Upper bounds for multiple-size spherical cap packings

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Multiple-size spherical cap packing problem

Given a fixed set \(\{\alpha_1, \ldots, \alpha_N\}\) of spherical cap angles:
What is the maximal spherical cap packing density?

\[ C(x, \alpha) = \{y \in S^{n-1} : x \cdot y \geq \cos \alpha\} \]
Spherical cap packing graph

\[ V = S^{n-1} \times \{1, \ldots, N\} \]
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\[(x, i) \sim (y, j) \iff \cos(\alpha_i + \alpha_j) < x \cdot y \text{ and } (x, i) \neq (y, j)\]
Spherical cap packing graph

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\[(x, i) \sim (y, j) \iff \cos(\alpha_i + \alpha_j) < x \cdot y \text{ and } (x, i) \neq (y, j)\]

\[ w(x, i) = \frac{\omega_{n-1}(S^{n-2})}{\omega_n(S^{n-1})} \int_{\cos \alpha_i}^{1} (1 - u^2)^{(n-3)/2} du \]
Spherical cap packing graph

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- Stable sets correspond to packings
- Weighted stability number gives the maximal packing density
The weighted theta number for finite graphs

- Computing the weighted stability number is NP-hard
- The weighted theta (prime) number gives upper bounds:

\[ \vartheta'_w(G) = \min \left\{ M : \begin{aligned} &K - \sqrt{w} \sqrt{w}^T \in S^V_{\succeq 0} \\ &(K - MI)(u, v) \leq 0 \text{ when } u \not\sim v \end{aligned} \right\} \]

- This can be computed in polynomial time using semidefinite programming
Infinite graphs

Hilbert-Schmidt kernels:
\[ \mathcal{C}(V \times V) = \{ K : V \times V \to \mathbb{R} : K \text{ continuous} \} \]
Infinite graphs

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  \[ \mathcal{C}(V \times V) = \{ K : V \times V \to \mathbb{R} : K \text{ continuous} \} \]
- \( K \in \mathcal{C}(V \times V) \) is positive if it is symmetric and
  \[ (K(u_i, u_j))_{1 \leq i, j \leq n} \succeq 0 \text{ for all } n \text{ and all } u_1, \ldots, u_n \in V \]
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- Generalization of the theta number:
  \[ \vartheta'_w(G) = \inf \left\{ M : \begin{array}{c} K - \sqrt{w} \otimes \sqrt{w} \in C_{\geq 0}(V \times V) \vspace{1mm} \\ (K - MI)(u, v) \leq 0 \text{ when } u \not\sim v \end{array} \right\} \]

- Infinitely many variables/constraints: how to compute this?
Using symmetry

Group action: $O(n) \times V \rightarrow V$, $g(x, i) = (gx, i)$
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Observation:
If \((K, M)\) is feasible for
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\]
then \((\overline{K}, M)\) is also feasible, where
\[
\overline{K}(u, v) := \int_{O(n)} K(gu, gv) \mu(dg)
\]
and where \(\mu\) is the normalized Haar measure on \(O(n)\).
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Symmetry reduction:
In the infimum we can restrict to \(O(n)\)-invariant kernels
Positive invariant kernels

A kernel $K \in \mathcal{C}(V \times V)$ is positive and $O(n)$-invariant if and only if

$$K((x, i), (y, j)) = \sum_{k=0}^{\infty} f_{k,ij} P_k^n(x \cdot y),$$

where $(f_{k,ij})_{1 \leq i,j \leq N} \succeq 0$ for all $k$
(For $N = 1$ this is a result of Schoenberg)

Jacobi polynomials $P_k^n$:
Orthogonal with respect to the weight $(1 - s^2)^{(n-3)/2}$ on $[-1, 1]$
Normalized such that $P_k^n(1) = 1$
Simplified program

This gives the following simplified program

\[ \vartheta'_w(G) = \inf \left\{ M : \begin{array}{l} (f_{0,ij} - \sqrt{w(\alpha_i)} \sqrt{w(\alpha_j)})_{1 \leq i,j \leq N} \geq 0 \vb{1}_{i,j} \leq \sqrt{w(\alpha_i)} \sqrt{w(\alpha_j)} \geq 0, \ k = 1, 2, \ldots \ \quad \sum_{k=0}^{\infty} f_{k,ij} P^n_k(u) \leq 0, \ -1 \leq u \leq \cos(\alpha_i + \alpha_j) \ \quad \sum_{k=0}^{\infty} f_{k,ii} \leq M \end{array} \right\} \]

▶ Replace \( \infty \) by a large number \( d \)
▶ Finitely many variables, but still infinitely many constraints
▶ Use a sum of squares characterization to simplify further:
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(f_{k,ij})_{1 \leq i,j \leq N} \geq 0, \ k = 1, 2, \ldots \\
\sum_{k=0}^{\infty} f_{k,ij} P_{k}^{n}(u) \leq 0, \ -1 \leq u \leq \cos(\alpha_i + \alpha_j) \\
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If \( p \) is a real even univariate polynomial, then

[\[ p(x) \geq 0 \text{ for all } x \in [a, b] \Leftrightarrow p(x) = q(x) + (x - a)(b - x)r(x) \]

where \( q \) and \( r \) are SOS polynomials
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\[ p(x) \text{ is SOS } \iff p(x) = [x]^T Q[x] \text{ for some } Q \succeq 0 \]

\[ [x] = (1, x, \ldots, x^d)^T \]
A semidefinite program

This gives the semidefinite program

\[
\varphi'_w(G) = \inf \left\{ M : \begin{align*}
(f_{0,ij} - \sqrt{w(\alpha_i)}\sqrt{w(\alpha_j)} &\geq 0 \\
(f_{k,ij})_{1 \leq i,j \leq N} &\geq 0, \ k = 1, \ldots, d \\
Q^{ij} &\in S_{\geq 0}^{d/2+1}, \ R^{ij} \in S_{\geq 0}^{d/2}, \ 1 \leq i,j \leq N \\
\sum_{k=0}^{d} \langle P^n_i \rangle_k f_{l,ij} + \langle Q^{ij}, E_l \rangle + \langle R^{ij}, T_{l,ij} \rangle &\leq 0 \\
\sum_{k=0}^{d} f_{k,ii} &\leq M
\end{align*} \right\}
\]

- \(E_l\) is the 0/1 matrix with \((E_l)_{i+1,j+1} = 1\) when \(i + j = l\)
- \(T_{l,ij} = \cos(\alpha_i + \alpha_j)E_l + (-1 + \cos(\alpha_i + \alpha_j))E_{l-1} - E_{l-2}\)
Single size packings \((n = 3)\)
Single size packings ($n = 3$)

- SDP Bound (LP bound)
- Geometric bound (Florian 2001)
Single size packings \((n = 3)\)
Single size packings for $n = 3$

![Graph showing density vs. angle with various packings labeled: Tetrahedron, Octahedron, Icosahedron, Snubcube, and Twisted cube. The graph includes annotations for SDP Bound (LP bound), Geometric bound (Florian 2001), Packing configurations (Sloane), and Rounding down.]
Single size packings for $n = 4$
Single size packings for $n = 5$
Binary packings for $n = 3$
SDP bound / Geometric bound

![Graph showing SDP and Geometric bounds](image-url)
Binary packings for $n = 4$
Binary packings for $n = 5$