Upper Bounds for Non-Congruent Sphere Packings

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Abstract

We prove upper bounds on the average kissing number \( k(P) \) and contact number \( C(P) \) of an arbitrary finite non-congruent sphere packing \( P \), and prove an upper bound on the packing density \( \delta(P) \) of an arbitrary infinite non-congruent sphere packing \( P \).

Keywords: average kissing number, contact number, packing density, non-congruent sphere packing, linear programming bounds, upper bounds.

MSC 2010 Subject Classifications: Primary 52C17, Secondary 51F99.

1 Lexicon

Let

\[ P = \bigcup_{i=1}^{k} \bigcup_{j=1}^{n_i} (x_{ij} + r_i S^2) \]

be an arbitrary non-congruent sphere packing. Then

\[ \|x_{ij} - x_{i'j'}\| \geq r_i + r_{i'}, \forall 1 \leq i, i' \leq k, j \neq j' \]

is a necessary condition required for the spheres to be non-overlapping. Hence, the vertex set and edge set of the sphere packing \( P \) are

\[ V(P) = \{x_{ij} \in \mathbb{R}^3 \mid 1 \leq i \leq k, 1 \leq j \leq n_i\} \]

\[ E(P) = \{(x_{ij}, x_{i'j'}) \mid \|x_{ij} - x_{i'j'}\| = r_i + r_{i'}, x_{ij}, x_{i'j'} \in V(P)\} \]

The the average kissing number of \( P \) is \( k(P) = 2|E(P)|/n \), where \( n = \sum_{i=1}^{k} n_i \), and the contact number of \( P \) is \( C(P) = |E(P)| \).

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2 Upper Bounds on Average Kissing Numbers and Contact Numbers of Sphere Packings

Consider, as in Cohn-Zhao [3], a continuous function $g : [-1, 1] \to \mathbb{R}$ which is positive definite on $S^2$ with $g(t) \leq 0, \forall t \in [-1, \cos \theta]$ and

$$g = \frac{\int_{-1}^{1} g(t)(1-t^2)dt}{\int_{-1}^{1} (1-t^2)dt} > 0,$$

then

$$g \in F_\theta(S^2).$$

Furthermore, let $A(3, \theta)$ be the maximum size of a spherical $\theta$-code and recall that

$$A^{LP}(3, \theta) = \inf_{g \in F_\theta(S^2)} \frac{g(1)}{\mathcal{g}},$$

is the best upper bound on $A(3, \theta)$ that could be derived using Theorem 3.1 from Cohn-Zhao [3] (which appeals to the Delsarte-Goethals-Seidel [4] and Kabatiansky-Levenshtein [5] linear programming bounds). Let $\tau_{r_i}(r_j)$ be the maximum number of radius $r_i$ spheres which can touch a radius $r_j$ sphere; $\tau_{r_j}(r_i)$ is defined similarly, namely the maximum number of radius $r_j$ spheres which can touch a radius $r_i$ sphere.

**Theorem 1.** Let $P$ be a sphere packing with $n_i$ spheres of radius $r_i$ for $1 \leq i \leq k$. Then,

$$k(P) < 12 + \sum_{i \neq j} \min\{n_i \min\{n_j, \tau_{r_i}(r_j)\}, n_j \min\{n_i, \tau_{r_j}(r_i)\}\} - 1.85335 \sum_{i=1}^{k} n_i^{2/3} \sum_{i=1}^{k} n_i$$

where $\tau_{r_i}(r_j) \leq A^{LP}(3, \arccos\left(1 - \frac{2r_j^2}{(r_i + r_j)^2}\right))$ and $\tau_{r_j}(r_i) \leq A^{LP}(3, \arccos\left(1 - \frac{2r_i^2}{(r_i + r_j)^2}\right)).$
Proof. Decompose the vertex set and edge set of $\mathcal{P}$ as

$$V(\mathcal{P}) = \bigcup_{i=1}^{k} V_i(\mathcal{P}) := \bigcup_{i=1}^{k} \{x_{ij} \in V(\mathcal{P}) \mid 1 \leq j \leq n_i\}$$

$$|V(\mathcal{P})| = \sum_{i=1}^{k} |V_i(\mathcal{P})| = \sum_{i=1}^{k} n_i$$

$$E(\mathcal{P}) = \bigcup_{i=1}^{k} E_{ii}(\mathcal{P}) \cup \bigcup_{i \neq i'} E_{ii'}(\mathcal{P}) := \bigcup_{i=1}^{k} \{(x_{ij}, x_{ij'}) \mid \|x_{ij} - x_{ij'}\| = 2r_i, x_{ij}, x_{ij'} \in V_i(\mathcal{P})\} \cup \bigcup_{i \neq i'} \{(x_{ij}, x_{ij'}) \mid \|x_{ij} - x_{ij'}\| = r_i + r_{i'}, x_{ij}, x_{ij'} \in V_i(\mathcal{P})\}$$

$$|E(\mathcal{P})| = \sum_{i=1}^{k} |E_{ii}(\mathcal{P})| + \frac{1}{2} \sum_{i \neq j} |E_{ij}(\mathcal{P})|$$

Apply Theorem 1 (i) of Bezdek and the author [1] (Theorem 1.1.6 (i) in [2]) to bound the cardinality of each edge set and obtain $|E_{ii}| < 6n_i - 0.926n_i^{2/3}$, $\forall 1 \leq i \leq k$. By applying a homothetic transformation with a scaling factor of either $1/r_i$ or $1/r_j$ to $\mathcal{P}$, it is clear that $\tau_j(r_i) = \tau_i(r_j/r_j)$ and $\tau_i(r_j) = \tau_j(r_j/r_i)$. Hence, each $|E_{ij}(\mathcal{P})| + |E_{ji}(\mathcal{P})|$ counts the number of edges between spheres of radius $r_i$ and $r_j$, and thus by the above homothetic transformation of either type, counts the number of edges between spheres of radius 1 and radius $r_j/r_i$ or spheres of radius $r_i/r_j$ and radius 1, respectively. Therefore, by the law of cosines applied to the geometric embedding of the contact graph of two spheres of radius $r_j/r_i$ and a sphere of radius 1, and the geometric embedding of the contact graph of two spheres of radius $r_i/r_j$ and a sphere of radius 1, we obtain the $\theta$-code size desired in each case:

$$\theta_i^j = \arccos \left( 1 - \frac{2r_j^2}{(r_i + r_j)^2} \right)$$

$$\theta_j^i = \arccos \left( 1 - \frac{2r_i^2}{(r_i + r_j)^2} \right)$$

Hence, $\tau_i(r_i/r_j) = A(3, \theta_i^j) \leq A^{LP}(3, \theta_i^j)$ and $\tau_j(r_j/r_i) = A(3, \theta_j^i) \leq A^{LP}(3, \theta_j^i)$. From this we observe, from basic restrictions on the number of spheres of varying radii, that

$$|E_{ij}(\mathcal{P})| = |E_{ji}(\mathcal{P})| < \min \{n_i \min \{n_j, \tau_i(r_j)\}, n_j \min \{n_i, \tau_j(r_i)\}\} = \min \{n_i \min \{n_j, A^{LP}(3, \theta_j^i)\}, n_j \min \{n_i, A^{LP}(3, \theta_j^i)\}\}$$

Cumulatively, these observations combined with the definition of the average kissing number $k(\mathcal{P})$ prove the theorem.  

\[ \square \]
In practice, it is difficult to compute $A^{LP}(3, \theta)$ explicitly, but a weaker bound may be provided by nonnegative linear combinations of Gegenbauer polynomials $C^{\frac{2}{3}-1}_k$ as shown by Schoenberg’s characterization of continuous positive definite functions [7]. Gegenbauer polynomials, or ultraspherical polynomials, are a special case of the Jacobi polynomials, or hypergeometric polynomials, and for algorithmic implementations of the following theorem we can follow [3] and set

$$g(t) = \sum_{k=0}^{\infty} c_k C^{\frac{2}{3}-1}_k(t), g = c_0$$

For algorithmic implementation, tighter bounds on $A(n, \theta)$ may be found using de Laat-de Oliveira Filho-Vallentin semidefinite programming bounds [9], or Cohn-Elkies error-correcting codes bounds [8]. Furthermore, Theorem 1 can be considered a packing dependent generalization of the celebrated Kuperberg-Schramm bound on the supremal average kissing number $k$ of a sphere packing in $\mathbb{R}^3$ [6], which says that $12.566 < k := \sup_{\mathcal{P} \rightarrow \mathbb{R}^3} k(\mathcal{P}) < 8 + 4\sqrt{3} \approx 14.928$. Future research goals include the algorithmic implementation of Theorem 1 to compare with the Kuperberg-Schramm bound.

We now state Theorem 1 in terms of contact numbers which follows directly from the definition of $k(\mathcal{P})$, thus generalizing Theorem 1 (i) of Bezdek and the author [1] (Theorem 1.1.6 (i) in [2]), which states that if $\mathcal{P}$ is a packing of $n$ congruent spheres then $C(\mathcal{P}) < 6n - 9.26n^{2/3}$.

**Corollary 1.** Let $\mathcal{P}$ be a sphere packing with $n_i$ spheres of radius $r_i$ for $1 \leq i \leq k$. Then,

$$C(\mathcal{P}) < \sum_{i=1}^{k} (6n_i - 0.926675n_i^{2/3}) + \frac{1}{2} \sum_{i \neq j} \min \{n_i \min \{n_j, \tau_{r_i}(r_j)\}, n_j \min \{n_i, \tau_{r_j}(r_i)\}\}$$

where $\tau_{r_i}(r_j) \leq A^{LP}(3, \arccos \left(1 - \frac{2r^2}{(r_i+r_j)^2}\right))$ and $\tau_{r_j}(r_i) \leq A^{LP}(3, \arccos \left(1 - \frac{2r^2}{(r_i+r_j)^2}\right))$.

## 3 Upper Bounds on Infinite Sphere Packings’ Densities

We define the locally maximal tetrahedron $\Delta(r_i, r_j, r_k, r_l)$ to be the convex hull of the center points of spheres of radius $r_i, r_j, r_k, r_l$, which are maximally contracted; i.e., there does not exist a non-trivial contractive mapping of the spheres. We can use the geometric structure of the locally maximal tetrahedron to calculate an upper bound on the density of an infinite sphere packing of distinct radii $r_i, i \in S \subseteq \mathbb{N}$, by defining $\Delta(r_i, r_j, r_k, r_l) = \text{conv}\{\vec{w}_i, \vec{w}_j, \vec{w}_k, \vec{w}_l\}$ and intersecting spheres of the associated radii at each vertex of the locally maximal tetrahedron. By connecting spherical geometry and dihedral angles we arrive at the following theorem which holds for any sphere packing $\mathcal{P}$ in $\mathbb{R}^3$ whether or not it has finitely many distinct radii, or infinitely many distinct radii, although the theorem does not have a realizable algorithmic implementation in the case of infinitely many distinct radii.
Theorem 2. Let $\mathcal{P}$ be a sphere packing in $\mathbb{R}^3$ with distinct radii $r_i, i \in S \subseteq \mathbb{N}$, and let $
abla_{\text{max}}(\mathcal{P}_\Delta(r_i, r_j, r_k, r_l))$ be the maximal packing density of $\Delta(r_i, r_j, r_k, r_l)$ in $\mathbb{R}^3$. Then,

$$\delta(\mathcal{P}) < 2 \max_{r_i \leq r_j \leq r_k \leq r_l} \nabla_{\text{max}}(\mathcal{P}_\Delta(r_i, r_j, r_k, r_l)) \left( \left[ \sum_{m=i,j,k,l} r^3_m (A_m + B_m + C_m - \pi) \right] / \| \vec{\omega}_2 \cdot (\vec{\omega}_3 \times \vec{\omega}_4) \| \right),$$

where $\Delta(r_i, r_j, r_k, r_l) = \text{conv}\{\vec{\omega}_i, \vec{\omega}_j, \vec{\omega}_k, \vec{\omega}_l\}$ and

$$U_{ijk} = \vec{\omega}_j \times \vec{\omega}_k, \quad U_{ikl} = \vec{\omega}_k \times \vec{\omega}_l, \quad U_{ijl} = \vec{\omega}_j \times \vec{\omega}_l, \quad U_{jkl} = (\vec{\omega}_k - \vec{\omega}_j) \times (\vec{\omega}_l - \vec{\omega}_j).$$

Proof. Observe that

$$\text{vol}(\partial (\vec{\omega}_m + r_m \mathbb{S}^2) \cap \Delta(r_i, r_j, r_k, r_l)) = \frac{r_m}{3} \text{area}(\partial (\vec{\omega}_m + r_m \mathbb{S}^2) \cap \Delta(r_i, r_j, r_k, r_l)).$$

is the volume of a spherical wedge intersecting a sphere of radius $r_m$ and a locally maximal tetrahedron. By calculating the volume of each of these spherical wedges in terms of the spherical area of a triangle on $r_m \mathbb{S}^2$ and observing that the supremum of $\delta(\mathcal{P})$ is less than the supernal density of a locally maximal tetrahedron $\Delta(r_i, r_j, r_k, r_l)$, we obtain

$$\delta(\mathcal{P}) < \max_{r_i \leq r_j \leq r_k \leq r_l} \nabla_{\text{max}}(\mathcal{P}_\Delta(r_i, r_j, r_k, r_l)) \sum_{m=i,j,k,l} \text{vol}(\partial (\vec{\omega}_m + r_m \mathbb{S}^2) \cap \Delta(r_i, r_j, r_k, r_l)) / \text{vol}(\Delta(r_i, r_j, r_k, r_l)).$$

The apparatus for calculating the upper bound is self evident from the definition of dihedral angles, tetrahedral volumes, and areas of spherical triangles. \qed
References

[1] K. Bezdek, S. Reid. Contact graphs of unit sphere packings revisited. Journal of Geometry, April 2013.

[2] K. Bezdek. Lectures on Sphere Arrangements - the Discrete Geometric Side. Springer, 2013.

[3] H. Cohn, Y. Zhao. Sphere Packing Bounds via Spherical Codes. Duke Math. J., Volume 163, Number 10, 2004; pp. 1965 - 2002.

[4] P. Delsarte, J. M. Goethals, J. J. Seidel. Spherical codes and designs. Geometriae Dedicata, Volume 6, 1977; pp. 363 - 388.

[5] G. A. Kabatiansky, V. I. Levenshtein. Bounds for packings on a sphere and in space. [Russian] Problemy Pereda˘ci Informacii, Volume 14, 1978; pp. 3 - 25.

[6] G. Kuperberg, O. Schramm. Average kissing numbers for non-congruent sphere packings. Math. Res. Lett., Volume 1, 1994; pp. 339 - 344.

[7] I. J. Schoenberg. Positive definite functions on spheres. Duke Math. J., Volume 9, 1942; pp. 96 - 108.

[8] H. Cohn, N. Elkies. New upper bounds on sphere packings I. Annals of Mathematics, Volume 157, 2003; pp. 689 - 714.

[9] D. de Laat, F. M. de Oliveira Filho, F. Vallentin. Upper bounds for packings of spheres of several radii. Forum of Mathematics, Sigma, Volume 2, 2014; e23.