

Density of sphere packings: from coins to oranges

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supervised by

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Density of sphere packings



Plan

- What is a packing?
- Packing O in 2D and O in 3D
- Triangulated packings
- Proof for O
- Proof for Oo
- Proof strategies for O, O = and O
- Work in progress:

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Density of sphere packings

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$$\delta(P) = \limsup_{n \to \infty} \frac{\operatorname{area}([-n, n]^2 \cap P)}{\operatorname{area}([-n, n]^2)}$$



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Main Question

Given a finite set of discs (e.g., $\bigcirc \bigcirc \bullet$), which packing maximizes the density?

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Density of sphere packings

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Motivation

• Packing fruits and vegetables

Motivation

• 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.

Packing 🔵 in 2D and 🕘 in 3D



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

2D hexagonal 🔵 -packing:

Lagrange, 1772 Hexagonal packing maximizes the density among lattice 🔵 -packings. Thue, 1910 (Fejes Tóth, 1940)

Hexagonal packing maximizes the density.

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Packing o in 2D and o in 3D

The proof of the Kepler Conjecture

	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
• 18th problem of the Hilbert's list	1900
• Fejes Tóth: local density approach	1953
• Hsiang: close enough but judged incomp	plete 1990
• Hales' program: The Sphere Packing Pr	oblem . Comp. App. Math. 1992
 6 preprints by Hales and Ferguson > 50000 + 137000 lines of code 	ArXiv 1998
• reviewing: 13 reviewers, 3 years "99%	certain"
• 6 edited papers	Discrete & Computational Geometry 2006
 Flyspeck project: formal proof (HOL Lig 	ht and Isabelle) 2003–2014 Forum of Mathematics, Pi 2017

Density of sphere packings

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



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O Kennedy, 2006

(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.



Even more motivation







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tilings by triangles

with local rules

 $density = weighted \ proportion \ of \ tiles$

Even more motivation



density = weighted proportion of tiles

Triangulated Packing Problem



$\forall r_1, \cdots, r_k$ with triangu	lated packings, one is periodic	\Rightarrow		decidable
(Wang algorithm: search	n for a period)			
$\exists r_1, \cdots, r_k$ whose triangulated packings are all aperiodic		\Rightarrow	und	ecidable?
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Even more motivation



Dense Packing Problem

algebraic numbers represented by polynomials and intervals	excludes hexagonal packing
Cives / disc vedicionali	π
Given k disc radii r_1, \cdots, r_k , is there a	packing of density $> \frac{1}{2\sqrt{3}}$
	203

e!
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Density of sphere packings

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Thue, 1910 (Toth, 1940)

The hexagonal packing maximizes the density.





Thue, 1910 (Toth, 1940)

The hexagonal packing maximizes the density.



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



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 saturated

Density of sphere packings





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)

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Delaunay triangulation





 ${\it P}$ of density δ

Show that for any saturated packing P,

 $\delta^* \geq \delta$

Delaunay triangulation



Voronoi cell of a disc in a packing: set of points closer to this disc than to any other Voronoi diagram of a packing: partition of the plane into Voronoi cells

Delaunay triangulation





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Delaunay triangulation of a packing: dual graph of the Voronoi diagram

Delaunay triangulation



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Voronoi cell of a disc in a packing: set of points closer to this disc than to any other Voronoi diagram of a packing: partition of the plane into Voronoi cells

Delaunay triangulation of a packing: dual graph of the Voronoi diagram Main property: no points inside the circumscribed circle of any triangle

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Density of sphere packings

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Density of a triangle Δ in a packing = its proportion covered by discs

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





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Density of a triangle Δ in a packing = its proportion covered by discs $\delta_{\Delta} = \frac{\operatorname{area}(\Delta \cap P)}{\operatorname{area}(\Delta)}$



- The largest angle of any Δ is between $\frac{\pi}{3}$ and $\frac{2\pi}{3}$ $\hat{A} < \frac{\pi}{6} \Rightarrow R = \frac{|BC|}{2\sin\hat{A}} \ge \frac{1}{\sin\hat{A}} > 2$
- The density of a triangle Δ : $\delta_{\Delta} = \frac{\pi/2}{area(\Delta)}$
- The area of a triangle ABC with the largest angle \hat{B} is $\frac{1}{2}|AB|\cdot|BC|\cdot\sin\hat{B}$ which is at least $\frac{1}{2}\cdot2\cdot2\cdot\frac{\sqrt{3}}{2}=\sqrt{3}$
- Thus the density of *ABC* is less or equal to $\frac{\pi/2}{\sqrt{3}} = \delta_{\Delta^*}$
Density of a triangle Δ in a packing = its proportion covered by discs $\delta_{\Delta} = \frac{\operatorname{area}(\Delta \cap P)}{\operatorname{area}(\Delta)}$



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- Thus the density of *ABC* is less or equal to $\frac{\pi/2}{\sqrt{3}} = \delta_{\Delta^*}$



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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FM-triangulation of packing P^*

Density redistribution:





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

FM-triangulation of packing P^*

Density redistribution:



Dense triangles "share their density" with neighbors

Emptiness instead of density



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



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

Emptiness instead of density



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



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Emptiness instead of density



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



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



Emptiness of a triangle $\Delta \in \mathcal{T}$: $E(\Delta) = \delta^* \times area(\Delta) - area(\Delta \cap P)$

 $E(\Delta) > 0$ iff the density of Δ is less than δ^* $E(\Delta) < 0$ iff the density of Δ is greater than δ^*

Additive!

Emptiness instead of density



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



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



Emptiness of a triangle $\Delta \in \mathcal{T}$: $E(\Delta) = \delta^* \times area(\Delta) - area(\Delta \cap P)$

 $E(\Delta) > 0$ iff the density of Δ is less than δ^* $E(\Delta) < 0$ iff the density of Δ is greater than δ^*

Additive!

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

Redistribution: potential

(inspired by Kennedy 2005)

We construct a **potential**
$$U(\Delta) := \overbrace{\dot{U}_{\Delta}^{A} + \dot{U}_{\Delta}^{B} + \dot{U}_{\Delta}^{C}}^{\text{vertices}}$$
 such that

 $\forall \text{ triangle } \Delta \in \mathcal{T}, \ U(\Delta) \leq E(\Delta) \ (\Delta)$

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```

$$\forall \text{ vertex } v \in \mathcal{T}, \sum_{\Delta \in C_{v}} \dot{U}_{\Delta}^{v} \geq 0 \quad (ullet)$$



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$$\forall \text{ vertex } v \in \mathcal{T}, \sum_{\Delta \in \mathcal{C}_v} \dot{U}^v_\Delta \geq 0 \qquad (\bullet) \ \Rightarrow \sum_{\Delta \in \mathcal{T}} U(\Delta) \geq 0$$



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Redistribution: potential

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If such U exists then $\delta^* \geq \delta$

How to construct it and prove (Δ) , (\bullet) ?

Choosing *U* to assure (•)

(inspired by Kennedy 2005)

 Δ_{xyz} \widehat{xyz} V_{xyz} tight triangle: tangent discs of radii x, y, zangle of Δ_{xyz} in the center of the y-disc potential of Δ_{xyz} in the center of the y-disc



Choosing U to assure (•)

(inspired by Kennedy 2005)

 Δ_{xyz} \widehat{xyz} V_{xyz}

tight triangle: tangent discs of radii x, y, zangle of Δ_{xyz} in the center of the y-disc potential of Δ_{xyz} in the center of the y-disc

potential of a triangle Δ in v:

$$\dot{U}_{\Delta}^{v} \coloneqq V_{xyz} + m |\hat{v} - \widehat{xyz}|$$

measures how "far" Δ is from being tight



Choosing *U* to assure (•)

tight triangle: tangent discs of radii x, y, z angle of Δ_{xyz} in the center of the y-disc potential of Δ_{xyz} in the center of the y-disc

potential of a triangle Δ in v:

$$\dot{U}^{v}_{\Delta} \coloneqq V_{xyz} + m |\hat{v} - \widehat{xyz}|$$

measures how "far" Δ is from being tight

 $\begin{array}{l} \text{Choose } m \text{ to satisfy } \sum_{\Delta \in \mathcal{C}_{\nu}} \dot{U}_{\Delta}^{\nu} \geq \sum_{\substack{x,y,z \\ \text{disc radii of} \\ \Delta \in \mathcal{C}_{\nu}}} V_{xyz} + m \times |2\pi - \sum_{\substack{x,y,z \\ \text{disc radii of} \\ \Delta \in \mathcal{C}_{\nu}}} \widehat{xyz}| \geq 0 \text{ for all coronas } \mathcal{C}_{\nu} \end{array}$



Choosing U to assure (•)

bounded $|S(C_v)|$

28



$$\Delta_1$$

angle values do not matter \Rightarrow

FM-triangulation \Rightarrow

finite number of linear inequalities on m \Rightarrow computer search

sequence of disc radii $S(C_v)$

(inspired by Kennedy 2005)



Defining U, we make it as small as possible keeping it positive around any vertrex (ullet)

(Δ): How to check $E(\Delta) \ge U(\Delta)$ on each triangle Δ ? (there is a continuum of them)

(∆**)**

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



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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 $x \in I$.

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```
sage: x = RIF(0,1)
                                                                 # Interval [0,1]
sage: x<2</pre>
                                                                # \forall t \in [0,1], t < 2
True
sage: (x+x).endpoints()
                                                                    # [0,1]+[0,1]
(0.0, 2.0)
sage: Ipi = 4*arctan(RIF(1))
(3.14159265358979, 3.14159265358980)
                                                                # Interval for \pi
sage: sin(Ipi).endpoints()
(-3.21624529935328e-16, 1.22464679914736e-16)
                                                            # Interval for sin(\pi)
Two intersecting intervals are incomparable:
sage: sin(Ipi)<=x</pre>
False
sage: sin(Ipi)>=x
False
                                                    # These intervals intersect
```

Our proof worked for these cases:



53

66

93

118







56

















116











And these:

























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Density of sphere packings

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Steps of the proof

- δ^* denotes the maximal density

FM-triangulation

emptiness E

Steps of the proof

- δ^{\ast} denotes the maximal density

Steps of the proof

- δ^{\ast} denotes the maximal density
- FM-triangulation emptiness Epotential \dot{U} (•) choice of *m* in *U* check all possible local configurations run through all coronas ϵ -triangles which are usually configurations close to local maxima coronas of \mathcal{T}^*

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Space partition

2D, 🔵

Delaunay triangulation 2D, 🔵 💽 🔹

FM-triangulation \mathcal{T} (weighted Delaunay triangulation)





3D, 🔴

Voronoi cells + Delaunay simplices

 $\mathsf{HF}\text{-}\mathsf{partition}\ \mathcal{P}$

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 ↓

local configurations denser than δ^{\ast}

regular dodecahedron for Voronoi cells (as in dodecahedral conjecture)





Hales and McLaughlin 1998

Space partition

2D, 🔵

Delaunay triangulation 2D, 🔵 💽 🔹

FM-triangulation \mathcal{T} (weighted Delaunay triangulation)





3D, 🔴

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only Voronoi cells or only Delaunay simplices \downarrow local configurations denser than δ^* pentagonal prism for Delaunay simplices





Ferguson 2006

Suitable function to measure the density

2D, \bigcirc 2D, $\bigcirc \bullet \bullet$ density emptiness δ



compression

 $\textit{E}(\Delta) := \delta^* \times \textit{area}(\Delta) - \textit{area}(\Delta \cap \textit{P}) \quad \ \ \Gamma(R) := \textit{vol}(R \cap \textit{P}) - \delta_{\sf oct} \times \textit{vol}(R)$

 $\delta_{\mathsf{oct}} := \delta(\mathsf{tight regular octahedron}) < \delta^*$

$$\delta^* = \frac{\delta_{\text{tet}}}{3} + 2\frac{\delta_{\text{oct}}}{3}$$

Suitable function to measure the density

2D, 2D, 4 density δ emptiness $E(\Delta) := \delta^* \times area(\Delta) - area(\Delta \cap P)$ $E(\Delta) := \delta^* \times area(\Delta) - area(\Delta \cap P)$ $C(R) := vol(R \cap P) - \delta_{oct} \times vol(R)$ $\delta_{oct} := \delta(\text{tight regular octahedron}) < \delta^*$ $\delta^* = \frac{\delta_{\text{tet}}}{3} + 2\frac{\delta_{oct}}{3}$

An additive function reflecting the density:

 $\Gamma(R) < 0$ iff the density of *R* is less than δ_{oct} $\Gamma(R) > 0$ iff the density of *R* is greater than δ_{oct}

 $\delta \leq \delta^* \leftarrow \Gamma$ is "low enough" on each small region

Redistribution of emptiness and compression

2D, 🔵 💽 🔹

vertex potential

$$egin{array}{lll} ext{for } \Delta \in \mathcal{T}, m{v} \in \Delta, \ \dot{U}^{m{v}}_{\Delta} = V_{ ext{xyz}} + m{m} imes | \hat{m{v}} - \hat{m{v}}_{ ext{xyz}} | \end{array}$$

where x, y, z are disc radii of Δ \hat{v} is the angle of Δ in vand $V_{xyz}, m, \hat{v}_{xyz}$ are constants

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 = Vor(v)), then $\sigma(R, v) = 4\Gamma(R)$ and $\sigma(R, w) = 0$ for $w \neq v$

if R is a simplex, σ varies in function of its properties and depends on Γ

Redistribution of emptiness and compression

2D, 🔵 💽 🔹

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if R is a simplex, σ varies in function of its properties and depends on Γ

$$U(\Delta) = U_{\Delta}^{A} + U_{\Delta}^{B} + U_{\Delta}^{C} \leq E(\Delta)$$

i.e. U is easy to manipulate and is at most E (lower approximation)

$$\sum_{v\in R}\sigma(R,v)=4\Gamma(R)$$

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

2D, 🔵 💽 🔹

for each $v \in \mathcal{T}, \sum_{\Delta \in C_v} \dot{U}_{\Delta}^v \ge 0$

configuration around a vertex – corona C

combinatorial representation of C – sequence of disc radii S(C)

 $\sum_{\substack{x,y,z\\ \text{disc radii of}\\ \Delta \in C}} V_{xyz} + m \times |2\pi - \sum_{\substack{x,y,z\\ \text{disc radii of}\\ \Delta \in C}} \widehat{xyz} | \ge 0$

for all coronas *C*

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

(linear programming)

3D, 🔴

 $\begin{array}{l} \text{for each } v \in \mathcal{P}, \ \sum_{R \in D_v} \sigma(R, v) \leq 8 pt \\ \text{configuration around a vertex } - \\ \text{decomposition star } D \end{array}$

combinatorial representation of $D-{\rm graph}~G(D)$

conditions on geometry of D "easily" implying $\sigma(D) \leq 8pt$ (interval arithmetics)

(Sphere packings IV. Detailed bounds)

tame graphs – 25 000 graphs of the remaining D have restricted geometry $\Rightarrow \max \sigma(D) \le 8pt$ (linear programming)

(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)

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Density of sphere packings

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

2D, 🔵 💽 🔹

for each $v \in \mathcal{T}, \sum_{\Delta \in C_v} \dot{U}^v_\Delta \ge 0$ configuration around a vertex – corona C

combinatorial representation of C – sequence of disc radii S(C)

 $\sum_{\substack{x,y,z\\\text{disc radii of}\\\Delta\in C}} V_{xyz} + m \times |2\pi - \sum_{\substack{x,y,z\\\text{disc radii of}\\\Delta\in C}} \widehat{xyz}| \ge 0$

for all coronas C

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

(linear programming)

3D, 🔴

for each $v \in \mathcal{P}$, $\sum_{R \in D_v} \sigma(R, v) \le 8pt$ configuration around a vertex – decomposition star D

combinatorial representation of D – graph G(D)

conditions on geometry of D "easily" implying $\sigma(D) \leq 8 pt$ (interval arithmetics)

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FCC graph and HCP graph

(Sphere packings III. Extremal cases)

Extremal cases



 ϵ -triangles – triangles close to tight \Rightarrow potential close to emptiness



FCC and HCP decomposition stars have maximal score

 \Rightarrow close configurations have high score
Proof strategies for \bigcirc , $\bigcirc \bigcirc \circ$ and \bigcirc

3D, 🔴

Extremal cases



for tight triangles, $U(\Delta_{xyz}) := E(\Delta_{xyz})$

 ϵ -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)



FCC and HCP decomposition stars have maximal score

 \Rightarrow close configurations have high score

derivatives to prove that FCC and HCP are local $\ensuremath{\mathsf{maxima}}$

(Sphere packings III. Extremal cases)

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.

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Fernique, 2019

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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! :-)

How to find triangulated packings

A packing is triangulated



Each disc has a "corona"



How to find triangulated packings



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

Symbolic corona

(Fernique, Hashemi, Sizova 2019)

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How to find triangulated packings



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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: $U(\Delta) := \dot{U}_{\Delta} + \bar{U}_{\Delta}$

$$ar{U}_\Delta = ar{U}_\Delta^{e_1} + ar{U}_\Delta^{e_2} + ar{U}_\Delta^{e_3}$$

$$ar{U}^e_\Delta := egin{cases} q d_e & ext{if } |e| > l \ 0 & ext{otherwise} \end{cases}$$

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

