Information Processing Letters 32 (1989) 205–211
North-Holland
1 September 1989

APPROXIMATING THE DIAMETER OF A SET OF POINTS IN THE EUCLIDEAN SPACE

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Communicated by David Gries
Received 13 June 1988
Revised 21 December 1988

Given a set P with n points in $\mathbb{R}^k$, its diameter d_P is the maximum of the Euclidean distances between its points. We describe an algorithm that in $m \leqslant n$ iterations obtains $r_1 < r_2 < \cdots < r_m \leqslant d_P \leqslant \min\{\sqrt{3}\, r_1, \sqrt{5-2\sqrt{3}}\, r_m\}$. For k fixed, the cost of each iteration is $O(n)$. In particular, the first approximation r_1 is within $\sqrt{3}$ of d_P, independent of the dimension k.

Keywords: Computational geometry, diameter computation, approximation algorithm

1. Introduction

Given a set P with n points in $\mathbb{R}^k$, its diameter d_P is the maximum of the Euclidean distances between its points. For $k = 2$, the diameter can be calculated in $O(n \log n)$ time. For the algorithm, as well as other interesting properties of this problem see [3]. For general $k > 2$, the best known algorithm has complexity

$$O\left(n^{2-\alpha(k)}(\log n)^{1-\alpha(k)}\right),$$

where $\alpha(k) = 2^{-(k+1)}$, due to Yao [4]. A fast randomized algorithm for finding diameters in $\mathbb{R}^3$ appears in [2]. It may be of interest to find fast approximations to the diameter of P in arbitrary dimension. The notion of approximation in computational geometry is not new, e.g., see [1] for approximation of the convex hull of points.

If R is the tightest rectangle with respect to the coordinate axes that contains P and l its largest side, then it is easy to show that $l \leqslant d_P \leqslant \sqrt{k}\, l$. For k fixed, l may be obtained in $O(n)$ time. However, this upper bound is not satisfactory, since it depends on the dimension k.

2. Approximation of the diameter

For a given $p \in \mathbb{R}^k$, let $F(p, P)$ be a point in P that is farthest from p. Let d denote the Euclidean distance function. Starting with an arbitrary point $p \in P$ consider the following simple algorithm for the approximation of d_P.

Algorithm A

Step 1: Let $q = F(p, P)$ and $r_p = d(p, q)$.
Step 2: Let $q' = F(q, P)$ and $r_q = d(q, q')$.

2.1. Theorem. $r_q \leqslant d_P \leqslant \sqrt{3}\, r_q$.

Proof. We only need to show that $d_P \leqslant \sqrt{3}\, r_q$. For a given $y \in \mathbb{R}^k$ and $r \geqslant 0$, let $S(y, r) = \{x \in \mathbb{R}^k: d(x, y) \leqslant r\}$. Note that we immediately have $d_P \leqslant 2r_q$. To prove the tighter bound, we estimate the diameter of $S(p, r_p) \cap S(q, r_q)$, that is, $\max\{d(x, y): x, y \in S(p, r_p) \cap S(q, r_q)\}$. Let p'

* Supported in part by NSF under Grant No. DCR-8603722.
** Supported in part by a Faculty Fellowship at Rutgers University.

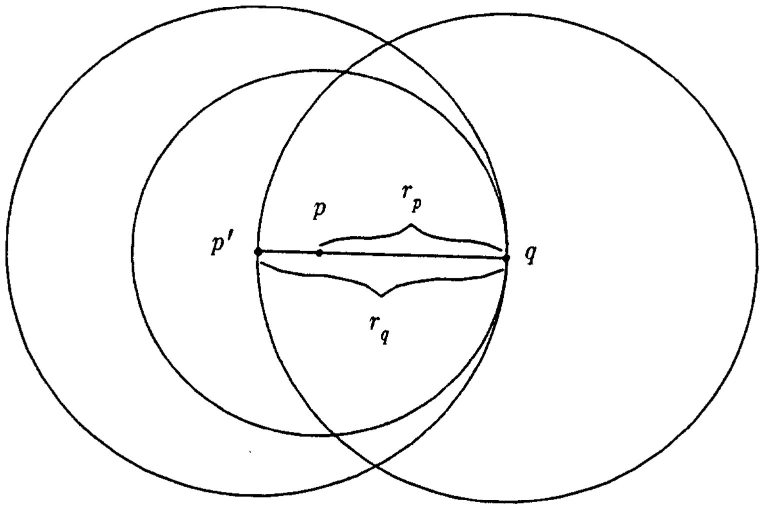

Fig. 1.

$= q + (r_q/r_p)(p - q)$. Note that $r_q \geqslant r_p$. If $x \in S(p, r_p)$, then

$$d(x, p') \leqslant d(x, p) + d(p, p') \leqslant r_p + (r_q - r_p).$$

Thus, $x \in S(p', r_q)$ (see Fig. 1).

We show that the diameter of $S(p', r_q) \cap S(q, r_q)$ equals $\sqrt{3}\, r_q$. Without loss of generality, we may assume $r_q = 1$, $p' = (-\frac{1}{2}, \ldots, 0)$, and $q = (\frac{1}{2}, \ldots, 0)$. The calculation of the diameter of $S(p', 1) \cap S(q, 1)$ may be cast as the following nonlinear optimization problem:

$$\text{(P1):} \quad \max d(x, y) \quad \text{s.t.}$$
$$\left(x_1 + \tfrac{1}{2}\right)^2 + x_2^2 + \cdots + x_k^2 \leqslant 1,$$
$$\left(x_1 - \tfrac{1}{2}\right)^2 + x_2^2 + \cdots + x_k^2 \leqslant 1,$$
$$\left(y_1 + \tfrac{1}{2}\right)^2 + y_2^2 + \cdots + y_k^2 \leqslant 1,$$
$$\left(y_1 - \tfrac{1}{2}\right)^2 + y_2^2 + \cdots + y_k^2 \leqslant 1,$$

where $x = (x_1, x_2, \ldots, x_k)$ and $y = (y_1, y_2, \ldots, y_k)$. Note that if x is feasible, so is $-x$. By the triangle inequality, it suffices to consider the following equivalent problem:

$$\max 2d(x, y) \quad \text{s.t.}$$
$$\left(x_1 + \tfrac{1}{2}\right)^2 + x_2^2 + \cdots + x_k^2 \leqslant 1,$$
$$\left(x_1 - \tfrac{1}{2}\right)^2 + x_2^2 + \cdots + x_k^2 \leqslant 1.$$

Let $g(x_1) = \min\{1 - (x_1 + \frac{1}{2})^2, 1 - (x_1 - \frac{1}{2})^2\}$. Then the previous problem is equivalent to

$$\max 2\sqrt{x_1^2 + g(x_1)} \quad \text{s.t.}$$
$$-\tfrac{1}{2} \leqslant x_1 \leqslant \tfrac{1}{2}.$$

The optimal value of the above is attained at 0 and is $\sqrt{3}$. □

The bound of Theorem 2.1 is also tight for each $k \geqslant 2$, as may be seen from Fig. 2. The figure also implies that no improvement is possible if one repeats Algorithm A, starting with q. This remains true even if one repeats the algorithm with a point different than both p and q, e.g., consider the case where many copies of p and q exist.

In what follows we describe Algorithm B, which either improves the lower bound or guarantees a tighter upper bound to d_P. Initially, the algorithm applies Algorithm A, starting with an arbitrary point $p \in P$, obtaining the estimate r_q. It then removes p and q from P and applies Algorithm A with the center of the line segment joining q and p' as the new starting point. Algorithm B terminates if the new estimate does not improve or if at most one point remains. Otherwise, the process is repeated. More formally the algorithm is as follows.

Algorithm B

Step 0: Let $P_1 = P$. Select $p_1 \in P$. Let $q_1 = F(p_1, P_1)$, $q_1' = F(q_1, P_1)$, $\rho_1 = d(p_1, q_1)$, and $r_1 = d(q_1, q_1')$. Set $j = 1$.

Step 1: Let $P_{j+1} = P_j - \{p_j, q_j\}$. If $|P_{j+1}| \leqslant 1$, stop. Otherwise, let

$$p_j' = q_j + (r_j/\rho_j)(p_j - q_j)$$

and $p_{j+1} = \frac{1}{2}(p_j' + q_j)$. Let $q_{j+1} = F(p_{j+1}, P_{j+1})$, $q_{j+1}' = F(q_{j+1}, P_{j+1})$, $\rho_{j+1} = d(p_{j+1}, q_{j+1})$ and $r_{j+1} = d(q_{j+1}, q_{j+1}')$.

Step 2: If $r_{j+1} \leqslant r_j$, stop. Otherwise, $j = j + 1$, go to Step 1.

Assume that the above algorithm terminates for $j = m$. Clearly, $m \leqslant n$. Also note that if $|P_{m+1}| \leqslant 1$, we have computed $r_m = d_P$ in $O(n)$ iterations. Since each iteration requires $O(n)$ steps, in this case Algorithm B computes the actual diameter in $O(n^2)$ time, which is no worse than the time complexity of the pedestrian algorithm of computing the distance between every pair of points in P.

2.2. Lemma. $r_m \leqslant d_P$.

Proof. We need to show that for $j = 2, \ldots, m$, $p_j \in H(P)$, where $H(P)$ is the convex hull of P. This, together with the fact that P and $H(P)$ have the same diameter, implies the result. By induction, we only need to prove this for $j = 2$. Note that $p_2 = \alpha_1 p_1 + \alpha_2 q_1$, where $\alpha_1 = \frac{1}{2} r_1/\rho_1$ and $\alpha_2 = 1 - \alpha_1$. Since $r_1 \leqslant 2\rho_1$, it follows that p_2 is a convex combination of p_1 and q_1. □

Next we obtain an upper bound to d_P. Since $r_{m+1} \leqslant r_m$, we may conclude that

$$P \subset S(p_m', r_m) \cap S(q_m, r_m) \cap S(q_{m+1}, r_m) \cap S(p_{m+1}, \rho_{m+1}). \quad (1)$$

We may assume $r_m = 1$, $p_m' = (-\frac{1}{2}, \ldots, 0)$ and $q_m = (\frac{1}{2}, \ldots, 0)$. The diameter of the intersection of these four hyperspheres is bounded above by the optimal value of the following optimization problem:

(P2): max $d(x, y)$ s.t.

$$(x_1 + \tfrac{1}{2})^2 + x_2^2 + \cdots + x_k^2 \leqslant 1,$$
$$(x_1 - \tfrac{1}{2})^2 + x_2^2 + \cdots + x_k^2 \leqslant 1,$$
$$(y_1 + \tfrac{1}{2})^2 + y_2^2 + \cdots + y_k^2 \leqslant 1,$$
$$(y_1 - \tfrac{1}{2})^2 + y_2^2 + \cdots + y_k^2 \leqslant 1,$$
$$(z_1 + \tfrac{1}{2})^2 + z_2^2 + \cdots + z_k^2 \leqslant 1,$$
$$(z_1 - \tfrac{1}{2})^2 + z_2^2 + \cdots + z_k^2 \leqslant 1,$$
$$x_1^2 + x_2^2 + \cdots + x_k^2 \leqslant z_1^2 + z_2^2 + \cdots + z_k^2,$$
$$y_1^2 + y_2^2 + \cdots + y_k^2 \leqslant z_1^2 + z_2^2 + \cdots + z_k^2,$$
$$(x_1 - z_1)^2 + \cdots + (x_k - z_k)^2 \leqslant 1,$$
$$(y_1 - z_1)^2 + \cdots + (y_k - z_k)^2 \leqslant 1.$$

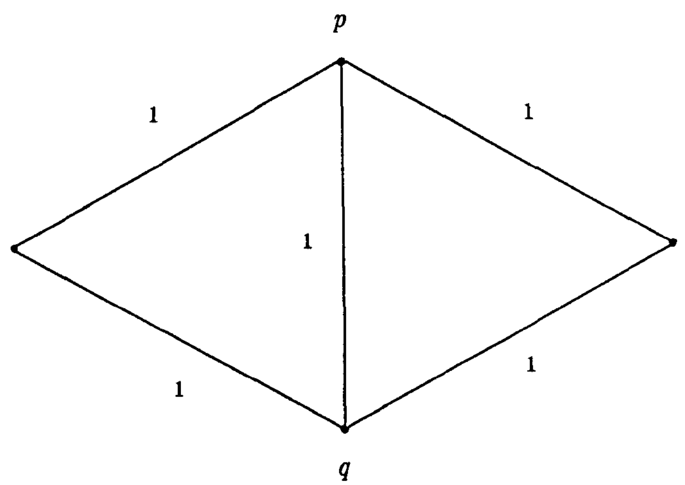

Fig. 2.

The point z in the above problem corresponds to q_{m+1}. Let $\delta(k)$ be the optimal value of (P2). We first obtain a lower bound to $\delta(k)$, and then using it we prove that the actual value coincides with this lower bound.

2.3. Lemma. $\delta(k) \geqslant \sqrt{5-2\sqrt{3}}$ *for all* $k \geqslant 2$.

Proof. For a given $z=(z_1, z_2, \ldots, z_k)$, let $z^1 = (-z_1, z_2, \ldots, z_k)$ and $z^2=(z_1, -z_2, \ldots, -z_k)$. We have $d(z^1, z^2)=2d(z, 0)$. Let us consider the restricted problem where $x=z^1$, and $y=z^2$. This problem reduces to

$$\max 2d(z, 0) \quad \text{s.t.}$$
$$(z_1+\tfrac{1}{2})^2+z_2^2+\cdots+z_k^2 \leqslant 1,$$
$$(z_1-\tfrac{1}{2})^2+z_2^2+\cdots+z_k^2 \leqslant 1,$$
$$4z_1^2 \leqslant 1,$$
$$4(z_2^2+z_3^2+\cdots+z_k^2) \leqslant 1.$$

The third equation is redundant and, without loss of generality, we may assume $z_i=0$ for $i=3, 4, \ldots, n$. Thus, the above problem has the same optimal value as the following:

$$\max 2\sqrt{z_1^2+z_2^2} \quad \text{s.t.}$$
$$(z_1+\tfrac{1}{2})^2+z_2^2 \leqslant 1,$$
$$(z_1-\tfrac{1}{2})^2+z_2^2 \leqslant 1,$$
$$4z_2^2 \leqslant 1.$$

It is not difficult to show that at an optimal solution of this new problem, the last equation and either the first or the second equations are tight. It follows that $(z_1^*, z_2^*)=(-\frac{1}{2}+\frac{1}{2}\sqrt{3}, \frac{1}{2})$ is an optimal solution. □

2.4. Theorem. $\delta(2)=\sqrt{5-2\sqrt{3}}$.

Proof. From Lemma 2.3 and Theorem 2.1, we only need to consider the case where

$$\tfrac{1}{2}\sqrt{5-2\sqrt{3}} \leqslant \rho \equiv \sqrt{z_1^2+z_2^2} \leqslant \tfrac{1}{2}\sqrt{3}.$$

Observe that we may assume $z_1, z_2 \geqslant 0$. Let $z^0=(z_1^0, z_2^0)$ be a fixed point with $z_1^0, z_2^0 \geqslant 0$ and $(z_1^0)^2+(z_2^0)^2=\rho^2$ with

$$\rho \in \left[\tfrac{1}{2}\sqrt{5-2\sqrt{3}}, \tfrac{1}{2}\sqrt{3}\right].$$

Let $S(z^0)$ be the intersection of the four circles in (1) with $k=2$, and let x, y, z, and w be the feasible intersection points. More specifically, $S(z^0)$ is the intersection of the circle of radius ρ centered at the origin and the circles of radius 1 centered at the points $(-\frac{1}{2}, 0)$, $(\frac{1}{2}, 0)$, and z_0 (see Fig. 3).

Let $d(u, v)$ be the diameter of $S(z^0)$ and put $A=\{x, y, z, w\}$. Note that the coordinates of x and z depend only on ρ but those of y and w will depend on ρ as well as the coordinates of z^0. We claim that $u, v \in A$. To prove this claim we first observe that since the maximum of a convex function over a convex set is attained at a boundary point, u and v lie on $\partial(S(z^0))$, the boundary of $S(z^0)$. Secondly, it suffices to show that one of the two points u, v must be in A because of the following simple property of a circle C: Suppose p is a point interior to C. If q is a boundary point of C where the tangent line at q is not orthogonal to the line segment connecting p and q, then q is not the farthest boundary point of C from p.

Suppose u is in A and v in $\partial(S(z^0))-A$. Then we apply the above property by letting the circle on which v lies play the role of C and u play the role of p. Thus $d(u, v)$ cannot be the diameter.

Now, suppose neither u nor v is in A. Let $C(u)$ and $C(v)$ denote the circles on which u and v lie respectively. Again, from the above argument, it follows that the line segment connecting u and v is orthogonal to the tangent line of $C(u)$ at u. Similarly, this line segment must be orthogonal to the tangent line of $C(v)$ at v. But this can happen only when $u=(-\frac{1}{2}, 0)$ and $v=(\frac{1}{2}, 0)$. But in this case we would replace u by either x or w, thus reducing it to the case where one of the points is in A. This proves the claim.

Thus for each fixed ρ and z^0 we need to consider six pairwise distances between points of A. First we consider the maximization of $d(x, y)$ as a function of ρ and the location of z^0. From the equations $(z_1+\frac{1}{2})^2+z_2^2=1$ and $z_1^2+z_2^2=\rho^2$,

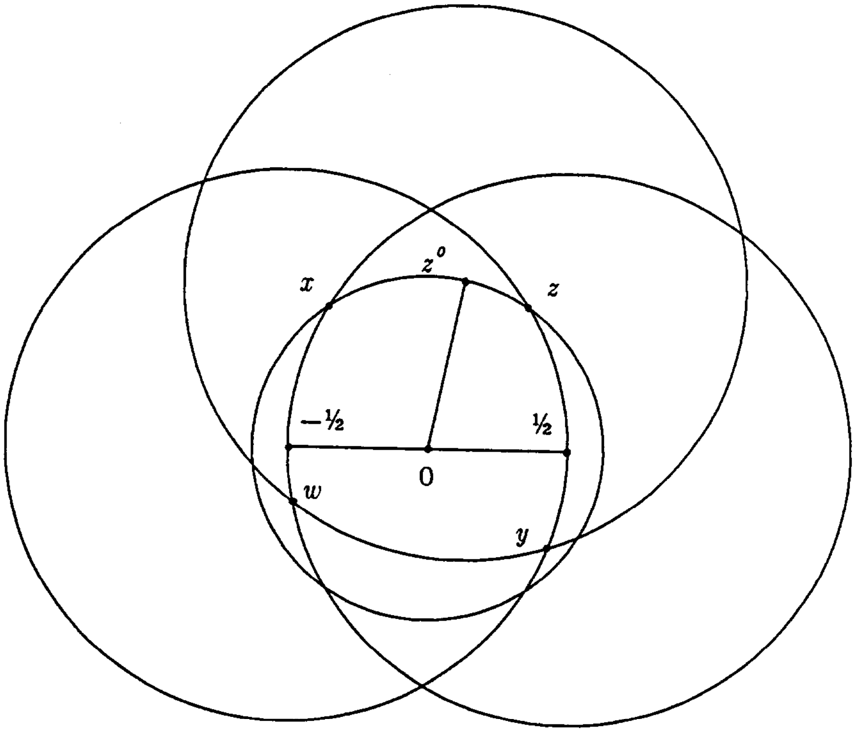

Fig. 3.

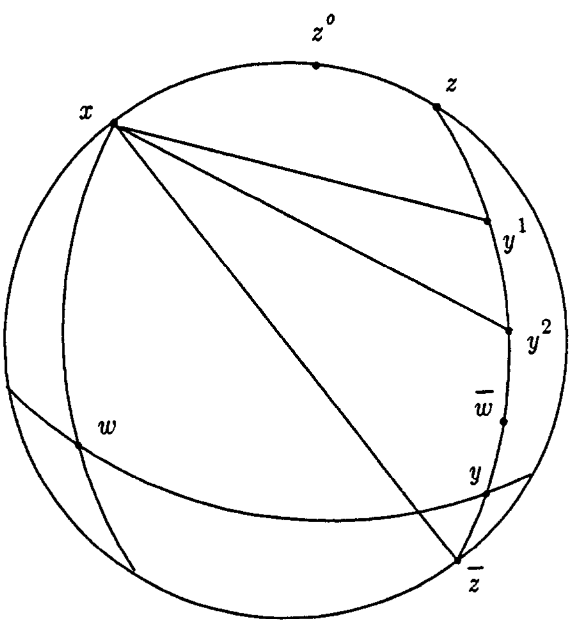

Fig. 4.

we obtain

$$z=(z_1,\ z_2)=\left(\tfrac{3}{4}-\rho^2,\ \sqrt{1-\left(\rho^2-\tfrac{5}{4}\right)^2}\right).$$

Note that $x=(-z_1,\ z_2)$. Let $\bar{z}=(z_1,\ -z_2)$. We have

$$\begin{aligned} d(z,\ \bar{z}) &= 2\sqrt{1-\left(\rho^2-\tfrac{5}{4}\right)^2} \\ &\geqslant 2\sqrt{1-\left(\tfrac{1}{4}(5-2\sqrt{3})-\tfrac{5}{4}\right)^2} \\ &= 1. \end{aligned} \tag{2}$$

Thus it follows that the point y that depends on z^0 will lie on the arc of the circle $\partial S((-\frac{1}{2}, 0), 1)$ from $\bar{z}$ to z. Now consider two points $y^1=(y_1^1,\ y_2^1)$ and $y^2=(y_1^2,\ y_2^2)$ on this arc with $y_1^1<y_1^2$ as in Fig. 4. Note that the angle $xy^1\bar{z}$ is obtuse since x and $\bar{z}$ are diametrically opposite. Therefore the angle xy^1y^2 is obtuse and it follows that $d(x,\ y^1) < d(x,\ y^2)$. This implies that for fixed ρ, $d(x,\ y)$

increases as z^0 moves clockwise. Thus $d(x, y)$ is maximized when $z^0 = z$. Taking $z^0 = z$, from the equation $(z_1 - y_1)^2 + (z_2 - y_2)^2 = 1$ we obtain $f(\rho) = d(x, y)^2 = 1 + 4z_1 y_1$. To compute y_1 we need to solve the equations $(y_1 + \frac{1}{2})^2 + y_2^2 = 1$, $(z_1 - y_1)^2 + (z_2 - y_2)^2 = 1$, and $z_1^2 + z_2^2 = \rho^2$. With elementary but tedious calculations it can be shown that

$$y_1 = \tfrac{1}{2}\left\{-(\rho^2 - \tfrac{1}{4}) + \sqrt{(\rho^2 - \tfrac{1}{4})(\tfrac{27}{4} - 3\rho^2)}\right\}.$$

Now making the transformation $\rho^2 - \frac{1}{4} = t$, $z_1 y_1$ turns into a product of two nonnegative decreasing functions of t on the interval $[1 - \frac{1}{2}\sqrt{3}, \frac{1}{2}]$. Thus f achieves its maximum for $\rho = \frac{1}{2}\sqrt{5 - 2\sqrt{3}}$. If $z_1^* = -\frac{1}{2} + \frac{1}{2}\sqrt{3}$ and $z_2^* = \frac{1}{2}$, an optimal solution is given by $x^* = (-z_1^*, z_2^*)$, $y^* = (z_1^*, -z_2^*)$ and $z^* = (z_1^*, z_2^*)$.

Note that it is easy to see geometrically that, for each ρ and fixed z^0, the diameter of A is $d(x, y)$. This fact can be verified analytically as follows. We need to show that the other five distances as functions of ρ and z^0 are bounded above by $d(x, y)$. Consider the triangle xzy. The angle xzy is obtuse since x and $\bar{z}$ are diametrically opposite. Thus $d(x, z) \leqslant d(x, y)$ and $d(z, y) \leqslant d(x, y)$. Let $\bar{w}$ be the reflection of w about the vertical axis. Considering the triangle $xz\bar{w}$ we may write $d(x, w) = d(z, \bar{w}) \leqslant d(x, \bar{w}) = d(z, w)$. Recalling the argument on $d(x, y^1)$ and $d(x, y^2)$ (see Fig. 4) we conclude that $d(z, w) \leqslant d(x, y)$. Since $d(x, y) \geqslant 1$, it suffices to prove that $d(w, y) \leqslant 1$. To prove this claim, we first observe that for every ρ, $d((-\frac{1}{2}, 0), z) = 1$. This implies that, for all z^0 in the first quadrant, the point w is below the x-axis. Similarly, the point y is always below the x-axis. Now $d(w, y)$ is bounded above by the diameter of the region defined by the intersection of the two spheres $S((-\frac{1}{2}, 0), 1)$, $S((\frac{1}{2}, 0), 1)$, and the lower half-plane. This diameter is easily seen to be 1. □

Finally, we show that the general case can be reduced to the analysis of $\delta(2)$.

2.5. Theorem. $\delta(k) = \delta(2)$ *for all* $k \geqslant 2$.

Proof. From Theorem 2.4, we observe that, for $k = 2$, the constraint $(x_1 - z_1)^2 + \cdots + (x_k - z_k)^2 \leqslant 1$ is redundant in (P2), i.e., if this constraint is removed, the resulting optimization problem has the same optimal value. Let (P3) denote this optimization problem that results once the above constraint is removed from (P2). We prove that (P3) has the same optimal value for all $k \geqslant 2$.

Let the triplet (x, y, z) with $x = (x_1, x_2, \ldots, x_k)$, $y = (y_1, y_2, \ldots, y_k)$, $z = (z_1, z_2, \ldots, z_k)$ be an optimal solution of (P3). Let $\bar{x} = (x_1, \overline{x_2}, 0, \ldots, 0)$, $\bar{y} = (y_1, \overline{y_2}, 0, \ldots, 0)$ and $\bar{z} = (z_1, \overline{z_2}, 0, \ldots, 0)$, where

$$\overline{x_2} = \sqrt{x_2^2 + \cdots + x_k^2}, \qquad \overline{y_2} = -\sqrt{y_2^2 + \cdots + y_k^2}$$

and

$$\overline{z_2} = -\sqrt{z_2^2 + \cdots + z_k^2}.$$

We show that $(\bar{x}, \bar{y}, \bar{z})$ is feasible with respect to (P3), and that $d(\bar{x}, \bar{y}) \geqslant d(x, y)$. The point $(\bar{x}, \bar{y}, \bar{z})$ is trivially feasible with respect to all but the last constraint of (P3). By the Cauchy-Schwarz inequality, $(\overline{y_2} - \overline{z_2})^2 \leqslant (y_2 - z_2)^2 + \cdots + (y_k - z_k)^2$. Since $(y_1 - z_1)^2 + \cdots + (y_k - z_k)^2 \leqslant 1$, it follows that $(\bar{x}, \bar{y}, \bar{z})$ satisfies the last constraint as well. Applying the Cauchy-Schwarz inequality once more, we get $(\overline{x_2} - \overline{y_2})^2 \geqslant (x_2 - y_2)^2 + \cdots + (x_k - y_k)^2$, implying that $d(\bar{x}, \bar{y}) \geqslant d(x, y)$. □

The main result of this paper may now be summarized as follows.

2.6. Theorem. $r_1 < r_2 < \cdots < r_m \leqslant d_P \leqslant \min\{\sqrt{3}\, r_1, \sqrt{5 - 2\sqrt{3}}\, r_m\}$, *where* $m \leqslant n$.

The worst-case bound of the algorithm is achievable by considering the five points $(-\frac{1}{2}, 0)$, $(\frac{1}{2}, 0)$, (z_1^*, z_2^*), $(-z_1^*, z_2^*)$, $(z_1^*, -z_2^*)$, where $z_1^* = -\frac{1}{2} + \frac{1}{2}\sqrt{3}$, $z_2^* = \frac{1}{2}$. If the first point is selected as p_1, then the second point is q_1 and $p_2 = (0, 0)$. If q_2 is the third point, the algorithm terminates with $r_1 = r_2 = 1$, while the actual diameter is $\sqrt{5 - 2\sqrt{3}}$. While the worst-case bound is achievable, we have not been able to determine the worst-case time complexity of Algorithm B.

However, based on empirical evidence described below, we are led to conjecture that for uniformly distributed points in $\mathbb{R}^k$ for fixed k, the worst-case time complexity of Algorithm B is $O(n)$.

Remarks. A computer implementation of Algorithm B was carried out and in what follows we present some of the results.

We considered sets of points of sizes $n = 50, 100, 150, 200, 250$ in each of the dimensions $k = 2, 3, 4, 5, 6$. For each possible pair of values of n and k, 100 sample sets P were generated by uniform distribution in the unit hypercube. For each test problem, Algorithm B was run and at the same time the actual diameter was computed by brute force. The average percentage error is produced in Table 1. For example, for $n = 150$ and $k = 4$, the mean error of the approximate diameters computed for 100 sample sets by Algorithm B was only 1.72%. Incidentally, during the runs, the maximum error reached was about 24%, showing that the theoretical error bound was attained ($\sqrt{5 - 2\sqrt{3}} \approx 1.24$). The maximum number of iterations m required by Algorithm B for the 100 sample sets considered for each pair n and k are given in Table 2. It appears difficult to justify the surprisingly small magnitude of these numbers.

Table 1
Average percentage error of Algorithm B

n	k				
	2	3	4	5	6
50	0.30	0.94	1.82	2.12	2.50
100	0.42	1.34	2.06	2.63	3.99
150	0.68	1.67	1.72	2.94	4.49
200	0.21	1.32	1.53	3.48	4.36
250	0.48	1.44	1.72	4.32	4.63

Table 2
Maximum number of iterations required by Algorithm B

n	k				
	2	3	4	5	6
50	4	5	5	4	4
100	3	3	4	5	4
150	3	4	5	4	5
200	3	4	6	4	4
250	3	5	5	5	5

Acknowledgment

We would like to thank the referees whose comments have greatly improved the readability of this paper.

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