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Workshop on Sphere Packing and Amorphous Materials

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Rigidity of Spherical Codes

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Rigidity of spherical codes

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We'll use the terms *jammed* and *rigid* interchangeably (cf. Bob Connelly's talk).

Recall that a sphere packing is rigid if it admits no local deformations, i.e. we can't move the spheres continuously without making them overlap (apart from using isometries of the ambient space).

If we can show a packing is not rigid, it might lead the way toward improving the sphere packing for density.

We'll be concerned with spherical codes, i.e. finite sets of points on the surface of a sphere. Think of these points as vertices of spherical caps. So want to study sphere packing on the surface of a sphere, and ask about local improvements and rigidity.

Previous work by Donev, Torquato, Stillinger and Connelly describes a linear programming algorithm to test infinitesimal jamming of sphere packings. We'll study the analogous algorithm for spherical codes.

In Euclidean space, infinitesimally jammed if and only if jammed (Roth, Whiteley, Connelly).

However, on the spherical code the proof does not work - so things are more complicated. Also, less complicated because finitely many points/no periodic boundary conditions.

The spherical codes we study are mathematically very interesting, and quite often related to dense sphere packings. Insights here may lead to insights in Euclidean space.

We also use these techniques to set new records for kissing numbers in dimensions 25 - 31.

Definition

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

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

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

Definition

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 $\theta(C) \ge \theta_0$?

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

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

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.

A central question is to find a/the densest packing in \mathbb{R}^n .

In low dimensions, the best sphere packings seem to come from lattices, as do some of the best kissing configurations.

- The simplex lattice $A_n = \{x \in \mathbb{Z}^{n+1} : \sum x_i = 0\}$ in the zero-sum hyperplane in \mathbb{R}^{n+1} .
- The checkerboard lattice $D_n = \{x \in \mathbb{Z}^n : \sum x_i \text{ even } \}.$
- The special root lattice $E_8 = D_8 \bigcup (D_8 + (\frac{1}{2}, \dots, \frac{1}{2}))$.
- E_7 , the orthogonal complement of an A_1 inside E_8 .
- E_6 , the orthogonal complement of an A_2 inside E_6 .
- The Leech lattice Λ_{24} , the densest lattice in \mathbb{R}^{24} .

The densest lattices in low dimensions are

n	1	2	3	4	5	6	7	8	24
Λ	A_1	A_2	A_3	D_4	D_5	E_6	<i>E</i> ₇	E_8	Leech

The best known kissing numbers in low dimensions are

n	1	2	3	4	5	6	7	8	24
Λ	2	6	12	24	40	72	126	240	196560

But in most dimensions (e.g. 10) the best known packings or kissing numbers come from non-lattices.

We may try to improve a given spherical code or sphere packing by local deformations.

Definition

We say C is locally jammed if no point of C can be continuously moved, while keeping the others fixed, and without decreasing the minimal distance of the code below $\theta(C)$.

Definition

We say C is collectively jammed if the only continuous motions of the points of C which do not decrease the minimum distance below $\theta(C)$, are the continuous rotations.

We can write a linear program to check whether any infinitesimal motions are allowed. The idea is due to Donev, Stillinger, Torquato and Connelly, who implemented it for sphere packings in Euclidean space.

Let x_1, \ldots, x_N be vectors describing the centers of N spheres of radius R. If spheres i and j are adjacent, we have $|x_i - x_j| = R$.

We take an infinitesimal motion $x_i + ty_i$ of these sphere centers. The condition for this to be admissible is

$$|x_i - x_j + t(y_i - y_j)| \geq R$$

for i, j in contact (the other constraints are irrelevant for t small).

This simplifies to

$$\langle x_i - x_j, y_i - y_j \rangle \geq 0$$

to first order.

This is a linear condition in the coordinates of the y_i .

It can be shown that a packing in Euclidean space is infinitesimally rigid if and only if it is rigid.

So we can test rigidity of sphere packings by an algorithm (among periodic packings with a fixed number of translates).

Essentially the same idea applies to spherical codes. Let C consist of x_1, \ldots, x_N . We use deformation vectors y_i which are in the tangent space. The infinitesimal constraint is that $\langle x_i, y_i \rangle = 0$, which is linear in the y_i .

The distance constraint is that $\langle x_i + ty_i, x_j + ty_j \rangle \leq \langle x_i, x_j \rangle$ whenever x_i and x_j are at the smallest distance. The first order condition is $\langle x_i, y_j \rangle + \langle x_j, y_i \rangle \leq 0$.

The linear program asks if some value $\langle x_i, x_j \rangle$ can be changed: the first order change in this quantity is $\langle x_i, y_j \rangle + \langle x_j, y_i \rangle$. This is the objective function.

We really have a collection of linear programs. If the objective function is always 0, we conclude that the spherical code is collectively jammed.

In practice, to try to unjam a code, we apply a random linear combination of these objective functions.

However, if we do get a nonzero answer, it does not necessarily mean that the code is not rigid. (Infinitesimal rigidity for spherical codes can be strictly stronger than rigidity)

Using dot products as above gets rid of orthogonal motions.

Let's begin with the kissing configurations of the root lattices A_n, D_n, E_6, E_7, E_8 .

Example

 A_2 : jammed, provably the best kissing configuration on S^1 , using angles.

Example

 A_3 : locally jammed, but not collectively. In fact, one can move the points around to achieve any permutation while still maintaining the minimum distance.

Similarly, we can contruct an explicit unjamming of the A_n kissing configuration for $n \ge 4$, using the one for n = 3.

A_3 unjamming by picture

Cuboctahedron:



Move pairs toward each other (twists the triangles).

Example

The kissing configuration of D_4 is jammed.

Proof.

This spherical code has 24 points. Normalize them to have length $\sqrt{2}$. Distinct vectors have inner products in $\{0, \pm 1, -2\}$. If $\langle x, y \rangle = \pm 1$, then x and y span a copy of A_2 , which is infinitesimally rigid. So their inner product does not change to first order. The -2 inner product occurs between antipodal vectors, so it does not change to first order. If $\langle x, y \rangle = 0$, we can "connect" them by intermediate vectors which have inner product 1 with x and y and use these to show that $\langle x, y \rangle$ does not change.

Example

The kissing configurations of D_n , n > 4 and E_6 , E_7 , E_8 are all jammed.

The proof is by "embedding" A_2 and D_4 into these lattices. The ± 1 inner products do not change because the vectors concerned span a copy of A_2 , and A_2 is jammed. Similarly, the 0 inner products do not change because for any two orthogonal vectors in D_n , there is a copy of D_4 inside D_n containing them.

The best known kissing configurations in these dimensions are not unique. There is one more 40-point kissing configuration in \mathbb{R}^5 , competing with that of D_5 .

There are three more 72-point kissing configuration in \mathbb{R}^6 , competing with that of E_6 .

There are three more 126-point kissing configuration in \mathbb{R}^7 , competing with that of E_7 .

Computer verification (rigorous, with rational numbers) shows they are all infinitesimally rigid.

Next is the E_8 kissing configuration of 240 points. This is the unique best code of its minimal angle, so it is rigid.

Example

In 9 dimensions, the best kissing configuration coming from a lattice is that of the laminated lattice Λ_9 . It consists of the 240 points from E_8 in the "equatorial" hyperplane, as well as points of the form $(0, \ldots, 0, \pm 1, 0, \ldots, 0, \pm 1)$.

These last 32 points lie above or below the "deep holes" of the E_8 kissing configuration, and they, along with the smallest vectors of $D_8 \subset E_8$, make up the root system of D_9 .

We know D_9 is infinitesimally jammed, so it's futile to try to move its minimal vectors. We are left with the half-integer vectors $(\pm \frac{1}{2}, \ldots, \pm \frac{1}{2}, 0)$, with an even number of minus signs.

It turns out that these points are not even locally jammed, so we can move them out of the equatorial plane, showing that the kissing configuration of Λ_9 is not rigid.

- \mathbb{R}^9 : 306 points from the non-lattice packing P_{9a} .
- \mathbb{R}^{10} : 500 points from the non-lattice packing P_{10b} .
- \mathbb{R}^{11} : 582 points from the non-lattice packings P_{11c} .
- \mathbb{R}^{12} : 840 points from the non-lattice packings P_{12a} .

These are eleven such spherical codes in dimension 11 and seventeen in dimension 12. We proved that they are all jammed.

Example

The best known lattice kissing configuration in \mathbb{R}^{12} is that of the Coxeter-Todd lattice K_{12} , which is the densest known lattice in that dimension. It has 756 minimal vectors.

The linear program gives a first-order unjamming of K_{12} , but the obvious motion $x_i \rightarrow (x_i + ty_i)/\sqrt{1 + t^2|y_i|^2}$ doesn't work. We can make a choice of first-order deformation, set up a linear program for a second order deformation, which also gives a non-trivial answer. But the obvious lift doesn't work ...

Thankfully, we can exploit the Eisenstein lattice structure of K_{12} to unjam this kissing configuration. It splits into 126 disjoint hexagons, which are far enough apart that they can be rotated independently through small angles, without changing the minimal distance.

The key property is that for distinct minimal vectors x, y of K_{12} (considered as a $\mathbb{Z}[\omega]$ lattice inside \mathbb{C}^6 , we have not just $\operatorname{Re} \langle x, y \rangle \leq 2$ but also the stronger property $\langle x, y \rangle = \sum x_i \overline{y_i} \leq 2$.

This fact is equivalent to an assertion about the 126-point code in \mathbb{CP}^5 obtained by taking the quotient by \mathbb{C}^{\times} or by the sixth roots of unity.

We have shown that the kissing configuration of K_{12} is not rigid.

Example

The densest lattice in \mathbb{R}^{16} is the Barnes-Wall lattice, a laminated lattice. Its kissing arrangement of 4320 vectors is also the best known in this dimension.

The linear program was too large to run on a computer. However, we showed by using A_2 and D_4 embeddings, and the automorphism group of this lattice, that the kissing configuration is jammed, so no local improvements are possible.

There is a very large number of competitors, which are not known to be rigid.

The Leech lattice kissing arrangement of 196560 vectors is an optimal code, unique for its size and minimal distance. Therefore it is certainly rigid.

The inner products between distinct vectors lies in $\{0, \pm 1/4, \pm 1/2, -1\}$.

Example

The (previous) record for kissing number in \mathbb{R}^{25} was 196560 + 96, from the kissing configuration of the laminated lattice Λ_{25} . It consists of taking the Leech minimal vectors on the equatorial hyperplane, along with the remaining vectors of D_{25} (a 24-dimensional cross-polytope above and below).

The kissing configuration of Λ_{25} is unjammed, just like that of Λ_9 . However, using this to try improve the kissing number is quite difficult. We found two different ways to beat the kissing number in \mathbb{R}^{25} .

One way is to look for a large kissing configuration which still contains $\mathcal{C}_{\mathrm{Leech}}$ as a cross-section. This leads to a small improvement. We describe the other method, which easily generalizes to give improvements in higher dimensions.

Within C_{Leech} , we searched by computer (simulated annealing) for a subset S such that for distinct x, y in S, the inner product is never 1/2, i.e. $\langle x, y \rangle \leq 1/4$.

The largest S we found has size 480. In fact, smaller S will also work. Here's one that's easy to describe. There is a copy of the Nordstrom-Robinson code of size 256 in the Barnes-Wall lattice (replace 0 by 1 and 1 by -1). In fact, together with the cross-polytope formed by twice the 32 standard coordinate directions and their negatives in \mathbb{R}^{16} , these generate the Barnes-Wall lattice.

Since the Barnes-Wall lattice is a cross-section of the Leech lattice, we obtain an S of cardinality 288. Then let

$$\mathcal{C}' = \Big\{ (x,0) : x \in \mathcal{C}_{\text{Leech}} \setminus S \Big\} \bigcup \Big\{ (x \cos \theta, \pm 2 \sin \theta) : x \in S \Big\}.$$

For $1/4 \leq \sin^2 \theta \leq 1/3$, this code has minimal angle at least $\pi/3$. Also $|C'| = |C_{\text{Leech}}| + |S| > 196560 + 96$. We beat the previous kissing numbers in all these dimensions (which are all from laminated lattices starting from Leech).

Example

In dimension 26, we obtain a kissing number of $196560 + 4 \cdot 480$, which beats the previous record by 768.

This uses the following fact:

Lemma

There exist two disjoint 1/2-avoiding sets S_1 and S_2 of size 480 in C_{Leech} .

Independent sets

Then let

$$egin{aligned} \mathcal{C}'' &= \left\{ (x,0): z \in \mathcal{C}_{ ext{Leech}} ackslash (S_1 \cup S_2)
ight\} \ &igcup \left\{ (x\cos heta, 2\omega^j\sin heta): x \in S_1, j = 0, 2, 4
ight\} \ &igcup \left\{ (x\cos heta, 2\omega^j\sin heta): x \in S_2, j = 1, 3, 5
ight\} \end{aligned}$$

Here ω is a primitive sixth root of unity in \mathbb{C} considered as \mathbb{R}^2 , and $\sin \theta = 1/\sqrt{3}$.

Proof.

Probabilistic method! Let S_1 be fixed. Then the expected number of elements of $S_1 \bigcap gS_1$ (where g runs over the elements of the automorphism group of the Leech lattice) is $480^2/196560 \approx 1.17$. So there exists $S_2 = gS_1$ which intersects S_1 in at most one element. S_1 can be chosen antipodal, so in fact they don't intersect at all.

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- Find an example of a spherical code which is rigid but not infinitesimally rigid.
- Find an algorithm to test whether a spherical code is rigid.
- Are there optimal (or near-optimal) kissing configurations in high dimensions which have no contacts at all?
- Are there exponentially large (in the dimension) kissing configurations which are jammed?

Reference: "Rigidity of spherical codes", Henry Cohn, Yang Jiao, Abhinav Kumar and Salvatore Torquato, arXiv:1102.5060.

Thank you!