## SUMS OF DISTANCES BETWEEN POINTS ON A SPHERE. II

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ABSTRACT. Given N points on a unit sphere in Euclidean m space,  $m \ge 2$ , we show that the sum of all distances which they determine plus their discrepancy is a constant. As applications we obtain (i) an upper bound for the sum of the distances which for  $m \ge 5$  is smaller than any previously known and (ii) the existence of N point distributions with small discrepancy. We make use of W. M. Schmidt's work on the discrepancy of spherical caps.

1. Introduction. For  $m \ge 2$  let d be a function on  $U \times U$  where  $U = U^m$ , the surface of the unit sphere of m dimensional Euclidean space  $E^m$ . Let  $M_n$  be a sequence of N points  $p_1, \dots, p_N \in U^m$ . Define

(1.1) 
$$S(N, m, M_p) = S(d; N, m, M_p) = \sum_{i < j} d(p_i, p_j)$$

and

(1.2) 
$$S(N, m) = S(d; N, m) = \max S(d; N, m, M_n)$$

where the maximum is taken over all sequences  $M_p$ . We wish to obtain estimates for S(N, m). Our main result, Theorem 2 of §2, shows in a very exact sense that for a certain class of functions d, including the usual Euclidean distance d(p,q)=|p-q|, the quantity  $S(N,m,M_p)$  is large or small depending upon whether  $D(M_p)$ , the discrepancy of  $M_p$ , is small or large. Since W. M. Schmidt [9] has obtained very good results on the discrepancy of point distributions on U, we can obtain (see Theorem 1 below) estimates on S(N,m) which are far better than any hitherto known. Earlier results can be found, inter alia, in [1], [2], [3, p. 261, Remark 1], [4], [5], [8, pp. 36–38], and [12]; however, this paper can be read independently of these. Also, by applying Lemma 2.4 of [1] we can show (see Theorem 3 of §4) that there exist finite sequences  $M_p$  having small discrepancy. A precise definition of the discrepancy  $D(M_p)$  is given after the statement of Theorem 2.

If  $d_0$  is the great circle metric then  $S(d_0; N, m) = (\pi/4)N^2$  for N even (see

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[7] and [11]; [7] also discusses the case N odd). For  $q_1, q_2 \in U$  define

(1.3) 
$$d_1(q_1, q_2) = \sigma(U)^{-1} \int |d_0(q_1, p) - d_0(q_2, p)| \, d\sigma(p)$$
$$\leq d_0(q_1, q_2) \leq (\pi/2) \, |q_1 - q_2|$$

where  $d\sigma(p)$  is the element of surface area on U, and the total surface area of U is denoted by  $\sigma(U)$ . Clearly  $d_1$  is a metric. Now (and henceforth) we let c(m),  $c_1(m)$ ,  $c_i(m, \varepsilon)$ , etc., denote positive constants depending on the indicated parameters. Here c(m) and  $c_1(m)$  equal the coefficient of  $N^2$  in (2.4), for the appropriate  $\rho$ .

THEOREM 1. For  $\varepsilon > 0$  and  $m \ge 3$  we have

$$c_1(m)N^2 - c_2(m)N^{1-1/(m-1)} < S(d_1; N, m) < c_1(m)N^2 - c_3(m, \varepsilon)N^{\theta_1(m)-\varepsilon}$$

where  $\theta_1(m) = (m^2 - 4m + 2)(m - 1)^{-2}$ . Similarly, when d is the Euclidean metric and  $m \ge 3$  we have

(1.5) 
$$c(m)N^{2} - c_{4}(m)N^{1-1/(m-1)} < S(d; N, m) < c(m)N^{2} - c_{5}(m, \varepsilon)N^{\theta(m)-\varepsilon}$$

where  $\theta(m) = (m^2 - 5m + 2)(m - 1)^{-2}$ .

The older results, when applied to d, yield at best

(1.6) 
$$S(d; N, m) < c(m)N^2 - c'(m)$$

for some constant c'(m)>0. In fact, aside from [1], they yield results weaker than (1.6). Thus for  $m \ge 5$  the result of (1.5) is stronger than any previously known. It suggests the following question: is there a positive constant h(m) such that

$$S(N, m) = c(m)N^{2} - h(m)N^{1-1/(m-1)} + o(N^{1-1/(m-1)})?$$

2. The main result. We let  $p_0 \in U$  denote the vector  $(1, 0, \dots, 0)$  and we denote the inner product of vectors  $p, q \in U$  by  $p \cdot q$ . Note that  $p \cdot \tau q = \tau^{-1} p \cdot q$  for any orthogonal transformation  $\tau \in SO = SO(m)$ , the special orthogonal group acting on  $U^m$ . We let  $\int \cdots d\tau$  denote a normalized Haar integral over this group. For integrals on the real line we let  $\int_{a,b}$  denote  $\int_a^b$  unless b < a, in which case it shall denote  $\int_b^a$ .

DEFINITION 2.1. For  $p_1, p_2 \in U$  and a function g=g(x) integrable in [0, 1] we define

(2.1) 
$$\rho(p_1, p_2) = \rho(g; p_1, p_2) = \iint_{\text{True True }} g(x) \, dx \, d\tau.$$

Clearly  $\rho$  is independent of  $p_0$ , and for  $\tau_1 \in SO$  we have

(2.2) 
$$\rho(\tau_1 p_1, \tau_1 p_2) = \rho(p_1, p_2).$$

Note that  $\rho$  is a metric if g(x)>0; however, our proof of Theorem 2 does not require this hypothesis. We call g the kernel of  $\rho$ . If g(x)=1 then  $\rho(p_1,p_2)$  is a constant multiple of the Euclidean distance  $|p_1-p_2|$ . The metric  $d_1$  of §1 has kernel  $(1-x^2)^{-1/2}$ . It is sometimes useful to relax the restriction on g to integrability on closed subintervals of the open interval (0,1) and consider  $\rho$  to be defined whenever the inner integral is integrable over SO. In particular this permits the kernel  $(1-x^2)^{-1}$ .

DEFINITION 2.2. Let  $\sigma(x) = \{p \in U | p \cdot p_0 \le x\}$ . We also denote the surface area of this set by the *same* symbol. Thus

(2.3) 
$$\sigma(x) = \int_{p \cdot p_0 \le x} d\sigma(p) \quad \text{and} \quad \sigma(1) = \sigma(U).$$

Set  $\sigma^*(x) = \sigma(x)/\sigma(U)$ . Next, let  $f_p = f(M_p, \tau, x) = |M_p \cap \tau\sigma(x)|$  where |T| denotes the cardinality of the set T. Thus  $f_p$  is the number of points of  $M_p$  which lie in a certain spherical cap congruent to  $\sigma(x)$ .

THEOREM 2.

(2.4) 
$$S(\rho; N, m, M_p) + \int_{-1}^{1} g(x) \int (f(M_p, \tau, x) - N\sigma^*(x))^2 d\tau dx = N^2 \cdot 2^{-1} \sigma(U)^{-2} \iint \rho(p, q) d\sigma(p) d\sigma(q).$$

This is our main result. The second term on the left of (2.4) clearly measures the discrepancy of  $M_p$ ; i.e. the extent to which it deviates from a uniform distribution. We denote it by  $D(M_p)$ , and call it the "discrepancy of  $M_p$  with respect to the weight (or kernel) g(x)". Theorem B of [9] shows that, for  $\varepsilon > 0$ ,

$$(2.5) D(M_n) \gg N^{1-1/(m-1)-\varepsilon}$$

for any  $M_p$  when  $g(x)=(1-x^2)^{-1}$ ; the implied constant depends on  $\varepsilon$ . Theorem 2 is perhaps best appreciated as an invariance principle: the sum of all distances determined by N points plus their discrepancy is constant.

3. The proof. First we prove a useful identity, various forms of which have already appeared explicitly or implicitly in the literature; see [1], [2], [6, p. 196, Theorem 3.1], [10], and [12].

LEMMA. If  $p_i$  and  $q_j$  are real numbers for  $1 \le i \le u$  and  $1 \le j \le v$  with  $p_1 \le \cdots \le p_u$  and  $q_1 \le \cdots \le q_v$  then

(3.1) 
$$\sum_{i,j} \int_{p_i,q_j} - \sum_{i$$

where  $\int_{a,b} = \int_{a,b} g(x) dx$  and

(3.2) 
$$G = \sum_{y_j \le x} 1 - \sum_{q_j \le x} 1.$$

*Note.* If u=v and g(x)=1 we have

$$\int_{-\infty}^{\infty} G^2 dx \ge \int_{-\infty}^{\infty} |G| dx = \sum_{i=1}^{u} |p_i - q_i|$$

and (3.1) becomes the inequality of Lemma 2.1 in Alexander's paper [1].

PROOF. Let x be a real number distinct from any  $p_i$  or  $q_j$ . Let s be the number of  $p_i$  to the left of x and t the number of  $q_j$  to the left of x. From the identity

$$s(v-t) + t(u-s) - s(u-s) - t(v-t) = (s-t)((s-t) - (u-v))$$

we see that g(x) occurs on the left of (3.1) the same net number of times as it occurs on the right. This proves the Lemma.

We begin our proof of Theorem 2 by letting u=v=N and letting  $M_p$  and  $M_q$  be the sequences  $p_1, \dots, p_N$  and  $q_1, \dots, q_N$  respectively. We let  $\phi_1, \phi_2$ , and  $\tau$  be elements of SO and

$$\sum = \sum_{i,j} \rho(\phi_1 p_i, \phi_2 q_j).$$

If R denotes the right side of (2.4) then

$$(3.3) 2R = \iint \sum d\phi_1 d\phi_2.$$

We now recall (2.1), apply the above lemma to  $\sum$  with  $p_i$  and  $q_j$  replaced by  $\tau \phi_1 p_i \cdot p_0$  and  $\tau \phi_2 q_j \cdot p_0$  respectively, and then apply (2.2). This, and an integration over  $\tau$ , yields

(3.4) 
$$\sum = \sum_{i < j} \rho(p_i, p_j) + \sum_{i < j} \rho(q_i, q_j) + \iint_{-1}^{1} g(x) \left( \sum_{\substack{r, h_1, q_1, r_0 \le x \\ r, h_2, q_2, r_0 \le x}} 1 - \sum_{\substack{r, h_2, q_2, r_0 \le x \\ r, h_2, q_2, r_0 \le x}} 1 \right)^2 dx d\tau.$$

Upon inserting (3.4) into (3.3) we obtain

(3.5) 
$$2R = S(N, m, M_p) + S(N, m, M_q) + \int_{-1}^{1} \iint g(x) (f(M_p, \phi_1, x) - f(M_q, \phi_2, x))^2 d\phi_1 d\phi_2 dx.$$

Now clearly

(3.6) 
$$\int (f_p - N^*) d\phi_1 = \int (f(M_p, \phi_1, x) - N\sigma^*(x)) d\phi_1 = 0$$

since  $N^* = N\sigma^*(x)$  is just the expected value of  $f_v = f(M_v, \phi_1, x)$ . Since

$$(3.7) \quad (f_p - f_q)^2 = (f_p - N^*)^2 - 2(f_p - N^*)(f_q - N^*) + (f_q - N^*)^2$$

and the integral of the middle term on the right of (3.7) is zero, the right side of (3.5) is the sum of the discrepancies of  $M_p$  and  $M_q$  with respect to g(x). The proof is completed by setting  $p_i = q_i$  for  $1 \le i \le N$  and dividing both sides of (3.5) by 2.

*Note*. One could obtain a result having a more general appearance than (2.4) by using the full strength of the lemma rather than the special case u=v. A comparison of this result with (2.4) yields the identity

(3.8) 
$$\int_{-1}^{1} g(x)\sigma(x)(\sigma(U) - \sigma(x)) \ dx = \frac{1}{2} \iint \rho(p, q) \ d\sigma(p) \ d\sigma(q).$$

4. Some applications. We first introduce some notation from [9]. Let  $\mu$  be the normalized Lebesgue measure on U; thus  $\mu(U)=1$ . Let C=C(r,p) be the spherical cap consisting of all points whose spherical distance from  $p \in U$  is at most r. Note that  $0 \le r \le \pi$ . Let  $\Delta = \Delta(r,p) = N\mu(C) - \nu(C)$  where  $\nu(C)$  denotes the number of  $p_1, \dots, p_N$  which lie in C. Let  $E(r) = \int_U \Delta^2 d\mu(p)$ . Schmidt's Theorem B is given on p. 59 of [9]. By replacing his n and  $\delta$  with m-1 and  $\pi/2$  respectively we obtain the

THEOREM. If  $m \ge 3$ ,  $\varepsilon > 0$ , and  $N > \varepsilon$  then

(4.1) 
$$\int_0^{\pi/2} r^{-1} E(r) dr \ge c_6(m, \varepsilon) N^{1 - 1/(m - 1) - \varepsilon}.$$

For later use we note the trivial estimate

$$(4.2) E(r) \le c_7(m) N^2 r^{m-1}.$$

(This is Lemma 4, p. 67 of [9]; set s=r and note that Schmidt's E(r, r) is our E(r).) We now obtain a result which shows that (4.1) is not too far from best possible in its dependence on N. For  $m \ge 3$  we have

THEOREM 3. There are points  $p_1, \dots, p_N$  on U such that

(4.3) 
$$\int_0^{\pi/2} r^{-1} E(r) dr \le c_8(m) N^{1-1/(m-1)}.$$

To prove this we need the following special case of a result of Alexander (Lemma 2.4 of [1]).

LEMMA. Let  $\rho(p_1, p_2)$  be a nonnegative function on  $U \times U$  and let  $\mu$  be a Borel measure for which  $\mu(U)=1$ . Let  $P=\{A_1, \dots, A_N\}$  be a collection of Borel subsets of U such that  $\mu(A_i \cap A_j)=\delta_{ij}N^{-1}$  where  $\delta_{ij}$  is 1 if i=j and 0

otherwise. Then

(4.4) 
$$N^2 \int_{IJ} \int_{IJ} \rho(p, q) \, d\mu(p) \, d\mu(q) - \sum_{i=1}^{N} \rho(A_i) \leq 2S(\rho; N, m)$$

where  $\rho(A_i)$  is the "diameter" of  $A_i$ ; i.e.  $\rho(A_i) = \sup \rho(p, q)$  for  $p, q \in A_i$  (Alexander has  $|p_1 - p_2|$  in place of  $\rho(p_1, p_2)$  but his proof required only the nonnegativity of this function).

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We now choose  $M_p$  so that  $S(\rho; N, m, M_p) = S(\rho; N, m)$ . It follows from (2.4) and (4.4) that

(4.5) 
$$\int_{-1}^{1} g(x) \int (f(M_{p}, \tau, x) - N\sigma^{*}(x))^{2} d\tau dx \leq c_{0}(m) N \inf_{P} \max_{i} \rho(A_{i}),$$

a result of interest in itself.

To prove Theorem 3 let  $g(x)=(1-x^2)^{-1}$  and set  $p_1 \cdot p = \cos \theta_1$  and  $p_2 \cdot p = \cos \theta_2$  where  $\theta_1$  and  $\theta_2$  are the great circle distances between  $p_1$ , p and  $p_2$ , p respectively. Then

$$\rho = \rho(p_1, p_2) = c_9(m) \iint_{p_1 \cdot p, p_2 \cdot p} g(x) \, dx \, d\sigma(p)$$

$$= c_{10}(m) \iint |\log \tan \frac{1}{2}\theta_1 - \log \tan \frac{1}{2}\theta_2| \, d\sigma(p).$$

It is easy to see that this integral is finite since  $\int |\log \tan \frac{1}{2}\theta_1| d\sigma(p)$  is finite. Now

$$\begin{split} |p_1-p_2|^{-1} \, \rho(p_1,\,p_2) &= c_{10}(m) \int \{|\theta_1-\theta_2|^{-1} \, (\log\tan \tfrac{1}{2}\theta_1 - \log\tan \tfrac{1}{2}\theta_2)\} \\ & \cdot \{|\theta_1-\theta_2| \cdot |p_1-p_2|^{-1}\} \, d\sigma(p) \\ & \leq c_{11}(m) \int |\theta_1-\theta_2|^{-1} \, (\log\tan \tfrac{1}{2}\theta_1 - \log\tan \tfrac{1}{2}\theta_2) \, d\sigma(p) \\ & \equiv \int_U . \end{split}$$

We will show that  $\int_U$  remains bounded as  $p_2 \rightarrow p_1$ . Let the great circle distance between  $p_1$  and  $p_2$  be  $\gamma \pi/10$  where  $\gamma$  is a small positive parameter. Let  $B_1 = B_1(\gamma)$  be the set of points  $p \in U$  such that  $\gamma \pi \leq \theta_i \leq (1-\gamma)\pi$  for i=1, 2. Then  $B_2$ , the complement of  $B_1$ , consists of two components, say  $B_3$  and  $B_4$ . The estimates we need for the integrals over  $B_3$  and  $B_4$  will be essentially identical, so we give details only for  $B_4$  which we take to be the component for which  $\theta_1$ ,  $\theta_2 \leq 2\gamma\pi$ . Write  $B_4 = B_5 \cup B_6$  where  $B_5$ ,  $B_6$  are disjoint and  $B_5$  consists of those points of  $B_4$  for which  $\theta_1 \leq 2\theta_2$ . Then

$$\int_{U} = \int_{B_{1}} + \int_{B_{3}} + \int_{B_{5}} + \int_{B_{6}} \ll \int_{B_{1}} + \int_{B_{5}} + \int_{B_{6}}$$

The following two estimates make use of the fact that  $d\sigma(p) \ll \theta_i^{m-2} d\theta_i$ , and require  $m \ge 3$ :

$$\int_{B_5} \ll \int_{B_5} |\sin(\min(\theta_1, \theta_2))|^{-1} d\sigma(p) \ll \int_{B_5} \theta_1^{-1} d\sigma(p) \ll \int_0^{\gamma \pi} d\theta = \gamma \pi$$

and

$$\int_{B_6} \ll \int_{B_6} |\theta_2^{-1} \log \theta_2| \ d\sigma(p) \ll \int_0^{\gamma \pi} |\log \theta| \ d\theta \ll \gamma \ |\log \gamma|.$$

Also,

$$\int_{B_1} \ll \int_{B_1} (|\sin \theta_1|^{-1} + |\sin \theta_2|^{-1}) \, d\sigma(p) \ll 2 \int_{U} |\sin \theta_1|^{-1} \, d\sigma(p) < \infty.$$

Thus  $\rho(p_1, p_2) \ll |p_1 - p_2|$ . Now extend the integral on the left of (4.5) only to 0, and make the change of variable  $x = -\cos r$ . This yields

(4.6) 
$$\int_0^{\pi/2} r^{-1} E(r) dr \le c_{12}(m) N \inf_P \max_i \rho(A_i).$$

Now clearly one can choose the  $A_i$  so that their Euclidean diameters are  $\gg \ll N^{-1/(m-1)}$  for  $1 \le i \le N$ . But  $\rho(p_1, p_2) \ll |p_1 - p_2|$  so the result follows.

An immediate consequence of Theorem 1 and the above is that if  $\rho$  has kernel  $(1-x^2)^{-1}$  then

$$\begin{aligned} c_{13}(m)N^2 - c_{14}(m)N^{1-1/(m-1)} &< S(\rho; N, m) \\ &< c_{13}(m)N^2 - c_{16}(m, \varepsilon)N^{1-1/(m-1)-\varepsilon}. \end{aligned}$$

We now prove Theorem 1. The left-hand inequalities are deduced from (4.4) as in the proof of Theorem 3. For the right-hand inequality of (1.5) we set  $g(x) \equiv 1$  and note that

(4.7) 
$$D(M_p) \ge c_{17}(m) \int_{-1}^0 E(\cos^{-1}|x|) dx = c_{17}(m) \int_0^{\pi/2} \sin r E(r) dr$$

$$\ge c_{18}(m) \int_0^{\pi/2} r E(r) dr \ge c_{18}(m) N^{-\alpha} \int_{N^{-\alpha}}^{\pi/2} E(r) dr$$

for any  $\alpha > 0$ . From (4.1) and (4.2) we obtain

$$(4.8) \quad c_7(m)N^2 \int_0^{N-\alpha} r^{m-2} dr + N^{\alpha} \int_{N-\alpha}^{\pi/2} E(r) dr \ge c_6(m, \varepsilon) N^{1-1/(m-1)-\varepsilon}.$$

Set  $\alpha=1/(m-1)+1/(m-1)^2+2\varepsilon/(m-1)$ . Then the term on the extreme left of (4.8) has lower order of magnitude than the term on the extreme right, so it follows that

(4.9) 
$$D(M_p) \ge c_{19}(m, \varepsilon) N^{1-(3+4\varepsilon)/(m-1)-2/(m-1)^2-\varepsilon}$$

To prove (1.4) we note that in this case

(4.10) 
$$D(M_p) \ge c_{20}(m) \int_{N^{-\alpha}}^{\pi/2} E(r) dr,$$
 so

(4.11) 
$$D(M_n) \ge c_{21}(m, \varepsilon) N^{1 - (2 + 2\varepsilon)/(m - 1) - 1/(m - 1)^2 - \varepsilon}.$$

This completes the proof of Theorem 1.

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