A macro-meso-microscopic view of disk packing

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(based on work with Aaron Abrams, Jamie Pommersheim,
Alex Russell, Henry Landau, and Zeph Landau,
and work with Henry Cohn and Omer Tamuz;
aided by helpful conversations with Tibor Beke,
Ilya Chernykh, David Feldman, Boris Hasselblatt,
Alex Iosevich, Sinai Robins, and MathOverflow)

Slides at http://jamespropp.org/paris20a.pdf

In 2016 there were breakthroughs in sphere-packing in 8 dimensions and 24 dimensions.

This work came on the heels of earlier work on sphere packing in 3 dimensions, from Johannes Kepler to Thomas Hales, as well as work on sphere packing in 2 dimensions, commenced by Axel Thue and László Fejes-Tóth.

But for other values of n, we know very little, and I suspect that we still aren't asking exactly the right question.

I want to take a fresh look at $n = 2$.

It's "obvious" that in two dimensions, the optimal packing is the six-around-one hexagonal close packing.

But is it obvious what "optimal" means, or what it should mean?

It's my hope that by sharpening our notion of what it means for something to be an *optimal* sphere-packing, we'll obtain a coherent notion of what it might mean to classify all the optimal packings in n dimensions.

Part I: Density and optimality for sphere-packings

A **sphere-packing** of $\mathbb{R}^n$ is a collection of balls in $\mathbb{R}^n$ with disjoint interiors.

The density of a packing is

$$\lim_{r \to \infty} \lambda(S \cap B_r)/\lambda(B_r),$$

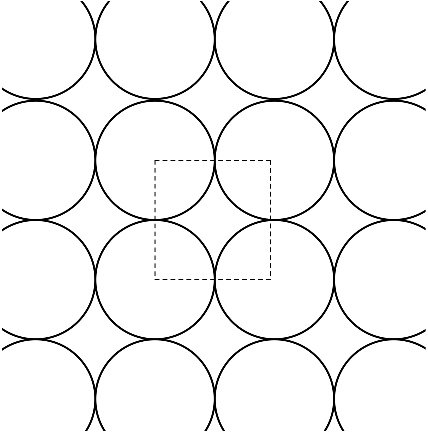
where B_r is the ball of radius r centered at 0,
S is the union of the balls in the packing, and
λ is n-dimensional Lebesgue measure.

Define Δ_n as the supremum of all densities of sphere-packings in $\mathbb{R}^n$ with all spheres having radius 1.

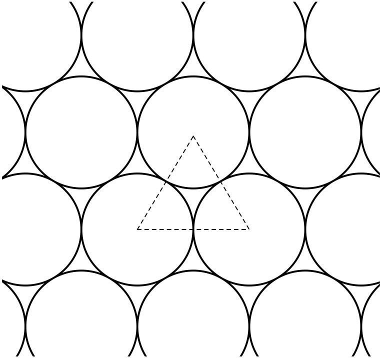
It's not hard to show that some packing achieves this supremum.

Trivially, $\Delta_1 = 1$.

The density of a 4-around-1 disk-packing is $\frac{\pi}{4} \approx 0.79$ (the fraction of a square joining 4 adjacent centerpoints covered by disks).



The density of a 6-around-1 disk-packing is $\frac{\pi}{\sqrt{12}} \approx 0.91$ (the fraction of a triangle joining 3 adjacent centerpoints covered by disks).



Axel Thue and László Fejes-Tóth's theorem: $\Delta_2 = \pi/\sqrt{12}$.

Let P be a packing of the plane by unit disks. If P is a hexagonal close packing, then P achieves density Δ_2.

Partial converse: Let P be a *periodic* packing of the plane by unit disks. If P achieves density Δ_2, then P is a hexagonal close packing.

Can we delete the word "periodic"?

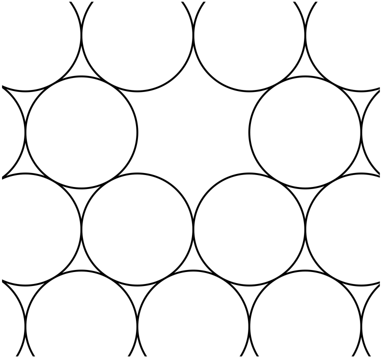
Let P be a packing of the plane by unit disks. If P is a hexagonal close packing, then P achieves density Δ_2.

Partial converse: Let P be a *periodic* packing of the plane by unit disks. If P achieves density Δ_2, then P is a hexagonal close packing.

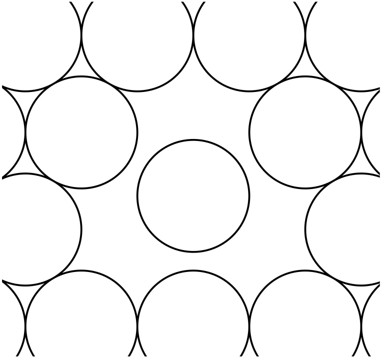
Can we delete the word "periodic"?

No.

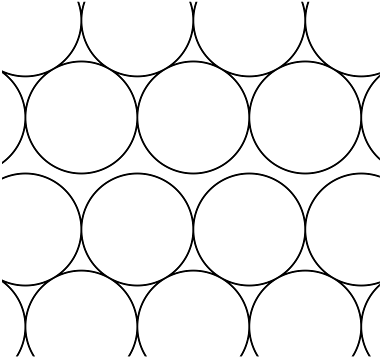
Counterexample 1:



Counterexample 2:



Counterexample 3:



Morally, these counterexamples seem like “cheats”.

How can we sharpen our notion of optimal packing to rule them out?

We’ll use an analytic trick of the sort that number-theorists have been using for over a century.

To see the analytic trick in action without geometric complications, let’s take things down a dimension first.

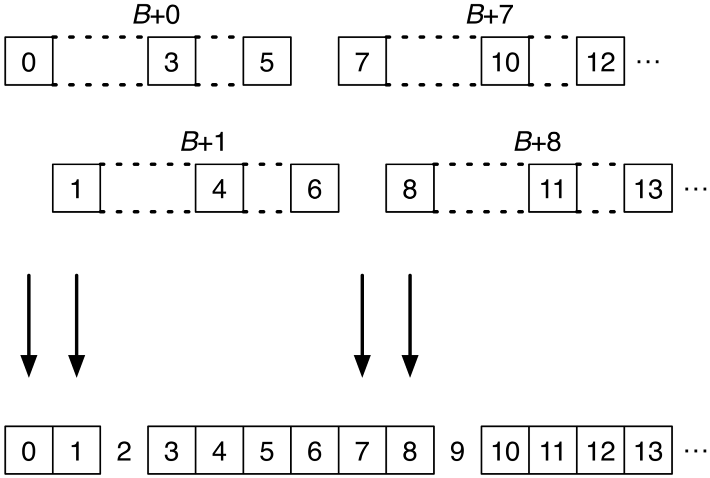
Part II: Packing problems in the natural numbers

(based on Germ Order for One-Dimensional Packing,
see also https://arxiv.org/abs/1807.06495 after Wednesday

Given a finite nonempty subset B of $\mathbb{N}$ (a *packing body*), say that a set $T \subseteq \mathbb{N}$ is a *translation set* for B iff the translates $B + n \ \ (n \in T)$ are disjoint.

The density of the packing is the density of the set $B + T$.

Running example: $B = \{0, 3, 5\}$, $T = \{0, 1, 7, 8, 14, 15, \dots\}$. The density of T is $2/7$; the density of $B + T$ is $|B| \times 2/7 = 6/7$.



B+0
B+7
0
3
5
7
10
12
B+1
B+8
1
4
6
8
11
13
0
1
2
3
4
5
6
7
8
9
10
11
12
13

Packings that achieve maximal density exist but are not unique.

(. . . because, for instance, deleting a translate of B, or shifting all the translates of B to the right, doesn't affect the density of the packing)

We need a more refined way of measuring density.

What we present here can be viewed as a way of measuring infinitesimal density, though it is more naturally thought of as a way of measuring infinite cardinality in $\mathbb{N}$.

The generating function of $S \subseteq \mathbb{N}$ is $|S|_q := \sum_{n \in S} q^n$, which converges for all $-1 < q < 1$.

T is a translation set for B iff $|B|_q \, |T|_q$ has all coefficients equal to 0 or 1.

$$
\begin{aligned}
|B|_q &= 1 + q^3 + q^5, \\
|T|_q &= 1 + q + q^7 + q^8 + q^{14} + q^{15} + \ldots, \\
|B|_q\,|T|_q &= 1 + q + q^3 + q^4 + q^5 + q^6 + q^7 + q^8 + q^{10} + \ldots.
\end{aligned}
$$

$|S|_q$ is the power series expansion of a rational function iff (the indicator sequence of) the set S is eventually periodic; i.e., iff there exist $N \geq 0$ and $d \geq 1$ such that for all $n \geq N$, $n \in S$ iff $n + d \in S$.

$$
\begin{aligned}
|T|_q &= 1 + q + q^7 + q^8 + q^{14} + q^{15} + \dots \\
&= \frac{1+q}{1-q^7} \\
&= \frac{2}{7}\;\frac{1}{1-q} + \frac{5}{7} + \dots
\end{aligned}
$$

The way we extend the notion of density is by paying attention to all the terms in the expansion, not just the first.

We say $S \succeq S'$ iff there exists $\epsilon > 0$ such that $|S|_q \geq |S'|_q$ for all $1 - \epsilon < q < 1$.

We call this the *germ-ordering* on (generating functions of) subsets of $\mathbb{N}$.

Write $S \succ S'$ iff $S \succeq S' \not\succeq S$.

Deleting an element from a set makes the set smaller:

$$\{0, 1, 7, 8, 14, 15, \dots\} \succ \{1, 7, 8, 14, 15, \dots\}$$

Increasing one or more elements of a set makes the set smaller:

$$\{0, 1, 7, 8, 14, 15, \dots\} \succ \{1, 2, 8, 9, 15, 16, \dots\}$$

The germs of rational generating functions are **totally ordered**.

Main result: **For every packing body B, every germ-maximal translation set for B is rational; hence the maximal T is unique if it exists.**

It is not necessarily true that the germ-maximal translation set is periodic; e.g., for $B = \{0, 7, 11\}$, the germ-maximal translation set is

$$\{0, 1, 3, 6, 9, \qquad 15, 18, 21, \ldots\},$$

which is infinitesimally bigger than the periodic set

$$\{0, \quad 3, 6, 9, 12, 15, 18, 21, \ldots\}$$

(since $\{1\}$ is infinitesimally bigger than $\{12\}$).

Proposition: T is a translation set for B iff the set $T - T := \{t - t' : t, t' \in T\}$ is disjoint from the set $D := \{|i - j| : i, j \in B,\ i \neq j\}$.

Thus finding the maximum packing of a body B in $\mathbb{N}$ is a special case of finding the maximal D-avoiding subset of $\mathbb{N}$, where D is a finite set of positive integers.

The prerint Germ Order for One-Dimensional Packing (at https://arxiv.org/abs/1807.06495 after Wednesday) by Abrams et al. proves: **For every finite distance-set D, every germ-maximal D-free set S is rational; hence the maximal S is unique if it exists.**

Open problems:

For every B, is there a maximal B-packing?

For every D, is there a maximal D-avoiding set?

The space of germs does not have a good topology, so setting up compactness arguments is tricky.

Packings that achieve germ-maximality are provably unique (and periodic) but for all we know there might be packing bodies B for which maximal packings do not exist.

Aside: We can use our $\sum_{n \in S} q^n$ trick to measure the sizes of sets of natural numbers not associated with packings or distance-avoiding sets.

Example: Let $S = \{0, 1, 4, 9, \dots\}$ and $T = \{0, 1, 3, 6, \dots\}$ (the sets of square numbers and triangle numbers). Then

$$|S|_q \, / \, |T|_q \to \sqrt{2}$$

and

$$|S|_q - \sqrt{2}\,|T|_q \to \sqrt{2}/2.$$

See the MathOverflow post on Comparing sizes of sets of natural numbers.

What about subsets of $\mathbb{Z}$, e.g., packings in $\mathbb{Z}$?

Here it's less obvious what should replace $\sum_{n \in S} q^n$.

$\sum_{n \in S} q^{n^2}$, perhaps?

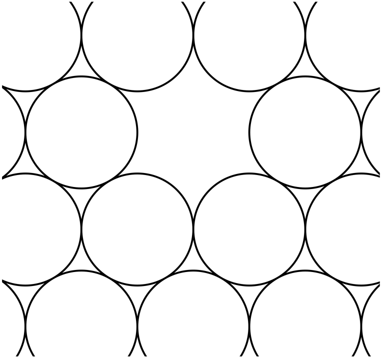
Such functions are not rational when S is periodic, so we haven't pursued the matter.

$q^{|n|}$ is more manageable but less natural.

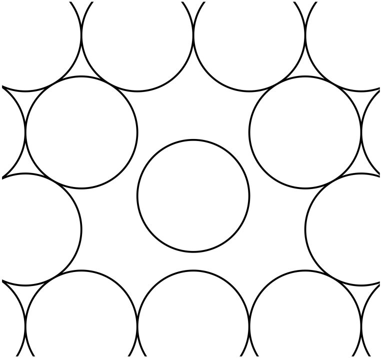
What seems clear is that some of the niceties of packings of $\mathbb{N}$ disappear, and maximal packings will be periodic, not just eventually periodic.

Part III: Optimal disk packing in two dimensions

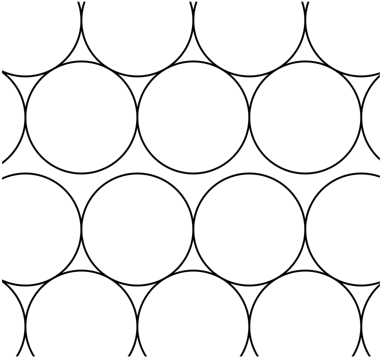
Counterexample 1:



Counterexample 2:



Counterexample 3:



Morally, these counterexamples seem like “cheats”.

Let’s sharpen our notion of optimal packing in $\mathbb{R}^2$ using the same trick we just used in $\mathbb{N}$.

I’ll show three possible approaches to doing this. Two are principled and one is tractable.

In the first approach, we replace disk packings by point packings P (using the centers of the disks, no two of which are at distance < 2).

The size of the infinite set P can be represented as the divergent infinite sum $\sum_{(x,y)\in P} 1$.

We'll regularize this sum by imposing a smooth cutoff at distance s from the origin, and then letting s go to infinity.

(Cf. the definition of density as $\lim_{r\to\infty} \lambda(S \cap B_r)/\lambda(B_r)$; this imposes a sharp cutoff at distance r, and gets rid of the divergence by a rescaling.)

Let $g_s(x, y) := \exp -(x^2 + y^2)/s^2$, so that

(1) for all $(x, y) \in \mathbb{R}^2$, $g_s(x, y) \to 1$ as $s \to \infty$, and

(2) for all $s > 0$, $\int_{\mathbb{R}^2} g_s < \infty$.

For P a discrete point-set in $\mathbb{R}^2$ containing no two points at distance ≤ 2 (so that the unit disks centered at points in P have disjoint interiors), let

$$|P|_s := \sum_{(x,y) \in P} g_s(x, y) < \infty.$$

If P is finite, $|P|_s \to |P|$ as $s \to \infty$.

Main idea: When P is infinite, $|P|_s$ diverges as $s \to \infty$, but the precise way it diverges gives information about the point set P.

In particular, for many non-optimal packings P,
we can expand $|P|_s$ as $\alpha s^2 + \beta s + \gamma + o(1)$, where

- α tells us about density,
- β tells us about line defects (see Counterexample 3), and
- γ tells us about point defects (see Counterexamples 1 and 2),

and moreover α, β, γ are independent of the choice of origin.

We'll come back to this later.

Theorem (Cohn): Let P be a point-packing of the plane.
If P is a hexagonal close packing, then $|P|_s = \Delta_2 s^2 + o(e^{-s})$.

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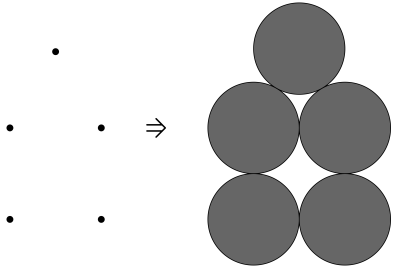
Conjectural converse: Let P be a point-packing of the plane.
If $|P|_s = \Delta_2 s^2 + o(1)$, then P is a hexagonal close packing.

"Evidence": The counterexamples I discussed above are not counterexamples to this conjecture.

But I've had trouble making progress with this definition.

Second approach: Go back to using disks instead of points. Let μ_P be Lebesgue measure restricted to the union of the disks.



Let

$$(P)_s = \int_{\mathbb{R}^2} g_s \, d\mu_P.$$

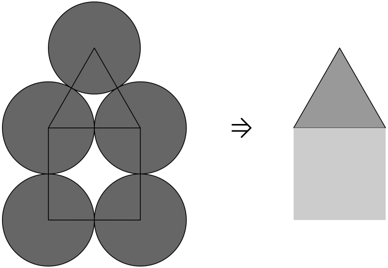
Compare: $|P|_s$ can be defined as the integral of g_s with respect to a "Dirac comb": a measure on $\mathbb{R}^2$ in which each point in P is assigned mass 1.

I will sometimes call $|P|_s$ the Dirac regularization of the divergent sum $\sum_{(x,y)\in S} 1$, in contrast to the disk regularization $(P)_s$ (and in contrast to the Delaunay regularization $[P]_s$ to be described next).

Third approach (“gerrymandering”): Redistribute the mass of the disks, so that the mass associated with a sector of a disk gets reapportioned uniformly throughout its Delaunay cell.

(Note: “Delaunay” = “Delone”.)

In a point-packing, a Delaunay cell is an inscriptible polygon whose vertices are points of the packing and whose circumcircle encircles no points of the packing.



Let $\bar{\mu}_P$ be the reapportioned measure, and let

$$[P]_s = \int_{\mathbb{R}^2} g_s \, d\bar{\mu}_P.$$

Main Theorem: Let P be a distance-2 point-packing. Then $[P]_s = \pi\Delta_2 s^2 + o(1)$ (i.e., $[P]_s - \pi\Delta_2 s^2 \to 0$) if and only if P is a hexagonal close packing.

Lemma (original source?): In a disk packing of the plane, no Delaunay cell can have local packing density exceeding $\pi/\sqrt{12}$. That is, the fraction of a Delaunay cell that is covered by disks of the disk-packing cannot exceed $\pi/\sqrt{12}$. Furthermore, equality holds if and only if the cell is an equilateral triangle.

Recall that $\bar{\mu}_P$ is Lebesgue measure of intensity 1 on the disks reapportioned uniformly over the Delaunay regions (yielding a "piecewise-Lebesgue" measure of intensity everywhere $\leq \Delta_2$), and that $[P]_s = \int_{\mathbb{R}^2} g_s \, d\bar{\mu}_P$.

If P^* is a hexagonal-close packing, $\bar{\mu}_P$ is the uniform measure $\Delta_2\lambda$ (where λ is Lebesgue measure) on $\mathbb{R}^2$.

Otherwise, $\bar{\mu}_P \leq \Delta_2\lambda$ everywhere (by the Lemma) AND there exists at least one Delaunay cell C whose $\bar{\mu}_P$ measure falls short of $\Delta_2\lambda(C)$ by some positive amount, say c; then $\liminf([P^*]_s - [P]_s) \geq c$, and since $[P^*]_s = \pi\Delta_2 s^2 + o(1)$, we cannot have $[P]_s = \pi\Delta_2 s^2 + o(1)$.

This completes the proof.

All three ways of regularizing $|S|$ (Dirac, disk, and Delaunay) give rise to germ-orderings with $s \to 1$; in each case, germ-maximality implies the complete saturation property.

(A packing is completely saturated if for no n is it possible to remove n disks and then add back $n+1$ disks.)

It is not known whether there exist completely saturated packings other than hexagonal close packings of disks.

Conjecture: Let P be a distance-2 point-packing. For each of the three orderings, P is germ-maximal if and only if P is a hexagonal close packing.

Note: the functions $|\cdot|_s$, $(\cdot)_s$, and $[\cdot]_s$ all extend to higher dimensions.

Part IV: Suboptimal disk packing in two dimensions

A **valuation** is a finitely-additive measure from a set-algebra into an abelian group: $v(A \cup B) = v(A) + v(B) - v(A \cap B)$, inclusion-exclusion, etc.

A **polyhedral set** in $\mathbb{R}^n$ is a set specified by some Boolean formula in n variables involving finitely many linear equations and inequalities.

Equivalently, it's a set that belongs to the set-algebra generated by open and closed half-planes.

Conjecture ("Throwing Gaussian darts at a polyhedral target"), proved for $n = 1$ and $n = 2$:

If S is a (not necessarily compact) polyhedral subset of $\mathbb{R}^n$, the probability that a Gaussian $N(0, \sigma)$ random variable lies in S is given by $p(\sigma)/\sigma^n$ plus an error term that goes to zero, where $p(\cdot)$ is a polynomial of degree n.

Proving this theorem is essentially equivalent to setting up a valuation v_n on polyhedral sets that assigns to each (not necessarily compact) polyhedral subset of $\mathbb{R}^n$ a generalized n-dimensional volume in a non-Archimedean ordered ring extension of $\mathbb{R}$.

If S is a compact polyhedral subset of $\mathbb{R}^n$, $v_n(S)$ will be the ordinary n-dimensional Lebesgue measure of S, but if S is a noncompact polyhedral set (of full dimension), v_n will be an "infinite" element of the non-Archimedean ordered ring $\mathbb{R}[\mathfrak{p}]$, where $\mathfrak{p}$ is a formal infinite element satisfying $1 << \mathfrak{p} << \mathfrak{p}^2 << \cdots << \mathfrak{p}^n$.

I'll sometimes informally call the valuation v_n a "measure" even though it's not countably additive or real-valued.

I'll focus on the cases of $\mathbb{R}$ and $\mathbb{R}^2$. I'll sometimes call v_1 "length" and v_2 "area", omitting the modifier "generalized".

Warning: Often a translation T carries a polyhedral set S into a proper subset or proper superset of itself.

E.g., $S = [0, +\infty)$ or $(-\infty, 0]$ in $\mathbb{R}$, $T : x \mapsto x + 1$.

In cases like this, we can't expect S and $T(S)$ to have the same measure.

But as we'll see there are compensations for this lack of symmetry.

The polyhedral subsets of $\mathbb{R}^1$ are unions of isolated points, finite open intervals and infinite open rays.

Isolated points have measure 0.

Define $v_1(I) :=$ length(I) if I is a finite interval, $v_1([x, +\infty)) = \mathfrak{p} - x$, and $v_1((-\infty, x)) = \mathfrak{p} + x$.

In particular, $v_1([0, +\infty)) = v_1((-\infty, 0]) = \mathfrak{p}$, $v_1((-\infty, +\infty)) = 2\mathfrak{p} > \mathfrak{p}$.

Theorem: There is a unique valuation on polyhedral sets in $\mathbb{R}^2$ taking values in the ordered ring $\mathbb{R}[\mathfrak{p}]$ satisfying the following four properties:

(1) Monotonicity: If S is a subset of S', $v_2(S) \leq v_2(S')$.

(2) Consistency with Lebesgue measure: If S is compact, $v_2(S)$ is the Lebesgue measure of S.

(3) Fubini property: If $S = A \times B$, $v_2(S) = v_1(A)v_1(B)$.

(4) Rotational invariance: If S and S' are related by rotation about the origin in $\mathbb{R}^2$, $v_2(S) = v_2(S')$.

Specifically, $v_2(S)$ is an element of $\mathfrak{p}^2\mathbb{R} + \mathfrak{p}\mathbb{R} + \mathbb{R}$ in which the coefficients of $\mathfrak{p}^2$, $\mathfrak{p}^1$, and $\mathfrak{p}^0$ are determined by the coefficients of s^2, s^1, and s^0 in the Laurent expansion of $\int_S e^{-(x^2+y^2)/s^2}\ dx\ dy$ in $1/s$ around $s = \infty$.

$\mathfrak{p}^2$ corresponds to $\frac{\pi}{4}s^2$,
$\mathfrak{p}^1$ corresponds to $\frac{\sqrt{\pi}}{2}s^1$, and
$\mathfrak{p}^0$ corresponds to $1s^0$.

What do properties (1)–(4) have to do with asymptotics of the integral of $e^{-(x^2+y^2)/s^2}$ over a set S?

(1) Monotonicity: The integrand is nonnegative.

(2) Consistency with Lebesgue measure: When S is compact, the integrand goes to 1 uniformly.

(3) Fubini property: The integrand factors as $e^{-x^2/s^2}e^{-y^2/s^2}$.

(4) Rotational invariance: The integrand is invariant under rotation.

Why is v_2 is uniquely determined by properties (1)-(4)?

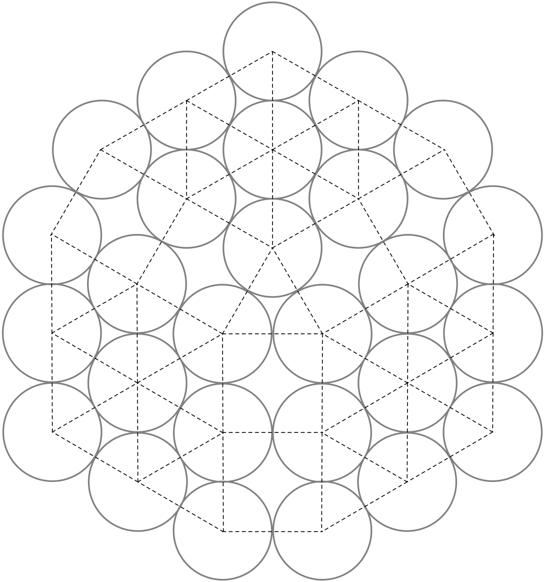
Proof sketch:

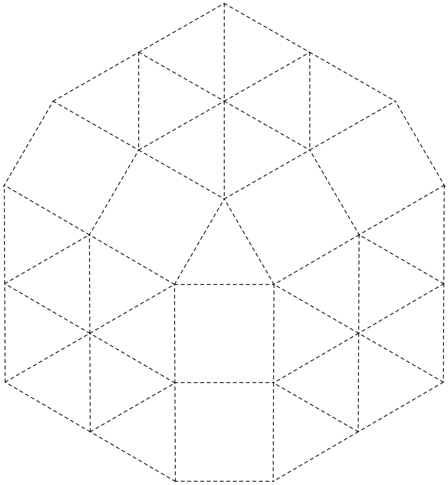
Triangulate S, using a mix of ordinary triangles, ideal triangles with 1 point at infinity, and ideal triangles with 2 points at infinity.

Show that for each kind of triangle T, properties (1)-(4) uniquely determine the generalized area of T.

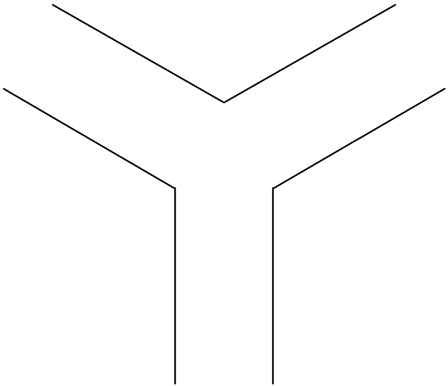
For some suboptimal packings, all the Delaunay cells are equilateral triangles and squares, each covered with its appropriate local packing density, and the union of the squares is a union of rectangles and half-strips (each full strip can be viewed as the union of two half-strips).

We call this special sort of polyhedral set a network of "hallways and junctions" (where a doubly-infinite hallway is considered to be two hallways):





A network with 3 hallways and 1 junction:



Theorem: Suppose that all the Delaunay cells of P are triangles and squares with side-length 2 forming a network of hallways and junctions. Then

$$[P]_s = (\Delta_2)\, s^2 - (W)(\delta\pi^{1/2})\, s + (A)(2\delta) + o(1),$$

where $\Delta_2 = \pi/\sqrt{12}$,

$\delta\ = \pi/\sqrt{12}\ -\ \pi/4$,

$W =$ the sum of the widths of the infinite hallways, and

$A =$ the total area of the junctions.

Note that the choice of origin makes no difference.

Application to crystal defects:

In a packing that's close to a hexagonal close packing,

point defects lead to networks with area on the order of 1,
line defects lead to networks with area on the order of $\mathfrak{p}$, and
density defects lead to networks with area on the order of $\mathfrak{p}^2$.

Can such a "defect calculus" be applied to other sorts of defects in 2D and 3D lattices?

Part V: The trouble with three dimensions

Conjecture: the $|P|_s$-optimal, $(P)_s$-optimal, and $[P]_s$-optimal 3D sphere packings are the Barlow packings (the uncountably many packings formed by layers of hexagonal close-packed spheres).

Theorem: There is NO valuation on polyhedral sets in $\mathbb{R}^3$ taking values in the ordered ring $\mathbb{R}[\mathfrak{p}]$ satisfying the following four properties:

(1) Monotonicity: If S is a subset of S', $v_3(S) \leq v_3(S')$.

(2) Consistency with Lebesgue measure: If S is compact, $v_3(S)$ is the Lebesgue measure of S.

(3) Fubini: If $S = A \times B$ with polyhedral sets $A \subseteq \mathbb{R}$ and $B \subseteq \mathbb{R}^2$, $v_3(S) = v_1(A)v_2(B)$.

(4) Rotational invariance: If S and S' are related by rotation about the origin in $\mathbb{R}^3$, $v_3(S) = v_3(S')$.

What's going wrong:

$$|[0,1]|_s = \int_0^1 e^{-x^2/s^2}\,dx = 1 - \frac{1}{3}s^{-2} + \frac{1}{10}s^{-4} - \cdots$$

The nonzero coefficient of s^{-2} in $|[0,1]|_s$ makes a nonzero contribution to the constant term of $|[0,1] \times [0,\infty) \times [0,\infty)|_s$.

So we lose the Fubini property when we truncate the $o(1)$ part of the germ.

Possible fix: Retain all the terms.

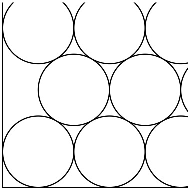
Part VI: Odds and ends

Lewis Bowen, Charles Holton, Charles Radin, and Lorenzo Sdun have an interesting approach to optimal packings whose philosophical motivations are similar to ours:

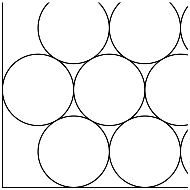
"Even though it would be intuitively satisfying to declare that the problem of optimally dense packings of E^2 by disks of fixed radius has the unique solution discussed above (Figure 1), there has been no satisfactory way to exclude some other packings of the same density, for instance those obtained by deleting a finite number of disks from this packing." (See also https://arxiv.org/pdf/math/0302056.pdf.)

However, the theory I've outlined today applies in situations where theirs doesn't. Here is one such situation.

Let P and P' be two disk-packings of a quadrant, as below. P is better at filling the quadrant than P' by exactly 1/4 of a disk, in the sense that $|P|_s - |P'|_s$, $(P)_s - (P')_s$, and $[P]_s - [P']_s$ all converge to 1/4.



P



P'

Is P the best packing of disks in a quadrant?

Do we even know there exists a best packing?

It's not clear to me how to employ compactness principles or contraction arguments or other analytic tools to prove existence of an optimum.

Going back to disk-packing of the whole plane, it's not obvious that there exists a best *non-optimal* disk-packing. But I believe there is one.

Gap conjecture: The most efficient non-optimal disk-packings are hexagonal close packings with one disk missing.

Note that Counterexample 3 from earlier does not disprove this; no matter how small ϵ is, if you displace a half-plane's worth of disks by ϵ, the amount of deficiency introduced corresponds to removal of infinitely many disks.

(Also, Kuperberg, Kuperberg, and Kuperberg have shown that packings like Counterexample 3 are not completely saturated.)

I'm hoping that other people, with various analytic and geometric insights, will help me figure out how to advance this point of view of packings.

Thank you!

These slides can be found at
http://jamespropp.org/paris20a.pdf.