LARGE REGULAR SIMPLICES CONTAINED IN A HYPERCUBE

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ABSTRACT. We prove that the n-dimensional unit hypercube contains an n-dimensional regular simplex of edge length $c\sqrt{n}$, where $c > 0$ is a constant independent of n.

Let $\ell\Delta_n$ be the n-dimensional regular simplex of edge length ℓ, and let ℓQ_n be the n-dimensional hypercube of edge length ℓ. For simplicity, we omit ℓ if $\ell = 1$, e.g., Q_n denotes the unit hypercube. We are interested in the maximum edge length of a regular n-dimensional simplex contained in Q_n.

Theorem. *For every $\varepsilon_0 > 0$ there is an N_0 such that for every $n > N_0$ one has*

$$\left(\frac{1-\varepsilon_0}{2}\sqrt{n}\right)\Delta_n \subset Q_n.$$

On the other hand, if $\ell\Delta_n \subset Q_n$, then $\ell \le \sqrt{(n+1)/2}$, which follows by comparing the circumscribed balls of $\ell\Delta_n$ and Q_n. (Recall that the circumradius of Δ_n is $\sqrt{n/(2n+2)}$.) This upper bound is reached iff there exists an Hadamard matrix of order $n+1$. Schoenberg [3] pointed out that this "readily established fact" went back to Coxeter, see also §4 of [1]. Our lower bound given by the theorem is approximately $1/\sqrt{2}$ of the upper bound.

Proof of Theorem. For a matrix (or a vector) $A = (a_{ij})$, let us define its norm by $\|A\| := \max_{ij} |a_{ij}|$. Let J_n be the $n \times n$ all one matrix.

Lemma 1. *Let $A = (a_{ij})$ be an $n \times n$ real orthogonal matrix, and let $c > 0$ be a constant. If*

$$\|A\| \le \frac{1}{c\sqrt{n}} \tag{1}$$

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and

$$\|J_n A\| \le \frac{1}{c}, \tag{2}$$

then we have $(c\sqrt{n/2})\Delta_n \subset Q_n$.

Proof. Let $p_i = (a_{i1}, \dots, a_{in})$ be the i-th row of the matrix A. Then the n points $p_1, \dots, p_n \in \mathbb{R}^n$ form a $\sqrt{2}\Delta_{n-1}$. By (1), we have $\|p_i\| \le 1/(c\sqrt{n})$ for all $1 \le i \le n$.

Let $g = (g_1, \dots, g_n) \in \mathbb{R}^n$ be the barycenter of the above $\sqrt{2}\Delta_{n-1}$, and let $p_{n+1} := (1-\sqrt{n+1})g$. Then a computation shows that the $p+1$ points $p_1, \dots, p_n, p_{n+1} \in \mathbb{R}^n$ form a $\sqrt{2}\Delta_n$. Moreover, it follows from (2) that $\|p_{n+1}\| = \|g\|(\sqrt{n+1}-1) \le 1/(c\sqrt{n})$. Thus we have $\sqrt{2}\Delta_n \subset (2/(c\sqrt{n}))Q_n$, as desired. □

Let us find orthogonal matrices satisfying (1) and (2). Let q be an odd prime power, and let $\mathbb{F}_q = \{b_0, \dots, b_{q-1}\}$ ($b_0 = 0$) be the finite field of order q. Define a character $\chi : \mathbb{F}_q \to \{0, \pm 1\}$ by $\chi(0) = 0$, $\chi(x) = 1$ if x is a square, and $\chi(x) = -1$ if x is a nonsquare. Define an $q \times q$ matrix $B = (b_{ij})$ by setting $b_{ij} := \chi(b_i - b_j)$. Then this matrix satisfies $BB^T = qI_q - J_q$, $BJ_q = J_qB = O$. (See pp. 202–203 in [2] for the proof and how to use this matrix to construct an Hadamard matrix of Paley type.) Finally we define an orthogonal $q \times q$ matrix A_q by

$$A_q := \frac{1}{\sqrt{q}}\Big(B + \frac{1}{\sqrt{q}}J_q\Big).$$

Then, it is easy to check that A_q satisfies $\|A_q\| \le \frac{1}{\sqrt{q}} + \frac{1}{q}$ and $J_qA_q = J_q$. Thus the matrix A_q satisfies (1) and (2) for $c = 1 - o(1)$, and this verifies the theorem for the case when the dimension is an odd prime power. (By using the fact that each entry a_{ij} of A_q satisfies $|a_{ij} - 1/q| \le 1/\sqrt{q}$, instead of (1), we can remove the $o(1)$, i.e., we actually get $\sqrt{q/2}\Delta_q \subset Q_q$.)

Now let $q_1, \dots, q_r$ be distinct odd prime powers, and let $n = q_1 \cdots q_r$ and $A_n := A_{q_1} \otimes \cdots \otimes A_{q_r}$. Then the matrix A_n is orthogonal with

$$\|A_n\| \le \frac{1}{\sqrt{n}} \prod_{i=1}^{r} \Big(1 + \frac{1}{\sqrt{q_i}}\Big). \tag{3}$$

Moreover, A_n satisfies $J_nA_n = J_n$ because $J_nA_n = (J_{q_1} \otimes \cdots \otimes J_{q_r})(A_{q_1} \otimes \cdots \otimes A_{q_r}) = (J_{q_1}A_{q_1}) \otimes \cdots \otimes (J_{q_r}A_{q_r}) = J_n$. We notice that

$$\prod_{i=1}^{r} \Big(1 + \frac{1}{\sqrt{q_i}}\Big) \le \prod_{p|n}\Big(1 + \frac{1}{\sqrt{p}}\Big) = \sum_{d|n} \frac{1}{\sqrt{d}} =: g(n), \tag{4}$$

where the product in the middle term is taken for all primes p dividing n. Thus (3) gives (1) with $c = 1/g(n)$, and Lemma 1 implies that

$$\Big(\frac{\sqrt{n}}{g(n)\sqrt{2}}\Big)\,\Delta_n \subset Q_n \tag{5}$$

for every odd integer n.

Lemma 2. *For every $\varepsilon, \delta > 0$ there is an n_0 with the following property. For every integer $n > n_0$ there are odd integers n_1, n_2 such that $2n = n_1 + n_2$, $(1-\varepsilon)n \le n_i \le (1+\varepsilon)n$ and $g(n_i) < 1 + \delta$ for each $i = 1, 2$.*

Proof. We will select an m, define

$$q = \prod_{p \le m} p$$

as the product of the primes up to m and select n_1, n_2 coprime to q. This guarantees that they are odd.

First we average $g(n)$ over integers coprime to q. Let $(q,r) = 1$. Write I_r for the set of integers $\{j \in [(1-\varepsilon)n, (1+\varepsilon)n] : j \equiv r \pmod{q}\}$. We have

$$\sum_{j \in I_r} (g(j) - 1) = \sum_{d > 1} \frac{1}{\sqrt{d}} N_d,$$

where N_d is the number of multiples of d in our set I_r. Clearly $N_d = 0$ if $(d,q) > 1$. If $(d,q) = 1$, then the multiples of d in this residue class form an arithmetic progression with difference qd, and we have the estimate

$$N_d \le \frac{2\varepsilon n}{qd} + 1.$$

Furthermore $N_d = 0$ if $d \ge 2n$.

Our choice of q implies that whenever $d > 1$ and $(d,q) = 1$, then $d > m$, so we have

$$\sum_{j \in I_r} (g(j) - 1) \le \sum_{m < d < 2n} \frac{1}{\sqrt{d}} \left(\frac{2\varepsilon n}{qd} + 1 \right).$$

We use the easy estimates

$$\sum_{d > m} d^{-3/2} < 2/\sqrt{m}, \quad \sum_{d < 2n} d^{-1/2} < 2\sqrt{2n} < 3\sqrt{n}$$

to conclude

$$\sum_{j \in I_r} (g(j) - 1) < \frac{4\varepsilon n}{q\sqrt{m}} + 3\sqrt{n}. \tag{6}$$

Now we define r as follows. Take a prime $p \le m$. If $2n \not\equiv 1 \pmod{p}$, we put $r \equiv 1 \pmod{p}$; if $2n \equiv 1 \pmod{p}$, let $r \equiv 2 \pmod{p}$. In this way both r and $r' = 2n - r$ will be coprime to q. Applying (6) for r and r' and summing we get

$$\sum_{j \in I_r} \big((g(j)-1) + (g(2n-j)-1)\big) < \frac{8\varepsilon n}{q\sqrt{m}} + 6\sqrt{n}.$$

The number of summands in the above sum is $\geq 2\varepsilon n/q - 1 > \varepsilon n/q$, assuming that $q < \varepsilon n$. Hence there is a value j such that

$$(g(j)-1) + (g(2n-j)-1) < \frac{8}{\sqrt{m}} + \frac{6q}{\varepsilon\sqrt{n}}.$$

If the right hand side is $< \delta$, we are done. To achieve this we make both summands $< \delta/2$. First we choose m so that $8/\sqrt{m} < \delta/2$, that is, $m > (16/\delta)^2$. This determines the value of q, and we choose n so large that $6q/(\varepsilon\sqrt{n}) < \delta/2$, that is, $n > (12q/(\varepsilon\delta))^2$. □

Lemma 3. *Let $\ell > 0$ be a real, and let s and t be positive integers with $\ell^2 \leq s \leq t$. If $\ell\Delta_s \subset Q_s$ and $\ell\Delta_t \subset Q_t$, then $\ell\Delta_{s+t+1} \subset Q_{s+t+1}$.*

Proof. Let $p_0, p_1, \dots, p_s$ be the vertices of $\ell\Delta_s$ inside Q_s, and let $q_0, q_1, \dots, q_t$ be the vertices of $\ell\Delta_t$ inside Q_t. We may assume that the origin is the centers of these regular simplices. Then the distance between p_i and the origin is given by $\ell\sqrt{s/(2s+2)}$. We will construct $\ell\Delta_{s+t+1}$ with vertices $u_0, \dots, u_s, v_0, \dots, v_t$ as follows. Define u_i for $0 \leq i \leq s$ and v_j for $0 \leq j \leq t$ by

$$u_i = (p_i, \vec{0}, x) \in \mathbb{R}^s \times \mathbb{R}^t \times \mathbb{R}, \quad v_j = (\vec{0}, q_j, 0) \in \mathbb{R}^s \times \mathbb{R}^t \times \mathbb{R}.$$

Choose $x > 0$ so that $|u_i - v_j| = \ell$ for all i, j. This can be done by solving

$$|u_i - v_j|^2 = \frac{s}{2s+2}\ell^2 + \frac{t}{2t+2}\ell^2 + x^2 = \ell^2,$$

which gives $x = \ell(\frac{1}{2s+2} + \frac{1}{2t+2})^{1/2} < \ell/\sqrt{s+1} < 1$. Namely, we have

$$u_i, v_j \in Q_s \times Q_t \times [0,1] = Q_{s+t+1},$$

for all i, j. □

We are ready to prove the theorem. Let $\varepsilon_0 > 0$ be given. Set $\varepsilon = \varepsilon_0/2$ and take $\delta > 0$ so that

$$1 - \varepsilon = \sqrt{1-\varepsilon}/(1+\delta). \tag{7}$$

Plug these ε and δ into Lemma 2 to get $k_0 = k_0(\varepsilon, \delta) > 0$ such that for every $k > k_0$ there are k_1, k_2 satisfying $2k = k_1 + k_2$, $k_i \geq (1-\varepsilon)k$, and $g(k_i) < 1 + \delta$. Choose $N_0 \geq 2k_0$ so that

$$(1-\varepsilon)\sqrt{n-1} > (1-\varepsilon_0)\sqrt{n} \tag{8}$$

holds for all $n > N_0$.

Now, let $n > N_0$ be given. First assume that n is odd, and write $n = 2k+1$. Lemma 2 gives a decomposition $2k = k_1 + k_2$. Then we have $\ell_i \Delta_{k_i} \subset Q_{k_i}$ for $i = 1, 2$, where

$$\ell_i \overset{(5)}{=} \frac{\sqrt{k_i}}{g(k_i)\sqrt{2}} > \frac{\sqrt{(1-\varepsilon)k}}{(1+\delta)\sqrt{2}} \overset{(7)}{=} \frac{(1-\varepsilon)\sqrt{k}}{\sqrt{2}} = \frac{1-\varepsilon}{2}\sqrt{n-1} \overset{(8)}{>} \frac{1-\varepsilon_0}{2}\sqrt{n}.$$

Applying Lemma 3 with $s = k_1, t = k_2$ and $\ell = \frac{1-\varepsilon_0}{2}\sqrt{n}$, we have the desired result $\ell\Delta_n \subset Q_n$.

Next assume that n is even, and write $n = 2k$. Lemma 2 gives $2k = k_1 + k_2$ and

$$\|A_{k_i}\| \overset{(3)(4)}{\leq} \frac{g(k_i)}{\sqrt{k_i}} < \frac{1+\delta}{\sqrt{(1-\varepsilon)k}} \overset{(7)}{=} \frac{\sqrt{2}}{(1-\varepsilon)\sqrt{n}} < \frac{\sqrt{2}}{(1-\varepsilon_0)\sqrt{n}} =: \frac{1}{c\sqrt{n}}.$$

Define an $n \times n$ orthogonal matrix C by

$$C = \begin{pmatrix} A_{k_1} & 0 \\ 0 & A_{k_2} \end{pmatrix}.$$

Then we have $\|C\| \leq \max \|A_{k_i}\| < 1/(c\sqrt{n})$ and $\|J_n C\| = \max \|J_{k_i} A_{k_i}\| = 1$. Thus, by Lemma 1, we have $(c\sqrt{n/2})\Delta_n = (\frac{1-\varepsilon_0}{2}\sqrt{n})\Delta_n \subset Q_n$. This completes the proof of the theorem. □

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