Universally optimal distribution of points on spheres

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Joint work with Henry Cohn

Copy of slides at

http://math.harvard.edu/~abhinav/calgary.pdf

Two familiar problems

<u>Sphere packing problem in $\mathbb{R}^n$</u>

What fraction of $\mathbb{R}^n$ can you cover by non-overlapping balls of equal size? What are the packings?

Answers:

$n = 1 : \mathbb{Z}$

$n = 2 : A_2$ (hexagonal lattice, Fejes Tóth 1940)

$n = 3 : A_3$ (face centred cubic, Hales 1998)

$n \geq 4$: not known. Conjectured to be E_8 and Λ_{24} in 8 and 24 dimensions.
For some evidence, see [Cohn-K,'03].

Dense spherical codes

How many points can you put in $S^{n-1} \subset \mathbb{R}^n$ such that any two distinct points are at least angle ϕ apart? i.e. How densely can you pack spherical caps of angle ϕ?

For $\phi = \pi/3$ this is the kissing problem: how many spheres of the same size can you pack around a central sphere in $\mathbb{R}^n$?

Answers to kissing problem:

$n = 2 : 6$

$n = 3 : 12$ (Gregory-Newton problem, Schütte-van der Waerden, Leech etc.)

$n = 4 : 24$ (Musin, 2003)

$n = 8 : 240, n = 24 : 196560$ (Odlyzko-Sloane and Levenshtein, 1979)

Linear programming (upper) bounds

For both these problems, there exist "linear programming bounds".

Cohn-Elkies bounds

Suppose $f : \mathbb{R}^n \to \mathbb{R}$ is an admissible function satisfying

- $f(0) = \widehat{f}(0) > 0$
- $f(x) \leq 0$ for $|x| \geq r$
- $\widehat{f}(t) \geq 0$ for all t.

Then the density of sphere packings in $\mathbb{R}^n$ is bounded above by vol$(B^n(r/2))$.

Remarks

- Schwartz functions are admissible

- Proof is essentially Poisson summation.

- In practice, take $f(x) = \text{poly}(x) e^{-\pi|x^2}$. Constraints on $f, \widehat{f}$ are linear on coefficients of the polynomial i.e. it becomes a convex programming problem.

Linear programming bounds for spherical codes

Let $n = 24$, $\lambda = n/2 - 1$, and let $C_i^\lambda(\mathrm{z})$ be the Gegenbauer or ultraspherical polynomials (up to normalization, same as certain Jacobi polynomials), $i = 0, 1, \ldots$

They satisfy $\sum_{x,y\in\mathcal{C}} C_i^\lambda(\langle x, y\rangle) \geq 0$ for any code $\mathcal{C} \subset S^{n-1}$.

Suppose we have $g(z) = \sum g_i C_i^\lambda(z)$ with

$$g(z) \leq 0 \text{ on } [-1, \cos\phi]$$

$$g_i \geq 0 \, \forall i$$

Then any code $\mathcal{C}$ with minimal angle $\geq \phi$ has $|\mathcal{C}| \leq g(1)/g_0$

Remarks

- Again the constaints on g become linear constrains on the coefficients g_i.

- For the kissing problem, get a bound of ≈ 13.16 for $n = 3$, ≈ 25.56 for $n = 4$. But sometimes you get exact integer bounds: 240 for $n = 8$, 196560 for $n = 24$.
Sloane and Bannai (1981) used this to show that the best kissing configurations in 8 and 24 dimensions are unique.

- Similarly for $n = 7$, $\phi = \arccos(1/3)$, get a bound of 56 exactly.
Many other configurations match the bounds, including a class of spherical codes which are spherical designs of sufficiently high degree.

Another concept of “good” spherical code.

Place N particles on S^{n-1} with a repulsive force between any two (e.g. $1/r^k$), where r is the Euclidean distance between two points. For instance, putting electrons on the surface of a sphere. Let the kinetic energy dissipate slowly, for example by a viscous force. They will settle in a configuration which is a local minimum for the associated potential energy. This provides a new measure for “goodness” of a spherical code, since we can argue that the particles are reasonably well distributed.

Define f-potential energy for a code $\mathcal{C}$ to be

$$\sum_{x,y\in\mathcal{C},x\neq y} f(|x-y|^2)$$

Linear programming bounds for potentials

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 non-negative coefficients $\alpha_0, \ldots, \alpha_d$ such that

$$h(t) = \sum_{i=0}^{d} \alpha_i C_i^{n/2-1}(t)$$

in terms of the Gegenbauer (i.e. ultraspherical) polynomials. Then every set of N points on S^{n-1} has potential energy at least

$$N^2 \alpha_0 - N h(1)$$

Note: the variable $t \in [-1, 1]$ represents the inner product, and $2-2t$ is the squared distance between two points on the unit sphere.

Yudin, Kolushov and Andreev used the linear programming bound to show that optimality for certain codes and certain (classes of) potentials.

- harmonic potential ($f(r) = 1/r^{n-2}$) optimized by simplex and cross polytope (Yudin),

- harmonic potential optimized by E_8 minimal vectors (Kolushov and Yudin),

- simplex and cross polytope optimize some slightly more general potentials (Kolushov and Yudin),

- minimal vectors of Leech lattice and vertices of icosahedron for two potentials (Andreev).

New developments

There are codes which optimize f-potential energy for all completely monotonic functions $f : (0, 4] \to \mathbb{R}$, i.e. f is C^∞ and $(-1)^k f^{(k)} \geq 0$ for all k.

We call this property **universal optimality** of the code.

Remarks

- If you write f as a function of the inner product instead of squared distance (i.e. compose with $t \mapsto 2 - 2t$), then completely monotonic translates to absolutely monotonic (all the derivatives are ≥ 0).

- Inverse power laws are completely monotonic.

- Universal optimality of a code implies it's an optimal spherical code (maximizes the minimal angle).

Recall that a spherical M-design is a finite subset of the sphere such that for polynomials of degree $\leq M$ on $\mathbb{R}^n$, the average over the sphere is the same as the average over the design.

A sharp configuration (also called Delsarte code by Levenshtein) is a spherical M-design with m inner products between distinct points in it, and $M \geq 2m - 1 - \delta$, where $\delta = 1$ if the configuration is antipodal and $\delta = 0$ otherwise. Levenshtein showed that they are optimal spherical codes.

<u>Theorem (Cohn-K, 04)</u>:
Sharp configurations are universally optimal.

We also prove the 600-cell in S^3 is universally optimal, even though it's not a sharp configuration.

Method of proof: Coming up with the $h(t)$ requires just Hermite interpolation of $f(2-2t)$ at the inner products. For the 600-cell, there's an extra twist: make a few of the ultrasperical coefficients of $h(t)$ vanish.

The sharp configurations actually match the bounds for any f as in the theorem!

We can also show in many of the cases that the spherical code is the unique spherical code of N elements minimizing the f-potential energy, given that for all k, $(-1)^k f^{(k)}(t)$ is strictly positive for all t in the interval $(0,4)$ (for instance, any inverse power law).

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

Each is unique optimum for each individual f (strictly completely monotonic) except in last line: those are **not** always unique.

Euclidean case

For a periodic configuration P in $\mathbb{R}^n$, can define f-potential energy of any point $x \in P$ to be

$$\sum_{y \in P, y \neq x} f(|x-y|^2)$$

and take the average over x: this gives a well-defined potential energy.

Theorem (Cohn-K, 05)
Suppose $h(x) \leq f(|x|^2)$ for $x \neq 0$ and h is the Fourier transform of a nonnegative function $g \in L^1(\mathbb{R}^n)$ that is continuous at 0. Then the f-potential energy for any periodic point configuration of density δ is at least $\delta g(0) - h(0)$

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.

Sarnak and Strömbergsson conjectured E_8 and Leech are global optima among lattices for $f(r) = 1/r^s$, and proved local optimality. Our conjecture is a generalization, and provides a potential (!) method of proof of global optimality.

As usual, universal optimality of a configuration implies that the associated sphere packing is a densest sphere packing in that dimension. We prove that the conjecture implies that E_8 and the Leech lattice are the unique densest periodic packings in 8 and 24 dimensions.

We also prove that $\mathbb{Z} \subset \mathbb{R}$ is universally optimal.

Summary and questions

Potential energy minimization as a more natural problem, a generalization of packing.

Universal optimality holds for a number of codes, and conjectured for some lattices.

Find other universally optimal spherical codes and periodic configurations in $\mathbb{R}^n$.

What do the local optima/their families look like?

Does D_4 kissing arrangement optimize f-potential energy for $f(r) = (1 - r/4)^k$, for all sufficiently large k? (it's conjectured to be an optimal spherical code).

Universally optimal distribution of points on spheres (with H.Cohn)

http://math.harvard.edu/~abhinav/potential.pdf

The D_4 root system is not universally optimal (with H.Cohn, J.H. Conway and N.D. Elkies)

http://math.harvard.edu/~abhinav/D4.pdf