The \(D_4\) Root System is Not Universally Optimal

THE D_4 ROOT SYSTEM IS NOT UNIVERSALLY OPTIMAL

HENRY COHN, JOHN H. CONWAY, NOAM D. ELKIES, AND ABHINAV KUMAR

Abstract. We prove that the D_4 root system (equivalently, the set of vertices of the regular 24-cell) is not a universally optimal spherical code. We further conjecture that there is no universally optimal spherical code of 24 points in S^3, based on numerical computations suggesting that every 5-design consisting of 24 points in S^3 is in a 3-parameter family (which we describe explicitly, based on a construction due to Sali) of deformations of the D_4 root system.

1. Introduction

In [Cohn and Kumar 07] the authors (building on work by Yudin, Kolushov, and Andreev in [Yudin 93, Kolushov and Yudin 94, Kolushov and Yudin 97, Andreev 96, Andreev 97]) introduce the notion of a *universally optimal code* in S^{n-1}, the unit sphere in $\mathbb{R}^n$. For a function $f\colon [-1,1) \to \mathbb{R}$ and a finite set $C \subset S^{n-1}$, define the *energy* $E_f(C)$ by

$$E_f(C) = \sum_{\substack{c,c' \in C \\ c \neq c'}} f\big(\langle c, c' \rangle\big),$$

where $\langle c, c' \rangle$ is the usual inner product. We think of f as a potential function, and $E_f(C)$ as the potential energy of the configuration C of particles on S^{n-1}. Note that because each pair of points in C is counted in both orders, $E_f(C)$ is twice the potential energy from physics, but of course this constant factor is unimportant.

A function $f\colon [-1,1) \to \mathbb{R}$ is said to be *absolutely monotonic* if it is smooth and it and all its derivatives are nonnegative on $[-1,1)$. A finite subset $C_0 \subset S^{n-1}$ is said to be *universally optimal* if $E_f(C_0) \le E_f(C)$ for all $C \subset S^{n-1}$ with $\#C = \#C_0$ and all absolutely monotonic f. We say that C_0 is an *optimal spherical code* if $t_{\max}(C_0) \le t_{\max}(C)$ for all such C, where

$$t_{\max}(C) := \max_{\substack{c,c' \in C \\ c \neq c'}} \langle c, c' \rangle$$

is the cosine of the minimal distance of C. A universally optimal code is automatically optimal (let $f(t) = (1-t)^{-N}$ or $(1+t)^N$ for large N).

In [Cohn and Kumar 07], linear programming bounds are applied to show that many optimal codes are in fact universally optimal. Notably absent from this list is the D_4 root system C_{D_4}, which is expected but not yet proved to be the unique optimal code of size 24 in S^3. This root system can also be described as the vertices of the regular 24-cell.

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It is shown in [Cohn and Kumar 07] that the vertices of any regular polytope whose faces are simplices form a universally optimal spherical code. The dodecahedron, 120-cell, and cubes in $\mathbb{R}^n$ with $n \geq 3$ are not even optimal spherical codes (see [Sloane 00]) and hence cannot be universally optimal. Thus the 24-cell was the only remaining regular polytope. Cohn and Kumar conjectured in an early draft of [Cohn and Kumar 07] that C_{D_4} was universally optimal, but reported the numerical result that for the natural potential function $f(t) = (1-t)^{-1}$ there was another code $C \subset S^3$ with $\#C = 24$ at which E_f has a local minimum only slightly larger than $E_f(C_{D_4})$ (668.1902+, compared with 668).

What makes this code noteworthy is that in simulations of particle dynamics on S^3 under the potential function f (along with a viscosity force to remove kinetic energy and cause convergence to a local minimum for E_f), 24 particles converge more than 90% of the time to C, rather than to C_{D_4}. Similar effects appear to occur for $f(t) = (1-t)^{-s}$ for other values of s. In other words, these codes have a much larger basin of attraction than C_{D_4}, despite being suboptimal.

In this paper we give a simple description of a one-parameter family of configurations C_θ that includes these codes, and exhibit choices of f (such as $f(t) = (1+t)^8$) and θ for which $E_f(C_\theta) < E_f(C_{D_4})$. We thus disprove the conjectured universal optimality of C_{D_4}.

We further conjecture that there is no universally optimal spherical code of 24 points in S^3. Any such code would have to be a 5-design, because C_{D_4} is. Numerical computations led us to a 3-parameter family of such designs that can be constructed using an approach introduced by Sali in [Sali 94]. The family contains C_{D_4} as a special case, and consists of deformations of C_{D_4}.

We exhibit these designs and prove that, within the family, C_{D_4} minimizes the energy for every absolutely monotonic potential function, and is the unique minimizer unless that function is a polynomial of degree at most 5. Our computations suggest that every 5-design of 24 points in S^3 is in the new family. If true, this would imply the nonexistence of a universally optimal design of this size in S^3 because we already know that C_{D_4} is not universally optimal.

One way to think about the D_4 root system's lack of universal optimality is that it explains how D_4 is worse than E_8. The D_4 and E_8 root systems are similar in many ways: they are both beautiful, highly symmetrical configurations that seem to be the unique optimal spherical codes of their sizes and dimensions. However, one striking difference is that linear programming bounds prove this optimality and uniqueness for E_8 but not for D_4 (see [Arestov and Babenko 97, Bannai and Sloane 81, Levenshtein 79, Odlyzko and Sloane 79]). This leads one to wonder what causes that difference. Is D_4 in some way worse than E_8? Our results in this paper show that the answer is yes: for E_8, linear programming bounds prove universal optimality (see [Cohn and Kumar 07]), while for D_4 universal optimality is not merely unproved but in fact false.

2. The codes C_θ

We computed the 24×24 Gram matrix of inner products between the points of the suboptimal but locally optimal configuration mentioned above for the potential function $f(t) = (1-t)^{-1}$. Each inner product occurred more than once, suggesting that the configuration had some symmetry. By studying this pattern we eventually identified the configuration with a code in the following family of 24-point codes

$C_\theta \subset S^3$. (We are of course not the first to use this approach of computing a code numerically and using its Gram matrix to detect symmetries and then find good coordinates. One recent case — also, as it happens, for codes in S^3 — is [Sloane et al. 03], where the method is called "beautification.")

We identify $\mathbb{R}^4$ with the complex vector space $\mathbb{C}^2$ so that

$$S^3 = \{(w_1, w_2) \in \mathbb{C}^2 : |w_1|^2 + |w_2|^2 = 1\}.$$

For $\theta \in \mathbb{R}/2\pi\mathbb{Z}$ such that $\sin 2\theta \neq 0$ and $\sin\theta \neq \cos\theta$ we set

$$C_\theta := \{(z,0), (0,w), (z\sin\theta, w\cos\theta), (z\cos\theta, w\sin\theta) : z^3 = w^3 = 1\}.$$

Thus C_θ consists of 24 unit vectors, namely $3+3$ of the form $(z,0)$ or $(0,w)$ and 3^2+3^2 of the form $(z\sin\theta, w\cos\theta)$ or $(z\cos\theta, w\sin\theta)$. Each of these codes has 72 symmetries (each complex coordinate can be independently conjugated or multiplied by cube roots of unity, and the two coordinates may be switched), forming a group G isomorphic to the wreath product of the symmetric group S_3 with S_2. This group does not act transitively: there are two orbits, one consisting of the six points $(z,0)$ and $(0,w)$ and the other consisting of the remaining 18 points.

Listing all possible pairs $c, c' \in C_\theta$ with $c \neq c'$, we find that there are in general 11 possible inner products, with multiplicities ranging from 18 to 84. We thus compute that

$$\begin{aligned} E_f(C_\theta) = {} & 18\big(f(0) + f(\sin 2\theta)\big) + 36\big(f(\sin\theta) + f(\cos\theta)\big) \\ & + 36\left(f\left(\sin^2\theta - \frac{1}{2}\cos^2\theta\right) + f\left(\cos^2\theta - \frac{1}{2}\sin^2\theta\right)\right) \\ & + 72\left(f\left(-\frac{\sin\theta}{2}\right) + f\left(-\frac{\cos\theta}{2}\right) + f\left(\frac{\sin 2\theta}{4}\right) + f\left(-\frac{\sin 2\theta}{2}\right)\right) \\ & + 84 f\left(-\frac{1}{2}\right). \end{aligned}$$

For C_{D_4} we have the simpler formula

$$E_f(C_{D_4}) = 24f(-1) + 192\left(f\left(\frac{1}{2}\right) + f\left(-\frac{1}{2}\right)\right) + 144f(0).$$

3. Failure of Universal Optimality

By Theorem 9b in [Widder 41, p. 154], an absolutely monotonic function on $[-1,1)$ can be approximated, uniformly on compact subsets, by nonnegative linear combinations of the absolutely monotonic functions $f(t) = (1+t)^k$ with $k \in \{0,1,2,\dots\}$. To test universal optimality of some spherical code C_0 it is thus enough to test whether $E_f(C_0) \le E_f(C)$ holds for all $C \subset S^{n-1}$ with $\#C = \#C_0$ and each $f(t) = (1+t)^k$. We wrote a computer program to compute $E_f(C_{D_4})$ and $E_f(C_\theta)$, and plotted the difference $E_f(C_{D_4}) - E_f(C_\theta)$ as a function of θ.

For $k \le 2$ the plots suggested that $E_f(C_{D_4}) = E_f(C_\theta)$ for all θ. This is easy to prove, either directly from the formulas or more nicely by observing that C_{D_4} and C_θ are both spherical 2-designs (the latter because G acts irreducibly on $\mathbb{R}^4$), so $E_f(C_{D_4}) + 24f(1)$ and $E_f(C_\theta) + 24f(1)$ both equal 24 times the average of $c \mapsto f\big(\langle c, c_0\rangle\big)$ over S^3 for any $c_0 \in S^3$.

For $k = 3$, the plot suggested that $E_f(C_{D_4}) \le E_f(C_\theta)$, with equality at a unique value of θ in $[0,\pi]$, numerically $\theta = 2.51674+$. We verified this by using the rational parametrization

$$\sin\theta = \frac{2u}{1+u^2}, \quad \cos\theta = \frac{1-u^2}{1+u^2}$$

of the unit circle, computing $E_f(C_{D_4}) - E_f(C_\theta)$ symbolically as a rational function of u, and factoring this function. We found that

$$E_f(C_{D_4}) - E_f(C_\theta) = -18\frac{(u^6 - 6u^4 - 12u^3 + 3u^2 - 2)^2}{(u^2+1)^6},$$

and thus that $E_f(C_{D_4}) \le E_f(C_\theta)$, with equality if and only if u is a root of the sextic $u^6 - 6u^4 - 12u^3 + 3u^2 - 2$. This sextic has two real roots,

$$u = -(0.51171+), \quad u = 3.09594-,$$

which yield the two permutations of $\{\sin\theta, \cos\theta\} = \{0.58498-, -(0.81105+)\}$ and thus give rise to a unique code C_θ with $E_f(C_{D_4}) = E_f(C_\theta)$. This code is characterized more simply by the condition that $\sin\theta + \cos\theta$ is a root of the cubic $3y^3 - 9y - 2 = 0$, or better yet that $\sin^3\theta + \cos^3\theta = -\frac{1}{3}$. The latter formulation also lets us show that this is the unique C_θ that is a spherical 3-design: the cubics on $\mathbb{R}^4$ invariant under G are the multiples of $\mathrm{Re}(w_1^3) + \mathrm{Re}(w_2^3)$, and the sum of this cubic over C_θ is $6 + 18(\sin^3\theta + \cos^3\theta)$. Since C_{D_4} and this particular C_θ are both 3-designs, they automatically minimize the energy for any potential function that is a polynomial of degree at most 3. We must thus try $k > 3$ if we are to show that C_{D_4} is not universally optimal.

For $k = 4$ through $k = 7$ the plot indicated that $E_f(C_\theta)$ comes near $E_f(C_{D_4})$ for $\theta \approx 2.52$ but stays safely above $E_f(C_{D_4})$ for all θ, which is easily proved using the rational parametrization. (For $k = 4$ and $k = 5$ we could also have seen that C_{D_4} minimizes E_f by noting that C_{D_4} is a 5-design.) However, for $k = 8$ the minimum value of $E_f(C_\theta)$, occurring at $\theta = 2.529367746+$, is $5064.9533+$, slightly but clearly smaller than $E_f(C_{D_4}) = 5065.5$. That is, this C_θ is a better code than C_{D_4} for the potential function $(1+t)^8$, so C_{D_4} is not optimal for this potential function and hence not universally optimal.

The maximum value of $E_f(C_{D_4}) - E_f(C_\theta)$ for $f(t) = (1+t)^k$ remains positive for $k = 9, 10, 11, 12, 13$, attained at values of θ that slowly increase from $\theta = 2.52937-$ for $k = 8$ to $\theta = 2.54122-$ for $k = 13$. Each of these is itself enough to disprove the conjecture that C_{D_4} is universally optimal. (Another natural counterexample is $f(t) = e^{6t}$ with $\theta = 2.53719+$.)

We found no further solutions of $E_f(C_{D_4}) > E_f(C_\theta)$ with $k > 13$. It is clear that $E_f(C_{D_4}) < E_f(C_\theta)$ must hold for all θ if k is large enough, because $t_{\max}(C_\theta) > t_{\max}(C_{D_4}) = \frac{1}{2}$: the smallest value t_0 of $t_{\max}(C_\theta)$ is $(\sqrt{7}-1)/3 = 0.54858+$, occurring when either

$$t_0 = \sin\theta = \cos^2\theta - \frac{1}{2}\sin^2\theta$$

with $\theta = 2.56092+$ or

$$t_0 = \cos\theta = \sin^2\theta - \frac{1}{2}\cos^2\theta$$

with $\theta = 5.29305+$. Quantifying what "large enough" means, and combining the resulting bound with our computations for smaller k, we obtained the following result:

Proposition 3.1. *For $8 \le k \le 13$, there exists a choice of θ for which*

$$E_f(C_\theta) < E_f(C_{D_4})$$

when $f(t) = (1+t)^k$. *For other nonnegative integers* k, *no such* θ *exists.*

Proof. If k is large enough that

$$18f\left(\frac{\sqrt{7}-1}{3}\right) > 24f(-1) + 192\left(f\left(\frac{1}{2}\right) + f\left(-\frac{1}{2}\right)\right) + 144f(0),$$

then $E_f(C_{D_4}) < E_f(C_\theta)$. This criterion is wasteful, but we have no need of sharper inequalities. Calculation shows that this criterion holds for all $k \geq 75$. This leaves only finitely many values of k. For each of them, we use the rational parametrization of the unit circle to translate the statement of Proposition 3.1 into the assertion of existence or nonexistence of a real solution of a polynomial in $\mathbb{Z}[u]$, which can be confirmed algorithmically using Sturm's theorem. Doing so in each case completes the proof. □

We cannot rule out the possibility that there exists a universally optimal 24-point code in S^3, but it seems exceedingly unlikely. If C_{D_4} is the unique optimal spherical code, as is widely believed, then no universally optimal code can exist. The same conclusion follows from the conjecture in the next section.

It is still natural to ask which configuration minimizes each absolutely monotonic potential function. We are unaware of any case in which another code beats C_{D_4} and all the codes C_θ for some absolutely monotonic potential function, but given the subtlety of this area we are not in a position to make conjectures confidently.

4. New Spherical 5-Designs

Spherical designs are an important source of minimal-energy configurations: a spherical τ-design automatically minimizes the potential energy for $f(t) = (1+t)^k$ with $k \leq \tau$. Conversely, if an N-point spherical τ-design exists in S^{n-1}, then every N-point configuration in S^{n-1} that minimizes the potential function $f(t) = (1+t)^\tau$ must be a τ-design. Thus, when searching for universally optimal configurations, it is important to study τ-designs with τ as large as possible.

For 24 points in S^3, the D_4 root system forms a 5-design. By Theorem 5.11 in [Delsarte et al. 77], every 6-design must have at least 30 points, so 24 points cannot form a 6-design. Counting degrees of freedom suggests that 24-point 4-designs are plentiful, but 5-designs exist only for subtler reasons. One can search for them by having a computer minimize potential energy for $f(t) = (1+t)^5$. Here, we report on a three-dimensional family of 5-designs found by this method. The D_4 root system is contained in this family, and all the designs in the family can be viewed as deformations of C_{D_4}. We conjecture that there are no other 24-point spherical 5-designs in S^3. We shall show that this conjecture implies the nonexistence of a universally optimal 24-point code in S^3.

Our construction of 5-designs slightly generalizes a construction of Sloane, Hardin, and Cara for the 24-cell (Construction 1 and Theorem 1 in [Sloane et al. 03]). The Sloane–Hardin–Cara construction also works for certain other dimensions and numbers of points, and can be further generalized using our more abstract approach. For example, one can construct a family of designs in S^{2n-1} from a design in $\mathbb{CP}^{n-1}$. We plan to treat further applications in a future paper. See also the final paragraph of this section.

Fix an "Eisenstein structure" on the D_4 root lattice, that is, an action of $\mathbb{Z}[r]$, where $r = e^{2\pi i/3}$ is a cube root of unity. (It is enough to specify the action of r, which can be any element of order 3 in $\mathrm{Aut}(D_4)$ that acts on $\mathbb{R}^4$ with no nonzero fixed points; such elements constitute a single conjugacy class in $\mathrm{Aut}(D_4)$.) Then $\mathbb{R}^4$ is identified with $\mathbb{C}^2$, with the inner product given by

$$\big\langle (z_1, z_2), (\zeta_1, \zeta_2) \big\rangle = \mathrm{Re}\big(z_1\overline{\zeta}_1 + z_2\overline{\zeta}_2\big).$$

The group $\boldsymbol{\mu}_6$ of sixth roots of unity (generated by -1 and r) acts on C_{D_4} and partitions its 24 points into four hexagons centered at the origin; call them H_0, H_1, H_2, H_3. In coordinates, we may take

$$\begin{aligned} H_0 &= \{(w, 0) : w \in \boldsymbol{\mu}_6\}, \\ H_1 &= \{(uiw, tiw) : w \in \boldsymbol{\mu}_6\}, \\ H_2 &= \{(uiw, rtiw) : w \in \boldsymbol{\mu}_6\}, \\ H_3 &= \{(uiw, \overline{r}tiw) : w \in \boldsymbol{\mu}_6\}, \end{aligned}$$

where $u = \sqrt{1/3}$ and $t = \sqrt{2/3}$. For any complex numbers a_0, a_1, a_2, a_3 with $|a_0| = |a_1| = |a_2| = |a_3| = 1$, we define

$$D(a_0, a_1, a_2, a_3) = a_0H_0 \cup a_1H_1 \cup a_2H_2 \cup a_3H_3.$$

We claim that $D(a_0, a_1, a_2, a_3)$ is a 5-design. That is, we claim that for every polynomial P of degree at most 5 on $\mathbb{R}^4$, the average of $P(c)$ over $c \in D(a_0, a_1, a_2, a_3)$ equals the average of $P(c)$ over $c \in S^3$. It is sufficient to prove that the average is independent of the choice of a_0, a_1, a_2, a_3, because $D(1, 1, 1, 1) = C_{D_4}$ is already known to be a 5-design. But this is easy: for each $m \in \{0, 1, 2, 3\}$, the restriction of P to the plane spanned by H_m is again a polynomial of degree at most 5, and a_mH_m is a 5-design in the unit circle of this plane, so the average of P over a_mH_m is the average of P over this unit circle, independent of the choice of a_m.

This construction via rotating hexagons is a special case of Lemma 2.3 in [Sali 94], where that idea is applied to prove that many spherical designs are not rigid. Sali rotates a single hexagon to prove that C_{D_4} is not rigid, but he does not attempt a complete classification of the 24-point 5-designs.

It is far from obvious that there is no other way to perturb the D_4 root system to form a 5-design. For example, if there were two disjoint hexagons in D_4 that did not come from the same choice of Eisenstein structure as above, then rotating them independently would produce 5-designs not in our family. However, one can check via a counting argument that every pair of disjoint hexagons does indeed come from some common Eisenstein structure. This supports our conjecture that there are no other 24-point spherical 5-designs in S^3.

The family of 5-designs of the form $D(a_0, a_1, a_2, a_3)$ is three-dimensional, for the following reason. One of the four parameters a_0, a_1, a_2, a_3 is redundant, because for every $\alpha \in \mathbb{C}^*$ with $|\alpha| = 1$ we have $D(\alpha a_0, \alpha a_1, \alpha a_2, \alpha a_3) \cong D(a_0, a_1, a_2, a_3)$. We may thus assume $\alpha_0 = 1$. We claim that for each (a_1, a_2, a_3) there are only finitely many (a_1', a_2', a_3') such that $D(1, a_1, a_2, a_3) \cong D(1, a_1', a_2', a_3')$. If this were not true, there would be an infinite set of designs $D(1, b_1, b_2, b_3)$ equivalent under automorphisms of S^3 that stabilize H_0 pointwise. But this is impossible, because such an automorphism must act trivially on the first coordinate z_1. Hence our 5-designs constitute a three-dimensional family, as claimed.

Some other known spherical designs can be similarly generalized. For instance, the 7-design of 48 points in S^3, obtained in [Sloane et al. 03] from two copies of C_{D_4}, has a decomposition into six regular octagons, which can be rotated independently to yield a five-dimensional family of 7-designs.

It is also fruitful to take a more abstract approach. A 24-point design with a $\boldsymbol{\mu}_6$ action is specified by four points, one in each orbit. Our new designs are characterized by the condition that under the natural map $\mathbb{C}^2 \setminus \{(0,0)\} \to \mathbb{CP}^1$ given by $(z_1, z_2) \mapsto z_1/z_2$, the four points must map to the vertices of a regular tetrahedron (if we identify $\mathbb{CP}^1$ with S^2 via stereographic projection, with $\mathbb{CP}^1 = \mathbb{C} \cup \{\infty\}$ and S^2 a unit sphere centered at the origin). In slightly different language, we have specified the image of the design under the Hopf map $S^3 \to S^2$. The fact that the regular tetrahedron is a spherical 2-design in S^2 plays a crucial role, and can be used to prove that this construction yields 5-designs. Likewise, the six octagons that make up each of our 7-designs map to the vertices of a regular octahedron, which is a spherical 3-design. Again, we intend to discuss this approach in more detail in a future paper.

5. Optimality of C_{D_4} among new 5-designs

In this section we prove that among all these new 5-designs, the 24-cell minimizes potential energy for each absolutely monotonic potential function. As before, it is sufficient to do this for $f(t) = (1+t)^k$. For $k \leq 5$ this follows immediately from the spherical design property, and for $k > 5$ we will show directly that C_{D_4} is the unique minimizer.

Within each hexagon H_m, the six points are in the same relative position in each design, and thus make the same contribution to the potential energy. Hence it suffices to show that the potential energy between each pair of hexagons is separately minimized for the D_4 configuration.

Let $a_0 = 1$, $a_1 = ie^{i\theta}$, $a_2 = ie^{i\phi}$, and $a_3 = ie^{i\psi}$. Because of the sixfold rotational symmetry of each H_m, the angles θ, ϕ, and ψ are determined only modulo $\pi/3$. In particular, $\theta = \phi = \psi = \pi/6$ yields the 24-cell (because $\pi/2 \equiv \pi/6 \pmod{\pi/3}$).

First, consider the pair (H_0, H_1). We find that the inner products between the points of H_0 and $a_1 H_1$ are $(1/\sqrt{3})\cos(\theta + j\pi/3)$ with $0 \leq j \leq 5$, each repeated six times. By Lemma 5.1 below, the sum is minimized exactly when $\theta \equiv \pi/6 \pmod{\pi/3}$. Similarly, considering (H_0, H_2) and (H_0, H_3) shows that the corresponding contributions to potential energy are minimized when $\phi \equiv \pi/6 \pmod{\pi/3}$ or $\psi \equiv \pi/6 \pmod{\pi/3}$, respectively.

Next, consider the pair (H_1, H_2). The dot products possible are of the form

$$\operatorname{Re}\big((u^2 + \overline{r}t^2)a_1\overline{a}_2 w^j\big) = \frac{1}{\sqrt{3}} \cos\left(\frac{3\pi}{2} + \theta - \phi + \frac{j\pi}{3}\right)$$

with $0 \leq j \leq 5$, each repeated six times. Once again we conclude from Lemma 5.1 that the potential energy is minimized when $\theta \equiv \phi \pmod{\pi/3}$. Similarly, considering the remaining pairs (H_1, H_3) and (H_2, H_3) shows that $\theta \equiv \phi \equiv \psi \pmod{\pi/3}$. Thus, it will follow from the lemma below that for each $k \geq 6$, the D_4 configuration with $\theta = \phi = \psi = \pi/6$ is the unique code in this family that minimizes the potential energy under the potential function $f(t) = (1+t)^k$.

Lemma 5.1. *Let k be a nonnegative integer. When $k \geq 6$, the function*

$$\theta \mapsto \sum_{j=0}^{5} \left(1 + \frac{\cos(\theta + j\pi/3)}{\sqrt{3}}\right)^k$$

has a unique global minimum within $[0, \pi/3]$*, which occurs at* $\theta = \pi/6$*. When* $k \leq 5$*, the function is constant.*

Proof. We must show that the coefficient of y^k in the generating function

$$\sum_{j=0}^{5}\sum_{k=0}^{\infty}\left(\left(1+\frac{\cos(\theta+j\pi/3)}{\sqrt{3}}\right)^k-\left(1+\frac{\cos(\pi/6+j\pi/3)}{\sqrt{3}}\right)^k\right)y^k$$

is zero if $k \leq 5$ or $\theta \equiv \pi/6 \pmod{\pi/3}$ and strictly positive otherwise. Explicit computation using the sum of a geometric series shows that the generating function equals

$$\frac{y^6\left(\cos^2\theta\right)\left(4\cos^2\theta-3\right)^2}{216}\left(\frac{1}{1-y}+\frac{2}{2-y}+\frac{2}{2-3y}\right)\prod_{j=0}^{5}\frac{1}{1-y\left(1+\frac{\cos(\theta+j\pi/3)}{\sqrt{3}}\right)}.$$

The factor of $\left(\cos^2\theta\right)\left(4\cos^2\theta-3\right)^2$ vanishes iff $\theta \equiv \pi/6 \pmod{\pi/3}$ and is positive otherwise. Clearly the factor

$$\frac{1}{1-y}+\frac{2}{2-y}+\frac{2}{2-3y}$$

has positive coefficients, as does

$$\prod_{j=0}^{5}\frac{1}{1-y\left(1+\frac{\cos(\theta+j\pi/3)}{\sqrt{3}}\right)},$$

because $1+\cos(\theta+j\pi/3)/\sqrt{3} > 0$ for all j. It follows that their product has positive coefficients, and taking the factor of y^6 into account completes the proof. □

6. Local Optimality

So far, we have not addressed the question of whether our new codes are actually local minima for energy. Of course that is not needed for our main result, because they improve on the 24-cell regardless of whether they are locally optimal, but it is an interesting question in its own right.

For the codes C_θ this question appears subtle, and we do not resolve it completely. To see the issues involved, consider the case of $f(t) = (1-t)^{-1}$. As θ varies, the lowest energy obtained is $668.1920+$ when $\theta = 2.5371+$. That code appears to be locally minimal among all codes, based on diagonalizing the Hessian matrix numerically, but we have not proved it. By contrast, the other two local minima within the family C_θ (with energy $721.7796+$ at $\theta = -(2.0231+)$ and energy $926.3218+$ at $\theta = 0.5320+$) are critical points but definitely not local minima among all codes; the Hessians have 22 and 36 negative eigenvalues, respectively.

We do not know a simple criterion that predicts whether a local minimum among the codes C_θ as θ varies will prove to be a local minimum among all codes, but it is not hard to prove that every critical point in the restricted setting is also an unrestricted critical point. Specifically, a short calculation shows that for every code C_θ and every smooth potential function, the gradient of potential energy on the space of all configurations lies in the tangent space of the subspace consisting of all the codes C_θ. It follows immediately that if the derivative with respect to θ of potential energy vanishes, then the gradient vanishes as well. Furthermore, such critical points always exist: starting at an arbitrary code C_θ and performing gradient descent will never leave the space of such codes and will always end at a critical point.

At this point one may wonder whether it is even clear that the regular 24-cell is a local minimum for all absolutely monotonic potential functions. It is straightforward to show that it is a critical point, but we know of no simple proof that it is actually a local minimum. The best proof we have found is the following calculation.

For each of the 24 points, choose an orthonormal basis of the tangent space to S^3 at that point, and compute the Hessian matrix of potential energy with respect to these coordinates. Its eigenvalues depend on the potential function, but the corresponding eigenspaces do not. There is a simple reason for that, although we will not require this machinery. Consider the space $\mathrm{Sym}^{24}(S^3)$ of all unordered sets of 24 points in S^3. The symmetry group of the 24-cell acts on the tangent space to $\mathrm{Sym}^{24}(S^3)$ at the point corresponding to the 24-cell, and this representation breaks up as a direct sum of irreducible representations. On each nontrivial irreducible representation the Hessian has a single eigenvalue, and these subspaces do not depend on the potential function. In practice, the simplest way to calculate the eigenspaces is not to use representation theory, but rather to find them for one potential function and then verify that they are always eigenspaces.

If the potential function is $f\colon [-1,1) \to \mathbb{R}$, then the eigenvalues of the Hessian are

$$
\begin{aligned}
&0,\\
&2f''\left(\frac{1}{2}\right) + 8f''(0) + 2f''\left(-\frac{1}{2}\right) - 12f'\left(\frac{1}{2}\right) + 12f'\left(-\frac{1}{2}\right),\\
&2f''\left(\frac{1}{2}\right) + 4f''(0) + 6f''\left(-\frac{1}{2}\right) - 8f'\left(\frac{1}{2}\right) - 4f'(0) + 8f'\left(-\frac{1}{2}\right) + 4f'(-1),\\
&5f''\left(\frac{1}{2}\right) + 4f''(0) + 3f''\left(-\frac{1}{2}\right) - 14f'\left(\frac{1}{2}\right) + 8f'(0) + 2f'\left(-\frac{1}{2}\right) + 4f'(-1),\\
&6f''\left(\frac{1}{2}\right) + 6f''\left(-\frac{1}{2}\right) - 12f'\left(\frac{1}{2}\right) + 12f'\left(-\frac{1}{2}\right),\\
&2f''\left(\frac{1}{2}\right) + 4f''(0) + 6f''\left(-\frac{1}{2}\right) + 4f'\left(\frac{1}{2}\right) + 8f'(0) + 20f'\left(-\frac{1}{2}\right) + 4f'(-1),\\
&6f''\left(\frac{1}{2}\right) + 8f''(0) + 6f''\left(-\frac{1}{2}\right) - 4f'\left(\frac{1}{2}\right) + 4f'\left(-\frac{1}{2}\right),\\
&8f''\left(\frac{1}{2}\right) + 4f''(0) - 8f'(1/2) - 4f'(0) + 8f'\left(-\frac{1}{2}\right) + 4f'(-1),
\end{aligned}
$$

with multiplicities 6, 9, 16, 8, 12, 4, 9, and 8, respectively.

One mild subtlety is that 0 is always an eigenvalue, so one might worry that the second derivative test is inconclusive. However, note that the potential energy is invariant under the action of the 6-dimensional Lie group $\mathrm{O}(4)$, which yields the 6 eigenvalues of 0. In such a case, if all other eigenvalues are positive, then local minimality still holds, for the following reason. Notice that $\mathrm{O}(4)$ acts freely on the space of ordered 24-tuples of points in S^3 that span $\mathbb{R}^4$, and it acts properly since $\mathrm{O}(4)$ is compact. The quotient space is therefore a smooth manifold, and the positivity of the remaining eigenvalues suffices for the potential energy to have a strict local minimum on the quotient space.

To complete the proof, we need only consider $f(t) = (1+t)^k$ with $k \in \{0, 1, 2, \dots\}$. For $k \leq 5$ the other eigenvalues are not all positive (some vanish), but because the 24-cell is a spherical 5-design it is automatically a global minimum for these energies. For $k \geq 6$ one can check that all the other eigenvalues are positive. That is obvious asymptotically, because they grow exponentially as functions of k; to prove it for all $k \geq 6$ one reduces the problem to a finite number of cases and checks each of them. It follows that the regular 24-cell locally minimizes potential energy for each absolutely monotonic potential function, and it is furthermore a strict local minimum (modulo orthogonal transformations) unless the potential function is a polynomial of degree at most 5.

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References

[Andreev 96] N. N. Andreev. "An Extremal Property of the Icosahedron." *East J. Approx.* 2 (1996), 459–462.

[Andreev 97] N. N. Andreev. "Location of Points on a Sphere with Minimal Energy." *Proc. Steklov Inst. Math.* 219 (1997), 20–24.

[Arestov and Babenko 97] V. V. Arestov and A. G. Babenko. "On the Delsarte Scheme for Estimating Contact Numbers." *Proc. Steklov Inst. Math.* 219 (1997), 36–65.

[Bannai and Sloane 81] E. Bannai and N. J. A. Sloane. "Uniqueness of Certain Spherical Codes." *Canad. J. Math.* 33:2 (1981), 437–449.

[Cohn and Kumar 07] H. Cohn and A. Kumar. "Universally Optimal Distribution of Points on Spheres." *J. Amer. Math. Soc.* 20 (2007), 99–148.

[Delsarte et al. 77] P. Delsarte, J. Goethals, and J. Seidel. "Spherical Codes and Designs." *Geometriae Dedicata* 6 (1977), 363–388.

[Kolushov and Yudin 94] A. V. Kolushov and V. A. Yudin. "On the Korkin–Zolotarev Construction." *Discrete Math. Appl.* 4:2 (1994), 143–146.

[Kolushov and Yudin 97] A. V. Kolushov and V. A. Yudin. "Extremal Dispositions of Points on the Sphere." *Anal. Math.* 23:1 (1997), 25–34.

[Levenshtein 79] V. I. Levenshtein. "On Bounds for Packings in n-Dimensional Euclidean Space." *Soviet Math. Dokl.* 20 (1979), 417–421.

[Odlyzko and Sloane 79] A. M. Odlyzko and N. J. A. Sloane. "New Bounds on the Number of Unit Spheres That Can Touch a Unit Sphere in n Dimensions." *J. Combin. Theory Ser. A* 26 (1979), 210–214.

[PARI 05] PARI/GP, version 2.1.7, Bordeaux. Available online (`http://pari.math.u-bordeaux.fr/`), 2005.

[Sali 94] A. Sali. "On the Rigidity of Spherical t-Designs That Are Orbits of Finite Reflection Groups." *Des. Codes Cryptogr.* 4 (1994), 157–170.

[Sloane 00] N. J. A. Sloane, with the collaboration of R. H. Hardin, W. D. Smith, and others. "Tables of Spherical Codes." Available online (`http://www.research.att.com/~njas/packings/`), 2000.

[Sloane et al. 03] N. J. A. Sloane, R. H. Hardin, and P. Cara. "Spherical Designs in Four Dimensions." In *Proceedings of the 2003 IEEE Information Theory Workshop*, pp. 253–258. Washington, DC: IEEE Press, 2003.

[Widder 41] D. V. Widder. *The Laplace Transform*. Princeton: Princeton University Press, 1941.

[Yudin 93] V. A. Yudin. "Minimum Potential Energy of a Point System of Charges." *Discrete Math. Appl.* 3:1 (1993), 75–81.

Microsoft Research, One Microsoft Way, Redmond, WA 98052-6399
E-mail address: cohn@microsoft.com

Department of Mathematics, Princeton University, Princeton, NJ 08544-1000
E-mail address: conway@math.princeton.edu

Department of Mathematics, Harvard University, Cambridge, MA 02138
E-mail address: elkies@math.harvard.edu

Department of Mathematics, Massachusetts Institute of Technology, Cambridge, MA 02139
E-mail address: abhinav@math.mit.edu