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Sphere packings of discs with two radii

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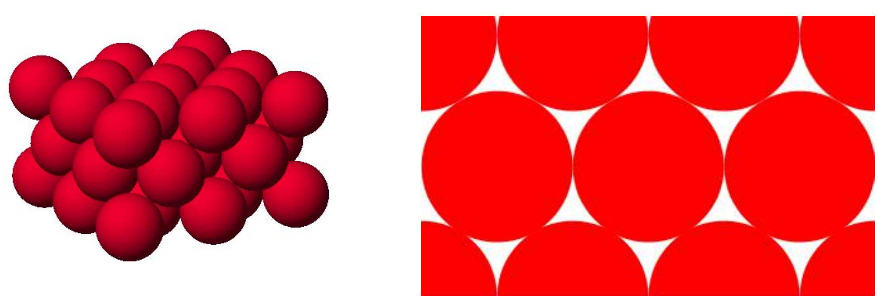
1 Abstract

In this paper we will take a look at sphere packings and we will try to find the highest density binary lattice packings in the 2-dimensional space $\mathbb{R}^2$. First we start with defining the properties of lattice packings of different convex bodies. Then we transform the problem into an optimization problem, which turns out to be a Non-Convex Quadratic Constrained Quadratic Program that can not be solved normally. Therefore a couple of relaxation techniques are used in order to find an upper bound on the highest density. Eventually only the option with two spheres in a unit tile have been examined for which also a lower bound for the highest density is given. Though the upper bounds and the lower bounds are equal, they are still lower bounds for the actual highest density of binary lattice packings.

Contents

2 Introduction

The mathematical view on sphere packings dates from the 16^{th} century when cannonballs took up space in ships. Stacking the cannonballs efficiently would save up space. This problem got the attention of Johannes Keppler to take a look at sphere packings, where one tries to leave the least possible space between the spheres. It was in 1611 that Keppler's stated his hypothesis that the highest density would be achieved by a face-centered cubic lattice packing, the arrangement used by grocers for stacking oranges, see figure 1(a). It was in the 19^{th} century when Carl Friedrich Gauss proved that this was true for all lattice packings. The prove for all packings, so including non-lattice packings, took some more time. Fejes Tóth reduced the problem to a finite number of calculations and finally in 1998 it was Thomas Callister Hales who got the prove with the help of computers. So the face-centered cubic lattice packing is the packing with the highest density, in this case the density is $\frac{\pi}{3\sqrt{2}} \approx 0.74$.
The 2-dimensional analog of the problem, in which case the sphere are discs was first proven by Axel Thue in 1890. He showed that the hexagonal lattice packing, as shown in figure 6(b), is the densest of all possible disc packings. His proof was considered by some to be incomplete. And it was Laśzló Fejes Tóth in 1940 who gave the first rigorous proof. The density achieved with the hexagonal packing is $\frac{\pi}{2\sqrt{3}}$ [1]. So far the packings consisted of spheres of equal size, but there has also been some research in unequal sphere packing, especially binary sphere packings. In the case of binary sphere packings there are only two different radii among the spheres.
In this report we will take a look at binary sphere packings but we reduce the problem to a 2-dimensional case and we only consider lattice packings.



(a) Face-Centered Cubic Packing (b) Hexagonal Packing

Figure 1: Optimal packings in the 3-dimensional and 2-dimensional space

3 What are the highest density binary lattice packings in 2-dimensions or ratio 1:1

Within the subject of sphere packings there are a lot of problems that can be solved. In this paper we take a look at densest sphere packings. We start with packings in general and lattice packings. Then we define define lattice packings of sphere's with different radii. Next we will reduce the problem to a 2-dimensional lattice packing problem of spheres with two different radii, also called a binary lattice packing. To be able to find the highest density packings, the problem will be translated to a Non-Convex Quadratic Constraint Quadratic Program, that can be solved by relaxation of the problem with Relaxation-Linearization Techniques and Semi-Definite Programming into a solvable Linear Program. This will give us upper bounds on the highest density, so to be able to know that it actually is the highest density we need to find packings that have a density equal to the density found.

3.1 Sphere Packings

To eventually give a definition of a binary lattice packing we will start with some basic definitions. Let K denote a *convex body* in n-dimensional Euclidean space E^n. K is a compact subset of E^n such that

$$\lambda \mathbf{x} + (1-\lambda)\mathbf{y} \in K,$$

whenever both $\mathbf{x}$ and $\mathbf{y}$ belong to K and $0 < \lambda < 1$. As usual, the interior, volume and diameter of K are denoted by $\mathrm{int}(K)$, $\mathrm{v}(K)$, $\mathrm{d}(K)$, respectively. An example of a convex body is the n-dimensional unit sphere

$$S^n = \{(x_1, x_2, \ldots, x_n) | \sum_{i=1}^{n} (x_i)^2 \leq 1\}$$

If $\mathbf{a}_i = (a_{i1}, a_{i2}, \ldots, a_{in})$, $i = 1, 2, \ldots, n$, are n linearly independent vectors in E^n, then the set

$$\Lambda = \left\{ \sum_{i=1}^{n} z_i \mathbf{a}_i : z_i \in \mathbb{Z} \right\},$$

is called a *lattice*, and we call $\{\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_n\}$ a basis for Λ. As usual, the absolute value of the determinant $\|a_{ij}\|$ is called the *determinant* of the lattice and is denoted by $\det(\Lambda)$. Let X be a set of discrete points in E^n. We shall call $K + X$ a *translative packing* of K if

$$\mathrm{int}(K + \mathbf{x}_1) \cap \mathrm{int}(K + \mathbf{x}_2) = \emptyset$$

whenever $\mathbf{x}_1$ and $\mathbf{x}_2$ are distinct points of X. In particular, we shall call it a *lattice packing* of K when X is a lattice. Let l be a positive number and let $m(K, l)$ be the maximum number of translates $K + \mathbf{x}$ that can be packed into the cube lI_n. We define

$$\delta(K) = \limsup_{l \to \infty} \frac{m(K, l) v(K)}{v(lI_n)},$$

the *density* of the *densest translative packings* of K in E^n. Similarly, the density $\delta^*(K)$ of the *densest lattice packings* of K is defined by restricting the translative vectors to those in a lattice. In this case, it can be deduced that

$$\delta^*(K) = \sup_{\Lambda} \frac{v(K)}{\det(\Lambda)},$$

where the supremum is over all lattices Λ such that $K + \Lambda$ is a packing. [5]

3.1.1 Multiple Convex Bodies

In order to be able to say something about binary lattice packings, we need to extend these definitions to multiple convex bodies. So in case of m convex bodies $K_i \subset E^n$ and vectors $d_i \in E^n$ and let $K = \bigcup(K_i + d_i)$ we shall call $K + \Lambda$ a lattice packing if

$$K_i + \Lambda \text{ is a lattice packing for all } i \text{ and}$$
$$(K_i + \Lambda + d_i) \cap (K_j + \Lambda + d_j) = \emptyset$$

for all distinct i and j. And we define the density of the lattice packing $K + \Lambda$ by

$$\delta^*(K) = \sup_{\Lambda, d_i} \frac{\sum_{i=1}^m v(K_i)}{\det(\Lambda)} \tag{1}$$

where the supremum is over all is over all lattices Λ and all possible $d_i \in E^n$ such that $K + \Lambda$ is a lattice packing.

3.1.2 Lattice Packings of Spheres in $\mathbb{R}^2$

From now on the Euclidean space will be $\mathbb{R}^2$ with Euclidean norm $||\cdot||$ and innerproduct $(\cdot, \cdot)$ and the convex bodies K_i will be spheres with radius $r_i \in \mathbb{R}$ and centre $\mathbf{c}_i = (c_1, c_2) \in \mathbb{R}^2$

$$S_{\mathbf{c}_i, r_i} = \{(x_1, x_2) | \sum_{k=1}^{2} (x_k - c_i)^2 \leq r_i\} \tag{2}$$

and of course the interior is given by

$$\text{int}(S_{c_i, r_i}) = \{(x_1, x_2) | \sum_{k=1}^{n} (x_k - c_k)^2 < r_i\} \tag{3}$$

the lattice $\Lambda = \langle \mathbf{a}, \mathbf{b} \rangle$ is supposed to be minimal, $||\mathbf{a}|| \leq ||\mathbf{b}||$ and $|(\mathbf{a}, \mathbf{b})| \leq ||\mathbf{a}||^2$ [6] and we will denote the lattice spherepacking by $S^n + \Lambda$.

Lemma 3.1. *Let Λ be a lattice with basis $\{\boldsymbol{a}, \boldsymbol{b}\}$ such that $2|(\boldsymbol{a}, \boldsymbol{b})| \leq ||\boldsymbol{a}|| \leq ||\boldsymbol{b}||$ and $\boldsymbol{x} \in \{\lambda\boldsymbol{a} + \mu\boldsymbol{b} | 0 \leq \lambda, \mu \leq 1\}$. Then one of $\boldsymbol{0}, \boldsymbol{a}, \boldsymbol{b}, \boldsymbol{a} + \boldsymbol{b}$ is the lattice point closest to $\boldsymbol{x}$, in other words* $\min_{l \in \{0, \boldsymbol{a}, \boldsymbol{b}, \boldsymbol{a}+\boldsymbol{b}\}} ||\boldsymbol{x} - \boldsymbol{l}|| = \min_{l \in \Lambda}(||\boldsymbol{x} - \boldsymbol{l}||)$

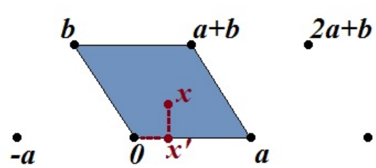


Figure 2: Maximum distance to lattice point is $\frac{\sqrt{2}}{2}||\mathbf{b}||$

Proof. First we determine an upper bound on the distance of $\mathbf{x}$ to the lattice point closest to $\mathbf{x}$. The minimal distance to at least one of the lines $n\mathbf{b} + \langle \mathbf{a} \rangle$, is the vector orthogonal to this line, and is at most $\frac{1}{2}||\mathbf{b}||$. And for any point $x' \in \{n\mathbf{b} + \langle \mathbf{a} \rangle\}$ to a lattice point is at most $\frac{1}{2}||\mathbf{a}||$, which can clearly be seen in figure 2. By the Pythagorian theorem we get

$$\min_{\mathbf{l}\in\Lambda} ||\mathbf{x}-\mathbf{l}|| \leq \sqrt{\frac{1}{4}\,||\mathbf{b}||^2 + \frac{1}{4}\,||\mathbf{a}||^2} \leq \sqrt{\frac{1}{4}\,||\mathbf{b}||^2 + \frac{1}{4}\,||\mathbf{b}||^2} \leq \frac{\sqrt{2}}{2}\,||\mathbf{b}|| \tag{4}$$

To eliminate some lattice points that are too far away to be the lattice point closest to $\mathbf{x}$ we take a look at the parallel lines $n\mathbf{b} + \langle \mathbf{a} \rangle$. The minimum distance between two parallel lines is the length of the vector between these parallel lines, orthogonal to these lines. This vector is $\mathbf{b} - \frac{(\mathbf{a},\mathbf{b})}{||\mathbf{b}||^2}\mathbf{a}$. We calculate the minimum length of this vector

$$\begin{aligned}
(\mathbf{b} - \frac{(\mathbf{a},\mathbf{b})}{||\mathbf{b}||^2}\mathbf{a}, \mathbf{b} - \frac{(\mathbf{a},\mathbf{b})}{||\mathbf{b}||^2}\mathbf{a}) &= (\mathbf{b},\mathbf{b}) - 2\frac{(\mathbf{a},\mathbf{b})^2}{||\mathbf{a}||^2} + \frac{(\mathbf{a},\mathbf{b})^2}{||\mathbf{a}||^2} \\
&= ||\mathbf{b}||^2 - \frac{(\mathbf{a},\mathbf{b})^2}{||\mathbf{a}||^2} \\
&= ||\mathbf{b}||^2 - \frac{(2\,|(\mathbf{a},\mathbf{b})|)^2}{4\,||\mathbf{a}||^2} \\
&\geq ||\mathbf{b}||^2 - \frac{||\mathbf{a}||^2\,||\mathbf{b}||^2}{4\,||\mathbf{a}||^2} \\
&= \frac{3}{4}\,||\mathbf{b}||^2
\end{aligned}$$

So we have that

$$||\mathbf{x} - m\mathbf{a} - n\mathbf{b}|| \geq \frac{\sqrt{3}}{2}\,||\mathbf{b}|| \text{ for } n \notin \{0,1\}$$

If we combine this result with the results from (4) we have reduced the problem to showing that

$$\min_{l\in\{0,\mathbf{a},\mathbf{b},\mathbf{a}+\mathbf{b}\}} ||\mathbf{x}-\mathbf{l}|| = \min\{||vectx - vectl||\,\|l = m\mathbf{a} + n\mathbf{b}, m \in \mathbb{Z}, n \in \{0,1\}\}$$

To show this last step we take a look at the case $n = 0$ and $m < 0$, and we will show that

$$||\mathbf{x} - m\mathbf{a}|| \geq ||\mathbf{x} - \mathbf{0}|| = ||\mathbf{x}||$$

We start with the orthogonal projection $\gamma\mathbf{a}$ of $\mathbf{x}$ on $\langle \mathbf{a} \rangle$,

$$\begin{aligned}
\gamma = \frac{(\mathbf{x},\mathbf{a})}{||\mathbf{a}||^2} &= \frac{(\mathbf{x},\mathbf{a})}{||\mathbf{a}||^2} \\
&= \frac{(\lambda\mathbf{a} + \mu\mathbf{b},\mathbf{a})}{||\mathbf{a}||^2} \\
&= \lambda + \frac{\mu(\mathbf{b},\mathbf{a})}{||\mathbf{a}||^2} \\
&\geq \lambda - \mu\frac{2\,|(\mathbf{b},\mathbf{a})|}{2\,||\mathbf{a}||^2} \\
&\geq \lambda - \frac{1}{2}\mu \geq -\frac{1}{2}
\end{aligned}$$

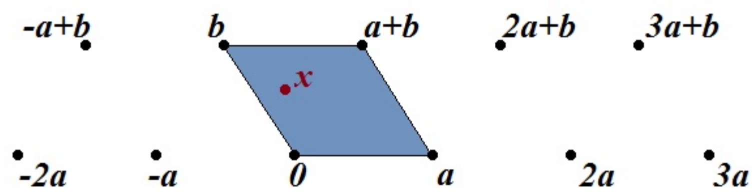


Figure 3: Either $\mathbf{0}$,$\mathbf{a}$,$\mathbf{b}$,$\mathbf{a}+\mathbf{b}$ is closest to $\mathbf{x}$

So we get

$$\begin{aligned}
||\mathbf{x}-m\mathbf{a}||^2 &= ||\mathbf{x}-\gamma\mathbf{a}+\gamma\mathbf{a}-m\mathbf{a}||^2 \\
&= ||\mathbf{x}-\gamma\mathbf{a}||^2 + ||\gamma\mathbf{a}-m\mathbf{a}||^2 \\
&= ||\mathbf{x}-\gamma\mathbf{a}||^2 + (\gamma-m)^2\,||\mathbf{a}||^2 \\
&\geq ||\mathbf{x}-\gamma\mathbf{a}||^2 + \gamma^2\,||\mathbf{a}||^2 \\
&= ||\mathbf{x}-\gamma\mathbf{a}||^2 + ||\gamma\mathbf{a}||^2 \\
&= ||\mathbf{x}-\gamma\mathbf{a}+\gamma\mathbf{a}||^2 \\
&= ||\mathbf{x}||^2
\end{aligned}$$

which implies that $||\mathbf{x}-m\mathbf{a}-n\mathbf{b}|| \geq ||\mathbf{x}-\mathbf{0}||$ for $n=0$ all $m<0$. Because of the symmetry of the problem, see figure 3, a reflection can map $\mathbf{a}$ on $\mathbf{0}$ and $(m+1)\mathbf{a}$ on $-m\mathbf{a}$, without changing the problem

$$||\mathbf{x}-m\mathbf{a}|| \geq ||\mathbf{x}-\mathbf{a}|| = ||\mathbf{x}||$$

holds for $m>1$. The case for $n=1$ can be shown by a rotation which maps $m\mathbf{a}$ on $(1-m)\mathbf{a}+\mathbf{b}$, which concludes our proof. □

Remark It is easy to generalize this result for $\mathbf{x} \in \{\lambda\mathbf{a}+\mu\mathbf{b} | l_\lambda \leq \lambda \leq u_\lambda, l_\mu \leq \mu \leq u_\mu\}$ with $l_\lambda, u_\lambda, l_\mu, u_\mu \in \mathbb{N}$. Then the closest vector is in the set $\{n\mathbf{a}+m\mathbf{b} | n,m \in \mathbb{N}, l_\lambda \leq n \leq u_\lambda, 1_\mu \leq m \leq u_\mu\}$

Theorem 3.2. *Let Λ be a lattice with basis $\{\boldsymbol{a},\boldsymbol{b}\}$ such that $2\,|(\boldsymbol{a},\boldsymbol{b})| \leq ||\boldsymbol{a}|| \leq ||\boldsymbol{b}||$, $S=\bigcup S_i = \bigcup S_{r_i,c_i}$ with $r_i \in \mathbb{R}$ and $\boldsymbol{c}_i \in \{\lambda\boldsymbol{a}+\mu\boldsymbol{b} | 0 \leq \lambda,\mu \leq 1\}$ for $i=1,\ldots,n$ and $Z=\{\boldsymbol{0},\boldsymbol{a},\boldsymbol{b},\boldsymbol{a}+\boldsymbol{b},\boldsymbol{a}-\boldsymbol{b}\}$. The following statements are equivalent.*

1. *$S+\Lambda$ is a lattice packing*
2. *(a) $||\boldsymbol{c}_i-\boldsymbol{c}_j-\boldsymbol{z}|| \geq r_i+r_j$ for $i \neq j$ and all $\boldsymbol{z} \in Z$*

   (b) $||\boldsymbol{a}|| \geq 2r_i$ for all i

note: the set Z is reduced from $Z=\{\boldsymbol{0},\boldsymbol{a},-\boldsymbol{a},\boldsymbol{b},-\boldsymbol{b},\boldsymbol{a}+\boldsymbol{b},-\boldsymbol{a}-\boldsymbol{b},\boldsymbol{a}-\boldsymbol{b},-\boldsymbol{a}+\boldsymbol{b}\}$ to $Z=\{\boldsymbol{0},\boldsymbol{a},\boldsymbol{b},\boldsymbol{a}+\boldsymbol{b},\boldsymbol{a}-\boldsymbol{b}\}$ because $||\boldsymbol{c}_i-\boldsymbol{c}_j-\boldsymbol{z}||$ for $i \neq j$ also contains $||\boldsymbol{c}_j-\boldsymbol{c}_i-\boldsymbol{z}|| = ||\boldsymbol{c}_i-\boldsymbol{c}_j+\boldsymbol{z}||$.

Proof. $1 \Rightarrow 2$ $\quad S+\Lambda$ is a lattice packing so for $i=1,\ldots,n$, $S_i+\Lambda$ is a lattice packing,so

$$\operatorname{int}(S_i+\mathbf{x}_1) \cap \operatorname{int}(S_i+\mathbf{x}_2) = \emptyset$$

for all distinct $\mathbf{x}_1$ and $\mathbf{x}_2$ in Λ. Suppose there is an i such that $||\mathbf{a}|| < 2r_i$ then also $||\mathbf{x}_1-\mathbf{x}_2|| < 2r_i$ for some $\mathbf{x}_1$ and $\mathbf{x}_2$. $\left|\left|\frac{1}{2}(\mathbf{x}_1-\mathbf{x}_2)\right|\right| < r_i$ then $\left|\left|\mathbf{x}_1-\frac{1}{2}(\mathbf{x}_1+\mathbf{x}_2)\right|\right| < r_i$ but also $\left|\left|\mathbf{x}_2-\frac{1}{2}(\mathbf{x}_1+\mathbf{x}_2)\right|\right| <$

r_i so $\frac{1}{2}(\mathbf{x}_1+\mathbf{x}_2) \in \text{int}(S_i+x_1)$ and $\frac{1}{2}(\mathbf{x}_1+\mathbf{x}_2) \in \text{int}(S_i+x_2)$ hence $\frac{1}{2}(\mathbf{x}_1+\mathbf{x}_2) \in (\text{int}(S_i+\mathbf{x}_1) \cap (\text{int}(S_i+\mathbf{x}_2))$, a contradiction, so $||\mathbf{x}_1-\mathbf{x}_2|| \geq ||\mathbf{a}|| \geq 2r_i$. Furthermore the following holds

$$\text{int}(S_i+\mathbf{y}_1) \cap \text{int}(S_j+\mathbf{y}_2) = \emptyset$$

for all $i \neq j$ and $\mathbf{y}_1$ and $\mathbf{y}_2$ in Λ. Suppose that there are i, j with $i \neq j$ and a $\mathbf{z} \in \mathbb{Z}$ such that $||\mathbf{c}_i - \mathbf{c}_j - \mathbf{z}|| < r_i + r_j$ but then

$$\left|\left|\mathbf{c}_i - \left(\frac{r_j}{r_i+r_j}\mathbf{c}_i - \frac{r_i}{r_i+r_j}(\mathbf{c}_j+\mathbf{z})\right)\right|\right| = \left|\left|\frac{r_i}{r_i+r_j}(\mathbf{c}_i-\mathbf{c}_j-\mathbf{z})\right|\right| < r_i,$$
$$\left|\left|\mathbf{c}_j - \left(\frac{r_j}{r_i+r_j}\mathbf{c}_i - \frac{r_i}{r_i+r_j}(\mathbf{c}_j+\mathbf{z})\right)\right|\right| = \left|\left|\frac{r_j}{r_i+r_j}(\mathbf{c}_i-\mathbf{c}_j-\mathbf{z})\right|\right| < r_j,$$

hence $\frac{r_j}{r_i+r_j}\mathbf{c}_i - \frac{r_i}{r_i+r_j}(\mathbf{c}_j+\mathbf{z}) \in \text{int}(S_i+\mathbf{y}_1) \cap \text{int}(S_j+\mathbf{y}_2)$ gives a contradiction, so for all i, j with $i \neq j$ and all $z \in \mathbb{Z}$ holds $||\mathbf{c}_i - \mathbf{c}_j - \mathbf{z}|| \geq r_i + r_j$.

$2 \Rightarrow 1$ We have $||\mathbf{a}|| \geq 2r_i$ and let S_i be a sphere in $\mathbb{R}^2$, $\mathbf{x}_1, \mathbf{x}_2 \in \Lambda$ with $\mathbf{x}_1 \neq \mathbf{x}_2$ and let $x \in \text{int}(S_i+\mathbf{x}_1)$ so $||\mathbf{c}_i+\mathbf{x}_2-\mathbf{x}|| < r_i$ then we need to proof that $x \notin \text{int}(S_i+\mathbf{x}_2)$

$$\begin{aligned}
||\mathbf{c}_i+\mathbf{x}_2-\mathbf{x}|| &= ||\mathbf{c}_i+\mathbf{x}_2-\mathbf{c}_i-\mathbf{x}_1+\mathbf{c}_i+\mathbf{x}_1-\mathbf{x}|| \\
&= ||(\mathbf{x}_2-\mathbf{x}_1)-(\mathbf{x}-\mathbf{c}_i-\mathbf{x}_1)|| \\
&\geq \big|||(\mathbf{x}_2-\mathbf{x}_1)||-||\mathbf{x}-\mathbf{c}_i-\mathbf{x}_1||\big| \\
&\geq ||\mathbf{a}||-||\mathbf{x}-\mathbf{c}_i-\mathbf{x}_1|| \\
&\geq 2r_i - r_i = r_i
\end{aligned}$$

so for all i, $S_i + \Lambda$ is a lattice packing.
The last thing left to prove is that $S+\Lambda$ is a lattice packing. We have that $||\mathbf{c}_i-\mathbf{c}_j-\mathbf{z}|| \geq r_i+r_j$ for $i \neq j$ and all $\mathbf{z} \in Z$ now let S_i and S_j be two spheres in $\mathbb{R}^2$ and $\mathbf{x}_1, \mathbf{x}_2 \in \Lambda$ then we need to show that if $x \in \text{int}(S_i+\mathbf{x}_1)$ implies that $x \notin \text{int}(S_j+\mathbf{x}_2)$. Or in other words $||\mathbf{c}_i+\mathbf{x}_1-\mathbf{x}|| < r_i$ implies $||\mathbf{c}_j+\mathbf{x}_2-\mathbf{x}|| \geq r_i$,

$$\begin{aligned}
||\mathbf{c}_j+\mathbf{x}_2-\mathbf{x}|| &= ||\mathbf{c}_j+\mathbf{x}_2-\mathbf{c}_i-\mathbf{x}_1+\mathbf{c}_i+\mathbf{x}_1-\mathbf{x}|| \\
&= ||(\mathbf{c}_i-\mathbf{c}_j-\mathbf{x}_2-\mathbf{x}_1)-(\mathbf{x}-\mathbf{c}_i-\mathbf{x}_1)|| \\
&\geq \big|||(\mathbf{c}_i-\mathbf{c}_j-\mathbf{x}_2-\mathbf{x}_1)||-||\mathbf{x}-\mathbf{c}_i-\mathbf{x}_1||\big|
\end{aligned}$$

Now we have to consider two cases, $\pm(\mathbf{x}_1+\mathbf{x}_2) \in Z$ and $\pm(\mathbf{x}_1+\mathbf{x}_2) \notin Z$. If $\pm(\mathbf{x}_1+\mathbf{x}_2) \in Z$ then

$$\big|||(\mathbf{c}_i-\mathbf{c}_j-\mathbf{x}_2-\mathbf{x}_1)||-||\mathbf{x}-\mathbf{c}_i-\mathbf{x}_1||\big| \geq r_j+r_i-r_i = r_j$$

If $\mathbf{x}_1+\mathbf{x}_2 \notin Z$ then we can use lemma 3.1 and its remark. Because $\mathbf{c}_i, \mathbf{c}_j \in \{\lambda\mathbf{a}+\mu\mathbf{b} \mid 0 \leq \lambda, \mu \leq 1\}$ then $\pm\mathbf{c}_i \mp \mathbf{c}_j \in \{\lambda\mathbf{a}+\mu\mathbf{b} \mid -1 \leq \lambda, \mu \leq 1\}$. So there is a $\mathbf{z}_0 \in Z$ such that $||\mathbf{c}_i-\mathbf{c}_j-\mathbf{z}_0|| \leq ||\mathbf{c}_i-\mathbf{c}_j-\mathbf{x}_1-\mathbf{x}_2||$ or $||\mathbf{c}_j-\mathbf{c}_i-\mathbf{z}_0|| \leq ||\mathbf{c}_i-\mathbf{c}_j-\mathbf{x}_1-\mathbf{x}_2||$ so we get

$$\begin{aligned}
\big|||(\mathbf{c}_i-\mathbf{c}_j-\mathbf{x}_2-\mathbf{x}_1)||-||\mathbf{x}-\mathbf{c}_i-\mathbf{x}_1||\big| &\geq ||(\mathbf{c}_i-\mathbf{c}_j-\mathbf{z}_0)||-||\mathbf{x}-\mathbf{c}_i-\mathbf{x}_1|| \\
&\geq r_j+r_i-r_i = r_j
\end{aligned}$$

□

3.2 Optimization Problem

Now we can look back at our problem, we want to optimize the density of a binary sphere packing. So we have the following problem

$$\begin{array}{ll} \text{minimize} & \det(\Lambda) \\ \text{subject to} & (S_{r_1,c_1} \cup S_{r_2,c_2}) + \Lambda \text{ is a lattice packing} \end{array}$$

More concretely say Λ has minimal basis $\{\mathbf{a}, \mathbf{b}\} = \{(a_1, a_2), (b_1, b_2)\}$, and $S_i = S_{\mathbf{c}_i, r_i} = \{\mathbf{x} \in \mathbb{R}^2 | \, ||\mathbf{c}_i - \mathbf{x}|| \leq r_i\}$ and $Z = \{\mathbf{0}, \mathbf{a}, \mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{a}-\mathbf{b}\}$

$$\begin{array}{ll} \text{minimize} & |a_1 b_2 - b_1 a_2| \\ \text{subject to} & (c_{i1} - c_{j1} - z_1)^2 + (c_{i2} - c_{j2} - z_2)^2 \geq (r_i + r_j)^2 \text{ for } i \neq j \text{ and all } (z_1, z_2) \in Z \\ & a_1^2 + a_2^2 \geq 4r_i^2 \text{ for } i = 1, \ldots, n \end{array}$$

3.2.1 Non-Convex QCQP's

Both the objective function and the constraint functions can be written as $\frac{1}{2}x^T P_i x + q_i^T x + s_i$ so

$$\begin{array}{ll} \text{minimize} & \frac{1}{2}x^T P_0 x + q_0^T x + s_0 \\ \text{subject to} & \frac{1}{2}x^T P_i x + q_i^T x + s_i \leq 0, i = 1, \ldots, m \end{array}$$

So we are dealing with a Quadratically Constrained Quadratic Programming problem [3]. If all the matrices P_i are positive semidefinite, the problem would be convex and can be solved efficiently. But in this case not all P_i are positive semidefinite, so the problem is a Non-Convex QCQP problem, which is at least as hard as a large number of other problems that also seem to be NP-hard. But this problem can be relaxed into a convex problem to find a lower bound on the optimal value of the objective function [4]. There are two well known relaxation methods, one is the Semidefinite Programming (SDP) and the other is the Reformulation-Linearization Technique [7]. The SDP relaxation is realized by using $x^T P x = \mathbf{Tr}(P(xx^T))$. The optimization problem can be rewritten as

$$\begin{array}{ll} \text{minimize} & \mathbf{Tr}(XP_0) + q_0^T x + s_0 \\ \text{subject to} & \mathbf{Tr}(XP_i) + q_i^T x + s_i \leq 0, i = 1, \ldots, m, \\ & X = xx^T. \end{array}$$

Now by replacing the equality constraint $X = xx^T$ with a positive semidefinite constraint $X - xx^T \succeq 0$ we relax this problem into a convex problem. This constraint can be formulated as a Schur complement, which gives us

$$\begin{array}{ll} \text{minimize} & \frac{1}{2}\mathbf{Tr}(XP_0) + q_0^T + r_0 \\ \text{subject to} & \frac{1}{2}\mathbf{Tr}(XP_i) + q_i^T + r_i \leq 0, i = 1, ..., m, \\ & \begin{bmatrix} X & x \\ x^T & 1 \end{bmatrix} \succeq 0 \end{array}$$

The RLT relaxation of QCQP is based on using all possible products of pairs of linear inequality constraints, including the bound constraints. Combining these two relaxation techniques in general gives a better result.

In order to say something about the best density we shall retrieve an upper bound and try to get it as low as possible. We shall show this on the problem with spheres of radius r_1 and r_2 with ratio 1 : 1.

3.3 Two Spheres with Ratio $1:1$ in a unit tile

We reduced the problem to an optimization problem with spheres in a parallelogram. This parallelogram, that we will call the unit tile, builds up the complete space. Let Λ be a lattice in $\mathbb{R}^2$ with minimal basis $\{(a_1, a_2), (b_1, b_2)\}$. Without loss of generality, because of the Euclidean plane isometries, we may assume that $a_2 = 0$, $a_1 > 0$, $b_2 > 0$. This gives us the following constraints

$$\begin{aligned} -b_2 &\leq 0 \\ a_1^2 - b_1^2 - b_2^2 &\leq 0 \\ 2a_1b_1 - a_1^2 &\leq 0 \\ -a_1^2 - 2a_1b_1 &\leq 0 \end{aligned}$$

Furthermore we have two spheres $S_1 = S_{(c_{11},c_{12}),r_1}$ en $S_2 = S_{(c_{21},c_{22}),r_2}$ with r_1 and r_2 given. So we can assume that $r_1 < r_2$ and also $(c_{11}, c_{12}) = (0, 0)$. We will call the set $\{\lambda(a_1, a_2) + \mu(b_1, b_2)|0 \leq \mu, \lambda \leq 1\}$ the unit tile. We want the centers of spheres to be in the unit tile, so we also use that $(c_{21}, c_{22}) \in \{\lambda(0, a_2) + \mu(b_1, b_2)|0 \leq \mu, \lambda \leq 1\}$. Then the following constraints arise

$$\begin{aligned} -c_{22} &\leq 0 \\ c_{22} - b_2 &\leq 0 \\ b_1c_{22} - b_2c_{21} &\leq 0 \\ b_2c_{21} - b_1c_{22} - a_1b_2 &\leq 0 \end{aligned}$$

Finally we need the constraints that make $S + \Lambda$ a lattice packing. Because $(c_{11}, c_{12}) = (0, 0)$ we only need the following constraints

$$\begin{aligned} (r_1 + r_2)^2 - c_{21}^2 - c_{22}^2 &\leq 0 \\ (r_1 + r_2)^2 - (c_{21} - a_1)^2 - c_{22}^2 &\leq 0 \\ (r_1 + r_2)^2 - (c_{21} - b_1)^2 - (c_{22} - b_2)^2 &\leq 0 \\ (r_1 + r_2)^2 - (c_{21} - a_1 - b_1)^2 - (c_{22} - b_2)^2 &\leq 0 \\ 2r_2 - a_1 &\leq 0 \end{aligned}$$

After using RLT and SDP to solve the problem and expanding the constraints by multiplying the constraints of degree one with each other, the result of the lower bound of the problem was 0. In 5 the results are given for $r_1 = r_2 = 1$ which should give us the hexagonal packing with $a_1 = 2, b_1 = 0, b_2 = 2\sqrt{3}, c_{21} = 1, c_{22} = \sqrt{3}$. The main cause for this result is the relaxation. For example, $a_1 = 2.14$, $b_2 = 0.88$ but $a_1b_2 = 0$. Also because of this relaxation, only a few constraints influence the variable a_1b_2. But there are several ways to improve this result.

$$\begin{pmatrix} 1 & a_1 & b_1 & b_2 & c_{21} & c_{22} \\ a_1 & a_1^2 & a_1b_1 & a_1b_2 & a_1c_{21} & a_1c_{22} \\ b_1 & a_1b_1 & b_1^2 & b_1b_2 & b_1c_{21} & b_1c_{22} \\ b_2 & a_1b_2 & b_1b_2 & b_2^2 & b_2c_{21} & b_2c_{22} \\ c_{21} & a_1c_{21} & b_1c_{21} & b_2c_{21} & c_{21}^2 & c_{21}c_{22} \\ c_{22} & a_1c_{22} & b_1c_{22} & b_2c_{22} & c_{21}c_{22} & c_{22}^2 \end{pmatrix} = \begin{pmatrix} 1.00 & 2.14 & 0.01 & 0.88 & -0.02 & 0.41 \\ 2.14 & 5.92 & -0.00 & 0.00 & -0.01 & 0.85 \\ 0.01 & -0.00 & 1.93 & 0.02 & -0.07 & -0.02 \\ 0.88 & 0.00 & 0.02 & 5.73 & -0.02 & 0.26 \\ -0.02 & -0.01 & -0.07 & -0.02 & 2.48 & -0.00 \\ 0.41 & 0.85 & -0.02 & 0.26 & -0.00 & 2.63 \end{pmatrix} \quad (5)$$

As shown in the results before we have to improve the results. There are two commonly used methods to do this. One of them is to suitably multiply appropriate constraints by nonnegative bound-factors, constraints-factors, or simply variables in order to derive a higher-dimensional lower bounding linear programming relaxation for the original problem. But the size of the resulting relaxation increases rapidly. Another option is *branch-and-bound* to find a globally optimal solution. This is done by successively partitioning the solution space of the original problem into smaller and smaller regions. Whenever a region is infeasible or its best-case bound is worse than some previously obtained worst-case solution, or if the regions subproblem is solved to optimality, we remove the region from any further consideration. Throughout the process, we track the best-known solution.[8]

Because most of the constraints were not influencing the result of a_1b_2 the option of successively partitioning the space would not give us the optimal solution of the original problem, the constraints that make sure that the result is a sphere packing would still not influence a_1b_2. So we decided to increase our problem to a 4^{th}-degree problem, by multiplying all possible combinations of constraints to create constraints of 3^{rd}- and 4^{th}-degree. We started with 4 constraints of degree 1 and 9 constraints of degree 2. Combining all these results give us a total of 289 constraints. The result for the case $r_1 = r_2 = 1$ was in this case $(a_1b_2)^2 = 12$ which gives a density of over 1. So we indeed managed to get a result closer to the actual optimum, but it is still not good enough. So we have again two options, we can either increase the degree of the problem to 6 or we can try the branch and bound. Because of the exponential increase in variables and constraints, increasing the degree even further would make it impossible for us to calculate the results with the hardware available. This leaves us to use branch and bound.

First we set bounds on all the variables such that anything outside these bounds will obviously give a worse solution or no solution at all. The bounds used are given in table 1. The lower-bound of a_1 is given by the constraints and the upper-bound is obtained by placing all spheres next to each other, such that they form a line. In this case it's obvious that if a_1 would become larger than this, it will give a worse result. The same arguments hold for b_2. The other bounds come directly from the bounds for a_1 and b_2 and the given constraints. So we have created a sub-space of the solution space and to be able to branch and bound, we cut this space in halve in every dimension, so we will get $2^5 = 32$ smaller regions, in which we are going to optimize the problem. To get back to our previous example in which $r_1 = r_2 = 1$ the results are given in table 2 for $(a_1b_2)^2$. We already know a packing that has $(a_1b_2)^2 = 48$ which means that most of the results can be disregarded, so we don't have to further partition those regions. Two of the regions contain results that imply further partitioning in order to get an optimal result. After partitioning these two regions the optimal solution was 48.00, so the upper bound for the density is equal to the density of the packing we already have, which was in this case, the hexagonal packing of which we already know that its the packing with the highest density. Next to getting the optimal solution we also get an impression of the values of the variables, in this case $a_1^2 = 4.0000, b_1^2 = 0.0000, b_2^2 = 12.0000, c_{21}^2 = 1.0000, c_{22}^2 = 3.0000$. These results are exactly the results we would expect for the hexagonal packing.

variable	lower bound	upper bound
a_1	2	$2(1+r)$
b_1	-(1+r)	1+r
b_2	$\sqrt{3}$	$2(1+r)$
c_1	$-(1+r)$	$3(1+r)$
c_2	0	$2(1+r)$

Table 1: lower- and upper bounds for the variables

63.95	47.98	55.71	64.00
63.95	47.98	55.68	55.71
78.18	99.21	104.84	125.34
79.04	99.21	83.60	99.21

Table 2: Results for the first bisection of $r_1 = r_2 = 1$. Half of the regions were infeasible.

Now we want to find upper bounds on density for different values of r_2, but to find these values we should first make some packings to be able to disregard any regions containing worse values. One way to create packings is to just randomly create one, but it would be more convenient to have a packing for every value of r_2. To start, we take the hexagonal packing and place a small sphere with radius r_2 in the space between the spheres, then slowly letting it increase and pushing the bigger spheres aside. In (6) the density, δ, is given for two radii, 1 and r, $0 \leq r \leq 1$ for which the graph is shown in figure 4.

$$\delta(r) = \begin{cases} \frac{(1+r^2)\pi}{2\sqrt{3}} & \text{if } 0 \leq r < \frac{2\sqrt{3}}{3} - 1 \\ \frac{(1+r^2)\pi}{2(\sqrt{2r+r^2} + \frac{4\sqrt{2r+r^2} - \sqrt{2r+r^2}(2r^2+4r-2)}{2(1+2r+r^2)})} & \text{if } \frac{2\sqrt{3}}{3} - 1 \leq r \leq \sqrt{2} - 1 \\ \frac{(1+r^2)\pi}{4\sqrt{r^2+2r}} & \text{if } \sqrt{2} - 1 < r \leq 1 \end{cases} \tag{6}$$

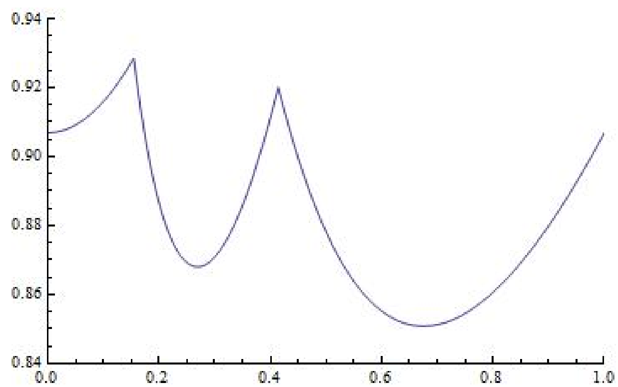
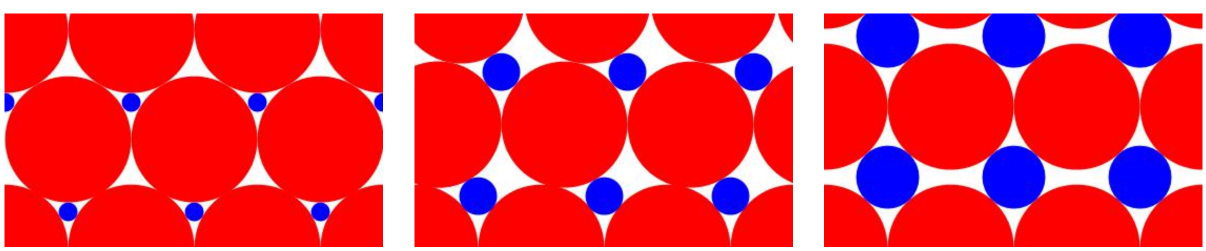


Figure 4: The density $\delta(r)$ for $0 \leq r \leq 1$

Now for every r_2 we know a packing with a certain density, which we can use to produce more results. Because getting results for a certain r_2 is somewhat time consuming we only take a look at 20 different values of r_2, in order to get an impression of what



$r_2 = 0.15$ $r_2 = 0.30$ $r_2 = 0.50$

Figure 5: sphere packings with optimal density

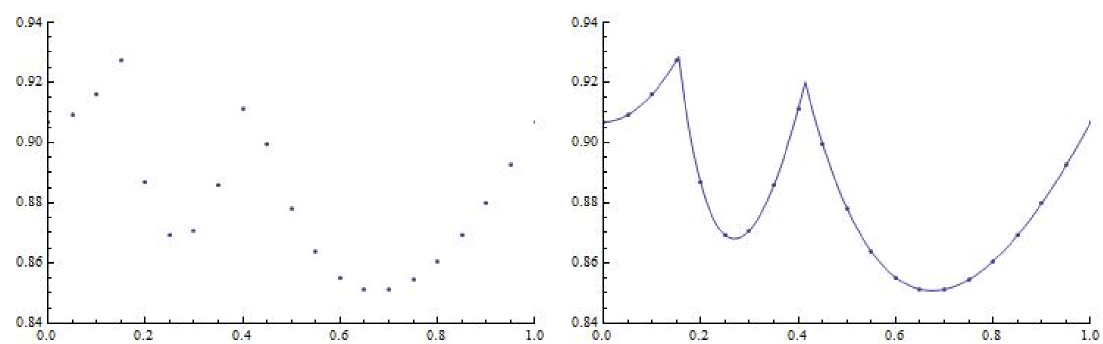
3.4 Results

The results of the RLT and DSP of the problem are upper bounds for the densities. Table 3 show the results for certain values of r. To be sure these are the optimal solutions of our problem, for each of the results we need to find a sphere packing that obtains this result. For some r these results are given in figure 5.

r	density	r	density
0.05	0.9092	0.55	0.8638
0.10	0.9160	0.60	0.8552
0.15	0.9273	0.65	0.8513
0.20	0.8866	0.70	0.8512
0.25	0.8693	0.75	0.8545
0.30	0.8709	0.80	0.8606
0.35	0.8858	0.85	0.8692
0.40	0.9113	0.90	0.8799
0.45	0.8995	0.95	0.8926
0.50	0.8781	1.00	0.9069

Table 3: upper bounds for the density of discs with radii 1 and r of ratio 1:1 in a unit cell

In figure 6(a) the upper bounds of the densities are shown and in figure 6 also the density $\delta(r_2)$ of known packings are shown. This graph gives the impression that these packings are actually the best packings for the problem.



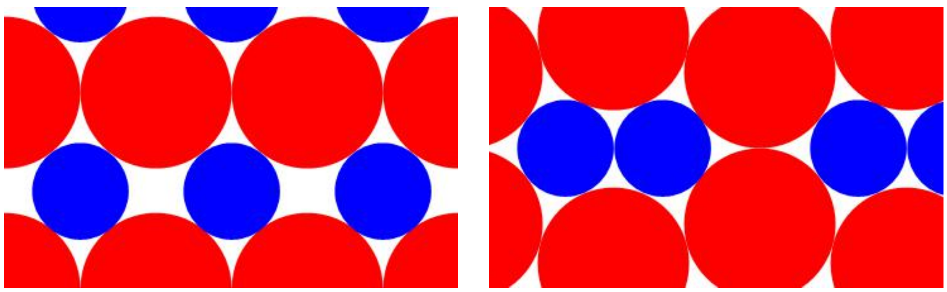
(a) Upper bounds of the density for different values of r_2

(b) Upper bounds and the density of known packings

Figure 6: Upper bounds for the highest density packings

4 Conclusion

The results found are still not the highest density possible for sphere packings with two spheres with ratio 1:1. Because these are the results of two spheres in a unit cell, but if the number of spheres in a unit sphere would be increased, the number of possible lattice packings increases, so a higher density might be obtained. An example is shown in figure 7, the density can be greatly improved by increasing the number of spheres in a unit cell, in this case this is the highest possible density for a sphere packing with radii 1 and 0.637556 [9]. So in order to get an answer to the problem *"What are the highest density binary lattice packings in 2-dimensions with ratio 1:1"* all possible numbers of spheres in a unit cell should be solved.



Density of 0.8518　　　　Density of 0.9107

Figure 7: Density of different number of spheres with radii 1 and 0.637559 in the unit cell

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