Numerical exploration in sphere packing, Fourier analysis, and physics

Lecture 1

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Sphere packing problem

How can we fill space as efficiently as possible w/ nonoverlapping, congruent balls?

$\mathcal{C} \subseteq \mathbb{R}^n$ w/ $\min\limits_{\substack{x,y \in \mathcal{C} \\ x \neq y}} |x-y| \geq 2r$

Center spheres of radius r at points of $\mathcal{C}$ to get $\mathcal{P} = \bigcup\limits_{x \in \mathcal{C}} B_r^n(x)$.

$$\begin{matrix}\text{upper} \\ \text{lower}\end{matrix} \text{ density} = \lim_{R \to \infty} \begin{matrix}\sup \\ \inf\end{matrix} \frac{\mathrm{vol}(\mathcal{P} \cap B_R^n(0))}{\mathrm{vol}(B_R^n(0))}$$

(independent of base point 0)

$$\Delta_n = \sup_{P} \limsup_{R \to \infty} \frac{\mathrm{vol}(P \cap B_R^n(0))}{\mathrm{vol}(B_R^n(0))}$$

<u>Thm (Grömer)</u> For each n, there exists a sphere packing $P \subseteq \mathbb{R}^n$ such that for all $x \in \mathbb{R}^n$,

$$\Delta_n = \lim_{R \to \infty} \frac{\mathrm{vol}(P \cap B_R^n(x))}{\mathrm{vol}(B_R^n(x))},$$

uniformly in x.

Why sphere packing?

- natural geometric problem
- toy model of granular materials
- error-correcting code for continuous communication channel

Continuous channel (e.g., radio)

Signal = point in $\mathbb{R}^n$
(n measurements)

corrupted by noise during transit

simple noise model:

send s

receive r

high prob $|r-s| \leq \varepsilon$

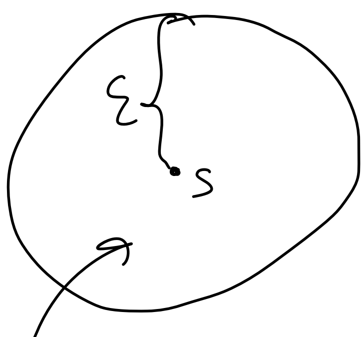
noise level

(central limit theorem)

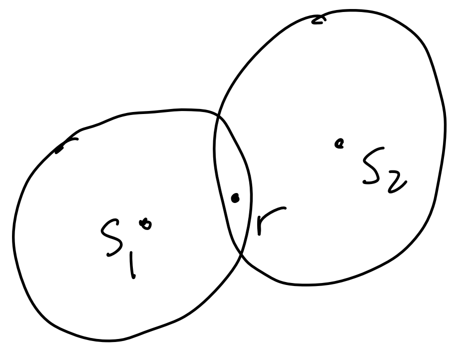
practical to send signals only in bounded subset of $\mathbb{R}^n$

say $B_R^n(0)$ w/ $R \gg \varepsilon$

Agree ahead of time on an
<u>error-correcting code</u>:
subset $\mathcal{C} \subseteq \mathbb{R}^n$
will send only $s \in \mathcal{C}$



error sphere of potential received signals



if error spheres overlap, ambiguous

To avoid ambiguity,

$$\bigcup_{x \in \mathcal{C}} B_\varepsilon^n(x)$$

should be a sphere packing.

To maximize the information transmission rate, maximize

$$\#\left(B_R^n(0) \cap \mathcal{C} \right).$$

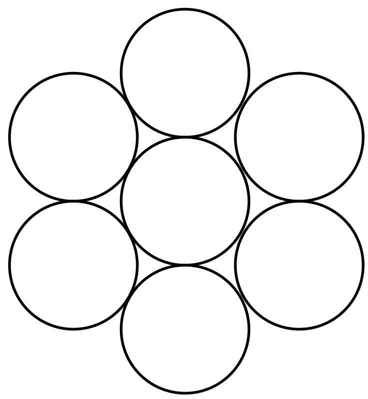
When R/ε is large, this converges to the sphere packing problem.

Note that n may be large. No reason we can't make many signal measurements.

What happens in low dimensions?

$n=1$ trivial

$n=2$ Thue (1892)



$n=3$ Hales (1998)

$n=8$ Viazovska (2016)
2022 Fields medal

$n=24$ Cohn, Kumar, Miller, Radchenko, Viazovska (2016)

In general:

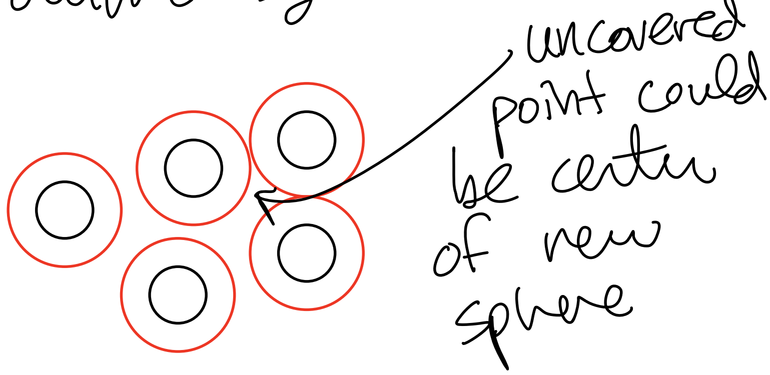
- no simple patterns
- stacking layers from the previous dimension does not always work
- upper/low bounds differ by exponential factor in $\mathbb{R}^n$ as $n \to \infty$
- completely unclear what the densest packings look like in high dimensions

Lower bounds for density

Def. A packing is saturated if no more spheres can fit.

Prop. Every saturated packing in $\mathbb{R}^n$ has density at least 2^{-n}.

Proof: Doubling the radius must cover space completely, and it multiplies volume by 2^n.



The lower bound of 2^{-n} is nearly the best known.

$cn\,2^{-n}$ from overlap

$cn \log\log n \; 2^{-n}$ Venkatesh 2013

for a sparse sequence of dimensions

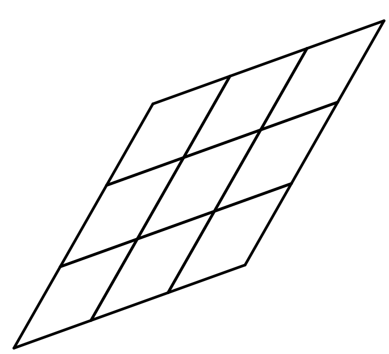
What do packings look like?

Simplest case: lattice packing

<u>Def.</u> A lattice $\Lambda \subseteq \mathbb{R}^n$ is a discrete subgroup of rank n.

i.e., the $\mathbb{Z}$-span of a basis of $\mathbb{R}^n$.

Center spheres at points of Λ.



Drawback: spheres only at corners of tiling.

Periodic packing

Sphere centers form finitely many orbits under translation by a lattice Λ.

$\Lambda \subseteq \mathbb{R}^n$

I.e., $\displaystyle\bigcup_{i=1}^{N} (\Lambda + x_i)$ w/ $x_1, \ldots, x_N \in \mathbb{R}^n$.

Periodic packings come arbitrarily close to the optimal density, but it's unclear whether they can achieve it exactly for large n.

lattice packing Λ

minimum vector length $\min_{x \in \Lambda \setminus \{0\}} |x|$.

Use radius

$$r = \frac{\min_{x \in \Lambda \setminus \{0\}} |x|}{2}$$

to avoid overlap.

Difficult to compute (see Silverman's course).

Density

$$\frac{\mathrm{vol}(B_r^n)}{\mathrm{vol}(\mathbb{R}^n/\Lambda)} = \frac{\pi^{n/2}}{(n/2)!} \cdot \frac{r^n}{|\det(B)|}$$

B = basis matrix for Λ

$(n/2)! = \Gamma(1+\frac{n}{2})$

How good are lattices?

Conj. If n is large enough, then there is no saturated lattice packing in $\mathbb{R}^n$.

(Intuition: exponential amount of space to fill, only quadratic # of degrees of freedom)

However, the best packings known in high dimensions are lattices.

Space of lattices

WLOG normalize so

$\mathrm{vol}(\mathbb{R}^n/\Lambda) = 1$.

I.e., can take basis matrix

B (columns are basis vectors)

w/ $\det B = 1$.

basis matrices

$$\mathcal{L}_n := SO_n(\mathbb{R}) \backslash SL_n(\mathbb{R}) / SL_n(\mathbb{Z})$$

rotations

change of lattice basis

Siegel observed that there is a canonical probability measure on $\mathcal{L}_n$.

$SL_n(\mathbb{R})$ has Haar measure (inv't measure) but it has infinite volume

Quotient space $\mathcal{L}_n$ has finite volume, so can normalize to get prob. measure.

(requires proof)

Call it μ_n.

We can determine certain properties of μ_n by symmetry.

Suppose $f: \mathbb{R}^n \to \mathbb{R}$ is integrable.

What is

expectation w.r.t. μ_n

$$\mathbb{E}_{\Lambda} \sum_{x \in \Lambda \setminus \{0\}} f(x) \ ?$$

We're computing pair correlations in a random lattice.

<u>Siegel mean value theorem</u>

$$\mathbb{E}_{\Lambda} \sum_{x \in \Lambda \setminus \{0\}} f(x) = \int_{\mathbb{R}^n} f(x)\, dx$$

Proof sketch

Check integrability.

$$\mathbb{E}_{\Lambda} \sum_{x \in \Lambda \setminus \{0\}} f(x)$$ is linear in f,

so

$$\int f \, d\nu$$

for some measure ν on $\mathbb{R}^n$.

By $SL_n(\mathbb{R})$-invariance, must be linear combination of δ_0 and Lebesgue measure (if regular).

Pin down coefficients via test functions.

Q.E.D.

$$\mathop{\mathbb{E}}_{\Lambda} \sum_{x \in \Lambda \setminus \{0\}} f(x) = \int_{\mathbb{R}^n} f(x)\,dx$$

same answer as Poisson point process (scatter points w/ density 1)

The algebraic structure has disappeared under averaging!

We can obtain dense lattices as follows.

Choose r so $\mathrm{vol}(B_r^n) = 2$.

Let
$$f(x) = \begin{cases} 1 & |x| \le r, \\ 0 & \text{else}. \end{cases}$$

By Siegel's theorem applied to f,

$$\mathbb{E}_{\Lambda} \underbrace{\#\left(B_r^n(0) \cap (\Lambda \setminus \{0\})\right)}_{\substack{\text{This \# must be even,} \\ \text{from } \pm x \text{ pairs.}}} = 2.$$

Some lattices have more than 2,

so
$$\exists \Lambda \text{ w/ } \begin{matrix} \det \Lambda = 1 \\ B_r^n(0) \cap \Lambda = \{0\} \end{matrix}$$

$$\text{density} = \mathrm{vol}(B_{r/2}^n) = 2 \cdot 2^{-n}.$$

$$\exists \Lambda \text{ w/ } \begin{array}{l} \det \Lambda = 1 \\ B_r^n(0) \cap \Lambda = \{0\} \end{array}$$

$$\text{density} = \mathrm{vol}(B^n_{r/2}) = 2 \cdot 2^{-n}$$

Here the extra factor of 2 comes from ± 1 symmetry.

Venkatesh gets a better factor by focusing on lattices w/ extra symmetry.

For the special case of lattice packings, the optimal density is known for dimensions 1–8 and 24.

Voronoi found a beautiful algorithm, although it's hard for 8 dimensions and has not been run above 8. Here's Ryshkov's geometric version of the algorithm.

Basis matrix B

act on left by $SO_n(\mathbb{R})$,

right by $SL_n(\mathbb{Z})$.

Gram matrix $G = B^t B$

matrix of inner products

specifies quadratic form

$GL_n(\mathbb{Z})$ acts on right by

$$G \longmapsto A^t G A$$

w/ $A \in GL_n(\mathbb{Z})$

could do $SL_n(\mathbb{Z})$, but might as well allow det -1 as well.

For $x \in \mathbb{Z}^n$, Bx is in lattice

$$|Bx|^2 = x^t B^t B x$$
$$= x^t G x$$
$$= \mathrm{Tr}(G x x^t)$$

$G \in \mathrm{Sym}^2(\mathbb{R}^n) = \{ n \times n \text{ symm. matrices} \}$

Inner product $\langle \cdot , \cdot \rangle$ on $\mathrm{Sym}^2(\mathbb{R}^n)$

$$\langle X, Y \rangle = \mathrm{Tr}(XY)$$

(check that this makes sense!)

Goal: (up to scaling) Minimize $|\det(B)|$ subject to $|Bx|^2 \geq 1$ for all $x \in \mathbb{Z}^n \setminus \{0\}$

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$$\det G = \det(B)^2$$

Goal: Minimize $\det(G)$
subject to $\langle G, xx^t \rangle \geq 1$
for all $x \in \mathbb{Z}^n \setminus \{0\}$

linear constraints!

Def. The Ryshkov polyhedron

$$\mathcal{P} = \{ G \in \mathrm{Sym}^2(\mathbb{R}^n) : G \text{ is pos. def. and } \langle G, xx^t \rangle \geq 1 \text{ for all } x \in \mathbb{Z}^n \setminus \{0\} \}$$

(lemma: locally finite polyhedron)

Thm (Minkowski)

$$G \longmapsto (\det G)^{1/n}$$

is strictly concave on symmetric, pos. def. $n \times n$ matrices

Thus, any locally optimal lattice must be a vertex of P ("perfect lattice"). Finitely many modulo $GL_n(\mathbb{Z})$.

Algorithm: enumerate all vertices by following edges until have explored all edges modulo $GL_n(\mathbb{Z})$.

$n=8$: Dutour Sikirič, Schürmann, Vallentin

Summary: the space of lattices has intricate and fruitful structure.

Questions

- Can we say more about lattices?
- Numerical exploration by computer? (under studied!)
- How can we get a handle on non-lattices?

  some ideas generalize to a <u>fixed</u> # of lattice translates, but that doesn't seem good enough