Sphere Packing with Limited Overlap

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Abstract

The classical sphere packing problem asks for the best (infinite) arrangement of non-overlapping unit balls which cover as much space as possible. We define a generalized version of the problem, where we allow each ball a limited amount of overlap with other balls. We study two natural choices of overlap measures and obtain the optimal lattice packings in a parameterized family of lattices which contains the FCC, BCC, and integer lattice.

1 Introduction

Sphere packing and sphere covering problems have been a popular area of study in discrete mathematics over many years. A sphere packing usually refers to the arrangement of non-overlapping n-dimensional spheres. A typical sphere packing problem is to find a maximal density arrangement, i.e., an arrangement in which the spheres fill as much of the space as possible. On the other hand, sphere covering refers to an arrangement of spheres that cover the whole space. Overlap is not only allowed in these arrangements, but inevitable. In this case, the aim is to find an arrangement that minimizes the density (i.e., the total volume of the spheres divided by the volume of the space).

In dimension 2, the densest circle packing and the thinnest circle covering are both attained by the hexagonal lattice [9]. In dimension 3, Hales [7] has recently given a computer-assisted proof showing that the face-centered cubic (FCC) lattice achieves the densest packing even when the sphere centers are not constrained to lie on a lattice. The thinnest covering in dimension 3 is achieved by the body-centered cubic (BCC) lattice [1], but it is not known yet if one can improve the covering by allowing non-lattice arrangements. In dimension 4 and higher, the situation is more complicated and even less is known; see [2] for a comprehensive summary.

Although sphere packing and sphere covering problems have attracted a lot of attention by mathematicians, the arrangements of spheres encountered for example in modeling in the biological sciences usually fall between sphere packing and sphere covering: Models consist of overlapping spheres, which do not fill the whole space, and one is often interested in maximal density configurations of spheres where we allow a certain amount of overlap. Examples are the spatial organization of chromosomes in the cell nucleus [3, 12], the spatial organization of neurons [10, 11], or the arrangement of ganglion cell receptive fields on the retinal surface [4, 8]. The wide applicability is also based on the fact that soft spheres can be modeled as hard spheres with limited overlap. In all these applications one would like to understand the optimal packing configuration of spheres when allowing a certain amount of overlap.

In this paper, we study this problem between sphere packing and sphere covering for the special case when the sphere centers lie on a particular family of lattices obtained by diagonally distorting the integer grid: Let $\delta > 0$ be a distortion parameter. Then the lattice $\mathcal{L}_\delta$ is defined by mapping each unit vector $e_i \in \mathbb{R}^n$, $i = 1, \ldots, n$, to

$$e_i^\delta := e_i + \frac{\delta - 1}{n}\mathbf{1}. \tag{1}$$

This family of lattices has been defined and studied in [6]. It is particularly interesting, since it contains the optimal packing lattices in dimensions 2 and 3 and the optimal covering lattices in dimensions 2–5. At the same time, it is simple enough (defined by one parameter only) allowing us to give a complete analysis of the density of sphere arrangements with limited overlap as a function of δ. In this paper, we prove that for dimension 2 and 3, the optimal packing and covering lattices are robust: even when allowing a certain overlap, either the optimal sphere packing lattice or the optimal sphere covering lattice attain the maximum density, depending on the amount of allowed overlap and how overlap is measured.

Our paper is organized as follows: In Section 2 we discuss two different measures of overlaps in sphere arrangements. The first one, called *distance-based overlap*, is simply a linear function of the distance between two sphere centers and has been used for the analysis in [12]. The second one, called *volume-based overlap* is based on the intersection volume of spheres. In Section 3 we give a complete description of the density of sphere arrangements with limited overlap for the distance-based overlap. In particular, we show that the FCC lattice results in the densest arrangement in the considered family of lattices, regardless of the amount of allowed overlap. In Section 4 we analyze the more complicated volume-based overlap measure: We derive an exact formula for

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the packing density for each lattice in the family and each overlap threshold by analyzing the Voronoi polytope of a lattice point. For planar lattices, we prove that the hexagonal lattice remains optimal for any overlap. In dimension 3, we show that the best choice depends on the allowed overlap and we provide numerical evidence that the optimal lattice is always either the FCC or the BCC lattice. We end with a short discussion in Section 5.

2 Measures of Sphere Arrangements

We let $B_r(p)$ denote the closed ball of radius r and center p. In particular we call the ball centered at the origin $B_r = B_r(0)$. Let $\mathcal{L}$ denote a lattice; w.l.o.g., we assume that the origin is a lattice point. We let $V_{\mathcal{L}}$ denote the Voronoi cell of the origin consisting of all points that are closer to the origin than to any other lattice point. The Voronoi cells of other lattice points are just translations of $V_{\mathcal{L}}$ and they tessellate $\mathbb{R}^n$.

A first measure of a sphere arrangement is the *density*. It is defined as the number of spheres that contain an average point and can be rephrased as

$$\mathcal{D}(\mathcal{L}, r) \;:=\; \frac{\operatorname{vol} B_r}{\operatorname{vol} V_{\mathcal{L}}}. \tag{2}$$

We define the *union* of a sphere arrangement to be

$$\mathcal{U}(\mathcal{L}, r) \;:=\; \frac{\operatorname{vol}\left(B_r \cap V_{\mathcal{L}}\right)}{\operatorname{vol} V_{\mathcal{L}}}. \tag{3}$$

The $\mathcal{U}$ denotes what fraction of the Voronoi cell is covered by the ball of radius r. Looking at the whole space, it also denotes what fraction of $\mathbb{R}^n$ is covered by the union of all balls of radius r. This follows because the Voronoi cells tessellate $\mathbb{R}^n$ and from the following statement:

Proposition 1 *Let p be a point that belongs to the Voronoi cell of c_1. If p is covered by a ball $B_r(c_2)$, then p is also covered by $B_r(c_1)$.*

A third measure of a sphere arrangement is the *overlap*. We define two measures of overlap. The *distance-based overlap* was used to model the spatial organization of chromosomes in [12] and is defined as the diameter of the largest sphere that can be inscribed into the intersection of two spheres, i.e.:

$$\mathcal{O}_{\text{dist}}(\mathcal{L}, r) \;:=\; \max\left(\frac{2r - \min_{\ell \in \mathcal{L}\setminus\{0\}}(\|\ell\|)}{2r}, 0\right). \tag{4}$$

A less simplified measure of overlap is the *volume-based overlap*, which we define as the fraction of a sphere that expands outside its Voronoi cell:

$$\mathcal{O}_{\text{vol}}(\mathcal{L}, r) := \frac{\operatorname{vol} B_r - \operatorname{vol}(B_r \cap \operatorname{vol} V_{\mathcal{L}})}{\operatorname{vol} V_{\mathcal{L}}}. \tag{5}$$

This value is equivalent to the fraction of all other spheres expanding into a Voronoi cell (i.e., the overlap with multiplicity inside a Voronoi cell).

We refer to the unnormalized version of $\mathcal{O}_{\text{vol}}$ as the *excess*:

$$\mathcal{E}(\mathcal{L}, r) := \operatorname{vol} B_r - \operatorname{vol}(B_r \cap \operatorname{vol} V_{\mathcal{L}}). \tag{6}$$

We observe that $\mathcal{D}(\mathcal{L}, \cdot)$, $\mathcal{U}(\mathcal{L}, \cdot)$ and $\mathcal{O}(\mathcal{L}, \cdot)$ (for both overlap measures) are non-negative, monotonously increasing functions with $\mathcal{U}(\mathcal{L}, \cdot)$ upper bounded by 1. The upper bound for $\mathcal{U}$ is reached exactly at the covering radius, the maximal distance of the origin to the boundary of V. The lower bound for $\mathcal{O}$ is reached exactly at the packing radius, the minimal distance of the origin to the boundary of V. Also, it holds that

$$\mathcal{O}_{\text{vol}}(\mathcal{L}, r) \;=\; \mathcal{D}(\mathcal{L}, r) - \mathcal{U}(\mathcal{L}, r). \tag{7}$$

Building upon these measures of sphere arrangements we can now define a relaxed packing and covering quality when allowing overlap and uncovered space, respectively. By fixing a threshold $\omega \in \mathbb{R}_{\geq 0}$, we define the *relaxed packing quality* of a lattice as

$$\mathcal{Q}_{\text{pack}}(\mathcal{L}, \omega) \;:=\; \max_{r \geq 0} \left\{\mathcal{D}(\mathcal{L}, r) \mid \mathcal{O}(\mathcal{L}, r) \leq \omega\right\}.$$

The goal is to find the lattice that maximizes $\mathcal{Q}_{\text{pack}}$. Note that for $\omega = 0$, this is equivalent to the classical sphere packing problem: We want to cover as much space as possible by balls without overlap. It is known that in dimension 3 the FCC lattice is the optimal solution to this problem.

Lemma 2 *The FCC lattice is not optimal w.r.t. $\mathcal{Q}_{\text{pack}}$ for some value of ω when measuring overlap by $\mathcal{O}_{\text{vol}}$.*

Proof. Let ω be the overlap of the BCC lattice when choosing the radius to be its covering radius. Note that the density of this covering is $1+\omega$ by (7). Assume that the FCC lattice attains the same density for ω. Then, again by (7), the union must be 1, so the FCC lattice yields a sphere covering with the same density as the BCC lattice. But this is a contradiction to the well-known fact that the FCC covering density is strictly larger than the BCC covering density. □

Interestingly, we will prove in Section 3 that the FCC lattice is in fact optimal for all values of ω when measuring overlap by $\mathcal{O}_{\text{dist}}$. Similarly, we can define a *relaxed covering quality* as

$$\mathcal{Q}_{\text{cover}}(\mathcal{L}, \omega) \;:=\; \min_{r \geq 0} \left\{\mathcal{D}(\mathcal{L}, r) \mid 1 - \mathcal{U}(\mathcal{L}, r) \leq \omega\right\}.$$

In words, we want as little overlap as possible while allowing only a certain amount of uncovered space. Note that for $\omega = 0$, this is equivalent to the classical covering problem: We want to cover the whole space by balls minimizing the density. Similarly as in Lemma 2 we can prove that the BCC lattice is not optimal w.r.t. $\mathcal{Q}_{\text{cover}}$ for all values of ω when measuring overlap by $\mathcal{O}_{\text{vol}}$. However, the BCC lattice is optimal for all values of ω when measuring overlap by $\mathcal{O}_{\text{dist}}$ as we will see in Section 3. For brevity, we concentrate on $\mathcal{Q}_{\text{pack}}$; our analysis easily extended to $\mathcal{Q}_{\text{cover}}$ with minor changes.

From now on, we focus on lattices $\mathcal{L}_\delta$ given by a diagonal distortion of the integer lattice in $\mathbb{R}^n$ as defined in (1). The parameter $\delta \in (0, \infty)$ defines the amount of distortion, with $\delta = 1$ denoting no distortion. For δ from 1 to 0, every point of the integer lattice undergoes a continuous motion towards its projection onto the plane with normal vector $(1, \ldots, 1)$. For $\delta \geq 1$, each lattice point moves continuously in the opposite direction. For $n = 2$, the hexagonal lattice corresponds to $\delta = 1/\sqrt{3}$ and $\delta = \sqrt{3}$, and for $n = 3$, the FCC lattice corresponds to $\delta = 2$ and the BCC lattice to $\delta = 1/2$; see [6] for more details. We will abuse notation and identify δ and the lattice $\mathcal{L}_\delta$ in the definitions of density, overlap and packing quality: for instance, we write $\mathcal{D}(\delta, r)$ instead of $\mathcal{D}(\mathcal{L}_\delta, r)$.

Fixing a threshold ω for the overlap, we would like to find the best lattice in the family such that $\mathcal{Q}_{\text{pack}}(\delta, \omega)$ is maximized. The approach we take is to compute $\mathcal{Q}_{\text{pack}}$ for a given δ in two steps:

1. Compute the largest ball radius $r(\delta, \omega)$ such that $\mathcal{O}(\delta, r(\delta, \omega)) \leq \omega$.

2. Compute $\mathcal{Q}_{\text{pack}}(\delta, \omega) = \mathcal{D}(\delta, r(\delta, \omega))$.

3 Distance-based overlap

In [12], an algorithm was developed for finding minimum overlap configurations of N spheres (or more generally ellipsoids) packed into an ellipsoidal container. In order to get an efficient algorithm, the simplified distance-based overlap measure was used, which could be computed as a convex optimization problem. One can easily check that the problem of finding minimal overlap configurations of spheres with a certain density is equivalent to finding maximal density configurations of spheres with a certain overlap, the problem we study in this paper. It was observed in a few examples (see Example 3.4 in [12]) that the optimal configuration of the spheres is invariant to scaling of the radii. This is in fact an important property for the application to chromosome packing, since the exact chromatin packing density is not known and one would hope that the positioning is robust to different scalings of the chromosomes. In the following, we prove that this scaling-invariance holds in infinite space when the sphere centers are restricted to lie on the 1-parameter distortion family defined in (1). In this case, the density simplifies to

$$\mathcal{D}(\delta, r) = \frac{V_n r^n}{\delta}, \tag{8}$$

where V_n denotes the (n-dimensional) volume of the n-dimensional unit ball. The packing radius of $\mathcal{L}_\delta$ has been computed in [6] as:

$$\min_{p \in \partial V} \|p\| = \begin{cases} \frac{1}{2}\delta\sqrt{n} & 0 \leq \delta \leq \frac{1}{\sqrt{n+1}}, \\ \frac{1}{2}\sqrt{1 + \frac{\delta^2 - 1}{n}} & \frac{1}{\sqrt{n+1}} \leq \delta \leq \sqrt{n+1}, \\ \frac{1}{2}\sqrt{2}, & \sqrt{n+1} \leq \delta. \end{cases} \tag{9}$$

Using these formulas we prove that the maximum density configuration is always attained by $\delta = \sqrt{n+1}$, regardless of the allowed overlap. This corresponds to the optimal packing lattice in the family for all $n \geq 2$ and over all lattices in dimension 2 and 3. The corresponding statement for the relaxed covering quality can be found in the appendix.

Theorem 3 *The lattice $\mathcal{L}_\delta$ which maximizes the relaxed packing quality w.r.t. $\mathcal{O}_{\text{dist}}$ is attained by $\delta = \sqrt{n+1}$ independent of the value of $\omega \in [0, 1)$.*

Proof. By plugging the packing radius given in (9) into the definition of $\mathcal{O}_{\text{dist}}$ in (4), we can solve for $r(\delta, \omega)$[1]. Then plugging $r(\delta, \omega)$ into the formula for the density given in (2) we get for the δ intervals given in (9):

$$\mathcal{D}(\delta, r(\delta, \omega)) = \begin{cases} \frac{n^{\frac{n}{2}} V_n}{2^n (1-\omega)^n} \, \delta^{n-1} \\ \frac{V_n}{2^n (1-\omega)^n} \, \delta^{-1} \left(1 + \frac{\delta^2 - 1}{n}\right)^{\frac{n}{2}} \\ \frac{V_n}{2^{\frac{n}{2}} (1-\omega)^n} \, \delta^{-1}. \end{cases} \tag{10}$$

The function $\mathcal{D}(\delta, r(\delta, \omega))$ for $n = 3$ and $\omega = 0.5$ is shown in Figure 1 (left). Since $\omega < 1$, the constants in the function $\mathcal{D}(\delta, r(\delta, \omega))$ in (10) are positive. By taking derivatives w.r.t. δ we find that for $0 < \delta \leq 1/\sqrt{n+1}$ the density is strictly increasing for all values of ω. Similarly, for the branch $1/\sqrt{n+1} \leq \delta \leq \sqrt{n+1}$ the density is strictly decreasing for $\delta < 1$, achieves a minimum at $\delta = 1$, and is strictly increasing for $\delta > 1$, independent of the value of ω. Finally, for $\delta \geq \sqrt{n+1}$ the density is strictly decreasing for all values of ω. As a consequence, the $\max_{\delta > 0} \mathcal{D}(\delta, r(\delta, \omega))$ is obtained in one of the interval boundaries $\delta \in \{\frac{1}{\sqrt{n+1}}; \sqrt{n+1}\}$.

Evaluating $\mathcal{D}$ using the first and last expressions from (10), we get $n^{\frac{n}{2}}(n+1)^{-\frac{n-1}{2}} \leq 2^{\frac{n}{2}}(n+1)^{-\frac{1}{2}}$ for all $n \geq 2$ with equality only for $n = 2$ where both lattices equal to the hexagonal lattice. Hence, the maximum is attained by $\delta = \sqrt{n+1}$. $\square$

[1] Note that $\min_{\ell \in \mathcal{L} \setminus \{0\}}(\|\ell\|) = 2 \cdot \min_{p \in \partial V} \|p\|$

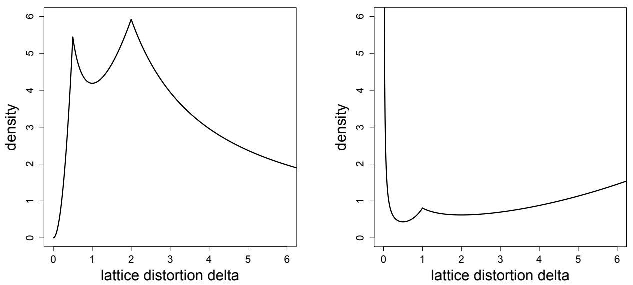

Figure 1: $\mathcal{Q}_{\text{pack}}$ (left) and $\mathcal{Q}_{\text{cover}}$ (right) as a function of the distortion parameter δ for $n = 3$ and $\omega = 0.5$.

4 Volume-based overlap

We next analyze $\mathcal{Q}_{\text{pack}}$ for the volume-based overlap measure in dimension 2 and 3. Because of Lemma 2, we cannot expect the same behavior as for the distance-based overlap measure from the previous section because the FCC lattice becomes worse than the BCC lattice for some value of ω. However, this does not rule out the possibility of other lattices being optimal. We perform a deeper investigation of the optimal lattice configurations, starting with the two-dimensional case.

4.1 Dimension 2

First of all, note that in dimension 2, the lattice for δ is a scaled version of the lattice for $\frac{1}{\delta}$. Because of this symmetry, it suffices to study all lattices with $0 < \delta \leq 1$.

Analyzing the volume-based overlap measure requires the investigation of $V := V_\delta$, the Voronoi cell of the origin in $\mathcal{L}_\delta$, in some detail. V is bounded by six bisectors: four of them with the lattice points $\pm e_1^{(\delta)}, \pm e_2^{(\delta)}$, and two with the lattice points $\pm(e_1^{(\delta)} + e_2^{(\delta)})$. We call the bisectors of type 1 and type 2, respectively. Their distances to the origin are given by r_1 and r_2, respectively, with

$$r_1 := \frac{\sqrt{\delta^2+1}}{2\sqrt{2}}, \qquad r_2 := \frac{\delta}{\sqrt{2}}.$$

We call $r_m = \min\{r_1, r_2\}$, and $r^m = \max\{r_1, r_2\}$. Note that $r_1 > r_2$ if and only if $\delta < \sqrt{\frac{1}{3}}$ (Figure 2).

There are six boundary vertices of V and they all have the same distance to the origin, namely

$$r_3 := \frac{\delta^2+1}{2\sqrt{2}},$$

which agrees with the covering radius computed in [6] (see also (13)). As expected, $r_3 \geq r^m$, with equality if and only if $\delta = 1$.

With this data we can directly derive a formula for the excess $\mathcal{E}$: If $r \leq r_m$, B_r is completely contained in V and the $\mathcal{E}$ equals 0. If $r \geq r_3$, B_r contains all boundary vertices of V and thus all of V (of volume δ), by convexity. In the last case where $r_m < r < r_3$, the part of B_r that is not in V is the union of up to six circular segments. Their area is given by

$$A = \frac{r^2}{2}(\Theta - \sin\Theta),$$

where Θ is the angle at the origin induced by the chord that bounds the circular segment. This angle can be expressed as

$$\Theta = 2\arccos\left(\frac{d}{r}\right),$$

where d is the smallest distance of the chord to the origin. In our case, the chord is given by a bisector. Depending on the type t of the bisector, d is either equal to r_1 or equal to r_2. So we define

$$\Theta_t := \begin{cases} 0 & r < r_t, \\ 2\arccos\left(\frac{r_t}{r}\right) & r \geq r_t, \end{cases}$$

Since the circular segments do not intersect for any $r < r_3$ (because an intersection would imply that a boundary vertex of V is part of B_r) and there are four bisectors of type 1 and two bisectors of type 2, it follows that for $0 \leq \delta \leq 1$:

$$\mathcal{E} = \begin{cases} 0 & 0 \leq r \leq r_m, \\ r^2(2\Theta_1 + \Theta_2 - 2\sin\Theta_1 - \sin\Theta_2) & r_m \leq r \leq r_3, \\ \pi r^2 - \delta & r_3 \leq r\ . \end{cases}$$

Recall that the overlap $\mathcal{O}_{\text{vol}}$ is simply the normalization of the excess; therefore, we obtain its formula after a division by δ. We can now prove:

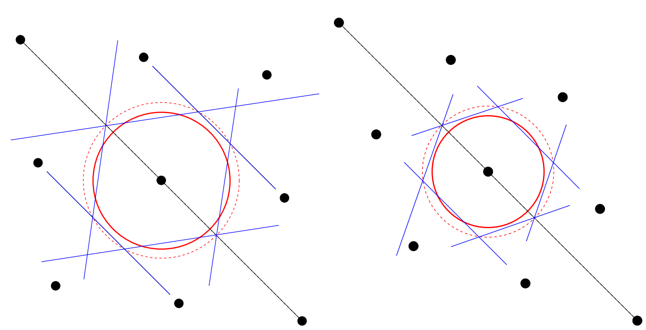

Figure 2: The Voronoi cell V for two different values of $\delta > \sqrt{\frac{1}{3}}$ (left) and $\delta < \sqrt{\frac{1}{3}}$ (right). On the left, the bisectors of type 1 are hit first, whereas in the right bisectors of type 2 are hit first. Note that all lattice points neighboring the origin lie on a common circle around the origin.

Theorem 4 *In dimension 2, the lattice $\mathcal{L}_\delta$ which maximizes the relaxed packing quality w.r.t. $\mathcal{O}_{\text{vol}}$ is attained by the hexagonal lattice (i.e. $\delta \in \{1/\sqrt{3}, \sqrt{3}\}$) independent of the value of $\omega \in \mathbb{R}_{\geq 0}$.*

Proof. Let ω and δ be fixed. Our goal is to compute $\mathcal{D}(\delta, r)$ where $r := r(\delta, \omega)$ is chosen maximally such that $\mathcal{O}_{\text{vol}}(\delta, r) \leq \omega$. Observe that the maximal r is certainly at least the packing radius r_m. This results in the packing density, which is maximized by the hexagonal lattice. Moreover, if ω is sufficiently large to allow a covering, i.e. $\omega \geq \mathcal{O}_{\text{vol}}(\delta, r_3)$, the maximal density is attained at the best covering. This is known to be the hexagonal lattice. So we can concentrate on the case $r_m \leq r \leq r_3$ where

$$0 \leq \mathcal{O}_{\text{vol}}(\delta, r) \leq \mathcal{O}_{\text{vol}}(\delta, r_3) = \frac{\pi(\delta^2+1)^2}{8\delta} - 1, \tag{11}$$

Consider the function $F(\delta, \omega, r) := \omega - \mathcal{O}_{\text{vol}}(\delta, r)$, with $\mathcal{O}_{\text{vol}} = \mathcal{E}/\delta$, which is defined for (ω, δ, r) in the limits of interest given in (11). By definition, $r = r(\delta, \omega)$ satisfies $F(\delta, \omega, r(\delta, \omega)) = 0$. The density is given by

$$\mathcal{D}(\delta, r(\delta, \omega)) = \frac{\pi \cdot r(\delta, \omega)^2}{\delta},$$

which we want to maximize w.r.t. δ. This requires computing the derivative of $r(\delta, \omega)$ w.r.t. δ. We do this by using the implicit function theorem

$$\frac{\partial r}{\partial \delta}(\delta, \omega) = -\frac{\frac{\partial F}{\partial \delta}(\delta, \omega, r)}{\frac{\partial F}{\partial r}(\delta, \omega, r)}.$$

After some calculations we find

$$\frac{\partial\, \mathcal{D}(\delta, r(\delta, \omega))}{\partial \delta} = \begin{cases} \frac{\pi\sqrt{2r^2-\delta^2}}{2\delta \arccos\left(\frac{\delta}{r\sqrt{2}}\right)}; \\[2em] \frac{\pi(\delta^2-1)\sqrt{8r^2-\delta^2-1}}{8\delta^2\sqrt{\delta^2+1}\arccos\left(\frac{\delta^2+1}{8r^2}\right)}; \\[2em] \frac{\sqrt{8r^2-\delta^2-1}(\delta^2-1)+2\delta\sqrt{2r^2-\delta^2}\sqrt{\delta^2+1}}{4r\sqrt{\delta^2+1}\left(2\arccos\sqrt{\frac{\delta^2+1}{8r^2}}+\arccos\left(\frac{\delta}{r\sqrt{2}}\right)\right)}; \end{cases}$$

for $r \leq r_m, 0 < \delta < \frac{1}{\sqrt{3}}$; $r \leq r_m, \frac{1}{\sqrt{3}} < \delta < 1$; and $r^m \leq r \leq r_3$, $0 < \delta < 1$, respectively.

One can easily check that the first derivative is non-negative for any δ, except if r equals the packing radius r_2 corresponding to $\omega = 0$, and we know the optimal packing for this case. Similarly, the second derivative is non-positive except if r equals the packing radius r_1. The third derivative is zero either if $\delta = \frac{1}{\sqrt{3}}$ or if r equals the covering radius r_3 corresponding to $\omega \geq \mathcal{O}_{\text{vol}}(\delta, r_3)$, in which case the hexagonal lattice is optimal as we argued above. Moreover, for $r < r_3$, the derivative is increasing for $\delta < \frac{1}{\sqrt{3}}$ and decreasing for $\delta > \frac{1}{\sqrt{3}}$. This concludes the proof. $\square$

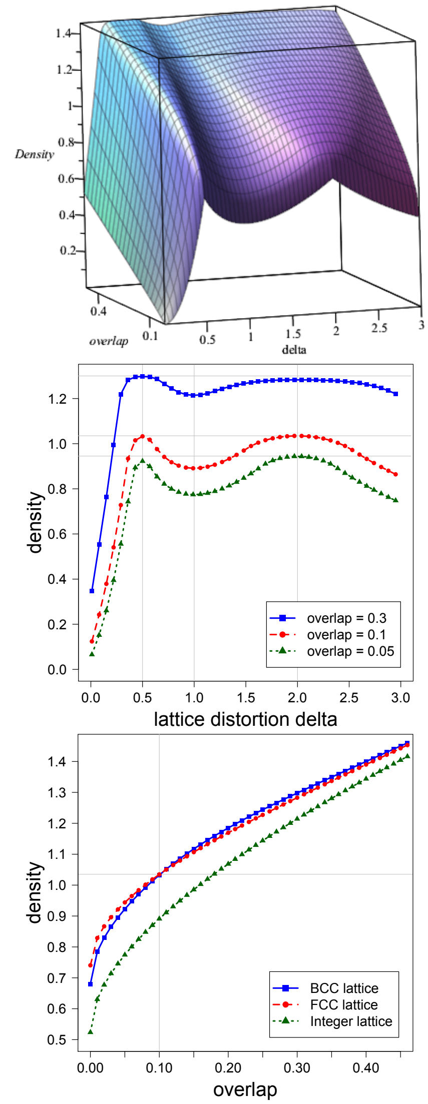

Figure 3: Relaxed packing quality.

4.2 Dimension 3

In three dimensions, we analyze the 3 dimensional Voronoi region V and measure the excess $\mathcal{E}$ by an inclusion-exclusion formula for spherical caps: for small radii, $B_r \subseteq V$ and the excess is zero. For increasing r, B_r starts to intersect facets of V, and the excess is the sum of spherical caps. When r further increases, B_r also intersects edges of V, and the intersection of two spherical caps must be subtracted from $\mathcal{E}$. Finally, when B_r includes vertices of V (but not all of V), the intersection of three spherical caps must be re-added to $\mathcal{E}$; we refer to the appendix for further details.

Formulas for the intersection of one, two and three spherical caps have been described in [5]. In combination with our analysis, they result in a branchwise-defined closed expression for $\mathcal{O}_{\text{vol}}(\delta, r)$. We have computed these expressions using the computer algebra system MAPLE.[2] A 3-dimensional plot of the function $\mathcal{Q}_{\text{pack}}(\delta,\omega)$ is shown in Figure 3 (top). In Figure 3 (middle and bottom) we highlight specific slices through the 3-dimensional plot to better explain the behavior. Figure 3 (middle) shows $\mathcal{Q}_{\text{pack}}(\delta,\omega)$ for three different values of ω. We can observe that the FCC lattice ($\delta = 2$) is indeed optimal for small values of allowed overlap ω. When $\omega = 0.1$, the BCC ($\delta = 0.5$) and the FCC lattice achieve approximately the same density, namely $\mathcal{D} = 1.03$. Interestingly, for larger values of ω the BCC lattice attains the maximal density and surpasses the FCC lattice. Also observe that both lattices always achieve a better relaxed packing quality than the integer lattice ($\delta = 1$). Looking at the density of the FCC and the BCC lattice depending on ω in Figure 3 (bottom), we can note that there is indeed only one switch of optimality (at $\omega \approx 0.1$).

Our analysis indicates that the *FCC* and the *BCC* lattice are always locally optimal configurations, and no other lattice from the family yields a better packing, independent of the allowed overlap. The natural next step would be to prove our observation. This problem can in theory be tackled with the same approach that we used in Section 4.1 in the $2D$ case by relating the derivative of $\mathcal{Q}_{\text{pack}}(\delta,\omega)$ to the partial derivatives of $\mathcal{O}_{\text{vol}}$ using the implicit function theorem. For small values of ω, we were able to verify the claim, that is, prove monotonicity of the function in all branches with a substantial amount of symbolic computations. However, as soon as the expression for $\mathcal{O}_{\text{vol}}$ involves intersections of 2 and 3 spherical caps, the derivatives seem to become too complicated to be handled analytically.

5 Discussion

This work has analyzed the problem of densest sphere packings while allowing some overlap among the spheres. We see our contributions as a first step towards an interesting and important research direction, given the numerous applications of spheres with overlap in the natural sciences. For example, our analysis of the distance-based overlap measure showing that the FCC lattice is optimal independent of the amount of overlap, and hence independent of the scaling of the spheres, lays the theoretical foundations for [12], i.e., for analyzing the spatial organization of chromosomes in the cell nucleus as a sphere arrangement. A major restriction of our approach is our focus on a one-dimensional sub-lattice, the diagonally distorted lattices. Can we hope for an analysis of more general lattice families? This question should probably first be considered in $2D$, given the extremely involved proof of optimality already for the classical packing problem in $3D$.

[2] `http://www.maplesoft.com`

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6 Appendix

6.1 Maximizing the Relaxed Covering Quality

We next briefly analyze the relaxed covering quality and show that in this case the optimum is always attained by the optimal covering configuration. Similarly as for $\mathcal{O}_{\text{dist}}$, we use a linearized measure of the uncovered space $1-\mathcal{U}$. We define it as the largest diameter of a sphere which can be inscribed into the free-space, i.e.:

$$\mathcal{F}(\delta, r) = \max\left(\frac{\max_{p\in\partial V}\|p\| - r}{r}, 0\right) \tag{12}$$

The $\max_{p\in\partial V}\|p\|$ has been computed in [6] for the 1-parameter family of lattices under consideration (it corresponds to the covering radius):

$$\max_{p\in\partial V}\|p\| = \begin{cases} \frac{\sqrt{n^2-1+(n^2+2)\delta^2+(n^2-1)\delta^4}}{\sqrt{12n}} & 0\le\delta\le 1,\\ \frac{\sqrt{n^2-1+\delta^2}}{2\sqrt{n}} & 1\le\delta;\ n \text{ odd},\\ \frac{\sqrt{n^2-2+\delta^2+\frac{1}{\delta^2}}}{2\sqrt{n}} & 1\le\delta;\ n \text{ even}. \end{cases} \tag{13}$$

Using these formulas we can show that the maximum density configuration does not depend on the amount of allowed free-space and is always attained by $\delta = 1/\sqrt{n+1}$, which corresponds to the optimal covering lattice in the family for all $n\ge 2$ and over all lattices in dimension 2-5.

Theorem 5 *The lattice $\mathcal{L}_\delta$ which minimizes the relaxed covering quality w.r.t. $\mathcal{F}$ is attained by $\delta = 1/\sqrt{n+1}$ independent of the value of $\omega\in\mathbb{R}_{\ge 0}$.*

Proof. The proof is analogous to the proof of Theorem 3. The function $\mathcal{D}(\delta, r(\delta,\omega))$ for $n=3$ and $\omega=0.5$ is shown in Figure 1 (right). □

6.2 Analyzing the 3D Voronoi Cell

In three dimensions, the symmetry between δ and $\frac{1}{\delta}$ is lost, and we need to analyze both branches.

We first discuss the case $0<\delta\le 1$: Imagine that r increases from 0 to ∞. Initially, the excess $\mathcal{E}$ is zero. When increasing the ball radius r, there are three possibilities w.r.t. the Voronoi cell $V := V_\delta$:

(i) We hit a bisector plane. From now on we have to add a spherical cap to the volume. There are a total of 14 bisector planes of three different types. Their distance to the origin and number of occurrences are:

$r_1 := \sqrt{\frac{\delta^2+2}{12}}$ (6 planes),
$r_2 := \sqrt{\frac{2\delta^2+1}{6}}$ (6 planes),
$r_3 := \frac{\delta\sqrt{3}}{2}$ (2 planes).

(ii) We hit a boundary edge of V, where two bisector planes are meeting. From now on, we have to subtract the volume of the intersection of the two spherical caps involved (because they are counted twice). There are a total of 36 trisector edges of two different types. Their distance to the origin, number of occurrences, and types of bisector planes between the 3 involved spheres are:

$r_4 := \frac{\delta^2+2}{3\sqrt{2}}$ (18 edges of type 1-1-2),
$r_5 := \frac{\sqrt{(\delta^2+2)(2\delta^2+1)}}{2\sqrt{3}}$ (18 edges of type 1-2-3).

However, note that the volume of the cap intersection depends on the type of the bisector plane between the two spheres that are not centered at the origin. We get 5 different subtypes, four of them appearing 6 times, and one appearing 12 times in the polytope.

(iii) We hit a boundary vertex of V. All 24 boundary vertices have the same distance to the origin, namely the covering radius $r_6 := \frac{1}{6}\sqrt{8\delta^4+11\delta^2+8}$.

When r exceeds r_6 the whole Voronoi cell V is covered, so the excess has volume $\operatorname{vol} B_r - \delta$.

Depending on the value of δ we have the following ordering of the critical radii:

$$\begin{array}{ll} r_3\le r_1\le r_2\le r_5\le r_4\le r_6 & 0\le\delta\le 1/2,\\ r_1\le r_3\le r_2\le r_4\le r_5\le r_6 & 1/2\le\delta\le\sqrt{\frac{2}{5}},\\ r_1\le r_2\le r_3\le r_4\le r_5\le r_6 & \sqrt{\frac{2}{5}}\le\delta\le\sqrt{\frac{19-\sqrt{(297)}}{4}},\\ r_1\le r_2\le r_4\le r_3\le r_5\le r_6 & \sqrt{\frac{19-\sqrt{(297)}}{4}}\le\delta\le 1. \end{array}$$

So $\mathcal{O}_{\text{vol}}(\delta, r)$ seen as a function in δ has 4 branches. In every branch, the interval which r falls into determines how many and which types of cap intersections have to be taken into account to compute the volume-based overlap.

For $\delta>1$, a similar analysis can be performed. However, there is one remarkable difference: The vertices of V are no longer arranged in the same distance around the origin. More precisely, there are 2 vertices at distance s_1 and 6 vertices at distance s_2 with

$$s_1 := \frac{\delta^2+2}{2\sqrt{3}\delta}, \qquad s_2 := \frac{\sqrt{\delta^2+8}}{2\sqrt{3}}.$$

Note that $s_1<s_2$ and s_2 is the covering radius. So for $\delta>1$ and $s_1<r<s_2$ we need to take into account also triple intersections of spherical caps.