: Semidefinite optimization, approximation and applications
Simons Institute for the Theory of Computing

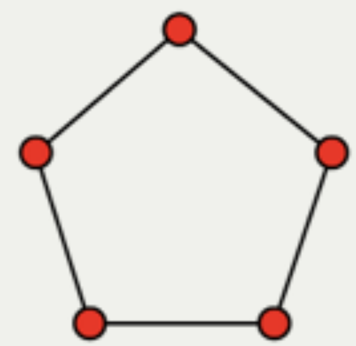
Independent sets in Cayley graphs

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

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

undirected graph on G

may contain loops



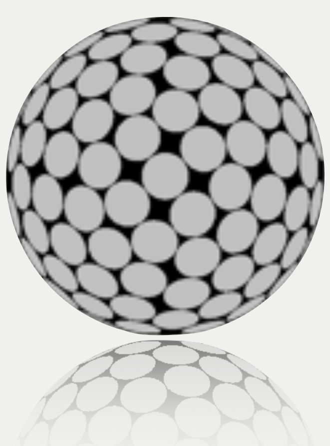
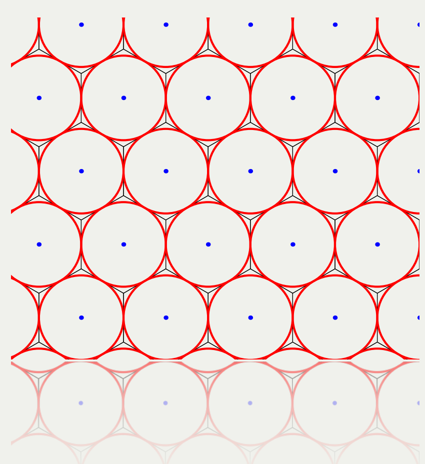
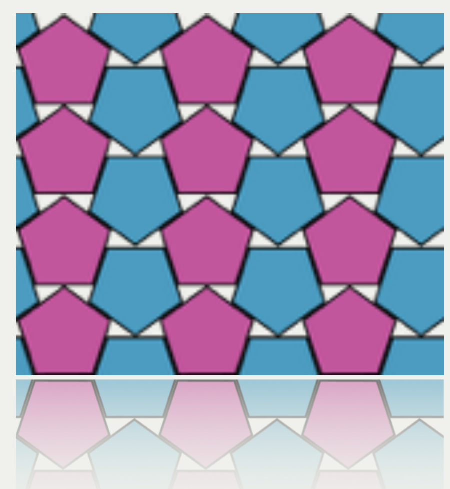
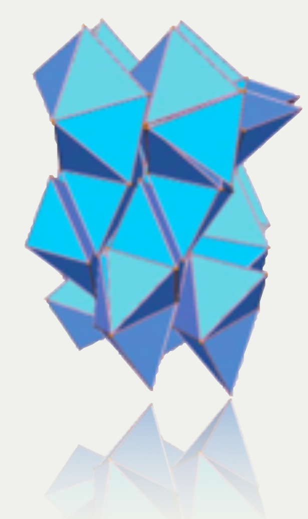
$\overline{\alpha} = 2/5$

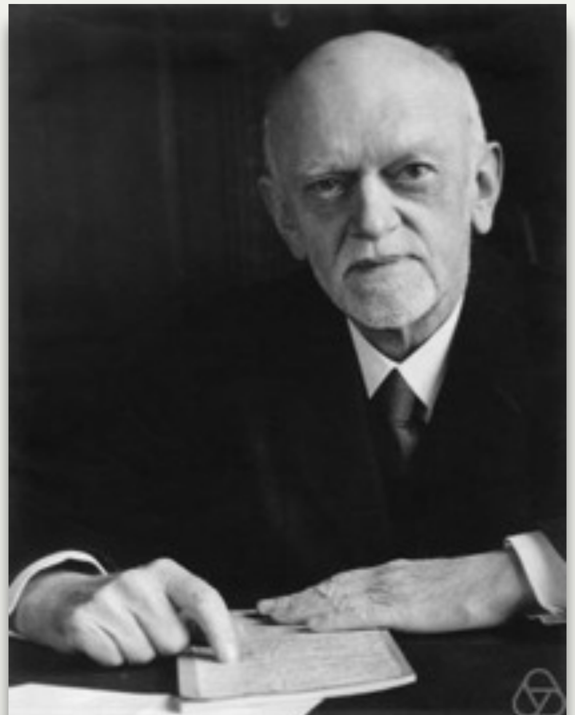
Cayley$(\mathbb{Z}/5\mathbb{Z}, \{1, 4\})$

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

find indep. sets in Cayley(G, Σ) which are as "large" as possible

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*

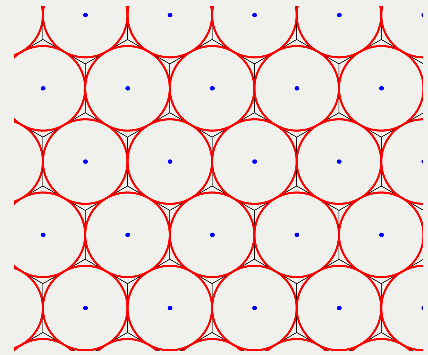


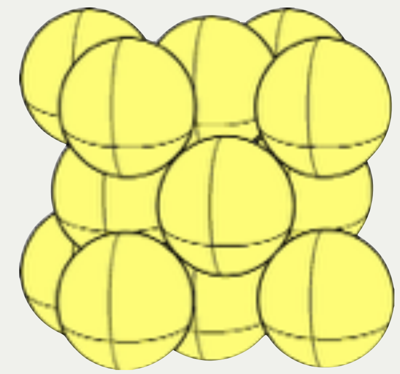
18. Building up of Space from Congruent Polyhedra

(. . .) How can one arrange most densely in space an infinite number of equal solids of given form, e.g., spheres with given radii or regular tetrahedra with given edges (or in prescribed position), that is, how can one so fit them together that the ratio of the filled to the unfilled space may be as great as possible?

'goal': solve Hilbert's problem (by computer) using an SOS proof system

$\mathcal{K}$ = unit ball





solved only for dimension 2, 3 (Hales, 1998/2014)

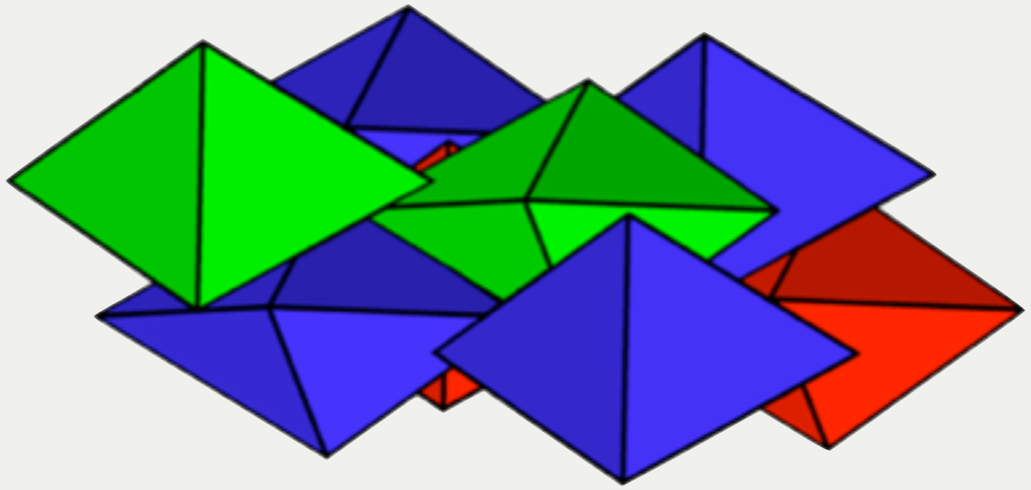
almost solved for dimension 8, 24 (Cohn-Elkies, 2003)

Dimension	*Lower bound*	*Cohn-Elkies bound*	*New upper bound*
4	0.12500	0.13126	0.130587
5	0.08839	0.09975	0.099408
6	0.07217	0.08084	0.080618
7	0.06250	0.06933	0.069193
9	0.04419	0.05900	0.058951

de Laat, Oliveira, V. (2012)

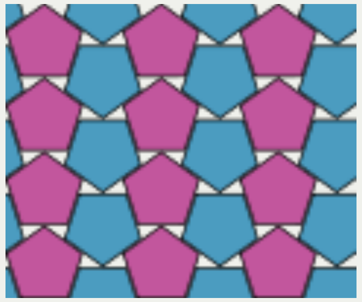
density given as point density (= # centers per unit volume)

$\mathcal{K}$ = regular tetradedron $\quad \overline{\alpha} \in [0.85, 1 - 10^{-26}]$



Chen, Engel, Glotzer (2010)
Gravel, Elser, Kallus (2011)

$\mathcal{K}$ = regular pentagon $\quad \overline{\alpha} \in [0.92, 0.98]$



Kuperberg^2 (1992)
Oliveira, V. (2013)

SOS proof systems for finite graphs

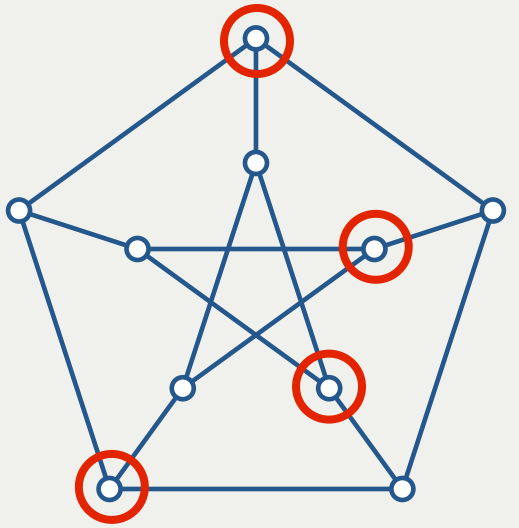
polynomial optimization formulation

$$\alpha(G) = \max \sum_{v \in V} x_v^2$$

$$x_v \geq 0$$

$$x_v^2 - x_v = 0 \text{ for } v \in V$$

$$x_u x_v = 0 \text{ if } u \sim v$$



t-th step of Lasserre's hierarchy

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

I_t = set independent sets with $\leq t$ 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}

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

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

Many variations possible:

- ⋆ consider ”interesting” principal submatrices
- ⋆ add more constraints

n-point bound: makes use of $y_{I \cup J}$ with $|I \cup J| \leq n$

Generalization of Lasserre's hierarchy

need topological assumptions

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

- $\star$ V is a Hausdorff topological space
- $\star$ 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

dual formulation

$$\mathrm{las}_t(G) = \inf \Big\{ K(\emptyset, \emptyset) : K \in \mathcal{C}(I_t \times I_t)_{\succeq 0}, \\ A_t K(S) \leq -1_{I_{=1}}(S) \text{ for } S \in I_{2t} \setminus \{\emptyset\} \Big\},$$

$$A_t \colon \mathcal{C}(I_t \times I_t)_{\mathrm{sym}} \to \mathcal{C}(I_{2t}), \quad A_t K(S) = \sum_{J, J' \in I_t : J \cup J' = S} K(J, J').$$

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

when G is a compact topological packing graph

Explicit computations

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 (spectral) bounds for Cayley(G, Σ)

$$\mathrm{las}_1(G) = \inf\left\{ \frac{f(e)}{\int_G f(x)\,d\mu(x)} : \begin{array}{l} f : G \to \mathbb{R} \text{ pos. type} \\ f(x) \leq 0 \text{ if } x \notin \Sigma \end{array} \right\}$$

f positive type:

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

$$\mathrm{las}_1(G) = \inf\left\{ \frac{f(e)}{\int_G f(x)\,d\mu(x)} : \begin{array}{l} f : G \to \mathbb{R} \text{ pos. type} \\ f(x) \le 0 \text{ if } x \notin \Sigma \end{array} \right\}$$

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.

Segal-Mautner 1950

If G is nice and if f is rapidly decreasing:

f is pos. type $\Longleftrightarrow$

optimization variable

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

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

$\widehat{G} = \{$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

relevant irred. rep. of $\mathbb{R}^n \rtimes \mathsf{SO}(n)$ for $n = 2$

$$\pi_a : G \to \mathsf{U}(L^2(S^1)) \qquad a > 0$$

$$\left[\pi_a(x, A)\varphi\right](\xi) = e^{2\pi i a x \cdot \xi}\varphi(A^{-1}\xi)$$

optimization variable

$\hat{f}(a) : L^2(S^1) \to L^2(S^1)$

$$f(x, A) = 2\pi \int_0^\infty \mathbf{trace}(\pi_a(x, A)\hat{f}(a))a\,da$$

Plancherel measure

in polar coordinates

$$f(\rho, \theta, \alpha) = \int_0^\infty \sum_{r,s\in\mathbb{Z}} \hat{f}(a)_{r,s} i^{s-r} e^{-i(s\alpha+(r-s)\theta)} J_{s-r}(2\pi a\rho)a\,da$$

$$x = \rho(\cos\theta, \sin\theta),\ A = \begin{pmatrix} \cos\alpha & -\sin\alpha \\ \sin\alpha & \cos\alpha \end{pmatrix}$$

the problem of finding an optimal function is an infinite-dimensional SDP

goal: reformulate and relax to a finite-dimensional SDP

solve this rigorously on a computer

When

$$\hat{f}(a)_{r,s} = \sum_{k=0}^{d} f_{r,s;k} a^{2k} e^{-\pi a^2}$$

and setting the right $\hat{f}(a)_{r,s}$ to zero

forces

$$f(\rho, \theta, \alpha) = \int_0^\infty \sum_{r,s \in \mathbb{Z}} \hat{f}(a)_{r,s} i^{s-r} e^{-i(s\alpha + (r-s)\theta)} J_{s-r}(2\pi a \rho) a \, da$$

to become a polynomial times exponential

If
$$e^{\pi a^2} \sum_{r,s=-N}^{N} \hat{f}(a) y_r y_s \in \mathbb{R}[a, y_{-N}, \ldots, y_N]$$

is a sum of squares, then f is pos. type

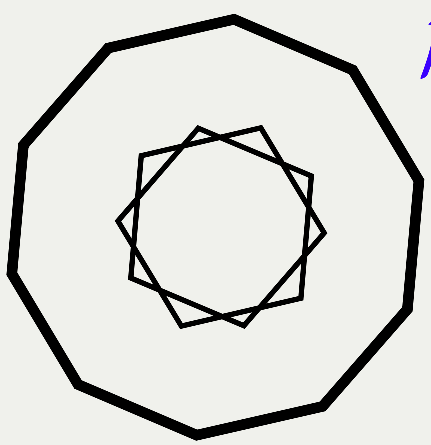
now formulate as a semidefinite program

geometric condition $f(x, A) \leq 0$ if $x \notin \mathcal{K} - A\mathcal{K}$

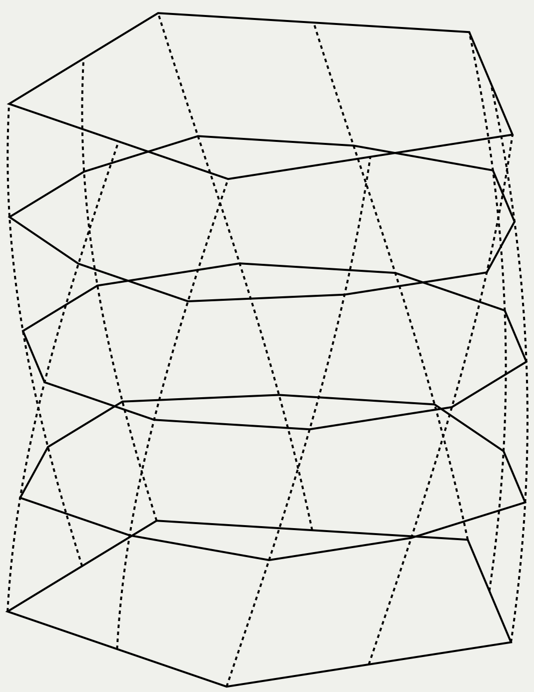
Fix $A \in \mathrm{SO}(n)$.

$x \in \mathbb{R}^n$ with $K^o \cap x + AK^o \neq \emptyset$ is Minkowski difference $K^o - AK^o$

If K is a polytope, this is a linear condition in x.



$\mathcal{K}^o - A\mathcal{K}^o$ is an open 10-gon



Rigorous computations

right choice of polynomial basis is extremely important

— using monomial basis fails badly, even for very small degrees

— our choice: $|\mu_k^{-1}| L_k^{n/2-1}(2\pi t)$

μ_k: coefficient of $L_k^{n/2-1}(2\pi t)$ with largest absolute value

— `SDPA-gmp` with 256 bits of precision: $d \leq 51$

— perform post processing of the floating point solution

— perturb to a rational solution

— analyze quality-loss of this perturbation

(by estimates of eigenvalues and condition numbers)

— custom made C++ library for SDPs with SOS constraints

Tetrahedra?

- ⋆ needs more automatization
  (also the harmonic analysis part)
- ⋆ needs more theory for numerical
  optimization with SOS constraints
  (condition numbers, special numerical solvers)
- ⋆ still a challenge