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Contact graphs of ball packings

Alexey Glazyrin*

Abstract

A contact graph of a packing of closed balls is a graph with balls as vertices and pairs of tangent balls as edges. We prove that the average degree of the contact graph of a packing of balls (with possibly different radii) in \mathbb{R}^3 is not greater than 13.955. We also find new upper bounds for the average degree of contact graphs in \mathbb{R}^4 and \mathbb{R}^5 .

1 Introduction

A packing of closed balls in \mathbb{R}^d is a finite set of balls with non-intersecting interiors. Each packing naturally entails a contact graph where graph vertices are the balls of the packing and two vertices are connected by an edge if and only if the corresponding balls are tangent.

The problem of characterizing contact graphs of planar disk packings is completely solved by the Koebe–Andreev–Thurston Theorem ([20, 2, 3, 31]).

Theorem 1 (Koebe–Andreev–Thurston). *For every simple planar graph G there is a set of non-intersecting closed disks on the plane whose contact graph is G .*

The natural question is to get a similar characterization of contact graphs in higher dimensions.

Question 1. *What graphs may be realized as contact graphs of closed balls in \mathbb{R}^d ?*

This question does not impose any restrictions on closed balls. One of such reasonable restrictions is to require balls in a packing to be congruent. An observation by Kirkpatrick and Rote (see [18] for more details) establishes that a graph G is a contact graph of a unit ball packing in \mathbb{R}^d if and only if the join $G \oplus K_2$ of the graph G with an edge K_2 is a contact graph of a general ball packing in \mathbb{R}^{d+1} . This observation combined with results for packings of unit balls imply that recognizing a contact graph of ball packings is NP-hard in dimensions 3, 4, 5, 9, 25 ([17, 8, 18], see also the survey [6]).

Since, as we can see, the general question is quite complicated, typically some characteristics of contact graphs are analyzed.

For each contact graph G of a closed ball packing in \mathbb{R}^d denote its average degree by $k(G)$. Define $k_d = \sup k(G)$ taken over all contact graphs. A simple way to bound k_d is by using kissing numbers. By a kissing number τ_d we mean the maximum number of non-overlapping closed unit balls tangent to a given unit ball in \mathbb{R}^d . As mentioned in [21], it is easy to show that $k_d \leq 2\tau_d$, since each ball cannot have more than τ_d larger or equal balls tangent to it.

The state-of-the-art bounds for τ_d imply the following bounds for k_d :

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$$k_3 \leq 24[30]; k_4 \leq 48[28]; k_5 \leq 88[26]; k_6 \leq 136[4]; k_7 \leq 268[26]; k_8 \leq 480[29, 23]$$

and the asymptotic (Kabatyanskii-Levenshtein) bound

$$k_d \leq 2^{0.401d(1+o(1))} [19].$$

Using the area argument Kuperberg and Schramm proved in [21] a non-trivial upper bound for k_3 . They also connected 600-cells in a chain and produced a ball packing with the average degree strictly greater than 12.

Theorem 2 (Kuperberg–Schramm [21]).

$$12.566 \approx 666/53 \leq k_3 < 8 + 4\sqrt{3} \approx 14.928.$$

In [13], the lower bound for k_3 was improved by a more intricate construction based on 600-cells.

Theorem 3 (Eppstein–Kuperberg–Ziegler [13]).

$$12.612 \approx 7656/607 \leq k_3.$$

In the general case, k_d can be bounded below by a lattice kissing number τ_d^* , the maximal number of balls tangent to one ball in a lattice packing of unit balls. Unfortunately, no general lower bounds for τ_d^* with exponential growth are known. For $d = 2^n$, it was shown that $\tau_d^* = 2^{\Omega(\log^2 d)}$ [22]. As for non-lattice packings, it was proven in [1] that there is a finite unit ball packing in dimension $d = 4^n$ such that each ball touches more than $2^{\sqrt{d}}$ others. This result implies $k_{4^n} > 2^{2^n}$.

Various studies were also dealing with certain characteristics of contact graphs of ball packings such as chromatic numbers ([24, 9]), graph separators ([25]), or with non-realizability of concrete graphs ([5]).

The main results of this paper are the new upper bounds $k_3 < 13.955$, $k_4 < 34.681$, $k_5 < 77.757$. The results in dimensions 4 and 5 are obtained by generalizing the method of Kuperberg and Schramm to higher dimensions. The improvement of the bound in \mathbb{R}^3 required a thorough analysis of packings of circular caps via the upper bounds from [15, 16].

The paper is structured as follows. In Section 2 we explain the approach of Kuperberg and Schramm with their upper bound for k_3 . In Section 3 we show how their approach works in higher dimensions. Section 4 is devoted to the proof of the new upper bound for k_3 . Finally, in Section 5 we raise some questions and discuss possible future advancements in this area.

2 Kuperberg-Schramm approach

In this section we will explain the approach of Kuperberg and Schramm which allowed them to prove the upper bound of $8 + 4\sqrt{3}$ for k_3 . Throughout the section we will use Archimedes' formula for areas of spherical caps: $A = 2\pi Rh$, where R is the radius of the sphere and h is the height of a cap.

For the sake of exposition, we will start with the following proposition.

Proposition 1.

$$\tau_3 \leq 8 + 4\sqrt{3}.$$

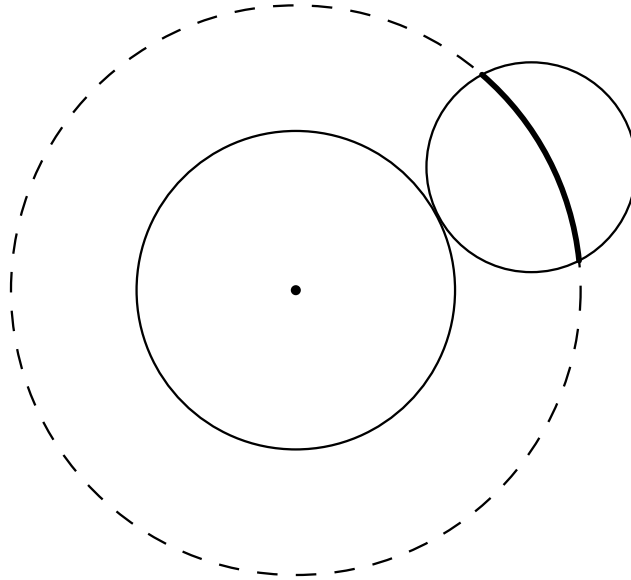
Proof. For a unit ball B in \mathbb{R}^3 , consider a concentric sphere with radius $\sqrt{3}$. Any unit sphere tangent to B intersects this concentric sphere by a spherical cap with the angular spherical radius of $\pi/6$. The height of this spherical cap is $\sqrt{3} - 3/2$. By Archimedes' formula, the area of this spherical cap is $2\pi\sqrt{3}(\sqrt{3} - 3/2) = (6 - 3\sqrt{3})\pi$. Since the area of the concentric sphere is 12π , no more than $\frac{12\pi}{(6-3\sqrt{3})\pi} = 8 + 4\sqrt{3}$ spherical caps may fit in the surface of the concentric sphere. \square

Remark 1. *Of course kissing numbers are integer so any upper bound may be substituted by its integer part and Proposition 1 also implies that $\tau_3 \leq 14$. The main purpose of the proposition is to emphasize the ideas to be transferred to the case of packings with different radii.*

The same idea of bounding the number of tangent spheres is not directly applicable when different radii are allowed. For a unit ball, one can construct any number of small balls tangent to it. However, for two tangent balls the smaller proportion of area taken by a smaller ball on a sphere concentric to a larger ball is compensated by a larger proportion of area taken by a larger ball on a sphere concentric to a smaller ball. This is the cornerstone of the approach by Kuperberg and Schramm.

Fix $\rho > 1$. For each closed ball B denote the concentric sphere with radius ρ times larger by $S_\rho(B)$. For two tangent balls B_1 with radius r_1 and B_2 with radius r_2 , define

$$a(B_1, B_2) = \frac{\text{area}(S_\rho(B_1) \cap B_2)}{\text{area}(S_\rho(B_1))}.$$



Remarkably, if both $S_\rho(B_1) \cap B_2$ and $S_\rho(B_2) \cap B_1$ are non-empty, $a(B_1, B_2) + a(B_2, B_1)$ depends only on ρ .

In order to prove this denote the height of a spherical cap $S_\rho(B_1) \cap B_2$ by h_1 and the height of $S_\rho(B_2) \cap B_1$ by h_2 (if an intersection is empty we use 0 for its height).

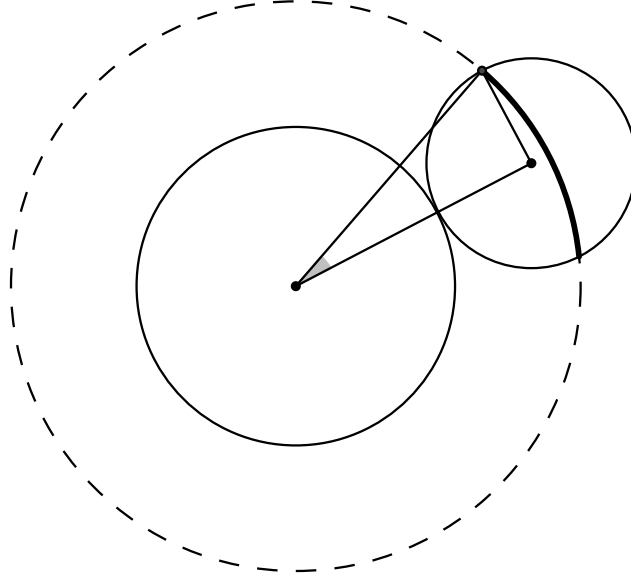
From this moment on, we consider only $\rho < 3$ because otherwise at least one of $a(B_1, B_2)$ and $a(B_2, B_1)$ is 0.

Lemma 2.1.

$$\frac{h_1}{\rho r_1} + \frac{h_2}{\rho r_2} = \frac{-\rho^2 + 4\rho - 3}{2\rho},$$

if both $S_\rho(B_1) \cap B_2$ and $S_\rho(B_2) \cap B_1$ are non-empty and the left hand side is greater than the right hand side otherwise.

Proof. $\frac{h_1}{\rho r_1} = 1 - \cos \alpha$, where α is the spherical radius of the cap.



We use the law of cosines for a triangle formed by the centers of B_1 and B_2 and any point on the boundary of the cap:

$$(\rho r_1)^2 + (r_1 + r_2)^2 - 2\rho r_1(r_1 + r_2) \cos \alpha = r_1^2,$$

$$\cos \alpha = \frac{(\rho r_1)^2 + (r_1 + r_2)^2 - r_1^2}{2\rho r_1(r_1 + r_2)} = \frac{(\rho^2 + 1)r_1 + 2r_2}{2\rho(r_1 + r_2)}. \quad (1)$$

Similarly, for the radius β of the second cap we get

$$\cos \beta = \frac{(\rho^2 + 1)r_2 + 2r_1}{2\rho(r_1 + r_2)}.$$

Therefore,

$$\cos \alpha + \cos \beta = \frac{(\rho^2 + 1)r_1 + 2r_2}{2\rho(r_1 + r_2)} + \frac{(\rho^2 + 1)r_2 + 2r_1}{2\rho(r_1 + r_2)} = \frac{\rho^2 + 3}{2\rho}, \quad (2)$$

$$\frac{h_1}{\rho r_1} + \frac{h_2}{\rho r_2} = 2 - (\cos \alpha + \cos \beta) = \frac{-\rho^2 + 4\rho - 3}{2\rho}.$$

Since $\rho < 3$, the equality still holds when the second spherical caps consists of one point, i.e. $r_1 + 2r_2 = \rho r_1$. Increasing r_1 , we keep the second term equal to 0 and only increase the first one. Therefore, in the case when one intersection is empty the inequality holds. \square

Lemma 2.2.

$$a(B_1, B_2) + a(B_2, B_1) = \frac{-\rho^2 + 4\rho - 3}{4\rho},$$

if both $S_\rho(B_1) \cap B_2$ and $S_\rho(B_2) \cap B_1$ are non-empty and the left hand side is greater than the right hand side otherwise.

Proof. This lemma follows immediately from the previous lemma and Archimedes' formula for areas of spherical caps. \square

Denote by $\text{dens}(\rho)$ the maximum of $\sum_i a(B, B_i)$, where the maximum is taken over all sets $\{B_i\}$ of closed balls with disjoint interiors such all B_i are tangent to B .

If $G = (V, E)$ is a contact graph of a ball packing then, on the one hand,

$$\sum_{\{X, Y\} \in E} (a(X, Y) + a(Y, X)) \geq \frac{-\rho^2 + 4\rho - 3}{4\rho} |E|.$$

On the other hand,

$$\sum_{\{X, Y\} \in E} (a(X, Y) + a(Y, X)) \leq \text{dens}(\rho) |V|$$

so

$$2|E|/|V| \leq \frac{8\rho}{-\rho^2 + 4\rho + 3} \text{dens}(\rho)$$

and, therefore, we proved the following bound.

Theorem 4.

$$k_3 \leq \inf_{1 < \rho < 3} \left\{ \frac{8\rho}{-\rho^2 + 4\rho - 3} \text{dens}(\rho) \right\},$$

where $\text{dens}(\rho)$ denotes the maximum proportion of area of $S_\rho(B)$ covered by non-overlapping balls tangent to B .

Kuperberg and Schramm used $\text{dens}(\rho) \leq 1$ and, taking the optimum $\rho = \sqrt{3}$, proved their upper bound.

3 Bounds in higher dimensions

We use the same notations $S_\rho(B)$, $a(B_1, B_2)$, etc as in Section 2. Throughout this section we use the following formula for the (d-1)-dimensional area of a spherical cap with spherical radius α on the unit sphere in \mathbb{R}^d :

$$A = \frac{\pi^{d/2}}{\Gamma(d/2)} \int_0^{\sin^2 \alpha} t^{\frac{d-3}{2}} (1-t)^{-\frac{1}{2}} dt. \quad (3)$$

For $d = 3$, this formula is equivalent to Archimedes' formula.

Lemma 3.1. For a fixed ρ , $1 < \rho < 3$, $a(X, Y) + a(Y, X)$ reaches its minimum when X and Y are congruent.

Proof. We begin with the case when both $a(X, Y)$ and $a(Y, X)$ are not 0. Denote the radii of the spherical caps $S_\rho(X) \cap Y$ and $S_\rho(Y) \cap X$ by α and β , respectively. Using formula (3) we get

$$a(X, Y) + a(Y, X) = K \left(\int_0^{\sin^2 \alpha} t^{\frac{d-3}{2}} (1-t)^{-\frac{1}{2}} dt + \int_0^{\sin^2 \beta} t^{\frac{d-3}{2}} (1-t)^{-\frac{1}{2}} dt \right),$$

where K is a constant depending only on d . Radii α and β must satisfy formula (2) showed in the proof of Lemma 2.1: $\cos \alpha + \cos \beta = C$, where C is a constant depending only on ρ , $C \in (1, 2)$. We denote $\cos \alpha$ by x , $x \in [C-1, 1]$ so that $x \leq 1$ and $C-x \leq 1$. Then $\cos \beta = C-x$ and the value to be optimized may be rewritten as

$$\begin{aligned} g(x) &:= \frac{1}{K}(a(X, Y) + a(Y, X)) = \int_0^{1-x^2} t^{\frac{d-3}{2}} (1-t)^{-\frac{1}{2}} dt + \int_0^{1-(C-x)^2} t^{\frac{d-3}{2}} (1-t)^{-\frac{1}{2}} dt. \\ g'(x) &= (-2x)(1-x^2)^{\frac{d-3}{2}} x^{-1} + 2(C-x)(1-(C-x)^2)^{\frac{d-3}{2}} (C-x)^{-1} = \\ &= 2(-(1-x^2)^{\frac{d-3}{2}} + (1-(C-x)^2)^{\frac{d-3}{2}}). \end{aligned}$$

Therefore, g is decreasing when $1-x^2 \geq 1-(C-x)^2$, i.e. when $x \in [C-1, C/2]$, and increasing when $x \in [C/2, 1]$. The only minimum is attained at $x = C/2$ or, in other words, when $\alpha = \beta$ and the radii of X and Y are the same.

The case when one of the intersections is empty can be explained using the same argument as in Lemma 2.1. The value of $a(X, Y) + a(Y, X)$ in the case one spherical cap consists of only one point, i.e. $\rho r_1 = r_1 + 2r_2$, is not smaller than the observed minimum. When we increase r_1 one of $a(X, Y)$ increases and the other retains its 0 value. Therefore, the total value is even larger. \square

Remark 2. Note that, for $d = 3$, $g'(x) = 0$ so $g(x)$ is constant and this lemma generalizes Lemmas 2.1 and 2.2

We can find the minimum established by Lemma 3.1 explicitly. By formula (2), $\cos \alpha = \cos \beta = \frac{\rho^2+3}{4\rho}$. The $(d-1)$ -dimensional area of the unit sphere by formula (3) can be found as

$$\frac{2\pi^{d/2}}{\Gamma(d/2)} \int_0^1 t^{\frac{d-3}{2}} (1-t)^{-\frac{1}{2}} dt.$$

Hence

$$a(X, Y) + a(Y, X) \geq \frac{1 - \left(\frac{\rho^2+3}{4\rho}\right)^2 \int_0^1 t^{\frac{d-3}{2}} (1-t)^{-\frac{1}{2}} dt}{\int_0^1 t^{\frac{d-3}{2}} (1-t)^{-\frac{1}{2}} dt}.$$

Denote this minimum by $f_d(\rho)$. Then, similarly to the 3-dimensional case, we get the general bound.

Theorem 5.

$$k_d \leq \inf_{1 < \rho < 3} \left\{ \frac{2}{f_d(\rho)} \text{dens}_d(\rho) \right\},$$

where $\text{dens}_d(\rho)$ denotes the maximum proportion of area of $S_\rho(B)$ covered by non-overlapping balls tangent to B .

Proof. For a contact graph $G = (V, E)$,

$$\begin{aligned} \sum_{\{X,Y\} \in E} (a(X,Y) + a(Y,X)) &\geq f_d(\rho)|E|, \\ \sum_{\{X,Y\} \in E} (a(X,Y) + a(Y,X)) &\leq \text{dens}_d(\rho)|V|. \end{aligned}$$

Therefore,

$$2|E|/|V| \leq \frac{2}{f_d(\rho)} \text{dens}_d(\rho).$$

□

$f_d(\rho)$, as a function of ρ , reaches its maximum when $1 - \left(\frac{\rho^2+3}{4\rho}\right)^2$ is maximal, i.e. $\rho = \sqrt{3}$ and $S_\rho(X) \cap Y$ is a spherical cap with radius $\pi/6$. Using $\text{dens}_d(\sqrt{3}) \leq 1$ and Theorem 5 for $\rho = \sqrt{3}$, we get the bound analogous to the Kuperberg-Schramm bound in higher dimensions.

Theorem 6.

$$k_d \leq a(d) = \frac{2 \int_0^1 t^{\frac{d-3}{2}} (1-t)^{-\frac{1}{2}} dt}{\int_0^{1/4} t^{\frac{d-3}{2}} (1-t)^{-\frac{1}{2}} dt}.$$

Remark 3. Just like the Kuperberg-Schramm upper bound is a generalization of Proposition 1, this theorem is a direct generalization of the upper bound for kissing numbers $\tau_d \leq a(d)$ based on area estimates.

For $d = 4, 5$, this theorem gives the new upper bounds on k_d .

Corollary 1. $k_4 < 34.681$, $k_5 < 77.757$.

Proof. We use MATLAB to calculate numerically $a(4)$ and $a(5)$: $a(4) < 34.681$, $a(5) < 77.757$. □

Starting from 6, upper bounds based on kissing numbers become better:

$$a(6) \approx 170.579; a(7) \approx 368.736; a(8) \approx 788.645.$$

As mentioned in Remark 3, the bound of Theorem 6 coincides with the bound for kissing numbers based on area estimates so it is asymptotically worse than the Kabatyanskii-Levenshtein bound from [19].

4 New bound in dimension 3

The area argument is arguably the easiest way to get upper bounds on kissing numbers. Sections 2 and 3 essentially explain how to extend this argument to the situation of packings with different radii. It is reasonable to try extending more sophisticated methods of analyzing kissing numbers to the more general case of different radii.

One of the fruitful approaches in this direction goes back to Fejes Tóth (see [14]). The idea consists of constructing a certain tiling associated with a packing (typically, a Delaunay-like or Voronoi-like tiling) and bounding the density of the packing in each tile of a tiling. This bound is then used as a general bound on the density.

In his original paper, Fejes Tóth showed that the density of a packing of congruent circles of spherical radius α in the unit sphere is not greater than the density of this packing in the regular spherical triangle of side length 2α with centers of circles at the vertices of this triangle. Coxeter in [10] conjectured that an analogous bound (sometimes also known as the simplex bound) will be true in higher dimensions as well and found an explicit expression for it. Finally, Böröczky in [7] proved this bound for all spaces of constant curvature using subdivisions into quasi-orthoschemes (refinements of Delaunay and Voronoi tilings).

We use the theorem that immediately follows from the results of Florian in [15, 16] generalizing [14] for the case of circular caps of different sizes.

Theorem 7. *Let $K(\alpha)$ be a non-decreasing function defined on $I = [\alpha_{min}, \alpha_{max}]$, $0 < \alpha_{min} \leq \alpha_{max} \leq \frac{\pi}{2}$. For a packing \mathcal{C} of a unit sphere with circles whose radii belong to I , the density is defined as*

$$d(\mathcal{C}) = \frac{1}{4\pi} \sum_{C \in \mathcal{C}} K(\text{radius}(C)).$$

For $x, y, z \in I$, we consider a spherical triangle Δ formed by centers of pairwise tangent circles of radii x, y, z . The density of this triangle is defined by

$$D(x, y, z) = \frac{1}{2\pi \cdot \text{area}(\Delta)} (K(x)\angle x + K(y)\angle y + K(z)\angle z).$$

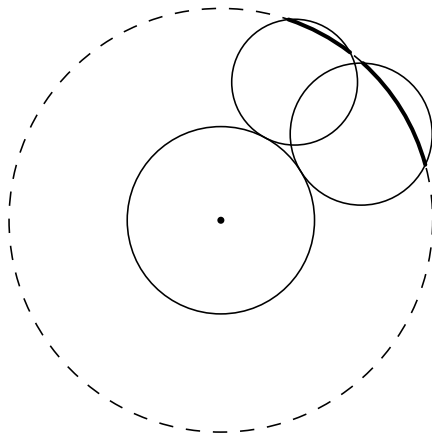
Then $d(\mathcal{C}) \leq \max_{x, y, z \in I} D(x, y, z)$.

The proof of this theorem essentially consists of two parts. First, we can show that for any saturated packing with caps of radii between α_{min} and α_{max} , there exists a Delaunay-like (Molnár) triangulation (see [27]). The second part consists of proving that the maximal density among Delaunay-like triangles is attained on a triangle defined by three pairwise tangent caps.

Remark 4. *Formally, Florian proved the theorem only for the case when I is a finite set of possible radii but Theorem 7 immediately follows from his results.*

We will couple this bound on the density with Theorem 4 to get the new bound in dimension 3. Just to recall the notation used in the previous sections, by $\text{dens}(\rho)$ we mean the maximum proportion of area of $S_\rho(B)$ covered by non-overlapping balls tangent to B .

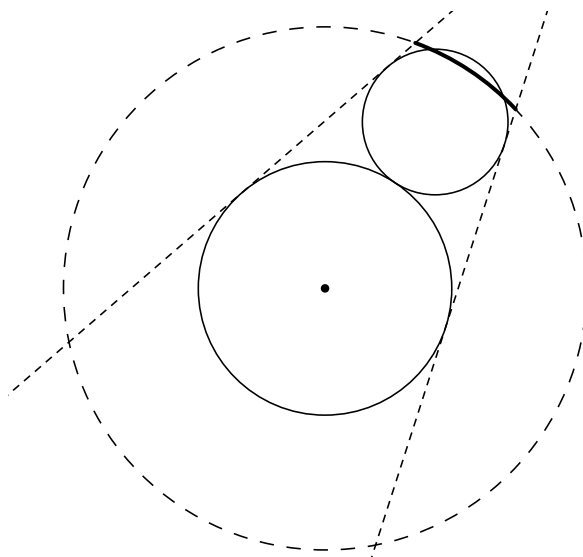
If we forget that circular caps on $S_\rho(B)$ were initially formed by non-overlapping balls and just try to find upper bounds for an arbitrary packing by circular caps, it is impossible to separate $\text{dens}(\rho)$ from 1. A spherical cap may have an arbitrarily small radius and thus the density of a packing may be arbitrarily close to 1.



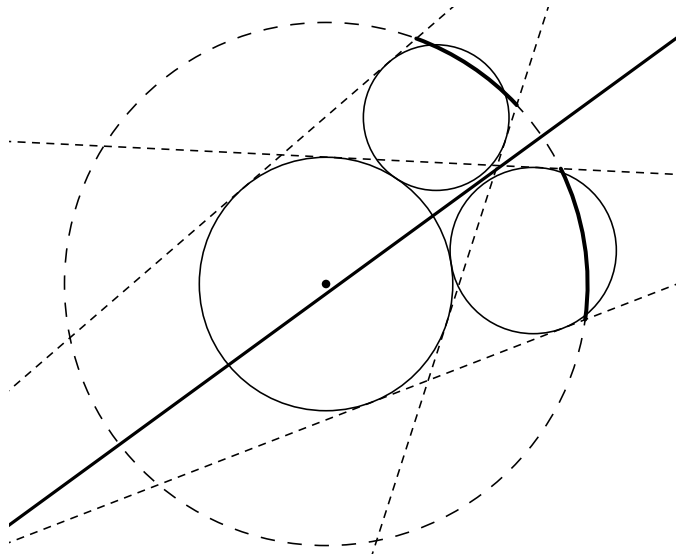
Relatively small caps may not be too close to each other.

The key idea under finding a meaningful upper bound for $dens(\rho)$ is to use an auxiliary circular packing which extends the original one and, most importantly, may not contain circular caps of arbitrarily small size.

For each ball X tangent to a ball B , we define a circular cap $C_\rho(B, X)$ as a cap on $S_\rho(B)$ defined by common tangent planes of B and X if a point of tangency of such common tangent plane with X is inside $S_\rho(B)$. Otherwise, $C_\rho(B, X) = S_\rho(B) \cap X$.



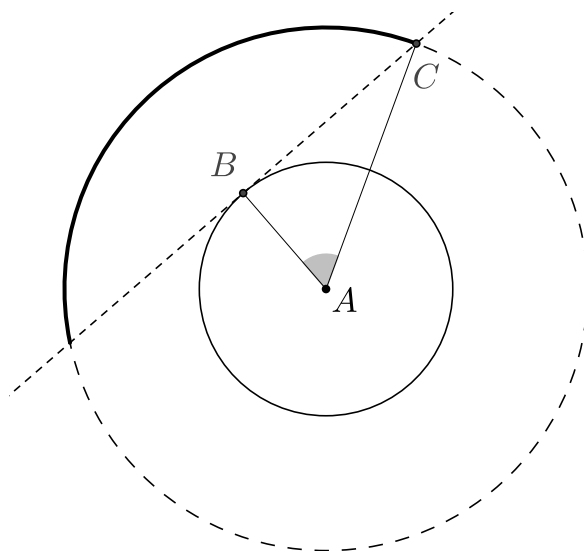
Lemma 4.1. *For any $\rho > 1$ and any non-overlapping balls X and Y tangent to B , spherical caps $C_\rho(B, X)$ and $C_\rho(B, Y)$ do not overlap.*



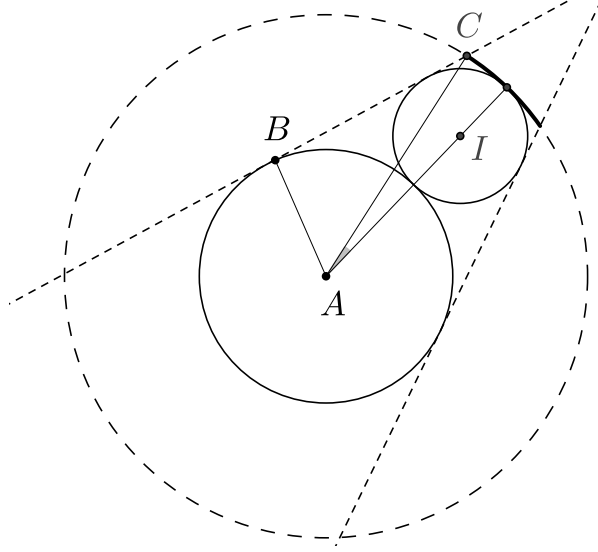
Proof. Consider a radical plane p of the boundaries of X and Y . We want to show that p separates $C_\rho(B, X)$ and $C_\rho(B, Y)$. Firstly, we note that p must intersect B . If this is not the case, one of the two half-spaces formed by p doesn't have a common point with B but it contains either X or Y both of which are tangent to B .

As a radical plane of two non-overlapping spheres, p may not contain interior points of X or Y . Therefore, in order to complete the proof of the lemma, it is sufficient for us to show that p doesn't have any interior points of $C_\rho(B, X)$ or $C_\rho(B, Y)$. We assume that p has an interior point of $C_\rho(B, X)$. We connect this point with an arbitrary point of $p \cap B$ by a line segment. This segment intersects X by an interior point so we get a contradiction to the fact that p contains no interior points of X . \square

Now we find all the functions needed to calculate the upper bound set by Theorem 7

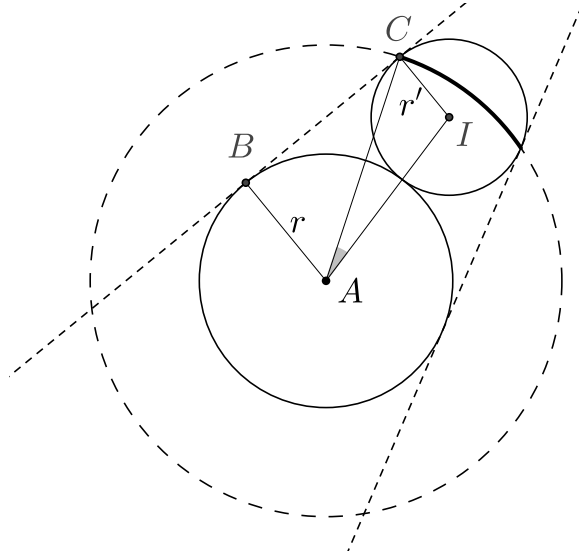


$$\alpha_{max} = \angle BAC = \arccos \frac{1}{\rho}. \quad (4)$$



$$\alpha_{min} = \angle BAI - \angle BAC = \arccos \frac{3-\rho}{1+\rho} - \arccos \frac{1}{\rho}. \quad (5)$$

Since we want to bound the density of the initial circular packing, the function $K(\alpha)$ should be equal to the area of the actual circular cap given the radius α of its auxiliary circular cap. By definition, these two caps coincide if the common tangent plane of a ball B and a ball X tangent to B lies inside $S_\rho(B)$. This will happen if α is greater or equal to a certain threshold α_0 , when the tangent point is exactly on $S_\rho(B)$.

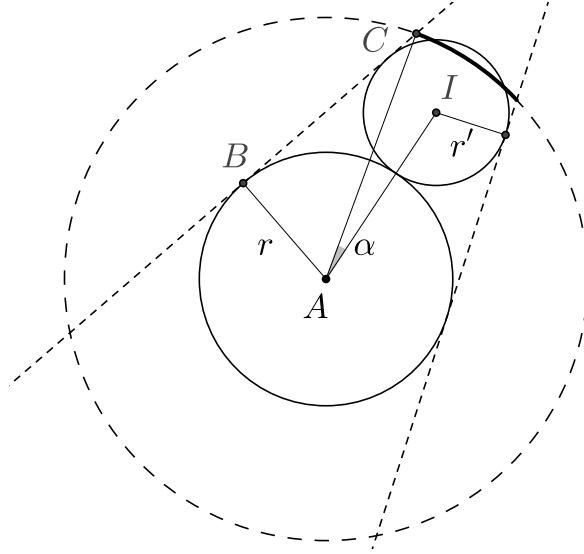


From $\triangle ABC$ we can find that $r' = \frac{\rho^2-1}{4}r$. Then, using formula (1), we get the formula for α_0 :

$$\alpha_0 = \arccos \frac{3\rho^2 + 1}{\rho(\rho^2 + 3)}. \quad (6)$$

Hence we can define $K(\alpha)$ as an area of a circular cap with the spherical radius α for $\alpha \in [\alpha_0, \alpha_{max}]$:

$$K(\alpha) = 2\pi(1 - \cos \alpha) \text{ if } \alpha \in [\alpha_0, \alpha_{max}]. \quad (7)$$



For the case when the initial cap and its auxiliary cap do not coincide, on the one hand, $\cos \angle BAI = \cos(\angle BAC + \alpha) = \frac{1}{\rho} \cos \alpha - \sqrt{1 - \frac{1}{\rho^2}} \sin \alpha$. On the other hand, $\cos \angle BAI = \frac{r-r'}{r+r'}$.

Hence $r' = \left(\frac{2}{\frac{1}{\rho} \cos \alpha - \sqrt{1 - \frac{1}{\rho^2}} \sin \alpha + 1} - 1 \right) r$. Combining this with formula (1), we find $K(\alpha)$ for $\alpha \in [\alpha_{min}, \alpha_0]$;

$$K(\alpha) = 2\pi \left(1 - \frac{(\rho^2 - 1) \left(\frac{1}{\rho} \cos \alpha - \sqrt{1 - \frac{1}{\rho^2}} \sin \alpha + 1 \right) + 4}{4\rho} \right) \text{ if } \alpha \in [\alpha_{min}, \alpha_0]. \quad (8)$$

The angles $\angle x, \angle y, \angle z$ are found by the Spherical Law of Cosines:

$$\angle x = \arccos \frac{\cos(y+z) - \cos(x+z) \cos(x+y)}{\sin(x+z) \sin(x+y)}; \quad (9)$$

$$\angle y = \arccos \frac{\cos(x+z) - \cos(x+y) \cos(y+z)}{\sin(x+y) \sin(y+z)}; \quad (10)$$

$$\angle z = \arccos \frac{\cos(x+y) - \cos(x+z) \cos(y+z)}{\sin(x+z) \sin(y+z)}. \quad (11)$$

Finally, we can formulate the general bound in dimension 3.

Theorem 8. For any $\rho \in (1, 3)$, we define $D_\rho(x, y, z)$ for all triples $x, y, z \in I_\rho = [\alpha_{min}, \alpha_{max}]$,

$$D_\rho(x, y, z) = \frac{1}{2\pi(\angle x + \angle y + \angle z - \pi)} (K(x)\angle x + K(y)\angle y + K(z)\angle z),$$

where $\alpha_{min}, \alpha_{max}, K(\alpha), \angle x, \angle y, \angle z$ are defined by formulas (4-11). Then

$$k_3 \leq \inf_{1 < \rho < 3} \left\{ \max_{x, y, z \in I_\rho} D_\rho(x, y, z) \frac{8\rho}{-\rho^2 + 4\rho - 3} \right\}$$

Proof. Using Theorems 4 and 7 we get

$$\begin{aligned} k_3 &\leq \inf_{1 < \rho < 3} \left\{ dens(\rho) \frac{8\rho}{-\rho^2 + 4\rho - 3} \right\} \leq \\ &\leq \inf_{1 < \rho < 3} \left\{ \max_{x, y, z \in I_\rho} D_\rho(x, y, z) \frac{8\rho}{-\rho^2 + 4\rho - 3} \right\}. \end{aligned}$$

□

We approximate the infimum in Theorem 8 numerically using MATLAB. The value of 13.908778... is attained at $\rho = 1.755$. Here we explain in more detail how this value was calculated.

In order to find the optimal ρ we exclude values where the function $D_\rho(\alpha_0, \alpha_0, \alpha_0) \frac{8\rho}{-\rho^2 + 4\rho - 3}$ is at least 14. These are found numerically using the *fzero* function in MATLAB. The interval for suitable ρ 's is subsequently narrowed down to [1.562, 1.928]. We go over ρ 's from this interval with the step 0.001. For each ρ , we find the maximal density numerically via the *fminsearch* function in MATLAB. The values of starting points of *fminsearch* are taken from the grid with 0.01 step for each coordinate of $(x, y, z) \in [\alpha_{min}, \alpha_{max}]^3$. These calculations show that the minimizing ρ is 1.755 and the minimal value is approximately 13.908778.

Now we can prove the new upper bound for k_3 with computer assistance.

Corollary 2.

$$k_3 < 13.955.$$

Proof. We use $\rho = 1.755$ and estimate $D_\rho(x, y, z)$ from above. Note that, over any compact region in \mathbb{R}^3 ,

$$\max D_\rho(x, y, z) \leq \frac{1}{2\pi \min area(x, y, z)} (\max K(x) \max \angle x + \max K(y) \max \angle y + \max K(z) \max \angle z). \quad (12)$$

We subdivide I_ρ^3 into cubes $[a, a + \delta] \times [b, b + \delta] \times [c, c + \delta]$. Straightforward calculations show that, over such a cube, the minimum area is attained at (a, b, c) , the maximum $K(x)$ is attained at $a + \delta$ (similarly, for the maxima of $K(y)$ and $K(z)$), the maximum $\angle x$ is attained at $(a, b + \delta, c + \delta)$ if $2x + y + z \leq \pi - 4\delta$, at $(a + \delta, b + \delta, c + \delta)$ if $2x + y + z \geq \pi$, and at one of these two points for rare cases when $\pi - 4\delta < 2x + y + z < \pi$ (similarly, for the maxima of $\angle y$ and $\angle z$).

Using $\delta = 0.0005$ and checking values from inequality (12) for all cubes of the subdivision via computer, we get that $D_\rho(x, y, z) \frac{8\rho}{-\rho^2 + 4\rho - 3} < 13.955$. □

Remark 5. Using better estimates than in inequality (12) or smaller values for δ one should get a bound closer to the actual value 13.908778... obtained numerically.

5 Discussion

In this section we would like to list several general observations and directions for research in this area.

1. First of all, we note that the approach utilized in the paper actually solves a more general problem. In a packing, any two elements do not overlap. Instead of this condition we can require a weaker condition: for any ball in a family \mathcal{F} , all balls from \mathcal{F} tangent to it do not overlap. All upper bounds for the average degree of contact graphs will be valid for such families as well. It will be interesting to find an argument taking into account the actual packing condition.
2. As we can see, some methods used for finding upper bounds can be transferred to bound the average degree of packings with different radii. Arguably, the most successful of these methods is based on zonal spherical functions and linear or semidefinite programming (see [19, 28, 4, 26]). It seems feasible to use some sort of averaging argument and extend the bounds obtained by Delsarte's method (see [11, 12]) to the case of different radii.
3. Unfortunately, there are no higher-dimensional analogues of Florian's results. The proof in [7] is quite heavy technically and cannot be directly extended to the case of different radii.
4. Since the kissing case for congruent balls is essentially a particular case of the average kissing number problem, any area-based approach cannot bring an upper bound better than ≈ 13.397 (Fejes Tóth – Coxeter – Böröczky simplex bound).

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