Compact ternary disc packings that maximize the density

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The general context

A *packing* of the plane is a collection of discs with disjoint interiors in $\mathbb{R}^2$. The *density* of a packing is a limit, if it exists, of the fraction of the area covered by these discs.

Since a long time, researchers are interested in the densest possible packings. Indeed, this problem has a lot of practical applications. How to fit as many oranges as possible in a huge box? How to assemble atoms in the most compact way? In materials sciences, self-assembly of hard spherical particles in two [6, 19] and three [18] dimensions is based on theoretical results (see Figures 4, 5 for an illustration).

Consider an infinite number of discs of the same size. How to arrange them in the densest possible way? Thue in 1890 proved that the maximal density is attained on the hexagonal packing shown in Figure 1. Notice that in this packing, any "hole" is bounded by three tangent discs. Such packings are called *triangulated*.

Suppose we have discs of two radii: 1 and r. It turns out that in this case, if the radii allow a triangulated packing, it maximizes the density [8]. There are 9 values of r permitting such packings [17], Figure 2 gives an example of triangulated packing for each of 9 radii.

In the case of three discs of radii 1, r, and s, there exists 164 pairs (r, s) admitting triangulated packings [10]. The example of a triangulated arrangement for the 54th pair is given in Figure 3. Do all of these packings maximize the density, as it happens for 1 and 2 discs? This is the central question of our work.

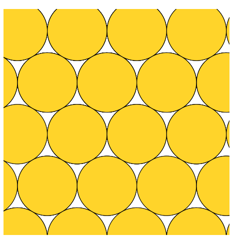


Figure 1: Hexagonal packing.

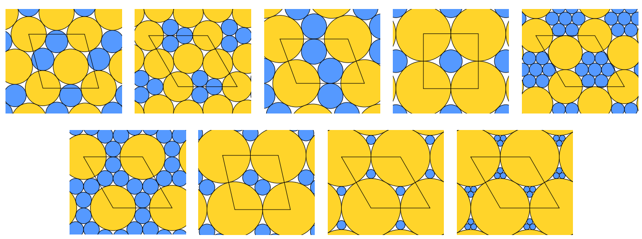


Figure 2: Compact binary packings.

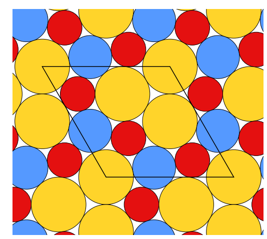


Figure 3: Triangulated ternary packing number 54.

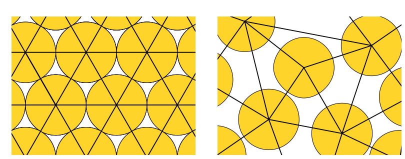
Results and my contribution

33 of the 164 cases are already known to not be the densest: some of them are not saturated and for others the density is maximized on packings with only 2 discs. However the remaining 131 pairs are good candidates maximize the density.

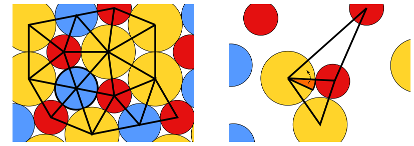
My first little challenge was to calculate the densities of each of the 164 packings out of a combinatorial encoding. This encoding contained values of r and s and a compact description of how to add discs one by one to get the whole domain of the packing. Having this information, I had to reproduce the geometrical configuration to calculate the densities. During this task, I got familiar with SageMath, especially its Arbitrary Precision Real Intervals to perform interval arithmetic and Polynomials to store algebraic numbers (as radii and densities).

The next step was to use the ideas given in [8] for binary packings to prove, if possible, the same results for the ternary packings, or to find counter examples.

Let me first introduce you with the very rough idea of this proof in the simplest case of 1 disc. Consider the hexagonal packing and the Delaunay triangulation of the disc centers, the density is equal to the density in each triangle: $\delta^* = \delta_{\triangle^*}$. Now take any other packing and its triangulation, you can easily see that the density of a triangle $\triangle'$ of this packing never exceeds the density of a triangle in the hexagonal packing: $\forall\, \triangle',\ \delta_{\triangle'} \le \delta_{\triangle^*} = \delta^*$.



Consider now a ternary periodic triangulated packing and its Delaunay triangulation. The densities in different triangles are different, and the all in all density is equal to the density of the domain: $\delta^* = \frac{\delta_{\triangle_1}+3\delta_{\triangle_2}+12\delta_{\triangle_3}}{16}$. Look now at an arbitrary packing and its triangulation. Here, the densities of some triangles might be higher than the densities of the triangles in the triangulated packing, so the previous proof does not work. However, it turns out that each "dense" triangle has a "sparse" neighbor. In our proof, we find a way to redistribute the density between such triangles and to get the required inequality for all triangles.



First of all, I proved that the packing number 54 maximizes the density following the technique used for the case 53 which was successfully treated before [9]. The proof is strongly based on the SageMath calculations that are explained in details further in this report. It roughly consists of two parts: choosing the parameters and verifying that these parameters satisfy the required inequality on all the triangles (here comes the interval arithmetic). I faced some issues of SageMath and had to take into account that some functions do not always give the right answers and others are precise but take a lot of time. My challenge was to combine the two in order to get a verified result without spending hours on calculations.

Then I started to extend the obtained proof to the other cases. The aim of this generalization was finding a way to minimize case analysis by hand and automatize the calculations as much as possible. This allowed me to get the proofs for the following cases: 51, 54, 55, 56, 58, 66, 77, 79, 93, 115, 116, 119, 123, 130. However, even more important part was discovering which cases are not eligible for this generalized proof and for which reasons. This allows us to move forward adjusting our strategy for the problematic cases and gives us an idea about hidden differences between the structures of those packings.

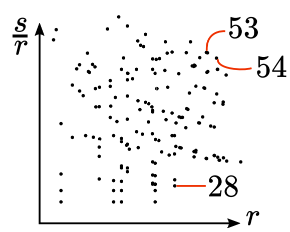
Finally, the last challenge was formalizing all of this in order to get a clear and formal proof. Computer calculations are getting more and more important in the purely theoretical results. Unfortunately, the proofs adopting computer calculations are still received with disbelief due to several reasons, the first being a difficulty in the presentation of such results. My last goal was to find a way to write down this proof which is strongly based on the computer assistance.

Besides that, I virtually participated in the Circle Packings and Geometric Rigidity workshop where I gave a short lightning talk describing my work [1].

Summary and future work

First of all, we plan to extend the proof to the remaining 116 cases assuming there are no counter examples (otherwise, our aim is to find them). This would provide us with a full description of triangulated ternary packings of the plane.

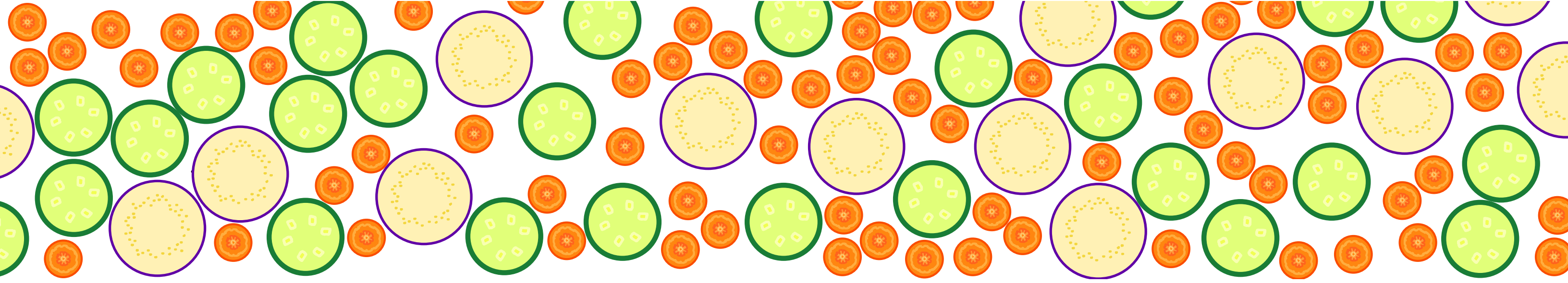
Nevertheless, the triangulated packings represent only 164 points out of an uncountable number of radii ratios schematically displayed on the right:



You can find a more detailed illustration in Figure 9. In order to get more information about the blank part of this map, we may try to vary the sizes of the discs continuously starting from a triangulated packing with the known maximal density. This technique was first used by Tóth [23] and showed itself to be a powerful tool. It was also applied to ternary packings by Connelly and Pierre in order to find a packing with s as close to 1 as possible that is however denser than the hexagonal packing [22]. Their packing is a perturbation of the packing number 53 (see Figure 9).

A good way to do that is by so-called flipping and flowing. This technique permits to go from one triangulated packing to another passing continuously trough "similar" non-triangulated packings [4]. Given that the two triangulated packings maximize the density, the intermediate packings are likely to be rather dense. This gives us a good lower bound of the density of packings with discs of these sizes and can potentially add a lot of information to our map.

To go deeper in the domain of the densest arrangements, one of our projects is to find a finite collection of discs such that the densest packing is aperiodic. This connects our study with the domain of tilings since any triangulated packing can be considered as a tiling by triangles. A progress in this question would be of interest to the experts in materials science in connection with the quasicrystals (locally ordered aperiodic structures) [20].



1 Introduction

You are given an infinite number of round zucchini slices of the same size:  . How to place them on an infinite frying pan without overlap to maximize the average covered area? You probably know the answer: this is called the hexagonal disc packing and a sketch of the formal proof is given in the previous section. What happens if you also need to fry slices of carrot  ? And if you have 3 sizes of slices: zucchinis , carrots  and eggplants  ? In this work, we are interested in the last question.

A disc packing of the plane is a set of discs placed in $\mathbb{R}^2$. A density of a packing D is the limit, if it exists, of the fraction of the area covered by the discs :

$$\delta(D) = \lim_{n\to\infty} \frac{S([-n,n]^2 \cap D)}{S([-n,n]^2)}$$

Since a long time people were interested in the densest packings of discs and spheres. In addition to frying vegetables and transporting oranges, these packings play a crucial role in materials science: in order to design dense materials, we need to find dense packings of particles [6, 18, 19] (see Figures 4, 5).

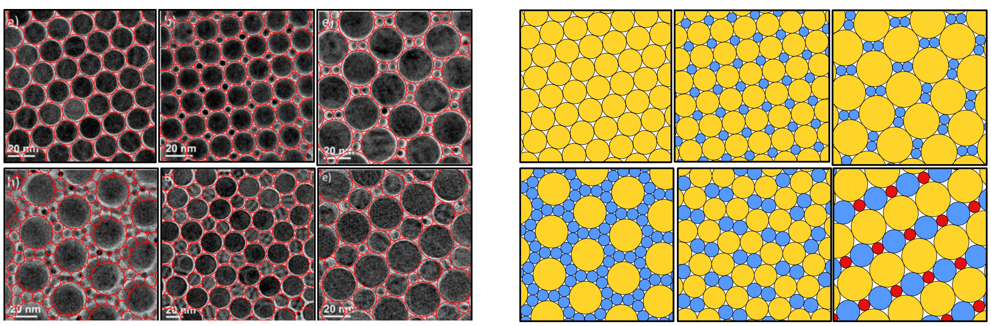


Figure 4: Binary and ternary superlattices from colloidal two-dimensional nanodisks and one-dimensional nanorods produced by experiments in [19] and their theoretical representation.

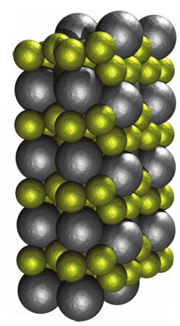
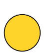


Figure 5: A high-density configuration of hard spherical particles [18].

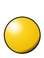
Given a set of discs, we consider two questions: what is the maximal density of a packing with these discs and which are the packings maximizing it.



Suppose first that we are given an infinite number of copies of a disc. In 1772, Lagrange proved that the maximal density of a lattice packing (i.e. a packing where the disc centers form a lattice) is $\frac{\pi}{2\sqrt{3}}$. This is the density of the hexagonal packing (see Figure 6 for an illustration). The first generalization of this result for any packing was only obtained in 1910 by Thue; a clear proof is given in [3].

Theorem 1 (Thue, 1910) The maximal density of a 1-disc packing on the plane is $\frac{\pi}{2\sqrt{3}}$.

It turned out that Thue's proof was incomplete: Toth published the rigorous complete version in 1940 [7].



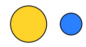
The packing problem seems to be even more practical in 3D : how to arrange oranges in the most compact way in a huge box? Kepler was apparently the first to study this question in depth: he conjectured that the 3D version of the hexagonal packing illustrated in Figure 7 maximizes the density.

Conjecture 2 (Kepler, 1611) The maximal density of a 1-sphere packing in the space is $\frac{\pi}{3\sqrt{2}}$.

Gauss in 1831 proved this conjecture to be true for lattice packings and only in 1998 Ferguson and Hales got the result for all packings.

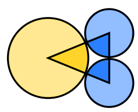
Theorem 3 (Ferguson, Hales, 1998 [12]) The maximal density of a 1-sphere packing in the space is $\frac{\pi}{3\sqrt{2}}$.

This was a 300 pages proof by exhaustion using computer calculations; it was hardly verifiable by experts. In 2014 Hales completed a formal proof using an automated proof assistant [13].



Suppose we are given discs of radii 1 and $r < 1$. Indeed, the maximal density $\delta(r)$ of a packing in this case is at least $\frac{\pi}{2\sqrt{3}}$ which is the density of the hexagonal packing (we get it just using only discs of one size). Florian in [11] derived an upper bound for the density of a two-discs packing:

Theorem 4 (Florian, 1960) The density of a packing with two sizes of discs never exceeds the density δ in a triangle formed by the centres of two small discs and one big disc, all mutually tangent:



$$\delta = \frac{\pi r^2 + 2(1-r^2)\sin^{-1}\left(\frac{r}{1+r}\right)}{2r\sqrt{1+2r}}$$

These bottom an upper bounds of the maximal density are marked red in Figure 8.

Blind in [2] found a constant $b \approx 0.74299$ such that for $b < r < 1$, the maximal density is $\frac{\pi}{2\sqrt{3}}$. That means that for such r the maximal density is achieved using only one of two disc sizes. The value of b is tagged green and the known precise values of $\delta(r)$ are traced blue in Figure 8.

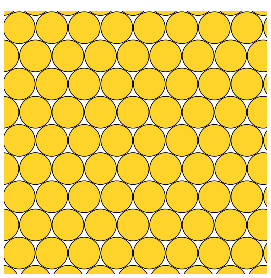


Figure 6: Hexagonal disc packing.

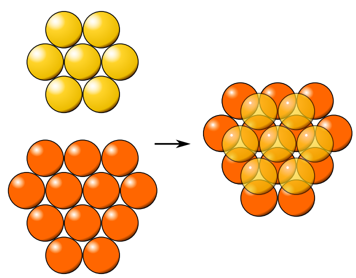


Figure 7: The structure of the hexagonal sphere packing.

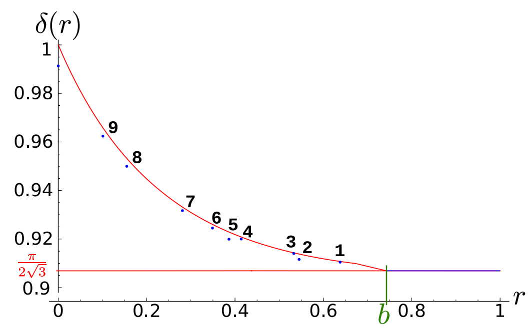


Figure 8: The density graph of binary disc packings.

Besides that, the maximal density is known only for 9 values of r (blue dots in Figure 8). These are exactly the values for which a triangulated packing exists. A packing is called *triangulated* (or, sometimes, *compact* like in [8]) if the graph formed by connecting the centers of any pair of adjacent discs is a triangulation. Find examples of triangulated packings in Figures 2 and 3.

All 9 radii with triangulated 2-discs packings were found by Kennedy [17]. 7 of them were proved to maximize the density in [14–16]. The complete proof where all 9 cases were shown to have the maximal density is given in [8].

Notice that the only triangulated 1-disc packing is the hexagonal packing which also maximizes the density. The fact that triangulated packings maximize the density for 1- and 2-discs packings seems quite intuitive. In such packings, all the "holes" are bounded by 3 discs, this arrangements seem to be rigid and triangulated.

The next question is: does this this still hold for 3-discs packings? This is the main direction of our research and we start talking about it in the next section.

We are given three disc radii: 1, r, and s, $1 > r > s$. In 2018, Fernique, Hashemi, and Sizova showed that there are 164 pairs of (r, s) permitting a triangulated 3-discs packing where circles of the three sizes appear [10]. Not all of these packings maximize the density. In cases 1–18 (marked blue in Figure 9), the densest triangulated packings have only two sizes of discs; in yet other 15 cases (24, 28–33, 37–44, marked green in Figure 9), the densest triangulated packings are not saturated (i.e. we can add more discs and get a denser packing).

All the 131 remaining cases are still good candidates to be densest.

Which of them do maximize the density? That is the central question of our study.

Connelly in [5] conjectured that if a finite set of discs allows a saturated packing then the density is maximized on this packing. As we saw, this is true for 1 and 2 discs and there are a few exceptions for 3 discs. Our aim is either to prove it for all the remaining cases or to find other counter examples.

The first step in this direction was made by Fernique who proved the packing 53 (marked violet in Figure 9) to have the maximal density [9]. This proof is based on a technique used in the case of 2 discs mentioned above [8] and strongly relies on computer calculations.

In our work, we obtained similar proofs for 14 other cases: 51, 54, 55, 56, 58, 66, 77, 79, 93, 115, 116, 119, 123, 130 (marked red in Figure 9) The scheme of the proof is given in Section 2: it contains the theoretical part of the result. Section 3 gives a detailed explication of the computational part of this proof.

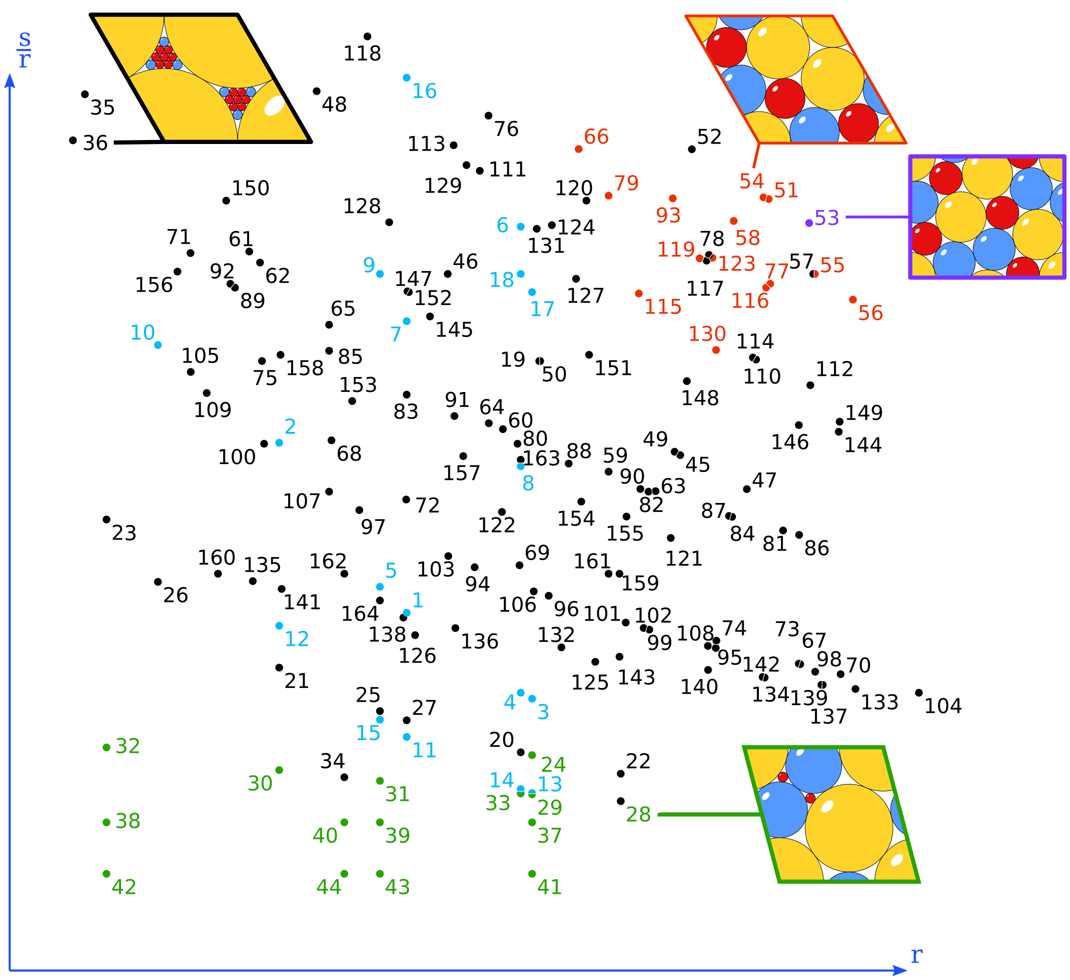


Figure 9: The map of the triangulated ternary packings.

2 Sketch of the proof

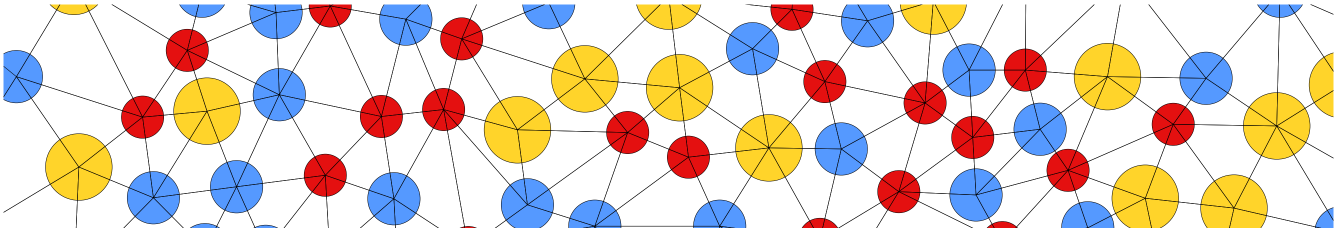


Figure 10: Example of an FM-triangulation.

First of all, we shall learn to triangulate circle packings since our proof is strongly based on the triangulation. A *Voronoi cell* of a disc in a packing is the set of points which are closer to this disc than to any other. Together, all the cells of the packing form a partition of the plane called the *Voronoi diagram*. The dual graph of this diagram is a triangulation with vertices in centers of the discs. It is called the *FM-triangulation* [24] or the *weighted Delaunay triangulation* with weights equal to the radii. An example of the FM-triangulation of a packing is given in Figure 10

A triangle [1] is called *tight* if its discs are mutually tangent (find an illustration in Figure 11). Notice that the FM-triangulation of any triangulated packing contains only tight triangles.

Consider a triangle T in the FM-triangulation of a packing and consider the circle tangent to the three discs of this triangle. This circle is called the *support circle* of T. Notice that if the packing is saturated then the radius of the support circle of each triangle is less than s.

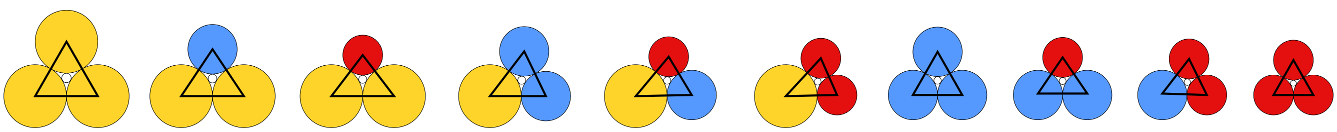


Figure 11: All types of tight triangles with their support circles.

Suppose we are given discs of radii $1, r$ and s and a triangulated packing with these discs which we call the target packing. This packing together with its FM-triangulation are denoted by $\mathcal{T}^*$. Our aim is to prove that it maximizes the density. Consider any other packing with its FM-triangulation $\mathcal{T}$ (without loss of generality, we assume $\mathcal{T}$ to be saturated). We shell prove that its density never exceeds the density of $\mathcal{T}^*$. Let us introduce the folloing value called the *sparsity* of a triangle $T \in \mathcal{T}$:

$$S(T) = \delta \times area(T) - cov(T)$$

where δ denotes the density of $\mathcal{T}^*$, $cov(T)$ denotes the area covered by the discs and $area(T)$ is the area of the triangle without discs. Notice that $S(T) > 0$ iff the density of covering of T is less than the density of the target packing. $S(T) < 0$ iff it is greater than the density of the target packing. Thus, to show that the a packing $\mathcal{T}$ is not denser than the target packing, it is enough to prove that $\sum_{T \in \mathcal{T}} S(T) \geq 0$.

To do this, we introduce a potential U over triangles in a packing satisfying two following inequalities: for any triangle $T \in \mathcal{T}$,

$$S(T) \geq U(T) \qquad (\triangle)$$

and

$$\sum_{T \in \mathcal{T}} U(T) \geq 0 \qquad (U)$$

[1]We consider the triangulation together with its packing, so by "triangle", we mean a triangle with the discs in its vertices.

Instead of proving directly the last one, we will define so-called vertex potentials $\dot{U}_T^v$ (the dot represents a vertex) and edge potentials $\bar{U}_T^e$ (the bar represents an edge) for each triangle T. So the potential of a triangle T with vertices x, y, z and edges a, b, c is the sum of its vertex potentials and edge potentials:

$$U(T) = \sum_{v \in T} \dot{U}_T^v + \sum_{e \in T} \bar{U}_T^e = \dot{U}_T^x + \dot{U}_T^y + \dot{U}_T^z + \bar{U}_T^a + \bar{U}_T^b + \bar{U}_T^c$$

Rather than showing that the total potential on all triangles is nonnegative (U), we prove it both for all local vertex potentials and all local edge potentials:
for any vertex $v \in \mathcal{T}$

$$\sum_{T \in \mathcal{T} | v \in T} \dot{U}_T^v \geq 0 \tag{$\bullet$}$$

and for any edge $e \in \mathcal{T}$

$$\sum_{T \in \mathcal{T} | e \in T} \bar{U}_T^e \geq 0 \tag{$-$}$$

Our aim now is to construct vertex and edge potentials satisfying the three inequalities $\triangle$, $\bullet$ and $-$. In Section 3.2, we choose the parameters to meet $\bullet$, in Section 3.3, we do it for $-$ and Section 3.4 eventually describes how we check that $\triangle$ is satisfied on all triangles.

3 Choosing the potentials, with the help of a computer

In this section, we explain in details how we find the potentials. This process is strongly based on computer calculations. In order to stay formal, we will first clarify how the constants are stored in the computer memory and what kind of computations we perform.

3.1 Dealing with constants

We implement all our computations in SageMath [2]. This tool is specifically useful for us as it provides libraries to work with interval arithmetic and polynomials. Thus, some values are stored as intervals and some as roots of polynomials. To keep track of different variable types, we use the following color notation in this document.

- Exact real values: x, 42, 3.1415[3]
- Algebraic numbers: r, s, δ represented by their characteristic polynomials
- Intervals (from Real Interval Field): a, V_{111}, π represented by intervals

Let us say a few words about interval arithmetic [21]. Intervals are used to store numbers in a computer memory when the precise value takes too much memory or performing operations on this value cost a lot of computation time. There are two conditions that shell hold to work with intervals.

- A representation of a number x is an interval I whose endpoints are exact values representable in a computer memory and such that $x \in I$.
- After performing an operation $\bullet$ on two intervals I, J, we get as a result an interval $I \bullet J$ containing all values that could be obtained: $\forall x \in I,\ y \in J,\ \ x \bullet y \in I \bullet J$.

[2] `https://doc.sagemath.org/`
[3] Notice that it is an exact real value, different from π.

Thesse two conditions guarantee that during computations, each number is contained in its interval.

In the SageMath implementation of interval arithmetic [4], an interval $I = [a, b]$ represents a set $\{x : a \leq x \leq b\}$. An interval has methods `endpoints()` that returns a pair of its endpoints, as well as `upper()` and `bottom()` returning each of them. The arithmetic operations on intervals in Sage satisfy the property given above. Comparison operations (`==,!=,<,<=,>,>=`) on I, J return `True` if every value in I has the given relation to every value in J. Find below an example of utilisation of interval arithmetic is SageMath.

```
sage: I = RealIntervalField()
sage: I42 = I(41.5, 42.5)
sage: I42.endpoints()                                  # An interval around 42
(41.5, 42.5)
sage: (I42 + 1).endpoints()                                           # Add 1
(42.5, 43.5)
sage: (I42 * 2).endpoints()                                   # Multiply by 2
(83.0, 85.0)
sage: Ipi = I(pi)                                          # An interval for π
sage: Ipi.endpoints()
(3.14159265358979, 3.14159265358980)
sage: (Ipi + I42).endpoints()                   # Interval(π) + Interval(42)
(44.6415926535897, 45.6415926535898)
```

Each of 164 triangulated ternary packings is given by a pair of radii (r, s) such that $1 > r > s$, coronas[5] for each of disc sizes and the density divided by π, δ (we store this value since it is algebraic unlike the density). These constants are given as algebraic numbers. We however keep them as intervals, and denote them by r, s and δ.

3.2 Vertex potentials

Tight triangles

For all triangles that are not far from tight, we choose to take into account only the vertex potential: we define $\bar{U}_T^e$ in a way that it equals zero in this case. So for now we take care only of the vertex potentials of nearly tight triangles.

Notice that by $\triangle$, $S(T) - U(T) \geq 0$ for any triangle T. Besides that, if $\mathcal{T}^*$ is the target packing triangulation then all its triangles are tight and, by definition of the sparsity, $\sum_{T \in \mathcal{T}^*} S(T) = 0$. Therefore we get

$$\sum_{T \in \mathcal{T}^*} (S(T) - U(T)) = \sum_{T \in \mathcal{T}^*} S(T) - \sum_{T \in \mathcal{T}^*} U(T) = - \sum_{T \in \mathcal{T}^*} U(T) \leq 0$$

Thus, for any tight triangle T present in $\mathcal{T}^*$, $U(T) = S(T)$ and $\sum_{T \in \mathcal{T}^*} U(T) = 0$.

There are 10 tight triangles depending on the triples of their disc radii. They provide us with 18 vertex potentials; the sums of vertex potentials of the tight triangles are respectively:

$$\begin{array}{lll}
\dddot{U}_{111} = 3\dot{U}_{111}^1 & \dddot{U}_{11r} = 2\dot{U}_{11r}^1 + \dot{U}_{11r}^r & \dddot{U}_{11s} = 2\dot{U}_{11s}^1 + \dot{U}_{11s}^s \\
\dddot{U}_{rrr} = 3\dot{U}_{rrr}^r & \dddot{U}_{1ss} = 2\dot{U}_{1ss}^r + \dot{U}_{1ss}^1 & \dddot{U}_{1rr} = 2\dot{U}_{1rr}^r + \dot{U}_{1rr}^1 \\
\dddot{U}_{sss} = 3\dot{U}_{sss}^s & \dddot{U}_{rrs} = 2\dot{U}_{rrs}^r + \dot{U}_{rrs}^s & \dddot{U}_{rss} = 2\dot{U}_{rss}^s + \dot{U}_{rss}^r
\end{array}$$
$$\dddot{U}_{1rs} = \dot{U}_{1rs}^1 + \dot{U}_{1rs}^r + \dot{U}_{1rs}^s$$

[4] https://doc.sagemath.org/html/en/reference/rings_numerical/sage/rings/real_mpfi.html

[5] A corona of a disc is a list of discs tangent to it in the packing.

By the reasoning above, those of them which are present in $\mathcal{T}^*$ are forced to be equal to the respective sparsities. Suppose there are t tight triangles present in $\mathcal{T}^*$, then it gives us t equations on vertex potentials.

Consider a disc in the target packing and all the triangles formed by it and the discs tangent to it. We call this sequence the *corona* of the disc. The inequality $\bullet$ and the fact that and $\sum_{T\in\mathcal{T}^*} U(T) = 0$ yield that the sum of vertex potentials of the triangles in each corona equals 0. Suppose, there are c different coronas in $\mathcal{T}^*$.

Notice now that all triangulated packings are periodic: there are two period vectors such that shifting the packing by them, we get the same packing. Thus we can choose a domain D of each packing: a smallest collection of discs such that we can get the whole packing by shifting this collection by period vectors. The domain completely characterize the packing and since the whole packing is the repetitions of the domain, $\sum_{T\in D} S(T) = \sum_{T\in D} U(T) = 0$. Thus, the previous equations are dependent and we got at most $t + c - 1$ independent equations on 18 variables.

In practice, $t + c$ never exceeds 13 and for most of the cases $t \leq 4$ and $c \leq 3$ so we have many free variables. For the sake of simplicity, for all the cases considered below, we complete our equations in a trivial way explained in details for the case 54 just below. Finding the right equations for the remaining variables is the most promising way to treat the cases that are not covered in this work.

54

The sparsity of a tight triangle of type abc is denoted by S_{abc}. Notice, that the sparsities depend on r, s and δ and are thus represented as RIFs.

In the packing number 54, there are 3 types of tight triangles present in the domain of $\mathcal{T}^{54}$: one of type 111, three of type $11s$, and 12 of type $1rs$, they are shown in Figure 12. So we get 3 equations for 3 types of tight triangles:

$$3\dot{U}^1_{111} = S_{111}, \quad 2\dot{U}^1_{11s} + \dot{U}^s_{11s} = S_{11s}, \quad \dot{U}^1_{1rs} + \dot{U}^r_{1rs} + \dot{U}^s_{1rs} = S_{1rs}$$

There are three coronas (see Figure 13): 1-corona $11srsrs$, r-corona $1s1s1s$, and s-corona $11r1r$. The equations of the last two are:

$$6\dot{U}^r_{1rs} = 0, \quad \dot{U}^s_{11s} + \dot{U}^s_{1rs} = 0$$

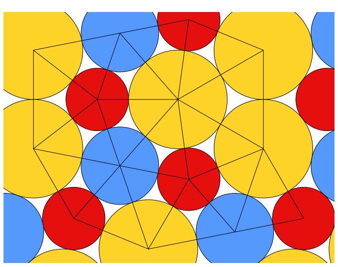


Figure 12: Tight triangles of the packing 54.

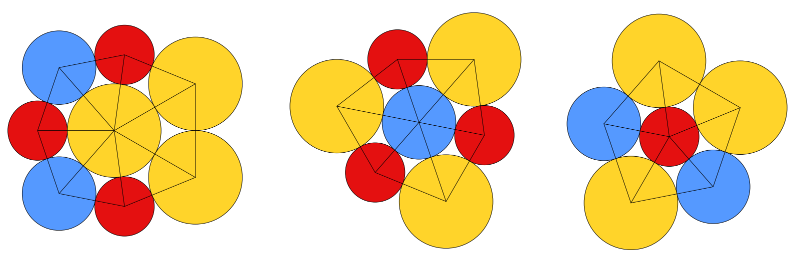


Figure 13: Coronas of the packing 54.

We thus got 5 equations on 18 variables. We complete them in the following way: first, we set the sums of vertex potentials of all the remaining tight triangles equal to their sparsities which provides us with 7 additional equations. And eventually, we set the vertex potential of the isoleces triangles equal zero which gives us yet 6 more equations:

$$\forall a \neq b \ \in \{1, r, s\}, \ \dot{U}^a_{abb} = 0$$

All in all, we have 18 independent equations and can thus resolve the system and fix the 18 values of vertex potentials of tight triangles.

Other vertex potentials

As in [9], we define the vertex potential of an arbitrary triangle T in v as follows:

$$\dot{U}_T^v = \min(\dot{U}_{abc}^a + m_a|\widehat{v} - \widehat{a}|,\ Z_a)$$

where $a \in \{1, r, s\}$ is the radius of the disc with the center in v; b and c are the disc radii of the two remaining vertices of T [6]; Z_a and m_a are the constants defined below; $\widehat{v}$ is the angle of v in T and $\widehat{a}$ is the angle of a in the tight triangle abc. These values are illustrated in Figure 14.

First, let us define m_1, m_r, and m_s. We choose these constants in a way that $\bullet$ holds if potentials were equal to $\dot{U}_{abc}^a + m_a|\widehat{v} - \widehat{a}|$ (we forget about Z_a for now). Let us denote by $\{T_i\}_{i\in I}$ the set of tight triangles containing a vertex a. It turns out that if m_a satisfies

$$m_a \geq -\frac{\sum_{i\in I} \dot{U}_{T_i}^a}{|2\pi - \sum_{i\in I} \widehat{a}(T_i)|}$$

then $\bullet$ holds for all vertices of type a in $\mathcal{T}$ (check [9] for the proof). We thus choose m_1, m_r, and m_s as the lesser values satisfying this inequality. Since the value to the right side is a RIF, we just take its upper bound.

Our aim is to take the vertex potentials as small as possible (to satisfy $\triangle$) still keeping the total potential around any vertex positive ($\bullet$). It turns out that we can "improve" the previously built structure by capping the potential of each by a constant depending only on the vertex type in a way that $\bullet$ remains satisfied.

$$Z_a := 2\pi \left| \min_{b,c\in\{1,r,s\}} \frac{\dot{U}_{abc}^a}{\widehat{a}} \right|$$

The detailed proof is given in [8].

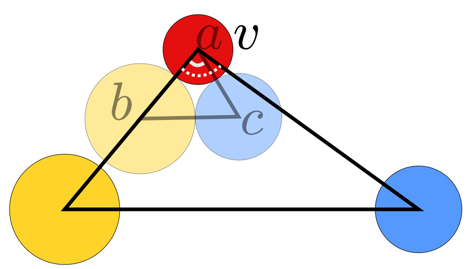


Figure 14: Illustration of a vertex potential for an arbitrary triangle.

3.3 Edge potentials

Let T be a triangle in $\mathcal{T}$ and e be its edge, then we define the edge potential of T on e as follows.

$$\bar{U}_T^e := \begin{cases} 0, & \text{if } |e| < l_{ab} \\ q_{ab} \times d_e(T), & \text{otherwise} \end{cases} \tag{1}$$

where abc is the type of T and ab is the type of e, $l_{ab} > 0$ and $q_{ab} > 0$ are constants described later and $d_e(T)$ is the signed distance of the center of the support circle of T to the edge e (it is positive if T and the center are on the same side of e and negative otherwise).

The support circle geometric position depends on the the radii of the discs so $d_e(T)$ is an interval. The details of how to compute it, as well as the proof of the next Lemma can be found in [8].

[6] We say that v is of *type* a and T is of *type* abc

Lemma 5 If e is an edge common to two triangles T_1 and T_2 of an FM-triangulation, then $\bar{U}^e_{T_1} + \bar{U}^e_{T_2} \geq 0$.

That means the inequality $-$ is always satisfied.

The constant $l_{ab} > 0$ controls the length of an edge starting from which the edge potential is taken into account while $q_{ab} > 0$ controls its intensity. We choose l_{ab} in a way that the edge potential becomes nonzero when $d_e(T)$ becomes negative. We choose q_{ab} so that $U(T')$ is slightly less than $S(T')$ where T' is a stretched triangle (i.e. only two pairs of its discs are tangent and the edge between the third pair is tangent to the remaining disc).

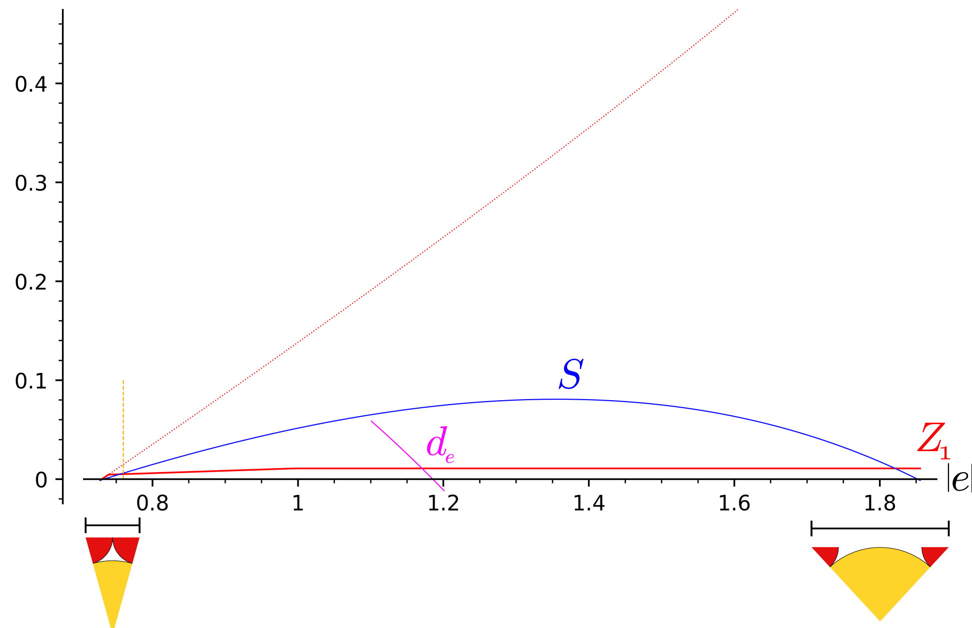


Figure 15: The value of ϵ (orange vertical line) together with Z_1 (red), d_e (violet), S (blue), and the vertex potential without capping (red dotted) in the case 118 as functions of the length of the side of type ss in the triangle of type $s1s$.

Figure 15 illustrates how the values of the vertex potential, the sparsity and d_e vary for a triangle of type $s1s$ in the case 118, from the tight to the stretched triangle.

3.4 Checking $\triangle$ on all triangles

We constructed the potentials in a way that the inequalities $\bullet$ and $-$ are satisfied. All that remains is to check $\triangle$. We will do it with the help of the computer by checking this inequality on all the possible triangles. First we have to restrict the number of triangles: the next two subsections are dedicated to this.

Epsilon-tight triangles

By definition, the potentials of tight triangles were set to be equal to their sparsities. In this section we show that in a neighbourhood of any tight triangle, U never exceeds E so $\triangle$ holds.

A triangle is called ϵ-tight if the distance between each pair of its discs is at most ϵ. Let T be a tight triangle, then T_ϵ denotes the set of ϵ-tight triangles of the same type as T. Our aim is to find ϵ such that on the set T_ϵ, the upper bound of the variation of the potential ΔU is not greater than the lower bound of ΔS.

First, notice that

$$\Delta S = \sum_{1 \leq i \leq 3} \frac{\partial S}{\partial x_i} \Delta x_i \geq \sum_{1 \leq i \leq 3} \min_{T_\epsilon} \frac{\partial S}{\partial x_i} \Delta x_i$$

where x_i are the side lengths of the triangle. On the other hand,

$$\Delta U = \sum_{1\leq i\leq 3} \frac{\partial S}{\partial x_i}\Delta x_i \leq \sum_{1\leq i\leq 3} \max_{T_\epsilon} \frac{\partial U}{\partial x_i}\Delta x_i$$

Thus, the inequality $\triangle$ holds on all triangles in T_ϵ for any ϵ such that

$$\forall i \in \{1,2,3\},\ \max_{T_\epsilon} \frac{\partial U}{\partial x_i} \leq \min_{T_\epsilon} \frac{\partial S}{\partial x_i}$$

Notice that we consider only ϵ small enough so that the edge potential equals zero (check Section 3.3). To check the above inequality, we use the interval arithmetic considering the side lengths x_i as intervals: if T has type abc, then $x_1 = [a+b, a+b+\epsilon]$, $x_2 = [b+c, b+c+\epsilon]$, $x_3 = [a+c, a+c+\epsilon]$.
Then we calculate the derivatives using these intervals:

$$\max_{T_\epsilon} \frac{\partial U(x_1,x_2,x_3)}{\partial x_i} = \left(\frac{\partial U(x_1,x_2,x_3)}{\partial x_i}\right)\texttt{.upper()}$$

$$\min_{T_\epsilon} \frac{\partial S(x_1,x_2,x_3)}{\partial x_i} = \left(\frac{\partial S(x_1,x_2,x_3)}{\partial x_i}\right)\texttt{.lower()}$$

Finally, to find the maximal value of ϵ, we use dichotomy.

Non-feasible triangles

Some triangles can never appear in an FM-triangulation of a saturated packing, so we also do not need to consider them. To eliminate those triangles, we use the following properties of FM-triangulations:

Lemma 6 If a triangle is in an FM-triangulation of a saturated packing by discs of radii 1, r, and s, then

- the radius of its support disc is less than s
- its area is at least $\frac{1}{2}\pi s^2$
- the altitude of any vertex is at least s

The proof of this Lemma is rather simple and is given in [8]. Now we do not need to consider triangles not satisfying at least one of these conditions.

All the others

Now we should check the inequality $\triangle$ over all the remaining triangles. By Lemma 6, if the triangle T of type abc appear in an FM-triangulation of $\mathcal{T}$ then the radius of its support disc is less than s and thus the center of a disc of radius q is at distance at most $q+s$ from the center of the support disc. Then, using the triangle inequality, we get that the side between discs a and b, for example, is shorter than $a+s+b+s$. The same holds for the other sides, so we get that the lengths of the edges of T are in the set $[a+b, a+b+2s] \times [b+c, b+c+2s] \times [a+c, a+c+2s]$.
We thus consider the side lengths equal to these intervals:

$$x_1 = [a+b, a+b+2\bar{s}],\ x_2 = [b+c, b+c+2\bar{s}],\ x_3 = [a+c, a+c+2\bar{s}]$$

where $\bar{s}$ is the upper bound of s. So the values of a potential U and sparsity S calculated on the triangle with these edges are also intervals.

1. If they do not intersect and $U < S$ then the inequality $\triangle$ is proven for triangles of type abc.
2. If they do not intersect and $U > S$ then the potential does not satisfy $\triangle$.
3. If they intersect then we need more precision to derive a result.

Thus, out strategy is to use recursion: we divide x_1, x_2, x_3 until we get 1, 2 or we are in the case of tight or non-feasible triangles.

4 Conclusion

The 15 cases for which the current version of the proof worked well are all among the 28 cases with the greatest values of s (the radius of the smallest disc). Among these 28 cases, there are also 3 cases where the calculations were not terminated because the recursion was too deep. Our next step is to find a strategy for the lesser s.

This proof is very flexible: many free parameters of the potentials were chosen arbitrary. We aim to use these parameters in order to redistribute the potential differently depending on the problematic triangles found during testing. We hope to be able to extend the proof to all the remaining cases, otherwise, we shall find counter examples. I will pursue a PhD in this domain and that is my first objective.

Next, we will try to fill the blank area in the map shown in Figure 9. If we slightly modify the radii of discs in a triangulated packing, we get similar packings which are not triangulated but are probably dense: this gives us a good lower bound on the maximal density. Flipping and flowing is an efficient way to do this [4].

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