Lattices, sphere packings and spherical codes: geometric optimization problems

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Sphere packings

Definition

A sphere packing in $\mathbb{R}^n$ is a collection of spheres/balls of equal size which do not overlap (except for touching). The density of a sphere packing is the volume fraction of space occupied by the balls.

The main question is to find a/the densest packing in $\mathbb{R}^n$.

Good sphere packings

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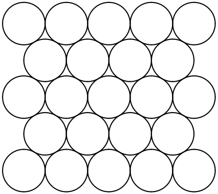
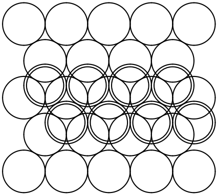


Good sphere packings II

In dimension 3, the best possible way is to stack layers of the solution in 2 dimensions. [Hales, $\sim$ 1998]



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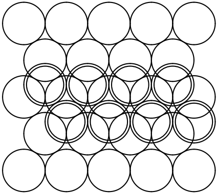

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Lattices

Definition

A lattice Λ in $\mathbb{R}^n$ is a discrete subgroup of rank n, i.e. generated by n linearly independent vectors of $\mathbb{R}^n$.

Example

- $\mathbb{Z}^n \subset \mathbb{R}^n$
- Root lattices A_n, D_n, E_8

Lattices are related to quadratic forms: if $b_1, \ldots, b_n$ is a basis of the lattice $\Lambda \subset \mathbb{R}^n$, then $Q(x_1, \ldots, x_n) = ||x_1 b_1 + \cdots + x_n b_n||^2$ is a positive definite quadratic form.

$$\{\text{Lattices up to isometry}\} \leftrightarrow \{\text{Quadratic forms mod change of coords}\}$$

$$O_n(\mathbb{R})\backslash GL_n(\mathbb{R})/GL_n(\mathbb{Z}) \cong Sym^2(\mathbb{R}^n)^+/SL_n(\mathbb{Z}).$$

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Lattice packings

If $m(\Lambda)$ is the shortest length of a non-zero vector of Λ, then we can put spheres of radius $m(\Lambda)/2$ at each point of the lattice.

Density is equal to

$$\mathrm{vol}(B_n(1))\frac{m(\Lambda)^n}{2^n \det(\Lambda)}$$

where $\det(\Lambda)$ is the volume of the fundamental cell of Λ.

Lattice packings II

The lattice packing problem asks for the densest lattice(s) in $\mathbb{R}^n$.

This is equivalent to the following question about quadratic forms/geometry of numbers:

What's the largest positive real number γ_n such that *every* positive definite quadratic form $Q(x)$ of determinant 1 in n variables represents a positive value less or equal to γ_n? (i.e. $\exists x \in \mathbb{Z}^n$ such that $0 < Q(x) \leq \gamma_n$)

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Dense lattices

What are the densest lattices in every dimension?

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
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Dimensions 8 and 24

Theorem (Cohn-K, $\sim$ 2005)

The Leech lattice is the unique densest lattice packing in $\mathbb{R}^{24}$*, and its density is optimal* (among all sphere packings) *up to an error of at most* $1.65 \cdot 10^{-30}$*. The* E_8 *lattice is the unique densest lattice packing in* $\mathbb{R}^8$*, and its density is optimal among all sphere packings up to an error of at most* 10^{-14}*.*

Note: The error bounds have since been improved quite a lot (in particular, the error for E_8 is less than 10^{-30} as well.

A key ingredient in the proof is the use of linear programming bounds for sphere packing density. We also use a criterion of Voronoi for local optimality in the space of lattices, and some combinatorial and geometric arguments.

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Dense lattices II

The lattice packing problem has a finite solution (Voronoi's theorem implies a finite list of local optima), but the number of these seems to grow very rapidly, so this approach is impracticable beyond $n = 8$ at the current time.

dimension	1	2	3	4	5	6	7	8	9
# local optima	1	1	1	2	3	6	30	2408	?

Strangeness in high dimensions

Even starting in $\mathbb{R}^9$, interesting phenomena emerge. For example, the best packings known in dimension 9 are a continuous family, one of which is a lattice, and the others are obtained by moving half the spheres relative to the other half (the fluid diamond packings).

In dimension 10, the current record is held by the Best packing (40 translates of a lattice, obtained as the inverse image of a non-linear binary code in $\mathbb{F}_2^{10}$ under the reduction $\mathbb{Z}^{10} \to \mathbb{F}_2^{10}$).

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Covering and quantizer problems

The covering radius of a lattice (or more generally, discrete set) $\Lambda \subset \mathbb{R}^n$ is the smallest r such that spheres of radius r centered at points of Λ cover all space. The thinness of a covering is the fraction of space wasted. The covering problem asks for the thinnest lattice covering of $\mathbb{R}^n$.

The Voronoi cell of a point of Λ is the set of points of $\mathbb{R}^n$ closer to it than to any other point of Λ. The quantizer problem asks for Λ (with one point per unit volume on average) such that the (average) moment of inertia of the Voronoi cell is smallest.

Both of these problems arise naturally in communication theory.

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Energy minimization

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

Let $f(r)$ be a potential energy function, e.g. $f(r) = 1/r^{2k}$ or $f(r) = e^{-cr^2}$.

If $\mathcal{P}$ is a periodic configuration in $\mathbb{R}^n$ then 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 $x \in \mathcal{P}$ (it's a finite average).

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

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Theta and zeta functions

For instance, if $f(r) = 1/r^s$ then for a lattice Λ we get

$$E_f(\Lambda) = \sum_{0 \neq x \in \Lambda} \frac{1}{|x|^s}$$

which is the Epstein zeta function of the lattice (converges for $s > n$).

If $f(r) = e^{-cr^2}$ then for a lattice Λ we get

$$E_f(\Lambda) = \sum_{0 \neq x \in \Lambda} e^{-c|x|^2} = \Theta_\Lambda(ic/\pi) - 1$$

where

$$\Theta_\Lambda(z) = \sum_{x \in \Lambda} e^{\pi i |x|^2 z}$$

is the theta function of the lattice.

Completely monotonic potentials

The potential functions we consider are completely monotonic functions of squared distance.

That is, $f(r) = g(r^2)$ where $g(x) \geq 0, g'(x) \leq 0, g''(x) \geq 0, \dots$, i.e. derivatives alternate in sign.

This is a natural extension of positive, decreasing, convex functions, and includes Gaussians and inverse power laws. So it's a fairly broad class of functions. But still strong enough to allow us to prove something interesting!

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Spherical codes

A spherical code $\mathbb{C}$ is a finite subset of a sphere $S^{n-1} \subset \mathbb{R}^n$.

Some symmetrical examples:

1. N vertices of a regular N-gon on S^1.
2. Vertices of Platonic solids on S^2 (tetrahedron, octahedron, cube, icosahedron, dodecahedron).
3. Vertices of a 24-cell, 600-cell or 120-cell in S^3.
4. 240 roots of E_8 lattice on S^7.

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Spherical codes II

The angular distance $\theta(C)$ of the code C is the minimal angular separation between distinct points.

We may ask, given N, how to place the points of C such that $\theta(C)$ is maximized. Conversely, given θ_0, what is the maximum number of points N in a code C with $\theta(C) \geq \theta_0$?

The spherical code problem is the same as packing spherical caps on the surface of a sphere.

For $\theta_0 = \pi/3$, the latter problem becomes the kissing number problem.

Answers only known in dimensions $1, 2, 3$ (Schutte and van der Waerden), 4 (Musin), 8 and 24 (Odlyzko-Sloane and Levenshtein).

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Connection with potential energy minimization

One way to make good spherical codes is to put N electrons on the surface of a sphere, and let them repel under electrostatic force (Thomson's plum pudding model of the atom).

When they come to equilibrium, expect them to be far apart, i.e. form a good spherical code.

In other words, we can study the problem of energy minimization (in this case $1/r$ potential energy), and expect the ground states to be related to good spherical codes or packings.

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Energy minimization for spherical codes

Basic question: Find configuration(s) of N points on S^{n-1} which minimize f-potential energy.

Again, we consider completely monotonic functions of squared distance. The cone of such functions is spanned by the functions $A_\ell(r) = (4 - r)^\ell$, for non-negative integers ℓ.

Limits

The spherical coding problem (or sphere packing problem) is a limit case of the energy minimization problem, for e^{-cr^2} as $c \to \infty$ or of $1/r^k$ as $k \to \infty$.

This is because the dominant term comes from the minimal distance, and the contribution of other terms become negligible in proportion as the parameters c or k go to infinity.

In fact, the limit problem contains finer information (e.g. about the number of minimal vectors, if the answer to the packing density problem is degenerate).

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Examples

Energy minimization for harmonic potential, for $1/r$ potential.

4 points in S^2: regular tetrahedron.

6 points in S^2: regular octahedron.

8 points in S^2: skew-cube!

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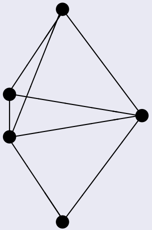
□

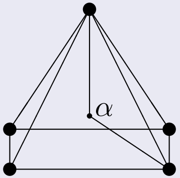
Examples II

5 points in S^2: two competing configurations.

A : triangular bipyramid



B_θ : square pyramid



$$\alpha = \pi/2 + \theta$$

Examples III

For the function $A_\ell = (4 - r)^\ell$, the configuration A wins for $1 \leq \ell \leq 6$, whereas some B_θ wins for $\ell \geq 7$.

Note that A maximizes angular distance, as does B_0.

For inverse power laws, B wins for steep power laws $1/r^k$ for $k > 7.524+$, but A wins for smaller k.

Recently, R. Schwartz proved that for $1/r$ and $1/r^2$, the triangular bipyramid (configuration A) is the global optimum.

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Universal optimality

We say a spherical code is universally optimal if it minimizes f-potential energy (among codes of its size) for all completely monotonic f.

There are examples of universally optimal codes, though their existence is *very uncommon*. The typical situation is that we have one or more families of N-point configurations, each being optimal for A_ℓ in a certain range of ℓ.

Similarly, we say a periodic configuration $\mathcal{P}$ in $\mathbb{R}^n$ is universallly optimal if it minimizes potential energy for all completely monotonic functions f, among point configurations with the same density as $\mathcal{P}$.

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Examples of universal optima on spheres

Known universally optimal configurations of N points on S^{n-1}:

n	N	Name
2	N	N-gon
n	$n+1$	simplex
n	$2n$	cross polytope
3	12	icosahedron
4	120	600-cell
8	240	E_8 root system
7	56	spherical kissing
6	27	spherical kissing/Schläfli
5	16	spherical kissing/Clebsch
24	196560	Leech lattice minimal vectors
23	4600	spherical kissing
22	891	spherical kissing
23	552	regular 2-graph
22	275	McLaughlin
21	162	Smith
22	100	Higman-Sims
$q\frac{q^3+1}{q+1}$	$(q+1)(q^3+1)$	Cameron-Goethals-Seidel

Examples of universal optima on spheres II

Theorem (Cohn-K)

These are sharp for the linear programming bounds for potential energy and hence universally optimal. All the examples except for the 600-cell are sharp configurations.

Definition

A spherical M-design is a code C for which we have

$$\frac{1}{|C|}\sum_{x\in C} p(x) = \frac{1}{vol(S^{n-1})}\int_{S^{n-1}} p(x)d\omega(x)$$

for any polynomial p of degree at most M.

We say C is a sharp configuration if there are m different inner products between distinct points, and it is a $2m-1$ design.

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Positive definite kernels

Fix $n \geq 2$. We say $f : [-1,1] \to \mathbb{R}$ is a positive definite kernel if for every code $C \subset S^{n-1}$, the $|C| \times |C|$ matrix $\left(f(\langle x,y\rangle)\right)_{x,y\in C}$ is positive semidefinite.

In particular, $\sum_{x,y\in C} f(\langle x,y\rangle) \geq 0$.

Schönberg (1930s) classified all the positive definite kernels. He showed that the ultraspherical or Gegenbauer polynomials $C_i^\lambda(t), i = 0,1,2,\ldots$ are PDKs and that any PDK is a non-negative linear combination of them. Here $\lambda = n/2 - 1$.

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Gegenbauer polynomials

The Gegenbauer polynomials arise from representation theory/harmonic analysis. They are given by the generating function

$$(1 - 2tz + z^2)^{-\lambda} = \sum_{i=0}^{\infty} C_i^{\lambda}(t) z^i$$

So we have

1. $C_0(t) = 1$
2. $C_1(t) = (n-2)t$
3. $C_2(t) = (n-2)(nt^2 - 1)/2$

and so on.

Linear programming bounds

The linear programming bounds of Delsarte for the spherical code problem (maximize N for a given θ), were adapted by Yudin to give LP bounds for potential energy.

Theorem (Yudin)

Let $f : (0,4] \to \mathbb{R}$ be any function. Suppose $h : [-1,1] \to \mathbb{R}$ is a polynomial such that $h(t) \leq f(2-2t)$ for all $t \in [-1,1]$, and suppose there are nonnegative coefficients $\alpha_0, \ldots, \alpha_d$ such that $h(t) = \sum_{i=0}^{d} \alpha_i C_i^{\lambda}(t)$ in terms of the Gegenbauer (i.e. ultraspherical) polynomials. Then every set of N points on S^{n-1} has potential energy at least $N^2\alpha_0 - Nh(1)$.

Proof of LP bound for Potential energy

Proof.

$$
\begin{aligned}
E_f(C) &= \sum_{x,y\in C, x\neq y} f(|x-y|^2) \geq \sum_{x,y\in C, x\neq y} h(\langle x,y\rangle) \\
&= -Nh(1) + \sum_{x,y\in C} h(\langle x,y\rangle) \\
&= -Nh(1) + \sum_{x,y\in C}\sum_i \alpha_i C_i(\langle x,y\rangle) \\
&= -Nh(1) + \sum_i \alpha_i \sum_{x,y\in C} C_i(\langle x,y\rangle) \\
&= -Nh(1) + N^2\alpha_0 + \sum_{i>0}\alpha_i \sum_{x,y\in C} C_i(\langle x,y\rangle) \\
&\geq -Nh(1) + N^2\alpha_0
\end{aligned}
$$

□

Proof of universal optimality

Proof idea.

We construct $h(t)$ to be the Hermite interpolation of $f(2-2t)$ to order 2 at the set of inner products of distinct points of the code (except at -1, where we interpolate to order 1).
Show $h(t) \leq f(2-2t)$ and that $h(t)$ is positive definite (which is also used in the proof of uniqueness).
The 600-cell involves an extra twist: we need a polynomial of somewhat higher degree with some vanishing Gegenbauer coefficients. □

Apart from sphere packing bounds and universal optimality, LP bounds have been used in many other settings, for instance by Odlyzko-Sloane and Levenshtein to solve the kissing number problem in 8 and 24 dimensions, and by Musin to solve it in 4 dimensions.

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Linear programming bounds for Euclidean space

Bochner's Theorem: A function on $\mathbb{R}^n$ is positive definite exactly when its Fourier transform in non-negative.

Theorem (Cohn-K)

Let $f : (0, \infty) \to [0, \infty)$ *be any function. Suppose* $h : \mathbb{R}^n \to \mathbb{R}$ *satisfies* $h(x) \leq f(|x|^2)$ *for all* $x \in \mathbb{R}^n \setminus \{0\}$ *and is the Fourier transform of a function* $g \in L^1(\mathbb{R}^n)$ *such that* g *is continuous at* 0 *and* $g(t) \geq 0$ *for all* $t \in \mathbb{R}^n$. *Then every periodic configuration in* $\mathbb{R}^n$ *with density* δ *has* f*-potential energy at least*

$$\delta g(0) - h(0).$$

Dimensions $1, 2, 8, 24$

We can show that the LP bound is sharp for $\mathbb{Z} \subset \mathbb{R}$ (nontrivial!).

Conjecture

This LP bound is sharp for the hexagonal lattice, E_8, and the Leech lattice, for all completely monotonic potential functions which decay sufficiently rapidly.

This implies universal optimality of these lattices. We prove that the conjecture implies that E_8 and the Leech lattice are the unique densest periodic packings in 8 and 24 dimensions.

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Survey of results, conjectures

Sarnak and Strömbergsson have shown that D_4, E_8 and the Leech lattice are locally optimal among lattices for potential energy for all completely monotonic functions.

Coulangeon showed that any lattice Λ whose shells are all 4-designs is locally optimal for the Epstein zeta function,

$$\zeta(\Lambda, s) = \sum_{x \in \Lambda - \{0\}} \frac{1}{|x|^{2s}}$$

which is the f-potential energy for $f(r) = 1/r^s$.

In particular, this holds for A_2, D_4, E_8 and Leech. Recent result of Coulangeon and Schürmann extends this to local optimality of these among all periodic configurations.

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Energy minimization for periodic configurations

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.
- Gaussian is more general since $1/r^k$ is Mellin transform of a Gaussian.

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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.
- $n = 3$: For $c >> 1$ get A_3. For $c \approx 0$ get A_3^* (duality).
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Optimizers in dimension 5

In each of these dimensions, the experimentally observed minima seem to occur in a family of periodic configurations obtained by glueing together two lattices along their holes.

Let $D_5^+ = D_5 \bigcup (D_5 + (1/2, \ldots, 1/2))$, and $D_5^+(\alpha)$ $= \{(x_1, \ldots, x_4, \alpha x_5) \,|\, x \in D_5^+\}$.

These are non-lattices (union of 2 translates of a lattice).

For $c >> 1$ we get $D_5^+(2)$ and for c close to zero we get $D_5^+(1/2)$.

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Dimension 6

Get E_6 for $c \to \infty$, and E_6^* for $c \to 0$.

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

Let 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 $(-1/2, -1/2, -1/2, 1, 1, 1)$.

Let $P_6(\alpha)$ be obtained by scaling the first three coordinates of P_6 by α and the last three by $1/\alpha$.

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Dimensions 7 and 8

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: More interesting phenomena, but calculations get much harder.

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For $n = 9$, seem to always get D_9^+ (no scaling!)

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Duality

For any lattice Λ, we have its dual lattice
$\Lambda^* = \{y \in \mathbb{R}^n \mid \langle x, y\rangle \in \mathbb{Z} \quad \forall\, x \in \Lambda\}$.

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

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

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

(Useful for establishing functional equation for zeta function, etc.)

Formal duality

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

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

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

$$\Sigma'(f,\mathcal{P}) = \mathrm{Average}_{x\in\Lambda}\left[\sum_{y\in\Lambda, y\neq x} f(x-y)\right]$$

where Σ' means diagonal terms (with $x = y$) are omitted, and only differences of lattice vectors matter.

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Formal duality, contd.

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

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 $D_n^+(1/\alpha)$.

Similarly, $P(\alpha)$ is formally self-dual.

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

In joint work with Cohn, Reiher and Schürmann, we have found some other examples of formal duality.

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Inverse problem

What happens if we evolve 8 points on S^2 under a $1/r^k$ potential?

The minimum for energy is not a cube. Rather, it's a skew cube (antiprism), where the distance between the two square faces varies as k varies.

Similarly, 20 points on S^2 don't settle down to a regular dodecahedron under the inverse power laws or Gaussians.

Can we design a potential function which is minimized by the cube?

Can do it with potential wells, but we want a nicer function.

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Inverse problem II

Theorem (Cohn-K)

Let $f(r) = 1/r + r/3 - 8r^2/11 + 2r^3/9 - r^4/50$. The cube is the unique global minimum for f-potential energy among 8-point codes in S^2.

Proof.

Linear programming bounds! We engineer f so that it's easy to come up with an h that works and gives a sharp bound for the cube. But note that f is in fact decreasing and convex as a function of distance (even though not completely monotonic). □

Similarly, we can design a potential function for the regular dodecahedron, the 4-dimensional hypercube and the 120-cell. Would like to do this for nice lattices (e.g. $\mathbb{Z}^n$).

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Some open problems/to-do list

- Are there only finitely many universal optima in a given dimension?
- How many local optima are there? Systematic upper/lower bounds?
- Is it possible to beat the D_4 lattice for energy among lattices or periodic configurations?
- Show A_2 is universally optimal among all periodic configurations in $\mathbb{R}^2$.
- Find the "magic functions" for E_8 and the Leech lattice to show that they are the densest sphere packings in their dimensions. More generally, to show they're universally optimal.

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- H. Cohn and A. Kumar, *Optimality and uniqueness of the Leech lattice among lattices*, Ann. of Math. 170 (2009), No. 3, 1003–1050. `arXiv:math.MG/0403263`.
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