Inverse problems in potential energy minimization

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Joint work with Henry Cohn

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We'll see some answers to this question, which involve a design-like property of the target structures.

Outline

- Spherical codes, potential energy minimization.

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- Open questions.

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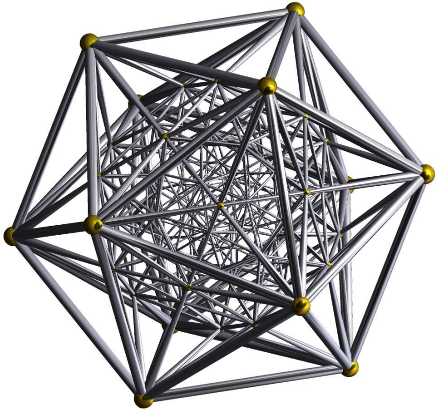
Good spherical codes: have large angular distance between distinct points.

600-cell



(Schlegel projection of a 600-cell to 3D. Image from Wikipedia)

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Newton-Gregory problem: $n = 3, \theta = \pi/3$. Maximum size of a code is 12 or 13.

Newton was correct (Schütte and van der Waerden 1953).

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If f is chosen appropriately (e.g. $f(r) = 1/r^k$ for k large), global minima for f tend to be good spherical codes.

Note that we may actually obtain such codes by computer simulation (such as gradient descent). $\square$

Potential Energy minimization

Functions such as $f(r) = 1/r^k = 1/(r^2)^{k/2}$ are completely monotonic functions of squared distance.

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However, today we will allow much broader classes of functions, especially when we are interested in mathematical feasibility.

Examples

Let's look at the solution to the energy minimization problem with $f(r) = 1/r$ on the 2-sphere for small numbers of points.

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- 6 points: octahedron.
- 8 points: not a cube. The square faces are unstable for $1/r$ potential energy. Minimum seems to be achieved by a skew-cube. □

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For general $\mathcal{C}$, it's not even clear that there exists such an f.

Some motivation

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But no proofs. The compact case (sphere) is easier to handle, and techniques should be useful in the Euclidean case. So we consider design of structures on the surface of a sphere.

Feasibility: necessary conditions

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- C is the only spherical code with its distance distribution d (since d and f determine the potential energy $E_f(C)$).
- d must be extremal: i.e. it cannot be written as a weighted average of other C-point distance distributions (since otherwise one of them is at least as good as d, for any choice of potential energy).

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Theorem (Cohn-K)

These two necessary conditions are also sufficient.

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Find a function ℓ defined on the support $\mathrm{supp}(d)$ such that d is the unique minimum of $t \mapsto \sum_r \ell(r)t(r)$ among C-point distributions with $\mathrm{supp}(t) \subset \mathrm{supp}(d)$. This is possible because d is extremal.

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Now for $\epsilon > 0$ choose a smooth function f_ϵ such that

$$f_\epsilon(s) > \sum_r \ell(r)d(r)$$

whenever s is not within ϵ of a point in $\mathrm{supp}(d)$, and also such that f_ϵ has strict local minima at the points of $\mathrm{supp}(d)$. For ϵ small enough, f_ϵ will have a strict global minimum at d, and therefore at $\mathcal{C}$. □

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Note that being decreasing and convex are linear conditions on the function, if we fix a linear space of functions.

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 $\big(f(\langle x, y\rangle)\big)_{x,y \in C}$ 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 $P_i^{\lambda}(t), i = 0, 1, 2, \ldots$ are PDKs and that any PDK is a non-negative linear combination of them. Here $\lambda = n/2 - 1$.

Gegenbauer polynomials

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

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

So we have

1. $P_0(t) = 1$
2. $P_1(t) = (n-2)t$
3. $P_2(t) = (n-2)(nt^2 - 1)/2$

and so on.

Theorem (Yudin, Linear programming bound)

Let $f : (0, 2] \to \mathbb{R}$ *be a potential function and* $h : [-1, 1] \to \mathbb{R}$ *be a positive definite polynomial such that* $h(t) \le f(\sqrt{2-2t})$ *for all* $t \in [-1, 1)$. *Write* $h(t) = \sum_i \alpha_i P_i(t)$ *with* $\alpha_i \ge 0$ *for all* i. *Then for any* N*-point spherical code* $\mathcal{C}$, *we have*

$$E_f(\mathcal{C}) \ge \frac{1}{2}(N^2\alpha_0 - Nh(1)).$$

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Furthermore, equality holds for $\mathcal{C}$ if and only if $\mathcal{C}$ is compatible with h. Namely,

1. *$h(t) = f(\sqrt{2-2t})$ whenever t is the inner product between two distinct points in $\mathcal{C}$.*

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1. *$h(t) = f(\sqrt{2-2t})$ whenever t is the inner product between two distinct points in $\mathcal{C}$.*
2. *whenever $\alpha_i > 0$ for some $i > 0$, we have $\sum_{x,y\in\mathcal{C}} P_i(\langle x, y\rangle) = 0$.*

Proof

$$
\begin{aligned}
E_f(C) &= \frac{1}{2}\sum_{x \neq y \in \mathcal{C}} f(\sqrt{2 - 2\langle x, y\rangle}) \geq \frac{1}{2}\sum_{x \neq y \in \mathcal{C}} h(\langle x, y\rangle) \\
&= -\frac{Nh(1)}{2} + \frac{1}{2}\sum_{x,y \in \mathcal{C}} h(\langle x, y\rangle) \\
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&\geq -\frac{Nh(1)}{2} + \frac{\alpha_0}{2}\sum_{x,y \in \mathcal{C}} P_0(\langle x, y\rangle) \\
&= \frac{N^2\alpha_0 - Nh(1)}{2}.
\end{aligned}
$$

Universal optima

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

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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.

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Theorem (Cohn-K)

Sharp configurations are universally optimal.

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). □

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

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$q\frac{q^3+1}{q+1}$	$(q+1)(q^3+1)$	Cameron-Goethals-Seidel

All the examples except for the 600-cell are sharp configurations.

Other structures

So for a universal optimum $\mathcal{C}$ with N points on S^{n-1}, we just have to put N points on a sphere with potential energy say $1/r$ or $1/r^2$, and let it evolve. The configuration $\mathcal{C}$ will be the global minimum.

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Bad news: We cannot make it with a completely monotonic potential. Some skew cube will be better.

Other structures

So for a universal optimum $\mathcal{C}$ with N points on S^{n-1}, we just have to put N points on a sphere with potential energy say $1/r$ or $1/r^2$, and let it evolve. The configuration $\mathcal{C}$ will be the global minimum.

What about vertices of a cube or a dodecahedron, which are not universal optima, but are very nice symmetric structures?

Bad news: We cannot make it with a completely monotonic potential. Some skew cube will be better.

Good news: If we only want a decreasing and convex potential function, we can still win.

Example: making the cube

Theorem

Let $f : (0,2] \to \mathbb{R}$ *be the potential function*

$$f(r) = \frac{1}{r^3} - \frac{1.13}{r^6} + \frac{0.523}{r^9}.$$

The cube is the unique global minimum for f*-potential energy among all* 8*-point codes in* S^2*. The function* f *is decreasing and strictly convex.*

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Proof sketch: Let h be the unique polynomial of the form

$$h(t) = \alpha_0 + \alpha_1 P_1(t) + \alpha_2 P_2(t) + \alpha_3 P_3(t) + \alpha_5 P_5(t)$$

which agrees with $P(\sqrt{2-2t})$ to order 2 at $t = \pm 1/3$ and to order 1 at $t = -1$. One checks that h satisfies the conditions of Yudin's theorem and that the cube is compatible with h.

Proof cont'd

Similarly, to check uniqueness, suppose that $\mathcal{C}$ is compatible with h. Since h agrees with $f(\sqrt{2-2t})$ only at $\pm 1/3$ and -1, these are the only possible inner products between distinct points of $\mathcal{C}$. Now for $y \in \mathcal{C}$ and $1 \leq i \leq 3$, we have $\sum_{x \in \mathcal{C}} P_i(\langle x, y \rangle) = 0$. That is, $\mathcal{C}$ is a spherical 3-design. We can use these equations to compute that $N_{-1} = 1$ and $N_{\pm 1/3} = 3$, thus determining the valencies of each point. Finally, one shows by a direct geometric argument that this data forces $\mathcal{C}$ to be the cube. $\square$

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Simulation: $\square$

Note: We used the Gegenbauer polynomials P_1, P_2, P_3, P_5 because their corresponding sums vanish for the cube. But we cannot use P_4 because the cube is not a 4-design.

Remarks

In general the strategy is as follows: we can use only the Gegenbauer polynomials that sum to zero on $\mathcal{C} \times \mathcal{C}$.

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Then we try to find a function that is decreasing and convex, usually by adding on a term of the form $\prod_{t_i \in \mathrm{InP}(C)} (t - t_i)^2 / r$ or something similar, where $t = 1 - r^2/2$. Here $\mathrm{InP}(C)$ the set of inner products of distinct vectors in C.

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Still, one might not always be able to get a decreasing convex potential function.

Dodecahedron

Theorem

Let $f : (0, 2] \to \mathbb{R}$ be defined by

$$f(r) = (1+t)^5 + \frac{(t+1)^2(t-1/3)^2(t+1/3)^2(t^2-5/9)^2}{6(1-t)^2}$$

where $t = 1 - r^2/2$. The regular dodecahedron is the unique global minimum for E_f among all 20-point codes on S^2. The function f is decreasing and strictly convex.

Note: Here $h(t) = (1+t)^5$.

120-cell

Let $\mathcal{C}$ be the 120-cell, and $q(t) = \prod_{1 \neq t_i \in \mathrm{supp}(d(C))} (t - t_i)$.

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Let $m_1, \ldots, m_{29}$ be the integers
$2, 4, 6, 8, 10, 14, 16, 18, 22, 26, 28, 34, 38, 46,$
$1, 3, 5, 7, 9, 11, 13, 15, 17, 19, 21, 23, 25, 27, 29$ and $c_1, \ldots, c_{17}$ be
$1, 2/3, 4/9, 1/4, 1/9, 1/20, 1/20, 1/15, 1/15,$
$9/200, 3/190, 0, 7/900, 1/40, 1/35, 3/190, 1/285.$

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Theorem

The potential function $f : (0, 2] \to \mathbb{R}$ defined by

$$f(r) = \sum_{i=1}^{17} c_i P_i(t) + \sum_{i=1}^{29} \frac{P_{m_i}(t)}{10^6} + 10^5 \frac{q(t)^2}{1-t}$$

(where $t = 1 - r^2/2$) is decreasing and strictly convex. The regular 120-cell is the unique global minimum for E_f among 600-point codes on S^3.

Simulation-guided optimization

Now we look at a heuristic algorithm which tries to solve the inverse problem for a given target configuration $\mathcal{C}$ (which satisfies the necessary conditions).

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Suppose we are only allowed to choose a linear combination of a specified finite set of functions $f_1, \ldots, f_k$ for our potential function f, and we want to impose some additional conditions on $f = \sum_i \lambda_i f_i$ which we assume are finitely many linear conditions $\mathcal{P}$ on the λ_i. For conditions such as decreasing and convex, we can approximate the interval $(0, 2]$ by a fine enough set of points, to get finitely many conditions.

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To keep the potential funtion bounded, we add the constraints $-1 \leq \lambda_i \leq 1$ to $\mathcal{P}$.

At any stage of the algorithm, we will have a finite list of competitors $\mathcal{C}_1, \ldots, \mathcal{C}_\ell$.

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5. If we have produced sufficiently many competitors, and the result of the previous step is always $\mathcal{C}$, then stop and return f as a putative solution to the inverse problem. Else go to step 2 with the augmented list of competitors.

Open questions

- For which n can one make the n-dimensional hypercube with, say, a decreasing convex potential? (Should be reasonable to solve, but we haven't worked it out.)

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  So solving the inverse problem rigorously for say the cubic lattice in 3 dimensions is probably extremely hard.
- Really, we should be talking about local optima with a large basin of attraction. How do we achieve that?

Reference

Cohn-Kumar, *Algorithmic design of self-assembling structures*, Proceedings of the National Academy of Sciences 106 (2009) no. 24, 9570–9575.