Sphere packings in the regular crosspolytope

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1. Introduction

The problem of packing equal spheres inside a given container has been considered for a long time. Schaer, Meir and Wengerodt determined the densest circle packing for a small number of circles within a square, whereas Pirl, Kravitz, Goldberg and Fodor concluded the same within a circle (see Fodor [2] for references, and Melissen [4] for a detailed survey on circle packings inside a given domain). In the three space, sphere packings inside a cube were investigated by Schaer who determined the optimal arrangement for up to ten equal spheres (see Schaer [5]). In addition, Bezdek [1] and Golser [3] found the maximal radius of n equal non–overlapping spheres within a tetrahedron and an octahedron for small n.

Let $v_1, \ldots, v_d$ be an orthonormal base of the d–space, and we write O^d to denote the d–dimensional regular crosspolytope whose vertices are $\pm v_1, \ldots, \pm v_d$, and hence the edge length of O^d is $\sqrt{2}$. In this paper, we determine the maximal radius $r(n,d)$ of n equal non–overlapping spheres within O^d for $n \leq 2d+1$.

We note that it is equivalent to consider the maximum $\varphi(n,d)$ of the minimal distance of n points in O^d; more precisely,

$$r(n,d) = \frac{\varphi(n,d)}{\varphi(n,d)\sqrt{d}+2}.$$

We present the results and arguments in terms of point sets in O^d because the formulation and the proofs are more transparent this way.

In the planar case, it is an elementary exercise to show that $\varphi(3,2) = 2(\sqrt{3}-1)$, one of the points in the optimal configuration is a vertex of O^2, and the three points are vertices of some regular triangle. The optimal configuration of four points are the vertices of O^2, and hence $\varphi(4,2) = \sqrt{2}$. Finally, the centre and the vertices of O^2 form the optimal configuration of five points, thus $\varphi(5,2) = 1$.

It is probably surprising but these estimates generalize to any dimension d; namely, we verify that $\varphi(n,d)$ is $2(\sqrt{3}-1)$ if $n = 3$, equals $\sqrt{2}$ if $4 \leq n \leq 2d$, and equals one if $n = 2d+1$:

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Theorem 1. *For $d \geq 3$, let the minimal distance among three points in O^d be maximal. Then one of the points is a vertex, say v_i, and the three points form a regular triangle that is contained in the square with vertices $\pm v_i, \pm v_j$ for some $v_j \neq v_i$.*

Theorem 1 was proved in Golser [3] and Bezdek [1] if $d = 3$. Now if the number n of the points in O^d is between 4 and $2d$ then one can not do better than placing them at the vertices:

Theorem 2. *For $d \geq 3$, let the minimal distance among n points in O^d be maximal where $4 \leq n \leq 2d$. Then either each point is a vertex of O^d, or $n = 4$, three of the points are the vertices of a two–face of O^d, and the fourth point is the centroid of the opposite two–face.*

Theorem 2 was proved in Golser [3] and Bezdek [1] if $d = 3$. In case of ball packings, Theorem 2 has the following interesting corollary:

If a d–dimensional regular crosspolytope contains four equal solid balls then it can host even $2d$ solid balls of the same radius.

Finally there exists only one optimal configuration if $n = 2d + 1$:

Theorem 3. *For $d \geq 3$, let the minimal distance among $2d + 1$ points in O^d be maximal. Then one of the points is the centre of O^d, and the other points are the vertices of O^d.*

Theorem 3 was proved in Golser [3] and Bezdek [1] if $d = 3$.

Some of ideas in the proofs below are taken from Bezdek [1] and Golser [3]. In order to to simplify notation, we define

$$v_{i+d} = -v_i, \quad i = 1, \ldots, d.$$

The scalar product is denoted by $\langle \cdot, \cdot \rangle$, and the origin is denoted by o.

2. The case of three points

Let $x_1, x_2, x_3 \in O^d$ be in optimal position, and hence the minimal distance between any two of them is at least $2(\sqrt{3}-1)$. Only at most one out of x_1, x_2, x_3 is a vertex of O^d because two neighbouring vertices are too close to each other, and the spheres of radius $\sqrt{2}$ around two opposing vertices cover the whole crosspolytope.

First we suppose that the triangle x_1, x_2, x_3 is not regular, and seek a contradiction. We may assume that $d(x_1, x_2) > d(x_1, x_3)$ and x_1 is not a vertex.

Then x_1 can be moved into a position $x_1' \in O^d$ such that both distances $d(x_1', x_2)$ and $d(x_1', x_3)$ are larger than $d(x_1, x_3)$. Now either x_2 or x_3 is not a vertex, and this point can be moved into a new position such that the distances between the pairs of the resulting system of three points in O^d are larger than $\varphi(3, d)$. This contradiction yields that any optimal triple determines a regular triangle.

Next we suppose that x_1 lies in the relative interior of a k–face F of O^d with $k \geq 2$, and seek a contradiction. Let H be the hyperplane that is the perpendicular bisector of the segment x_2x_3, and let G be the $(d-2)$–plane that is orthogonal to the two–plane $x_1x_2x_3$, and passes through x_1. Now G is contained in H, and we write G^+ to denote the half–hyperplane of H that is bounded by G and does not intersect the segment x_2x_3. Then $\mathrm{aff} F \cap G^+$ contains a half line h emanating from x_1, and hence translating x_1 along h we obtain an optimal triangle that is not regular. This is absurd; therefore each x_i is contained in an edge e_i, $i = 1, 2, 3$.

Since the convex hull of e_i and e_j is of diameter greater than $\sqrt{2}$, we deduce that

$$e_i \cap -e_j \neq \emptyset. \qquad (*)$$

First we consider the case when e_1, e_2, e_3 are pairwise disjoint. Then we may assume that e_1, e_2 and e_3 are the segments v_1v_{d+2}, v_2v_{d+3} and v_3v_{d+1}, respectively, and x_1 is not further from v_1 than from v_{d+2}. We write m_1 and m_2 to denote the midpoints of the segments v_1v_{d+2} and v_2v_{d+3}, respectively, and define $m_3 = \frac{3}{4} \cdot v_3 + \frac{1}{4} \cdot v_{d+1}$. Since x_1 is contained in the segment v_1m_1, and the diameter of the tetrahedron $v_1m_1v_3m_3$ is

$$d(v_1, m_3) = \frac{\sqrt{34}}{4} < 2 \cdot (\sqrt{3} - 1),$$

we deduce that x_3 is contained in the segment $v_{d+1}m_3$. Similarly, the diameter of the tetrahedron $v_1m_1v_{d+3}m_2$ is $\sqrt{2}$, and hence x_2 is contained in the segment v_2m_2. On the other hand, the diameter of the tetrahedron $v_2m_2v_{d+1}m_3$ is $\sqrt{2}$, therefore $d(x_2, x_3) < 2 \cdot (\sqrt{3} - 1)$. This contradiction yields that say e_1 and e_2 have a common vertex v_1.

According to $(*)$, we may assume that the other endpoints of e_1 and e_2 are v_2 and v_{d+2}, respectively. Now one endpoint of e_3 is $-v_1$. If x_3 is not contained in the square S with vertices $\pm v_1, \pm v_2$ then we may assume that the other endpoint of e_3 is v_3. Now for $i = 1, 2$, the longest side of the triangle $x_ix_3v_3$ is x_ix_3, and hence the angle $\angle x_ix_3v_{d+1}$ is obtuse. It follows that $d(x_i, x_3) < d(x_i, v_{d+1})$, or in other words, the triangle $x_1x_2v_{d+1}$ is optimal but not regular. Therefore x_3 does lie in S. If S has a side e that does not contain any of x_1, x_2, x_3 then the triangle $x_1x_2x_3$ can be translated orthogonally to e in a way that one of the x_i's arrives into the interior of S. We conclude that one of the x_i's is a vertex of S, which in turn yields Theorem 1.

3. The case when $4 \le n \le 2d$

In order to verify Theorem 2, it is sufficient to consider the case $n = 4$. Therefore let $x_1, x_2, x_3, x_4 \in O^d$ be an optimal set of four points, and hence $d(x_i, x_j) \ge \sqrt{2}$ holds for any $i \ne j$.

Let G_i denote the convex hull of v_i and the midpoints of the edges of $v_i v_j$, $j \ne i + d$, and we define

$$P_0 = O^d \setminus \cup_{i=1}^{2d} G_i.$$

Then the closure of P_0 is a polytope whose vertices are the midpoints of the edges of O^d but these midpoints do not belong to P_0. Since the maximal distance between the midpoints of the edges of O^d is $\sqrt{2}$, we deduce that at most one x_i is contained in P_0.

Now the diameter of any G_j is one, and hence any G_j contains at most one x_i. Thus we may assume that $x_1 \in G_1$ and $x_2 \in G_2$. For $0 \le t \le \frac{1}{2}$ and $i = 1, \ldots, 2d$, we write G_i^t to denote the image of G_i by the homothety whose centre is v_i, and the quotient is $2 \cdot t$. Therefore the vertices of G_i^t are

$$v_i \qquad \text{and} \qquad (1-t) \cdot v_i + t \cdot v_j \ \text{ for } \ v_j \ne \pm v_i.$$

Now we distinguish two cases:

a) Either x_3 or x_4 is contained in some G_j with $j \ne d+1, d+2$.

We may assume that $x_3 \in G_3$. Let $1 - t$ be the minimum of $\langle x_i, v_i \rangle$ for $i = 1, 2, 3$, where $0 \le t \le \frac{1}{2}$. We assume that $\langle x_1, v_1 \rangle = 1 - t$ and $\langle x_1, v_2 \rangle \ge \langle x_1, v_3 \rangle$. Then x_1 is contained in the part F of the facet of G_1^t opposite to v_1 such that the second coordinate of its points is not less than the third coordinate. Thus F is the $(d-1)$–polytope with vertices

$$\begin{cases} (1-t) \cdot v_1 \pm t \cdot v_i & \text{for } i = 4, \ldots, d \\ (1-t) \cdot v_1 + t \cdot v_2 & \\ (1-t) \cdot v_1 - t \cdot v_3 & \\ (1-t) \cdot v_1 \pm \frac{t}{2} \cdot (v_2 + v_3). & \end{cases}$$

On the other hand, x_2 is contained in G_2^t. If $0 < t \le \frac{1}{2}$ then some elementary calculations show for any vertex of F and any vertex of G_2^t that the distance between the two points is less than $\sqrt{2}$. Therefore $t = 0$; namely, $x_i = v_i$ for $i = 1, 2, 3$. It follows that x_4 is either another vertex of O^d or the centre of the two face $v_{d+1} v_{d+2} v_{d+3}$.

b) Neither x_3 nor x_4 is contained in some G_j with $j \ne d+1, d+2$.

Then we may assume that $x_3 \in G_{d+1}$.

We suppose that $x_4 \in P_0$, and seek a contradiction. We may assume that $\langle x_4, v_1\rangle \geq \langle x_4, v_{d+1}\rangle$, and hence x_4 lies in the convex hull of the midpoints of edges of O^d that do not contain v_{d+1}. Since the distance of any of these midpoints from the vertices of G_1 is at most $\sqrt{2}$, and x_4 does not coincide with any of these midpoints, we deduce that $d(x_1, x_4) < \sqrt{2}$. This is absurd, and hence $x_4 \in G_{d+2}$.

The rest of the argument is similar to the one in a). Let $1-t$ be the minimum of $\langle x_1, v_1\rangle$, $\langle x_2, v_2\rangle$, $\langle x_3, v_{d+1}\rangle$ and $\langle x_4, v_{d+2}\rangle$ where $0 \leq t \leq \frac{1}{2}$. We may assume that $\langle x_1, v_1\rangle = 1-t$ and $\langle x_1, v_2\rangle \geq \langle x_1, v_{d+2}\rangle$. Then x_1 is contained in the part F' of the facet of G_1^t opposite to v_1 such that the second coordinate of its points is non–negative, and hence F' is the $(d-1)$–polytope with vertices

$$(1-t)\cdot v_1 + t\cdot v_2 \qquad \text{and} \qquad (1-t)\cdot v_1 \pm t\cdot v_i \ \text{ for } \ i = 3, \ldots, d.$$

On the other hand, x_2 is contained in G_2^t. If $0 < t \leq \frac{1}{2}$ then some simple calculations show for any vertex of F' and any vertex of G_2^t that the distance between the two points is less than $\sqrt{2}$. Therefore $t = 0$; namely, $x_1 = v_1$, $x_2 = v_2$, $x_3 = v_{d+1}$ and $x_4 = v_{d+2}$.

4. The case of 2d+1 points

We define the Dirichlet-Voronoi cell D_i of v_i as

$$D_i := \left\{x \in O^d : \ \langle x, v_i\rangle \leq \langle x, v_j\rangle \quad \text{for all } j \neq i\right\}.$$

Then the vertices of D_i are the centroids of the faces of O^d that contain v_i (including O^d as a d–face). We note that if F is an $(m-1)$–face with vertices $v_{i_1}, \ldots, v_{i_m}$ for some $2 \leq m \leq d$ then its centroid is $\frac{v_{i_1}+\ldots+v_{i_m}}{m}$.

Lemma *Let $x, y \in D_i$. Then $d(x,y) \leq 1$, and $d(x,y) = 1$ occurs only if either $\{x,y\} = \{o, v_i\}$ or $\{x,y\} = \{\frac{v_i+v_j}{2}, \frac{v_i-v_j}{2}\}$ where $v_j \neq \pm v_i$.*

Proof: The points o, v_i, $\frac{v_i+v_j}{2}$ and $\frac{v_i-v_j}{2}$ are all vertices of O^d, thus we may assume that x and y are vertices of O^d, as well. We may also assume that $i = 1$.

If either x or y is the origin or v_1 then the Lemma readily holds, and hence let x and y be contained in an $(m-1)$–face F and $(k-1)$–face G of O^d for $2 \leq m, k \leq d$, respectively. We assume that $k \leq m$. We write p to denote for the number of common vertices of F and G, and q to denote for the number of vertices of F whose opposite is a vertex of G. Then

$$d(x,y)^2 = p\cdot\left(\frac{1}{k} - \frac{1}{m}\right)^2 + q\cdot\left(\frac{1}{k} + \frac{1}{m}\right)^2 + \frac{m-q-p}{m^2} + \frac{k-q-p}{k^2}.$$

Now $p \geq 1$, and hence for given k and m, the possible maximum of $d(x,y)^2$ is attained if $p = 1$ and $q = k - 1$; namely, when

$$d(x,y)^2 = \frac{1}{m} \cdot \left(3 - \frac{4}{k}\right) + \frac{1}{k} \leq \frac{4}{k} \cdot \left(1 - \frac{1}{k}\right).$$

Therefore $d(x,y)^2$ is maximal if $m = k = 2$, and F is an edge $v_i v_j$, while G is the edge $v_i(-v_j)$. Q.E.D.

Let us prove Theorem 3. For $x \in O^d$ and $i = 1, \ldots, 2d$, we define the weight $w_i(x)$ of x as

$$w_i(x) = \begin{cases} \frac{1}{\#\{j\colon x \in D_j\}} & \text{if } x \in D_i \\ 0 & \text{if } x \notin D_i \end{cases}.$$

We note that $\sum_{i=1}^{2d} w_i(x) = 1$ holds for any $x \in O^d$.

Now the vertices and the centre of O^d form $2d + 1$ points whose mutual distances are at least one. Thus let $x_1, \ldots, x_n$ be n points in O^d such that the mutual distances are at least one. The Lemma yields for any $i = 1, \ldots, 2d$ that

$$\sum_{j=1}^{n} w_i(x_j) \leq 1 + \frac{1}{2d},$$

and equality holds if and only if the points of $\{x_1, \ldots, x_n\}$ in D_i are the origin and v_i. Therefore

$$n = \sum_{i=1}^{2d} \sum_{j=1}^{n} w_i(x_j) \leq 2d + 1,$$

and equality holds if and only if $x_1, \ldots, x_n$ consists of the vertices and the centre of O^d.

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