Numerical exploration in sphere packing, Fourier analysis, and physics

Lecture 2

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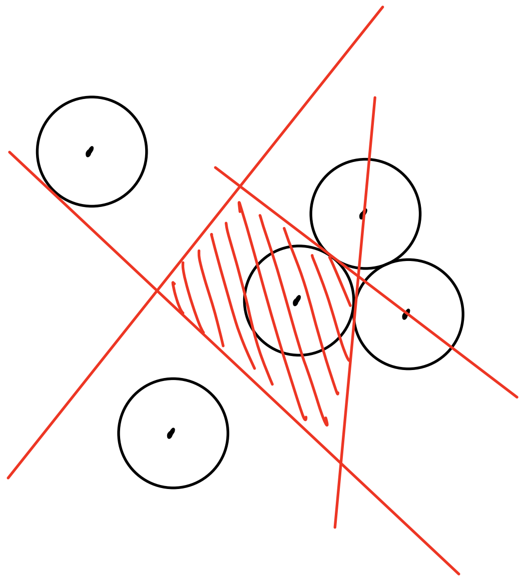
How can we prove upper bounds on the optimal packing density Δ_n in $\mathbb{R}^n$?

Let's examine $n=2$, unit disk packing in $\mathbb{R}^2$.

The proof will use just elementary geometry, graph theory, and calculus.

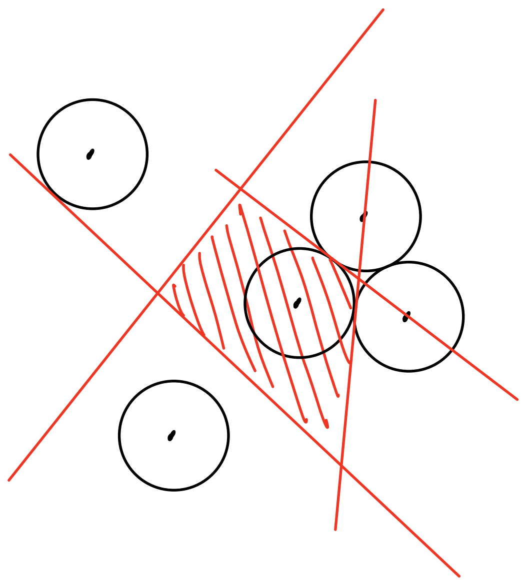
Now look at the <u>Voronoi cell</u> of a disk center, the points closer to it than any other disk center.



How small can its volume be?

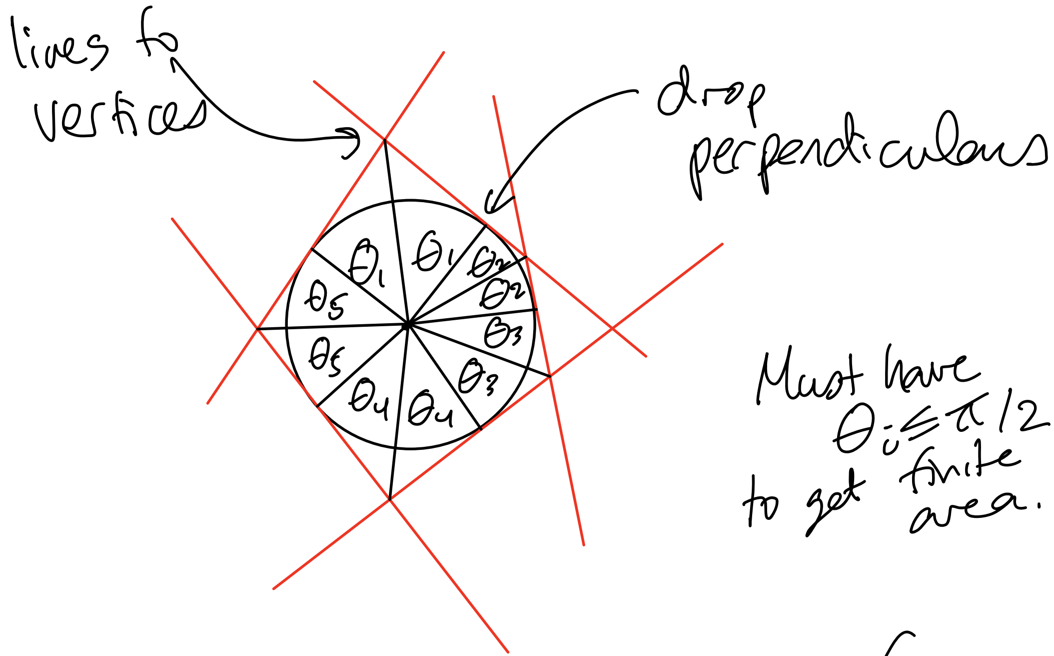
Define a graph w/
vertices = disk centers
adjacency = share edge of Voronoi cell

This graph is planar, so the average degree is at most 6.
(Euler's Thm. See exercises.)



How small can the average area be? (Small cells = high density.)

We can decrease the area by moving the disks to be tangent, so we get a circumscribed polygon.

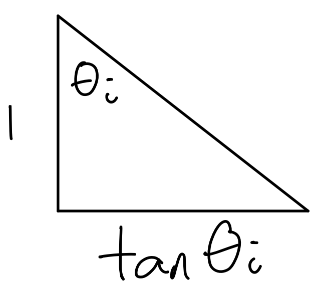


Must have $\theta_i \leq \pi/2$ to get finite area.

How small can the area of a cirumscribed k-gon be?

$$\text{area} = 2\sum_{i=1}^{k} \frac{1}{2}\cdot 1 \cdot \tan\theta_i$$

w/ $\theta_1 + \cdots + \theta_k = \pi$



By the convexity of the tangent function on $[0, \pi/2)$,

the smallest case is $\theta_1 = \cdots = \theta_k$

$$\text{area} = k \tan\frac{\pi}{k}$$

Now the area of a Voronoi cell w/ k edges is at least $k\tan\left(\frac{\pi}{k}\right)$.

Take a big chunk of packing, with n_k k-edge cells.

$$\text{density} \le \frac{\overset{\text{disk area}}{\pi} \cdot \overset{\#\text{ disks}}{(n_1 + \cdots + n_k + \cdots)}}{\underset{\text{lower bound for total area}}{n_1 a_1 + \cdots + n_k a_k + \cdots}}$$

where $a_k = k \tan\frac{\pi}{k}$.

By planarity, $\dfrac{n_1 + 2n_2 + \cdots}{n_1 + n_2 + \cdots} \le 6$

(Strictly speaking, we should take a limit as the chunk gets big.)

$$\text{density} \le \frac{\pi \cdot (n_1 + \cdots + n_k + \cdots)}{n_1 a_1 + \cdots + n_k a_k + \cdots}$$

where $a_k = k \tan \frac{\pi}{k}$

By planarity, $\frac{n_1 + 2n_2 + \cdots}{n_1 + n_2 + \cdots} \le 6$.

$$\Longrightarrow$$

$$\frac{n_1 a_1 + n_2 a_2 + \cdots}{n_1 + n_2 + \cdots} \ge a_6$$

since $k \mapsto k \tan \frac{\pi}{k}$ is convex (exercise).

So $\text{density} \le \frac{\pi}{a_6} =$ density of hexagonal packing

Q.E.D.

Why does this get really difficult in higher dimensions?

- The combinatorics of adjacency gets harder.

- We were lucky that Euler's theorem gave exactly 6.

- Polyhedra are <u>much</u> more complex than polygons.

- No simple analogue of the convexity arguments.

What can we do instead?

Fourier analysis.

From 2003 paper by Cohn and Elkies, based on ideas going back to Delsarte (1972).

For an integrable fn.

$$f : \mathbb{R}^n \to \mathbb{C},$$

define its Fourier transform

$$\hat{f} : \mathbb{R}^n \to \mathbb{C}$$

by

$$\hat{f}(y) = \int_{\mathbb{R}^n} f(x) e^{-2\pi i \langle x, y \rangle} dx$$

$\langle \cdot , \cdot \rangle$ = usual inner product on $\mathbb{R}^n$ (dot product)

People don't agree on where to put the 2π factors, but all other conventions are bad.

Fourier inversion:

$$f(x) = \int_{\mathbb{R}^n} \hat{f}(y)\, e^{2\pi i \langle x, y \rangle}\, dy$$

if $\hat{f}$ is itself integrable.

So $\hat{f}$ tells how to decompose f into complex exponentials.

Parseval / Plancherel:

$$\int_{\mathbb{R}^n} |f(x)|^2 \, dx = \int_{\mathbb{R}^n} |\hat{f}(y)|^2 \, dy.$$

$$\int_{\mathbb{R}^n} f(x) \overline{g(x)} \, dx = \int_{\mathbb{R}^n} \hat{f}(y) \overline{\hat{g}(y)} \, dy.$$

$$\langle f, g \rangle = \langle \hat{f}, \hat{g} \rangle$$

(reusing the $\langle \cdot, \cdot \rangle$ notation)

The Fourier transform extends to a unitary operator from $L^2(\mathbb{R}^n)$ to itself.

$$f(x) = \int_{\mathbb{R}^n} \hat{f}(y)\, e^{2\pi i \langle x, y \rangle}\, dy$$

Shifting x by t multiplies $\hat{f}(y)$ by $e^{2\pi i \langle y, t \rangle}$.

I.e., the Fourier transform <u>diagonalizes</u> the action of $\mathbb{R}^n$ by translation on functions.

More generally (but equivalently), the Fourier transform diagonalizes all linear operators that commute w/ the translation action.

E.g., translation-inv't differential operators,

time-inv't operators in signal processing.

Sphere packing does not correspond to just analyzing a linear operator, but if we're going to linearize the problem to obtain bounds, Fourier analysis should play a role.

Our key technical tool will be

Poisson summation.

Suppose $f : \mathbb{R}^n \to \mathbb{C}$ is smooth and rapidly decreasing, and $\Lambda \subseteq \mathbb{R}^n$ is a lattice. Then

$$\sum_{x \in \Lambda} f(x) = \frac{1}{\mathrm{vol}(\mathbb{R}^n/\Lambda)} \sum_{y \in \Lambda^*} \hat{f}(y)$$

Λ^* = "dual lattice"

This is a fundamental symmetry of the Fourier transform.

Λ basis $b_1, \dots, b_n$

dual basis $b_1^*, \dots, b_n^*$
with respect to $\langle \cdot, \cdot \rangle$

$$\langle b_j^*, b_k \rangle = \begin{cases} 1 & \text{if } j = k, \\ 0 & \text{else.} \end{cases}$$

Then $b_1^*, \dots, b_n^*$ are a basis of Λ^*.

Equivalently,

$$\Lambda^* = \{ y \in \mathbb{R}^n : \langle x, y \rangle \in \mathbb{Z} \text{ for all } x \in \Lambda \}.$$

not obviously basis-independent

not obviously a lattice

How can we prove Poisson summation?

Let's prove the seemingly more general

$$\underbrace{\sum_{x \in \Lambda} f(x+t)}_{\text{Call this } F(t).} = \frac{1}{\mathrm{vol}(\mathbb{R}^n/\Lambda)} \sum_{y \in \Lambda^*} \hat{f}(y) e^{2\pi i \langle y, t \rangle}$$

Call this $F(t)$.
It's f made periodic under Λ!

The right side is the Fourier series of $F(t)$.

The complex exponentials
$t \mapsto e^{2\pi i \langle y, t \rangle}$
w/ $y \in \Lambda^*$ are exactly those that are periodic mod Λ.

$$F(t) = \sum_{y \in \Lambda^*} c_y \, e^{2\pi i \langle y, t \rangle}$$

where

$$c_y = \frac{1}{\mathrm{vol}(D)} \int_D F(t) e^{-2\pi i \langle y, t\rangle} dt$$

some fundamental parallelotope for Λ (fund. domain for translation action)

$$= \frac{1}{\mathrm{vol}(\mathbb{R}^n/\Lambda)} \sum_{x \in \Lambda} \int_D f(x+t) e^{-2\pi i \langle y, t\rangle} dt$$

$$= \frac{1}{\mathrm{vol}(\mathbb{R}^n/\Lambda)} \int_{\mathbb{R}^n} f(t) e^{-2\pi i \langle y, t\rangle} dt$$

$$= \frac{1}{\mathrm{vol}(\mathbb{R}^n/\Lambda)} \hat{f}(y)$$

QED

Thm. (Cohn and Elkies)

Suppose $f: \mathbb{R}^n \to \mathbb{R}$ is smooth and rapidly decreasing, $r > 0$, and

- $f(0) = \hat{f}(0) = 1$
- $f(x) \leq 0$ for $|x| \geq r$, and
- $\hat{f}(y) \geq 0$ for all y.

Then

$$\Delta_n \leq \mathrm{vol}(B^n_{r/2})$$
$$= \frac{\pi^{n/2}}{(n/2)!} \left(\frac{r}{2}\right)^n.$$

[WLOG f is radial]

Proof for lattice packings

$\Lambda \subseteq \mathbb{R}^n$ WLOG min. vector length r

density $\dfrac{\mathrm{vol}(B^n_{r/2})}{\mathrm{vol}(\mathbb{R}^n/\Lambda)}$.

$$\sum_{x \in \Lambda} f(x) = \frac{1}{\mathrm{vol}(\mathbb{R}^n/\Lambda)} \sum_{y \in \Lambda^*} \hat{f}(y)$$

$\leq f(0)$ since $f(x) \leq 0$ for $|x| \geq r$

$\geq \hat{f}(0)$ since $\hat{f}(y) \geq 0$ for all y

$$1 = f(0) \geq \frac{\hat{f}(0)}{\mathrm{vol}(\mathbb{R}^n/\Lambda)} = \frac{1}{\mathrm{vol}(\mathbb{R}^n/\Lambda)}$$

so $\mathrm{vol}(\mathbb{R}^n/\Lambda) \geq 1$

QED.

Proof for more general packings is similar, with a little more algebra (see orignal paper or expository papers).

Some motivation:

extract information from Poisson summation by making two sides as different as possible

Throw away terms we don't understand (and hope they are small).

Suitable auxiliary functions f give packing bounds.

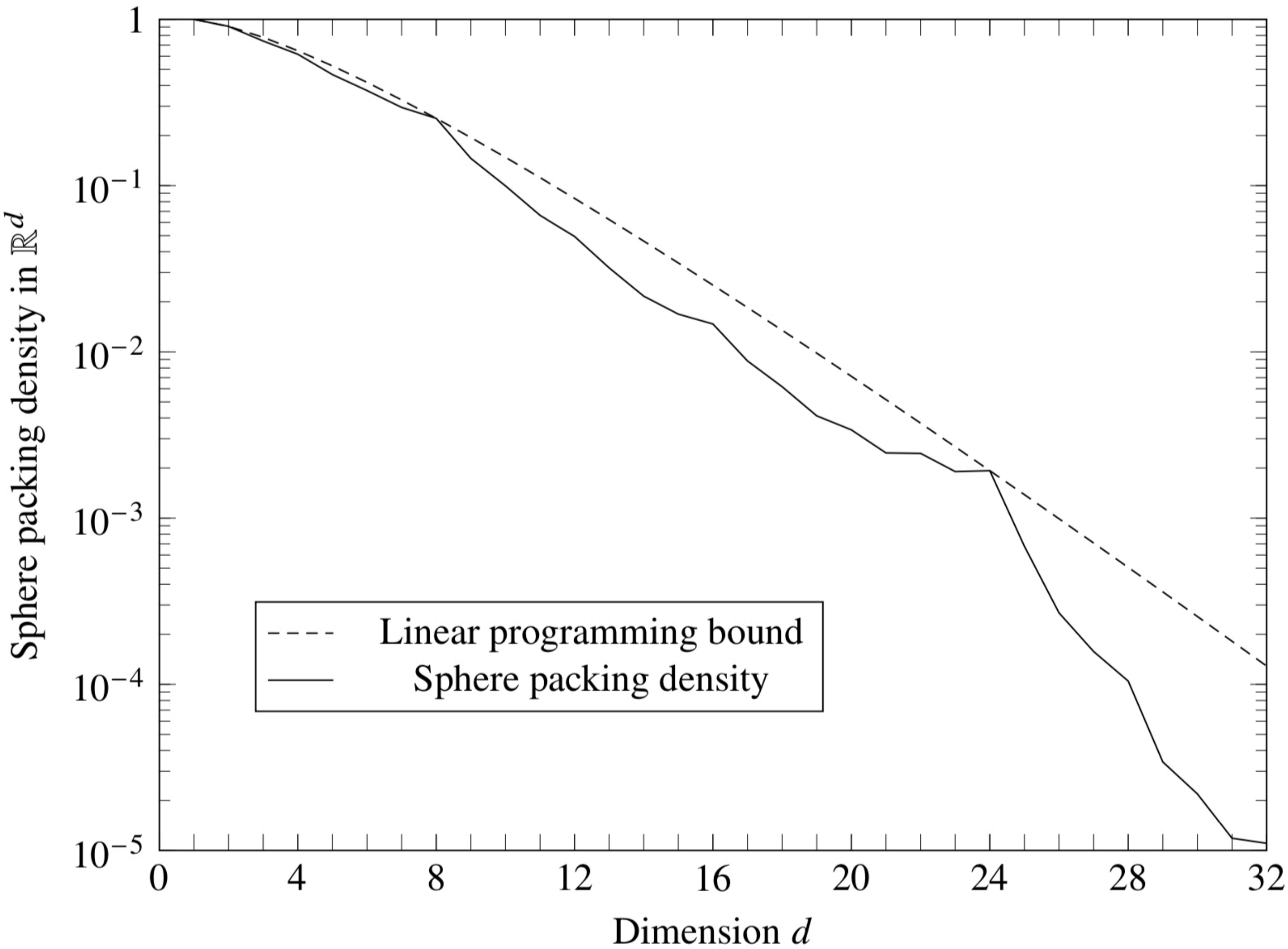
Not every bound can be obtained in this way.

E.g., cannot solve $\mathbb{R}^3$ or $\mathbb{R}^4$ (Rupert Li 2022).

How can we optimize the choice of f? Solved only for $n = 1, 8,$ and 24.

infinite-dimensional linear programming problem

We can optimize this bound numerically:



Sharp for 8 and 24 dims. Conjectured but had to wait for Viazovska for a proof.

Next time we'll study how this bound could be sharp.

How can we get numerics?

Use $f(x) = p(|x|^2)\, e^{-\pi|x|^2}$ where $p =$ polynomial.

This is convenient since

$$x \mapsto L_k^{n/2-1}(2\pi|x|^2)\, e^{-\pi|x|^2}$$

Laguerre poly of deg k w/ parameter $n/2-1$

is an eigenbasis with eigenvalues $(-1)^k$.

Orthogonal polynomials can look intimidating, but this is actually simple.

- $x \mapsto e^{-\pi|x|^2}$ is fixed by Fourier transform.

- $x \mapsto e^{-\pi\alpha|x|^2}$ has F.T.

  $y \mapsto \alpha^{-n/2} e^{-(\pi/\alpha)|y|^2}$

  by rescaling.

- Taking $(\partial/\partial\alpha)^k$ w/ $\alpha = 1$ shows that $x \mapsto |x|^{2k} e^{-\pi|x|^2}$ has F.T. $x \mapsto p(|x|^2)\, e^{-\pi|x|^2}$ where p has degree k and leading coeff. $(-1)^k$.

- Let $\mathcal{P}_k = \{x \mapsto p(|x|^2)e^{-\pi|x|^2}$ with $\deg(p) \le k\}$.

Because the Fourier transform is unitary, it must preserve the 1-dim'l orthogonal complement of $\mathcal{P}_{k-1}$ in $\mathcal{P}_k$. It must be spanned by an eigenfunction w/ eigenvalue $(-1)^k$.

A change of variables turns this orthogonality into the defining orthogonality of Laguerre polys:

$$\int_0^\infty L_j^\alpha(x)\, L_k^\alpha(x)\, x^\alpha e^{-x}\, dx = 0$$

if $j \ne k$.

It's not obvious how best
to carry out this optimization,
and we'll return to this topic.