Energy minimization for lattices and periodic configurations, and formal duality

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joint work with Henry Cohn and Achill Schürmann

Sphere packings

Sphere packing problem: What is (a/the) densest sphere packing in n dimensions?

In low dimensions, the best densities known are achieved by lattice packings.

n	1	2	3	4	5	6	7	8	24
Λ	A_1	A_2	A_3	D_4	D_5	E_6	E_7	E_8	Leech
due to	Gauss			Korkine-Zolotareff		Blichfeldt			Cohn-K.

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$n = 1$: lay intervals end to end (density 1).

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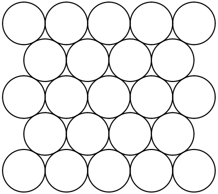

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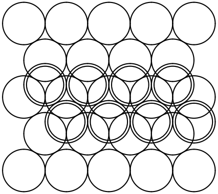
Barlow packings

$n = 3$: stack layers of the solution in 2 dimensions. [Hales 1998]



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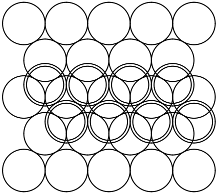

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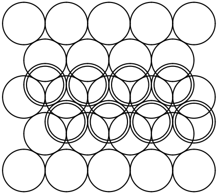

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Root lattices

- A_n (simplex lattice) $= \{x \in \mathbb{Z}^{n+1} \mid \sum x_i = 0\}$,
  inside the zero-sum hyperplane $\{x \in \mathbb{R}^{n+1} \mid \sum x_i = 0\} \cong \mathbb{R}^n$.
- D_n (checkerboard lattice) $= \{x \in \mathbb{Z}^n \mid \sum x_i \equiv 0 \pmod 2\}$
- $E_8 = D_8 \bigcup (D_8 + (1/2, \ldots, 1/2))$.
- $E_7 =$ orthogonal complement of A_1 inside E_8.
- $E_6 =$ orthogonal complement of A_2 inside E_8.

High dimensions

In higher dimensions, we believe the densest sphere packings don't come from lattices.

Example

In $\mathbb{R}^{10}$ the densest known is the Best packing, 40 translates of a lattice.

But do believe the densest packings can be achieved by periodic packings (Zassenhaus conjecture). Can provably come arbitrarily close for packing density.

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Periodic packings

Conway-Sloane describe densest known packings in low dimensions.

For $n = 3$, Barlow packings: stack layers of A_2. Two classes of deep holes, so three translates to play with, say A, B, C.

- Face-centered cubic A_3: $\dots ABCABC \dots$.
- Hexagonal close-packed: $\dots ABABAB \dots$.

Periodic iff string is periodic.

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Periodic packings, dimension 5

Three classes of deep holes in D_4, so four translates in all A, B, C, D (correspond to D_4^*/D_4).

Strings of these 4 letters, with no consecutive letters identical, correspond to the densest packings (conjecturally).

$D_5 = \Lambda_5^1$ corresponds to $\ldots ABAB \ldots$.

Other uniform packings (i.e. local configurations are isometric)

- Λ_5^2: corresponds to $\ldots ABCDABCD \ldots$
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Dimensions 6 through 8

Fiber over D_4.

Dimension 6: color the hexagonal lattice with 4 colors.

Dimension 7: color a Barlow packing with 4 colors.

Dimension 8: color D_4 with 4 colors (only one way).

Energy minimization

Energy minimization from physics is a good way to make dense arrangements.

Example

To make an optimal spherical code of N points in S^{n-1}, define

$$E_k = \sum_{i \neq j} \frac{1}{|v_i - v_j|^k}$$

and minimize. Corresponds to a repulsive force.

The limit $k \to \infty$ corresponds to the spherical coding problem (the dominant term is the one for minimal distance).

Energy minimization in $\mathbb{R}^n$

Take a lattice $\Lambda \subset \mathbb{R}^n$ and N translate vectors $0 = v_1, \ldots, v_N$.

Let $\mathcal{P} = \bigcup_i (\Lambda + v_i)$ be a periodic configuration.

Let $f(r)$ be a potential energy function, e.g. $f(r) = 1/r^{2k}$ or $f(r) = e^{-cr^2}$ (usually want a completely monotonic function of squared distance.

Define f-potential energy of $x \in \mathcal{P}$ to be

$$E_f(x, \mathcal{P}) = \sum_{x \neq y \in \mathcal{P}} f(|x - y|)$$

The f-potential energy of $\mathcal{P}$ is the average of $E_f(x, \mathcal{P})$ over the finitely many translates v_i, $i = 1, \ldots, N$.

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Energy minimization in $\mathbb{R}^n$, contd.

Stipulate that the center density $\delta(\mathcal{P})$ is fixed, and ask for $\mathcal{P}$ which minimizes the potential energy.

[Cohn-K-Schürmann '09]: computer simulations for $f = e^{-cr^2}$ for various c, dimension $n \leq 8$, $N \leq 10$. Gradient descent on space of periodic configurations with fixed number of translates.

Remarks:

- $c \to \infty$ is the sphere packing limit. But for large c, this has has more information. Between competitors of same density, break ties by favoring lower kissing number.
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- $n = 1$: [Cohn-K] proved $\mathbb{Z}$ is always optimal and unique.
- $n = 2$: We can't prove it, but expect A_2 to be always optimal, and experiments confirm this. Montgomery proved optimal among lattices.
- $n = 3$: For $c >> 1$ get A_3. For $c \approx 0$ get A_3^* (duality). In between, for a range we get phase coexistence!
- $n = 4$. Always seem to get D_4. No proof!

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For $c >> 1$ we get Λ_5^2 (not D_5!), one of the periodic packings described by Conway-Sloane. Corresponds to sequence $\ldots ABCDABCD \ldots$.

Let $D_5^+ = D_5 \bigcup (D_5 + (1/2, \ldots, 1/2))$, and

$D_5^+(\alpha) = \{(x_1, \ldots, x_4, \alpha x_5) \mid x \in D_5^+\}$.

Then $D_5^+(\alpha)$ is formally dual to $D_5^+(1/\alpha)$.

Also $\boxed{D_5^+(2) \cong \Lambda_5^2}$, the minimizer for $c \to \infty$.

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But in the middle we get a non-lattice, obtained by "gluing" D_3 and D_3 along their holes, and stretching.

Let $\mathcal{P}_6$ be $D_3 \oplus D_3$ along with its three translates by $(1/2, \ldots, 1/2)$, $(1, 1, 1, -1/2, -1/2, -1/2)$ and $(-1/2, -1/2, -1/2, 1, 1, 1)$.

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Dimension 7: We get $D_7^+(\alpha)$ where α varies depending on c. As $c \to \infty$ we get $D_7^+(\sqrt{2}) \cong E_7$.

Dimension 8: Get E_8 always, in accordance with [Cohn-K] conjecture of universal optimality.

Dimensions 9 and above: Calculations get much harder, but probably a lot of interesting phenomena.

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$\Lambda^* = \{y \in \mathbb{R}^n \,|\, \langle x, y\rangle \in \mathbb{Z} \quad \forall\, x \in \Lambda\}$.

We know $\mathrm{vol}(\mathbb{R}^n/\Lambda^*) = 1/\mathrm{vol}(\mathbb{R}^n/\Lambda)$, $(\Lambda^*)^* = \Lambda$, etc.

Poisson summation formula: For any nice function $f : \mathbb{R}^n \to \mathbb{R}$ (e.g. Schwartz function),

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

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Formal duality

Can the same hold for periodic configurations $\mathcal{P}$ and $\mathcal{Q}$? i.e. Can we have

$$\sum_{x \in \mathcal{P}} f(x) = \delta(\mathcal{P}) \sum_{y \in \mathcal{Q}} \widehat{f}(y)$$

A theorem of Cordoba says this cannot happen for all Schwartz functions f: it would force $\mathcal{P}$ to be a lattice.

But we're really only interested in

$$\Sigma(f, \mathcal{P}) = \frac{1}{N} \sum_{i,j} \sum_{x \in \Lambda} f(x + v_i - v_j).$$

Say $\mathcal{P}$ and $\mathcal{Q}$ are formal duals if $\Sigma(f, \mathcal{P}) = \delta(\mathcal{P}) \Sigma(\widehat{f}, \mathcal{Q})$.

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Formal duality, contd.

Theorem (Cohn-K-Schürmann)

D_n^+ is formally self-dual when n is odd or n is a multiple of 4. If $n \equiv 2 \pmod 4$, then D_n^+ is formally dual to an isometric copy of itself.

Corollary

$D_n^+(\alpha)$ is formally dual to an isometric copy of $D_n^+(1/\alpha)$.

So if f is radially symmetric, the Gaussian potential energies are related.

Now we're trying to get a classification, to show D_n^+ is "essentially" the only example.

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Thank you!