# Density of sphere packings: from coins to oranges 

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$$
20 / 3 / 2023
$$

## Plan

(1) What is a packing?
(2) Packing $\bigcirc$ in 2D and $\bigcirc$ in 3D
(3) Triangulated packings
4. Proof for
(5) Proof for $\bigcirc \bigcirc$
(6) Proof strategies for $\bigcirc, \bigcirc \bigcirc \bullet$ and $\bigcirc$
(7) Work in progress: 00


## Discs:



Packing $P$ : (in $\mathbb{R}^{2}$ )


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\delta(P)=\limsup _{n \rightarrow \infty} \frac{\operatorname{area}\left([-n, n]^{2} \cap P\right)}{\operatorname{area}\left([-n, n]^{2}\right)}
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Main Question
Given a finite set of discs (e.g., ○○•), which packing maximizes the density?

What is a packing?

## Motivation

- Packing fruits and vegetables



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- Packing fruits and vegetables

- Making compact materials


Binary and ternary superlattices self-assembled from colloidal nanodisks and nanorods. Journal of the American Chemical Society, 137(20):6662-6669, 2015.

2D hexagonal $\bigcirc$-packing:


$$
\delta=\frac{\pi}{2 \sqrt{3}}
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Lagrange, 1772
Hexagonal packing maximizes the density among lattice $\bigcirc$-packings.
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## Packing $O$ in 2D and $O$ in 3D

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$\delta=\frac{\pi}{3 \sqrt{2}}$

Gauss, 1831
Hexagonal compact packings maximize the density among lattice -packings.
Hales, Ferguson, 1998-2014
(Conjectured by Kepler, 1611)
Hexagonal compact packings maximize the density.

## Packing $\bigcirc$ in 2D and $O$ in 3D

## The proof of the Kepler Conjecture

- 18th problem of the Hilbert's list
- Fejes Tóth: local density approach

Mathematics as we practice it is much more formally complete and precise than other sciences, but it is much less formally complete and precise for its content than computer programs
W. P Thurston 1994


- Hsiang: close enough but judged incomplete 1990
- Hales' program: The Sphere Packing Problem

Comp. App. Math. 1992

- 6 preprints by Hales and Ferguson

ArXiv 1998
$>50000+137000$ lines of code

- reviewing: 13 reviewers, 3 years... " $99 \%$ certain"
- 6 edited papers

Discrete \& Computational Geometry 2006

- Flyspeck project: formal proof (HOL Light and Isabelle) 2003-2014
Forum of Mathematics, Pi 2017


A packing is called triangulated if each "hole" is bounded by three tangent discs:


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(Packings by discs of radii $1, r$ ) There are 9 values of $r$ allowing triangulated packings.


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○○• Fernique, Hashemi, Sizova 2019
(Packings by discs of radii $1, r, s$ ) There are 164 pairs $(r, s)$ allowing triangulated packings.


Triangulated packings

## Even more motivation

triangulated packings


tilings by triangles with local rules
density $=$ weighted proportion of tiles

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## Triangulated Packing Problem

algebraic numbers represented by polynomials and intervals
Given $k$ disc radii $\overbrace{r_{1}, \cdots, r_{k}}$, is there a triangulated packing of density $\overbrace{>\frac{\pi}{2 \sqrt{3}}}$
$\forall r_{1}, \cdots, r_{k}$ with triangulated packings, one is periodic (Wang algorithm: search for a period)
$\exists r_{1}, \cdots, r_{k}$ whose triangulated packings are all aperiodic

## Even more motivation

## triangulated packings




density $=$ weighted proportion of tiles

## Dense Packing Problem

algebraic numbers represented by polynomials and intervals
Given $k$ disc radii $\overbrace{r_{1}, \cdots, r_{k}}$, is there a
excludes hexagonal packing packing of density $\overbrace{>\frac{\pi}{2 \sqrt{3}}}$
$\Rightarrow$
decidable (interval arithmetic and subdivision until needed precision)
$\exists r_{1}, \cdots, r_{k}$ whose dense packings are all aperiodic

Thue, 1910 (Toth, 1940)

The hexagonal packing maximizes the density.

Heppes 2000,2003; Kennedy 2004; Bedaride, Fernique, 2019


All these 9 triangulated packings maximize the density.

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Conjecture (Connelly, 2018)
If a finite set of discs allows a saturated triangulated packing then the density is maximized on a saturated triangulated packing.

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triangulated saturated

non triangulated saturated

triangulated non saturated

non triangulated non saturated

Triangulated packings
3 discs:

$164(r, s)$ allowing triangulated packings:
(Fernique, Hashemi, Sizova 2019)

- 15 cases: non saturated
- 40 cases: a binary non triangulated packing is denser (Fernique, P 2022)
- case 53: a ternary triangulated packing is densest
(Fernique 2019)
- $15+15$ more cases: a ternary or binary triangulated packing is densest
(Fernique, P 2022)



## Delaunay triangulation



Show that for any saturated packing $P$,

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\delta^{*} \geq \delta
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Delaunay triangulation of a packing: dual graph of the Voronoi diagram Main property: no points inside the circumscribed circle of any triangle

Density of a triangle $\Delta$ in a packing $=$ its proportion covered by discs

$$
\delta_{\Delta}=\frac{\operatorname{area}(\Delta \cap P)}{\operatorname{area}(\Delta)}
$$


$\delta^{*}=\delta_{\Delta^{*}}=\frac{\pi}{2 \sqrt{3}}$

$\forall \Delta, \delta_{\Delta} \leq \delta_{\Delta^{*}}=\delta^{*}$

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- The largest angle of any $\Delta$ is between $\frac{\pi}{3}$ and $\frac{2 \pi}{3} \quad \hat{A}<\frac{\pi}{6} \Rightarrow R=\frac{|B C|}{2 \sin \hat{A}} \geq \frac{1}{\sin \hat{A}}>2$
- The density of a triangle $\Delta: \delta_{\Delta}=\frac{\pi / 2}{\operatorname{area}(\Delta)}$
- The area of a triangle $A B C$ with the largest angle $\hat{B}$ is $\frac{1}{2}|A B| \cdot|B C| \cdot \sin \hat{B}$ which is at least $\frac{1}{2} \cdot 2 \cdot 2 \cdot \frac{\sqrt{3}}{2}=\sqrt{3}$
- Thus the density of $A B C$ is less or equal to $\frac{\pi / 2}{\sqrt{3}}=\delta_{\Delta^{*}}$

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FM-triangulation of packing $P^{*}$

Triangles in $P^{*}$ have different densities:


Hopeless to bound the density in each triangle... What to do?


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Density redistribution:



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Hopeless to bound the density in each triangle... What to do?

Density redistribution:


Dense triangles "share their density" with neighbors

## Emptiness instead of density


saturated triangulated packing $P^{*}$ density $\delta^{*}$, FM-triangulation $\mathcal{T}^{*}$

saturated packing $P$ with the same discs density $\delta$, FM -triangulation $\mathcal{T}$

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Density function is not additive: $\delta(\infty)+\delta(\infty)$

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saturated packing $P$ with the same discs density $\delta$, FM -triangulation $\mathcal{T}$

Density function is not additive: $\delta$


Emptiness of a triangle $\Delta \in \mathcal{T}: \quad E(\Delta)=\delta^{*} \times \operatorname{area}(\Delta)-\operatorname{area}(\Delta \cap P)$
$E(\Delta)>0$ iff the density of $\Delta$ is less than $\delta^{*}$
$E(\Delta)<0$ iff the density of $\Delta$ is greater than $\delta^{*}$
Additive!

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Additive!

$$
\delta^{*} \geq \delta \Leftrightarrow \sum_{\Delta \in \mathcal{T}} E(\Delta) \geq 0
$$

We construct a potential $U(\Delta):=\overbrace{\dot{U}_{\Delta}^{A}+\dot{U}_{\Delta}^{B}+\dot{U}_{\Delta}^{C}}^{\text {vertices }}$ such that
$\forall$ triangle $\Delta \in \mathcal{T}, U(\Delta) \leq E(\Delta)(\Delta)$

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If such $U$ exists then $\delta^{*} \geq \delta$
How to construct it and prove $(\Delta),(\bullet)$ ?
tight triangle: tangent discs of radii $x, y, z$ angle of $\Delta_{x y z}$ in the center of the $y$-disc potential of $\Delta_{x y z}$ in the center of the $y$-disc


## Choosing $U$ to assure (॰)



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tight triangle: tangent discs of radii $x, y, z$ angle of $\Delta_{x y z}$ in the center of the $y$-disc potential of $\Delta_{x y z}$ in the center of the $y$-disc potential of a triangle $\Delta$ in $v$ :

$$
\dot{U}_{\Delta}^{v}:=V_{x y z}+m|\hat{v}-\widehat{x y z}|
$$

measures how "far" $\Delta$ is from being tight


Choose $m$ to satisfy $\sum_{\Delta \in C_{v}} \dot{U}_{\Delta}^{v} \geq \sum_{\substack{x, y, z \\ \text { disc } \\ \Delta \in C_{v} \\ \text { adi of }}} V_{x y z}+m \times\left|2 \pi-\sum_{\substack{x, y, z \\ \text { disc radii of } \\ \Delta \in C_{v}}} \widehat{x y z}\right| \geq 0$ for all coronas $C_{v}$

## Choosing $U$ to assure (॰)


angle values do not matter $\Rightarrow$
FM-triangulation $\Rightarrow$
sequence of disc radii $S\left(C_{v}\right)$ bounded $\left|S\left(C_{v}\right)\right|$
finite number of linear inequalities on $m$

$$
\Rightarrow \text { computer search }
$$

Defining $U$, we make it as small as possible keeping it positive around any vertrex $(\bullet)$
$(\Delta)$ : How to check $E(\Delta) \geq U(\Delta)$ on each triangle $\Delta$ ? (there is a continuum of them)

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FM-triangulation properties + saturation $\Rightarrow$ uniform bound on edge length


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interval arithmetic
verify $E\left(\Delta_{a, b, c}\right) \geq U\left(\Delta_{a, b, c}\right)$ where

$$
a=\left[r_{c}+r_{b}, r_{c}+r_{b}+2 s\right] b=\left[r_{a}+r_{c}, r_{a}+r_{c}+2 s\right] c=\left[r_{a}+r_{b}, r_{a}+r_{b}+2 s\right]
$$

not precise enough (intervals intersect) $\rightarrow$ dichotomy

## Proof for OO

## Inequalities and interval arithmetic

A representation of a number $x$ is an interval I whose endpoints are exact values representable in a computer memory and such that $x \in I$.

```
sage: x = RIF (0,1)
sage: x<2
True
sage: (x+x).endpoints()
(0.0, 2.0)
sage: Ipi = 4*arctan(RIF(1))
(3.14159265358979, 3.14159265358980)
sage: sin(Ipi).endpoints()
(-3.21624529935328e-16, 1.22464679914736e-16)
```

```
    # Interval for }
    # Interval [0,1]
    # \forallt [ [0,1], t<2
        # [0,1]+[0,1]
# Interval for sin(\pi)
```


## Proof for $\mathrm{OO}^{\circ}$

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Two intersecting intervals are incomparable:
sage: sin(Ipi)<=x
False
sage: sin(Ipi)>=x
False
# These intervals intersect
```


## Our proof worked for these cases:



## And these:



1


2


3


5


6


11


## Steps of the proof

$\delta^{*}$ denotes the maximal density

○|○०○ $\mid$ © partition space into "small" cells

○○○○ 0 (2) find a suitable function to represent the density

FM-triangulation
emptiness $E$

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o| $\circ \cdot 0$ (2) find a suitable function to represent the density
emptiness $E$
$\bigcirc \bullet \cdot$ (3) distribute the density among the vertices in each cell
potential $\dot{U}$
$\bigcirc \bullet \circ$ ( ) verify that the redistributed density $\leq \delta^{*}$
(•) choice of $m$ in $\dot{U}$
check all possible local configurations run through all coronas
©००| (0) treat special cases which can not be treated by this technique which are usually configurations close to local maxima

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○००| (O) treat special cases which can not be treated by this technique which are usually configurations close to local maxima
00.(2) verify that the sum of vertex densities in a cell $\geq$ its density interval arithmetic check all possible cells

## Space partition

2D,
Delaunay triangulation

2D, ○○•
FM-triangulation $\mathcal{T}$
(weighted Delaunay triangulation)

3D,
$\underbrace{\text { Voronoi cells + Delaunay simplices }}$
HF-partition $\mathcal{P}$
consists of several types of simplices and modified Voronoi cells
(Sphere packings II. A formulation of the Kepler Conjecture)
only Voronoi cells or only Delaunay simplices $\Downarrow$
local configurations denser than $\delta^{*}$ regular dodecahedron for Voronoi cells (as in dodecahedral conjecture)



Hales and McLaughlin 1998

## Space partition



2D, ○○•
FM-triangulation $\mathcal{T}$
(weighted Delaunay triangulation)

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only Voronoi cells or only Delaunay simplices $\Downarrow$
local configurations denser than $\delta^{*}$ pentagonal prism for Delaunay simplices


Ferguson 2006

## Suitable function to measure the density

| 2D, | 2D, Oo• | 3D, 0 |
| :---: | :---: | :---: |
| $\begin{aligned} & \text { density } \\ & \delta \end{aligned}$ | emptiness | compression |
|  | $E(\Delta):=\delta^{*} \times \operatorname{area}(\Delta)-\operatorname{area}(\Delta \cap P)$ | $\Gamma(R):=\operatorname{vol}(R \cap P)-\delta_{\text {oct }} \times \operatorname{vol}(R)$ |
|  |  | $\delta_{\text {oct }}:=\delta($ tight regular octahedron $)<\delta^{*}$ |
|  |  | $\delta^{*}=\frac{\delta_{\text {ret }}}{3}+2 \frac{\delta_{\text {oct }}}{3}$ |

## Suitable function to measure the density

$$
\begin{array}{lll}
2 \mathrm{D}, \bigcirc & 2 \mathrm{D}, \bigcirc 0 \bullet & \text { 3D, } \bigcirc \\
\text { density } & \text { emptiness } & \text { compression } \\
\delta & E(\Delta):=\delta^{*} \times \operatorname{area}(\Delta)-\operatorname{area}(\Delta \cap P) & \Gamma(R):=\operatorname{vol}(R \cap P)-\delta_{\text {oct }} \times \operatorname{vol}(R) \\
& \delta_{\text {oct }}:=\delta(\text { tight regular octahedron })<\delta^{*} \\
& \delta^{*}=\frac{\delta_{\text {tet }}}{3}+2 \frac{\delta_{o c t}}{3}
\end{array}
$$

An additive function reflecting the density:
$\Gamma(R)<0$ iff the density of $R$ is less than $\delta_{\text {oct }}$

$$
\Gamma(R)>0 \text { iff the density of } R \text { is greater than } \delta_{\text {oct }}
$$

$$
\delta \leq \delta^{*} \Leftarrow \Gamma \text { is "low enough" on each small region }
$$

## Redistribution of emptiness and compression

2D, ○○•
vertex potential
for $\Delta \in \mathcal{T}, v \in \Delta$,
$\dot{U}_{\Delta}^{v}=V_{x y z}+m \times\left|\hat{v}-\hat{v}_{x y z}\right|$
where $x, y, z$ are disc radii of $\Delta$ $\hat{v}$ is the angle of $\Delta$ in $v$ and $V_{x y z}, m, \hat{v}_{x y z}$ are constants

3D, $\bigcirc$
score
for $R \in \mathcal{P}, v \in R$,
$\sigma(R, v)$ depends on the type of $R$
if $R$ is a Voronoi cell of $v(R=\operatorname{Vor}(v))$,
then $\sigma(R, v)=4 \Gamma(R)$
and $\sigma(R, w)=0$ for $w \neq v$
if $R$ is a simplex, $\sigma$ varies in function of its properties and depends on $\Gamma$

## Redistribution of emptiness and compression

2D,
vertex potential
for $\Delta \in \mathcal{T}, v \in \Delta$,
$\dot{U}_{\Delta}^{\nu}=V_{x y z}+m \times\left|\hat{v}-\hat{v}_{x y z}\right|$
where $x, y, z$ are disc radii of $\Delta$ $\hat{v}$ is the angle of $\Delta$ in $v$ and $V_{x y z}, m, \hat{v}_{x y z}$ are constants
$U(\Delta)=U_{\Delta}^{A}+U_{\Delta}^{B}+U_{\Delta}^{C} \leq E(\Delta)$
i.e. $U$ is easy to manipulate and is at most $E$ (lower approximation)

3D,
score
for $R \in \mathcal{P}, v \in R$,
$\sigma(R, v)$ depends on the type of $R$
if $R$ is a Voronoi cell of $v(R=\operatorname{Vor}(v))$,
then $\sigma(R, v)=4 \Gamma(R)$
and $\sigma(R, w)=0$ for $w \neq v$
if $R$ is a simplex, $\sigma$ varies in function of its properties and depends on $\Gamma$
$\sum_{v \in R} \sigma(R, v)=4 \Gamma(R)$
i.e. score of a region always equals to
$4 \times$ compression
(Sphere packings II. A formulation of the Kepler Conjecture)

## Verify that redistribution $\leq \delta^{*}$ around each vertex

$$
\begin{aligned}
& \text { 2D, OO } \\
& \text { for each } v \in \mathcal{T}, \sum_{\Delta \in C_{v}} \dot{U}_{\Delta}^{v} \geq 0
\end{aligned}
$$

configuration around a vertex - corona C
combinatorial representation of $C$ sequence of disc radii $S(C)$
choose $m$ to satisfy


FM-triangulation $\Rightarrow$ bounded $|S(C)|$
$\Rightarrow$ finite number of inequalities on $m$
$\Rightarrow$ computer search

3D, $\bigcirc$ for each $v \in \mathcal{P}, \sum_{R \in D_{v}} \sigma(R, v) \leq 8 p t$ configuration around a vertex decomposition star $D$
combinatorial representation of $D$ graph $G(D)$
conditions on geometry of $D$ "easily" implying $\sigma(D) \leq 8 p t$ (interval arithmetics) (Sphere packings IV. Detailed bounds)
tame graphs - 25000 graphs of the remaining $D$ have restricted geometry $\Rightarrow \max \sigma(D) \leq 8 p t$ (linear programming)
(Sphere packings VI. Tame graphs and linear programs) except pentagonal prism graph,

## Verify that redistribution $\leq \delta^{*}$ around each vertex

| 2D, ○○• |
| :---: |
| for each $v \in \mathcal{T}, \sum \dot{U}_{\Delta}^{v} \geq$ |
| configuration around a vertex |
| corona C |
| combinatorial representation of C sequence of disc radii $S(C)$ |
|  |
| $\sum_{\substack{x, y, z \\ \text { disc radii of } \\ \Delta \in C}} V_{x y z}+m \times\left\|2 \pi-\sum_{\substack{x, y, z \\ \text { disc } \\ \Delta \in d i i \\ \Delta \in C}} \widehat{x y z}\right\| \geq 0$ |
| for all coronas $C$ |
| FM-triangulation $\Rightarrow$ bounded $\|S(C)\|$ <br> $\Rightarrow$ finite number of inequalities on $m$ <br> $\Rightarrow$ computer search |
| (linear programming) |

3D,
for each $v \in \mathcal{P}$,
configuration around a vertex decomposition star $D$
combinatorial representation of $D-$ graph $G(D)$
conditions on geometry of $D$ "easily" implying $\sigma(D) \leq 8 p t$ (interval arithmetics)
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(Sphere packings VI. Tame graphs and linear programs) except pentagonal prism graph,
(Sphere packing V. Pentahedral prisms)
FCC graph and HCP graph
(Sphere packings III. Extremal cases)

## Extremal cases

2D, ○○•


$$
\text { for the coronas of } \mathcal{T}^{*}, \sum_{\substack{x, y, z \\ \text { disc radii of } \\ \Delta \in y \text {-corona }}} V_{x y z}:=0
$$

for tight triangles, $U\left(\Delta_{x y z}\right):=E\left(\Delta_{x y z}\right)$
$\epsilon$-triangles - triangles close to tight $\Rightarrow$ potential close to emptiness

3D,


FCC and HCP decomposition stars have maximal score
$\Rightarrow$ close configurations have high score

## Extremal cases


for the coronas of $\mathcal{T}^{*}, \sum_{\substack{x, y, z \\ \text { disc radii of } \\ \Delta \in y-\text { orona }}} V_{x y z}:=0$
for tight triangles, $U\left(\Delta_{x y z}\right):=E\left(\Delta_{x y z}\right)$
$\epsilon$-triangles - triangles close to tight
$\Rightarrow$ potential close to emptiness
derivatives on side lengths $x_{i}$ :
$\min _{T_{\epsilon}} \frac{\partial E}{\partial x_{i}} \Delta x_{i} \geq \max _{T_{\epsilon}} \frac{\partial U}{\partial x_{i}} \Delta x_{i}$
(interval arithmetic)

$$
\text { 3D, } 0
$$



FCC and HCP decomposition stars have maximal score
$\Rightarrow$ close configurations have high score
derivatives to prove that FCC and HCP are local maxima
(Sphere packings III. Extremal cases)

## Work in progress:

## Locally halite packing

triangulated $\rightarrow$ simplicial
(contact graph is a pure simplicial 3-complex)
halite packing is formed by a close-packing of unit spheres where all octahedral holes are filled with spheres of radius $\sqrt{2}-1$

## Fernique, 2019

The only simplicial packings by two sizes of spheres in 3D are halite packings.

## Work in progress: $\bigcirc$

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## Fernique, 2019

The only simplicial packings by two sizes of spheres in 3D are halite packings.

## Conjecture

Halite packings maximize the density.

- simplicial partition
- vertex or edge potential?
- sphere triangulations or necklaces?
- bound density inside a tetrahedron (dimension reduction+derivatives)


## Thank you for your attention! :-)

A packing is triangulated


Each disc has a "corona"


## How to find triangulated packings

A packing is triangulated


Each disc has a "corona"


To find disc sizes with triangulated packings, we run trough all possible combinations of symbolic coronas of two discs (finite number)

Symbolic corona

$$
\begin{array}{lll}
r & \mathbb{I} \\
r^{r} & \mathbb{1} & r \\
\mathbb{1} & r & \mathbb{1}
\end{array}
$$

## How to find triangulated packings

A packing is triangulated


Each disc has a "corona"


To find disc sizes with triangulated packings, we run trough all possible combinations of symbolic coronas of two discs (finite number)

Symbolic corona



Value of $r$

$$
\begin{aligned}
& 6 \times \widehat{11 r}+1 \times \widehat{r 1 r}=2 \pi \\
& r \approx 0.63
\end{aligned}
$$

## Edge Potentials

Stretched triangles feature low emptiness but high vertex potential:


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Their neighbors feature high emptiness, so we can "balance" potential between them.

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Stretched triangles feature low emptiness but high vertex potential:


Their neighbors feature high emptiness, so we can "balance" potential between them. To do this, we introduce edge potential: $U(\Delta):=\dot{U}_{\Delta}+\bar{U}_{\Delta}$

$$
\begin{aligned}
& \bar{U}_{\Delta}=\bar{U}_{\Delta}^{e_{1}}+\bar{U}_{\Delta}^{e_{2}}+\bar{U}_{\Delta}^{e_{3}} \\
& \bar{U}_{\Delta}^{e}:= \begin{cases}q d_{e} & \text { if }|e|>/ \\
0 & \text { otherwise }\end{cases}
\end{aligned}
$$

## 40 counter examples



When the ratio of two discs is close enough to the ratio in a dense binary packing, we can pack these disc in a similar manner (non triangulated) and still get high density

## Examples:



counter example
using only 2 discs

triangulated
ternary pack ternary packing

counter example using only 2 discs


