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THE SUM OF THE DISTANCES TO N POINTS ON A SPHERE

KENNETH B. STOLARSKY

How can the sum of λth powers $(0 < \lambda < 2)$ of the Euclidean distances from the variable unit vector p to N fixed unit vectors $p_1, \cdots, p_N$ be maximized or minimized? By means of an integral transform used in distance geometry, the problem can be reduced in certain cases to minimizing or maximizing sums of integer powers of the inner products (p, p_i). In particular, a complete solution is obtained for the vertices of an m-dimensional octahedron.

1. Introduction. Let $|p - q|$ denote the Euclidean distance from p to q. Various authors [1-3, 7, 12, 14, 16, 17] have studied the problem of placing N points $p_1, \cdots, p_N$ on the unit sphere U of m-dimensional Euclidean space E^m so that

$$S(N, m) = \sum_{i<j} |p_i - p_j|^\lambda \qquad 0 < \lambda < 2 \tag{1}$$

is maximal. This suggests a second problem: If $p_1, \cdots, p_N$ are preassigned points of U, for what $p \in U$ is

$$T(p) = \sum_{i=1}^{N} |p - p_i|^\lambda \qquad 0 < \lambda < 2 \tag{2}$$

maximal? One can add to this, when is $T(p)$ minimal? For example, if $N = 3$ and p_1, p_2, p_3 are the vertices of an equilateral triangle, then $T(p)$ is maximal if and only if $p = -p_i$ for some i and minimal if and only if $p = p_i$ for some i. This is very easy to show for $0 < \lambda \leqq 1$, but is rather more difficult for $1 < \lambda < 2$.

In §2 we develop a method for attacking this second problem. Our main tools are (i) an integral transform introduced by Schoenberg (see [15, pp. 526-527] or [4, pp. 134-136]) to prove certain metric embedding theorems, and (ii) the concept of uniform power maxima introduced in §2. The results §§3-6 are applications of the theorem of §2 to various special cases. In §3 we determine the maxima and minima for $T(p)$ when the p_i are the vertices of a regular m-dimensional octahedron. In §4 we determine the maxima of $T(p)$ when the p_i are the vertices of an m-dimensional cube. In §5 we investigate the case where the p_i are the vertices of an m-dimesional simplex. We show that if a certain "elementary" inequality is valid, then $T(p)$ is minimal if and only if $p = p_i$ for some i. In §6 we determine the minima of $T(p)$ when the p_i are the vertices of a regular N-gon and U is the unit circle $x^2 + y^2 = 1$.

The general conclusion we draw from these results is that if the points p_i are "reasonably" uniformly distributed on U then $T(p)$ is large or small depending upon whether $\min_i |p_i - p|$ is large or small. It is interesting to contrast this with Theorem 2 of Björck [3, pp. 256-257]. Also, it can be shown that if p is constrained to be in the convex hull H of $p_1, \cdots, p_N$ and $1 \leqq \lambda$, then $T(p)$ will be *maximal* at some p_i.

In §7 we show that a modification of our method can be applied to the problem of minimizing $T(p)$ when λ is negative. This is related to the problem of stability configurations of electrons on a sphere; see [5-6, 8-10, 14, 18].

2. Uniform power maxima.

For vectors g and h in E^m, we let (g, h) denote their inner product.

DEFINITION. Let $p_1, \cdots, p_N$ be a set of points on the unit sphere U. We say $q_0 \in U$ is a uniform power maximum (minimum) for $p_1, \cdots, p_N$ if for every positive integer k, the sum

$$\sum_{i=1}^{N} (p_i, q)^k \tag{2.1}$$

achieves its absolute maximum (minimum) on U when $q = q_0$.

For example, let U be the unit circle $x^2 + y^2 = 1$. If $p_1 = (1, 0)$ and $p_2 = -p_1$, then the points p_1 and p_2 are themselves the uniform power maxima, while the points $(0, 1)$ and $(0, -1)$ are the uniform power minima. In general, uniform power maxima or minima may fail to exist.

If q_0 is a uniform power maximum, then we easily see that $q_0 = p_i$ for some i; let $k \to \infty$ through odd values in (2.1). Similarly, by letting $k \to \infty$ through even values, we see that $\max_i |(p_i, q_0)|$ must be minimal if q_0 is a uniform power minimum. For example, if N is even and $p_1, \cdots, p_N$ are the vertices of a regular N-gon inscribed in the unit circle U given by $x^2 + y^2 = 1$, then the only possibilities for uniform power minima are points on U which bisect the arc between adjacent p_i. The only possibilities for uniform power maxima are the p_i themselves.

The following result shows how the concepts of uniform power maxima and minima can be used.

THEOREM. *Let $p_1, \cdots, p_N$ have at least one uniform power maximum* (minimum). *Let $p \in U$. Then*

$$T(p) = \sum_{i=1}^{N} |p_i - p|^\lambda \qquad 0 < \lambda < 2 \tag{2.2}$$

is minimal (maximal) *if and only if p is a uniform power maximum* (minimum).

Proof. Let $p \in U$. Let q_0 be a uniform power maximum. Then

$$\sum_{i=1}^{N} (p_i, p)^k \leqq \sum_{i=1}^{N} (p_i, q_0)^k \tag{2.3}$$

for all integers $k \geqq 0$. If g and h are arbitrary unit vectors, then

$$2(g, h) = 2 - |g - h|^2 . \tag{2.4}$$

Hence

$$\sum_{i=1}^{N} (2 - |p_i - p|^2)^k \leqq \sum_{i=1}^{N} (2 - |p_i - q_0|^2)^k . \tag{2.5}$$

Set

$$E(p, t) = \sum_{i=1}^{N} \exp(-|p_i - p|^2 t^2) .$$

Multiply both sides of (2.5) by $t^{2k}/k!$ and sum over all k. This shows that

$$\begin{aligned} \exp(2t^2)E(p, t) &= \sum_{i=1}^{N} \exp(2t^2 - |p_i - p|^2 t^2) \\ &\leqq \sum_{i=1}^{N} \exp(2t^2 - |p_i - q_0|^2 t^2) \\ &= \exp(2t^2)E(q_0, t) . \end{aligned} \tag{2.6}$$

Note that here and throughout equality holds if and only if p is a uniform power maximum. Since $0 < \lambda < 2$, we can set

$$I_\lambda(s) = \int_0^\infty (1 - e^{-s^2 t^2}) t^{-1-\lambda} dt . \tag{2.7}$$

By making the change of variable $t \to t/s$ we see that

$$I_\lambda(s) = c(\lambda) s^\lambda \tag{2.8}$$

where $c(\lambda)$ is a positive constant depending only on λ; in fact,

$$c(\lambda) = \int_0^\infty (1 - e^{-t^2}) t^{-1-\lambda} dt .$$

Now replace s by $|p_i - q_0|$ in (2.7). From (2.6) and (2.8) we find that

$$\begin{aligned} c(\lambda) T(q_0) &= c(\lambda) \sum_{i=1}^{N} |p_i - q_0|^\lambda \\ &= \sum_{i=1}^{N} I_\lambda(|p_i - q_0|) \end{aligned}$$

$$(2.9) \qquad \begin{aligned} &= \int_0^\infty [N - E(q_0, t)] t^{-1-\lambda} dt \\ &\leqq \int_0^\infty [N - E(p, t)] t^{-1-\lambda} dt \\ &= c(\lambda) T(p) \ , \end{aligned}$$

with equality if and only if p is a uniform power maximum. The proof for uniform power minima is obtained simply by reversing all inequalities.

3. The octahedron. Let α_i denote that vector of E^m whose ith component is 1 and whose other components are 0. Let $\alpha_{N+i} = -\alpha_i$ for $1 \leqq i \leqq N$. Then we call $\alpha_1, \cdots, \alpha_{2N}$ the vertices of the standard N-dimensional octahedron.

COROLLARY 1. *Let $p \in U$. If $\alpha_1, \cdots, \alpha_{2N}$ are the vertices of the standard N-dimensional octahedron, and*

$$(3.1) \qquad p = \sum_{i=1}^{2N} |\alpha_i - p|^\lambda \qquad 0 < \lambda < 2$$

is minimal, then $p = \alpha_i$ for some i. If $T(p)$ is maximal, then

$$(3.2) \qquad p = \left(\sum_{i=1}^{N} \pm \alpha_i\right) \Big/ \sqrt{N} \equiv p^*$$

for some choice of plus and minus signs.

Before we prove this we need a simple inequality related to power means (for the basic properties of power means see, for example, [11, p. 26]).

LEMMA. *Let $s > 1$ and define*

$$f(u) = \sum_{i=1}^{N} u_i^s$$

for all N-tuples $u = (u_1, \cdots, u_N)$ satisfying

$$\sum_{i=1}^{N} u_i = 1$$

and

$$u_i \geqq 0 \qquad 1 \leqq i \leqq N \, .$$

Then $f(u)$ is minimal if and only if $u = (\sum_{i=1}^{N} \alpha_i)/N$ and maximal if and only if $u = \alpha_i$ for some i with $1 \leqq i \leqq N$.

Proof of Lemma. The sth power mean of $u_1, \cdots, u_N$ is non-decreasing as a function of s, so by letting $s \to 1$ and $s \to \infty$ we obtain

$$\frac{1}{N} \leqq \left[\frac{1}{N} f(u)\right]^{1/s} \leqq 1 .$$

The u_i must all be equal for equality to hold on the left, while for equality to hold on the right one of the u_i must equal 1.

Proof of Corollary 1. For $p \in U$ write $p = (x_1, \cdots, x_N)$. Thus $\sum x_i^2 = 1$. For every positive integer k we have

$$\textstyle\sum_k (p) \equiv \sum_{i=1}^{2N} (\alpha_i, p)^k = [1 + (-1)^k] \sum_{i=1}^{N} x_i^k . \tag{3.3}$$

Clearly $\sum_k (p)$ is zero unless $k = 2m$ for some positive integer m. Apply the above lemma with $u_i = x_i^2$ and $s = m$. It shows that the α_i are the uniform power maxima and the 2^N values of p given by (3.2) are the uniform power minima. Thus Corollary 1 follows from the theorem.

4. **The cube.** Let the β_i, for $1 \leqq i \leqq 2^N$, be the vectors in E^N whose components are either $N^{-1/2}$ or $-N^{-1/2}$. We call $\beta_1, \cdots, \beta_{2N}$ the vertices of the standard N-dimensional cube; this cube is inscribed in the unit sphere U.

COROLLARY 2. *Let $p \in U$. If $\beta_1, \cdots, \beta_M$ are the vertices of the standard N-dimensional cube, where $M = 2^N$, and*

$$T(p) = \sum_{i=1}^{M} |\beta_i - p|^\lambda \qquad 0 < \lambda < 2 \tag{4.1}$$

is maximal, then (in the notation of Corollary 1) *we have $p = \alpha_i$ for some i.*

Proof. For $p \in U$ write $p = (x_1, \cdots, x_N)$; thus $\sum x_i^2 = 1$. For every positive integer k we have

$$\begin{aligned} \textstyle\sum_k (p) &\equiv \sum_{i=1}^{M} (\beta_i, p)^k = N^{-k/2} \textstyle\sum^* (\pm x_1 \pm \cdots \pm x_N)^k \\ &\equiv N^{-k/2} \sum_{i=1}^{M} v_i^k \end{aligned} \tag{4.2}$$

where the asterisk indicates that the sum is extended over all M possible choices of plus and minus signs. Clearly $\sum_k (p)$ is zero unless $k = 2m$ for some positive integer m. Now

$$\sum_{i=1}^{M} v_i^2 = \sum{}^* (\pm x_1 \pm \cdots \pm x_N)^2 = M \sum_{i=1}^{N} x_i^2 = M \tag{4.3}$$

since all the mixed terms cancel. Now apply the lemma of §3 with $u_i = (v_i/\sqrt{M})^2$, with $s = m$, and with N replaced by M. It follows that

$$M^{1-m} = M\left(\frac{1}{M}\right)^m \leqq \sum_{i=1}^{M} u_i^m$$

so

$$M \leqq \sum_{i=1}^{M} v_i^{2m} \tag{4.4}$$

for every positive integer m. Thus every α_i is a uniform power minimum. For any $q = (x_1, \cdots, x_N) \in U$ which is not an α_i, it is easy to verify that

$$v^* \equiv \sum_{i=1}^{N} |x_i| > 1 . \tag{4.5}$$

But since $v^* = v_i$ for some i, this shows that q is not a uniform power minimum. The result now follows from the theorem.

We have no proof that the β_i are the uniform power maxima here. If they were, then $T(p)$ would be minimal if and only if $p = \beta_i$ for some i.

5. The simplex.

Let the γ_i, where $0 \leqq i \leqq N$, denote the vertices of a regular simplex inscribed in U. We now propose

Conjecture A. If m and N are integers with $m \geqq 0$ and $N \geqq 1$, then for $x \geqq 0$ we have

$$\begin{aligned} L_m(x) &\equiv \left(x + \frac{1}{N}\right)^{2m} + \left(1 + \frac{x}{N}\right)^{2m} + (N-1)\left(\frac{x-1}{N}\right)^{2m} \\ &\leqq \left(1 + \frac{1}{N^{2m-1}}\right)\left(x^2 + \frac{2}{N}\, x + 1\right)^m \equiv R_m(x) . \end{aligned} \tag{5.1}$$

If we set $P_m(x) = R_m(x) - L_m(x)$, then $P_0(x) \equiv P_1(x) \equiv 0$ and for $m = 2$ and $m = 3$ the coefficients of $P_m(x)$ are nonnegative. It seems likely, in fact, that the coefficients of $P_m(x)$ are always nonnegative.

COROLLARY 3. *Conjecture* A *implies that the uniform power maxima for the vertices of the regular simplex are simply the vertices themselves,* i.e., *the* γ_i *where* $0 \leqq i \leqq N$.

Proof. For $N = 1$ this is trivial. Assume true for all positive integers less than N. We shall examine

$$\sum\nolimits_k (p) \equiv \sum_{i=0}^{N} (\gamma_i, p)^k \tag{5.2}$$

where $p \in U$. Without loss of generality we may assume that $p = a_1\gamma_1 + \cdots + a_N\gamma_N$ where $a_i \geqq 0$ for $0 \leqq i \leqq N$. For any vector q, write $q = q_a + q_b$ where q_a is parallel to γ_0 and q_b is normal to γ_0. In particular, $(\gamma_i)_a \equiv \gamma_{ia} = -\gamma_0/N$. Thus

$$\begin{aligned}
\sum\nolimits_k (p) &= (\gamma_0, \gamma_a)^k + \sum_{i=1}^{N} [(\gamma_{ia}, \gamma_a) + (\gamma_{ib}, \gamma_b)]^k \\
&= (\gamma_0, \gamma_a)^k + \sum_{i=1}^{N} \left[-\frac{1}{N}(\gamma_0, \gamma_a) + (\gamma_{ib}, \gamma_b) \right]^k \\
&= (\gamma_0, \gamma_a)^k + \sum_{s=0}^{k} \binom{k}{s} \left[-\frac{1}{N}(\gamma_0, \gamma_a) \right]^{k-s} \sum_{i=1}^{N} (\gamma_{ib}, \gamma_b)^s \\
&= (\gamma_0, \gamma_a)^k + \sum_{s=0}^{k} c(k, s) \sum_{i=1}^{N} (\gamma_{ib}, \gamma_b)^s
\end{aligned} \tag{5.3}$$

where the coefficients $c(k, s)$ are all positive. By the induction hypothesis the last sum on the right can only become larger if p is rotated about an axis through γ_0 so that $\gamma_b = \gamma_{jb}$ for some j. Thus

$$\sum\nolimits_k (p) \leqq \sum_{i=0}^{N} (\gamma_i, p')^k \equiv J \tag{5.4}$$

where p' is a linear combination of γ_0 and γ_j, i.e. $p' = -x\gamma_0 + y\gamma_j$ where $x, y \geqq 0$. Now

$$1 = (p', p') = x^2 + \frac{2}{N}xy + y^2 \tag{5.5}$$

and

$$J = \left(y + \frac{x}{N}\right)^k + (-1)^k\left(\frac{y}{N} + x\right)^k + (N-1)\left(\frac{x-y}{N}\right)^k . \tag{5.6}$$

It suffices to show that J is maximal when $x = 0$ and $y = 1$ (in which case $J = 1 + (-1)^k N^{1-k}$) .

First we consider the case where k is odd, and write $k = 2m + 1$. The vector T, where

$$T = \left(-\left(\frac{x}{N} + y\right), \left(x + \frac{y}{N}\right)\right) , \tag{5.7}$$

is a counterclockwise tangent to the ellipse described by (5.5) in the first quadrant of the xy plane. We have

$$(5.8)\quad \begin{aligned} &(\operatorname{grad} J,\, T) \\ &= k(1 - N^{-2})\Big[x\Big(\frac{x}{N} + y\Big)^{2m} + y\Big(x + \frac{y}{N}\Big)^{2m} - (x + y)\Big(\frac{x}{N} - \frac{y}{N}\Big)^{2m}\Big] \\ &> 0 \end{aligned}$$

for $0 < x < 1$, so J achieves its maximal value at the endpoint $(0, 1)$. Next, let k be even and write $k = 2m$. Replace x by x/y in (5.1), and multiply both sides of (5.1) by y^{2m}. It follows that $J \leqq 1 + N^{1-2m}$ whenever (5.5) holds. Since a uniform power maximum must be one of the γ_i, this completes the proof.

COROLLARY 4. *Let $p \in U$. Let $\gamma_0, \cdots, \gamma_N$ be the vertices of the N-dimensional simplex, and assume the sum*

$$(5.9)\qquad T(p) = \sum_{i=0}^{N} |\gamma_i - p|^\lambda \qquad 0 < \lambda < 2$$

is minimal. If Conjecture A *is true, then $p = \gamma_i$ for some i.*

Proof. This follows from Corollary 3 and the theorem.

It seems reasonable to conjecture here that $T(p)$ is maximal if and only if $p = -\gamma_i$ for some i. But (see the comment towards the end of §6) the $-\gamma_i$ are not always uniform power minima.

We digress here to mention that an inductive procedure similar to that used in the proof of Corollary 3 shows that for *any* $p \in E^N$ we have

$$(5.10)\qquad \sum\nolimits_2 (p) \equiv \sum_{i=0}^{N} (\gamma_i, p)^2 = \frac{N+1}{N}(p, p)\ ,$$

where again the γ_i are the vertices of a regular simplex inscribed in U. The famous Selberg inequality [13, pp. 7-8] asserts that

$$(5.11)\qquad \sum_{i=0}^{N} (\gamma_i, p)^2 \Big[\sum_{j=0}^{N} |(\gamma_i, \gamma_j)|\Big]^{-1} \leqq (p, p)$$

for *any* nonzero vectors γ_i with $0 \leqq i \leqq N$. For the vertices of a regular simplex

$$(5.12)\qquad \sum_{j=0}^{N} |(\gamma_i, \gamma_j)| = 1 + N\Big(\frac{1}{N}\Big) = 2$$

so in this case the Selberg inequality yields

$$(5.13)\qquad \sum\nolimits_2 (p) \leqq 2(p, p)$$

which is somewhat weaker than (5.10). Also, the equality (5.10) has as a consequence that

$$(5.14)\qquad \sum_{i=0}^{N} |\gamma_i - p|^4 = 4(N+1)^2/N$$

for $p \in U$.

6. The regular N-gon. Let the ρ_i, where $0 \leqq i \leqq N-1$, denote the vertices of a regular N-gon inscribed in the unit circle U given by $x^2 + y^2 = 1$. We begin by establishing two lemmas; the first is well known, but we include it for the sake of completeness.

LEMMA 6.1. *For k a positive integer,*

$$\cos^k x = \sum_{s=0}^{k} a_{sk} \cos sx \tag{6.1}$$

where $a_{sk} \geqq 0$ and $a_{sk} = 0$ if $s \not\equiv k \bmod 2$.

Proof. Since $\cos^2 x = 1/2 + 1/2 \cos 2x$, this is true for $k = 1$ and $k = 2$. Assume true for integers less than k. For $k > 2$ we have

$$\begin{aligned} \cos^k x &= (\cos^{k-2} x)(\cos^2 x) \\ &= (\cos^{k-2} x)\left(\frac{1}{2} + \frac{1}{2} \cos 2x\right) \end{aligned}$$

and the result follows from the identity

$$\cos A \cos B = \frac{1}{2} \cos (A + B) + \frac{1}{2} \cos (A - B)$$

and the induction hypothesis.

LEMMA 6.2. *If k is a nonnegative integer, then for any real ϕ we have*

$$\sum_{j=0}^{N-1} \cos^k \left(\frac{2\pi j}{N} - \phi\right) \leqq \sum_{j=0}^{N-1} \cos^k \left(\frac{2\pi j}{N}\right) \tag{6.2}$$

with equality if and only if either $\phi = 2\pi m/N$ for some integer m, or $k < N$.

Proof. Let $d(N, s)$ be 1 if N divides s, and 0 otherwise. Then the left hand side of (6.2) is

$$\begin{aligned} &\sum_{j=0}^{N-1} \sum_{s=0}^{k} a_{sk} \cos \left(\frac{2\pi js}{N} - s\phi\right) \\ &= \sum_{s=0}^{k} a_{sk} \cos s\phi \sum_{j=0}^{N-1} \cos \frac{2\pi js}{N} + \sum_{s=0}^{k} a_{sk} \sin s\phi \sum_{j=0}^{N-1} \sin \frac{2\pi js}{N} \\ &= N \sum_{s=0}^{k} d(N, s) a_{sk} \cos s\phi \leqq N \sum_{s=0}^{k} d(N, s) a_{sk} \\ &= \sum_{j=0}^{N-1} \cos^k \frac{2\pi j}{N} \, . \end{aligned} \tag{6.3}$$

Equality holds only under the conditions stated, so the result is proved.

COROLLARY 5. *Let* $p = e^{i\phi} \in U$. *If* $\rho_j = e^{2\pi ij/N}$ *for* $0 \leqq j \leqq N-1$ *and*

$$T(p) = \sum_{j=0}^{N-1} |\rho_j - p|^\lambda \qquad 0 < \lambda < 2 \tag{6.4}$$

is minimal, then $p = \rho_j$ *for some* j.

Proof. The sum

$$\sum\nolimits_k (p) = \sum_{j=0}^{N-1} (\rho_j, p)^k = \sum_{j=0}^{N-1} \cos^k \left(\frac{2\pi j}{N} - \phi\right) \tag{6.5}$$

is maximal for *all* k if and only if $\phi \equiv 2\pi j/N \bmod 2\pi$ for some j with $0 \leqq j \leqq N-1$. In other words, if and only if $p = \rho_j$ for some j. The result now follows from the theorem.

Although the author has a proof that $T(p)$ is maximal if and only if $p = e^{\pi i(2j+1)/N}$ for some integer j, it is is *not* always true that these points are uniform power minima. The case $N = 3$ and $k = 6$ provides a counterexample.

Rather more can be proved here by means of certain differential inequalities associated with Sturm-Liouville problems. Namely, $T(p)$ is minimal if and only if p is a vertex, and maximal if and only if p lies half way between two vertices. Moreover, if λ is allowed to increase from 0 to $2N$, then every time λ passes through an even integer the points at which $T(p)$ was maximal will become the points at which it is minimal, and vice-versa. The present paper omits this proof.

7. Negative λ.

For $\lambda < 0$ define the integral transform

$$A_\lambda(s) = \int_0^\infty e^{-st} t^{-1-\lambda} dt = s^\lambda \Gamma(-\lambda) .$$

If q_0 is a uniform power minima, the proof of the theorem can be trivially modified, with $A_\lambda(s)$ in place of $I_\lambda(s)$, to show that $T(p)$ is minimal when $p = q_0$. So for λ negative, $T(p)$ is minimal for the octahedron when $p = p^*$ and minimal for the cube when $p = \alpha_i$.

Note added in proof. L. J. Yang has proved Conjecture A. Thus Corollary 4 is unconditionally valid. His method, essentially, is to analyze the cases (i) $0 < x < 1/4N$, (ii) $1/4N \leqq x < 2/N$; and (iii) $2/N \leqq x < 1$ separately. The details are somewhat lengthy, but require only elementary calculus.

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UNIVERSITY OF ILLINOIS