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PACKING OF POINTS INTO THE UNIT 6-DIMENSIONAL CUBE

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Abstract. The best known estimate for the packing of points into the 6-dimensional unit cube in mutual distances at least 1 is improved.

The following problem was stated in [10] and later repeated e.g. in [1], [6], [11], [12], [13].

> "Let $f(n)$ denote the maximum number of points that can be arranged in the n-dimensional unit cube so that all mutual distances are at least 1.
> Obviously, $f(n) = 2^n$ for $n \leq 3$. Many have shown that $f(n) \sim \frac{1}{2}n(\log n)$. Determine the exact values of $f(n)$ at least for small n."

Obviously, the problem could be formulated in the terms of packing equal balls in the cube.

In the paper [3] was proved $f(4) = 17$ and also the uniqueness of the extremal arrangement. An upper asymptotic estimate was proved in [3] and this was sharpened recently in [4] by [9] to

$$n^{n/2} \cdot 0.2419707^n \Omega\left(\sqrt{n}\right) \leq f\left(n\right) \leq n^{n/2} \cdot 0.63901^n e^{o(n)}.$$

Some results on $f(5)$ were proved in [5] and recently in [7] and [8]. The best known estimate $f(5) \leq 40$ can be found in [2].

In the paper [4] we showed many lower and upper estimates, besides others $f(6) \leq 192$, which is the best known estimate for this time. In this paper we give simple proof that $f(6) \leq 128$ using entirely different method. Further, we improve this upper estimate to $f(6) \leq 120$.

For the sake of brevity we say "points are *permissibly packed* in ..." instead of "points with mutual distances at least 1 are packed in ...".

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Lemma 1 (see [4]). *If three points are permissibly packed in a box of edge lengths* $w_1, w_2, \dots, w_n$ *then*

$$\sum_{i=1}^{n} w_i^2 \geq \frac{3}{2}.$$

Moreover, if $\sum_{i=1}^{n} w_i^2 = 3/2$ *then all three points lie in the vertices of the box.*

Proof. If $0 \leq x \leq y \leq z \leq w$, then

$$\begin{aligned}(x-y)^2 + (x-z)^2 + (y-z)^2 &\leq (0-y)^2 + (0-w)^2 + (y-w)^2 \\ &= 2w^2 - 2y(w-y) \leq 2w^2.\end{aligned}$$

Applying this inequality to every coordinate of three points $A = (a_1, a_2, \dots, a_n)$, $B = (b_1, b_2, \dots, b_n)$, and $C = (c_1, c_2, \dots, c_n)$ which are permissibly packed in the box $\prod_{i=1}^{n}[0, w_i]$ we get

$$\begin{aligned}3 &\leq |AB|^2 + |BC|^2 + |CA|^2 \\ &= \sum_{i=1}^{n} \left[(a_i - b_i)^2 + (b_i - c_i)^2 + (c_i - a_i)^2\right] \\ &\leq 2 \sum_{i=1}^{n} w_i^2.\end{aligned}$$

Clearly $3 = 2\sum_{i=1}^{n} w_i^2$ if and only if $a_i, b_i, c_i \in \{0, w_i\}$ for every i. □

We define a *small cube* by the following way. If we halve the n-dimensional unit cube $[0,1]^n$ by the hyperplanes $x_i = 1/2$ for $i = 1, 2, \dots, n$, we get 2^n small cubes. Each of these small cubes contains exactly one vertex of the n-dimensional unit cube, in other words every vertex uniquely determines the small cube containing it.

For a 6-dimensional small cube we have $w_1 = \dots = w_6 = 1/2$, consequently $\sum w_i^2 = 3/2$. Lemma 1 implies that three points can be permissibly packed in a 6-dimensional small cube only if the points lie in the vertices of the small cube. Of course, more than three points must be situated in the vertices of the small cube as well. It is easy to check that among five vertices of the small cube there are two at distance less than 1 apart. Thus we have the following lemma.

Lemma 2. *At most four points can be permissibly packed into a* 6*-dimensional small cube. Moreover, three or four points can be permissibly packed only into the vertices of the small cube.*

Now we define the *weight of the point* $X \in [0,1]^6$ as $w(X) = 1/2^k$ if exactly k co-ordinates of the point X are equal to $1/2$. It is easy to see that $f(6) = \sum w(C_i)$, where $w(C_i)$ is the sum of weights of all points packed in a small cube C_i. We will say "*the weight of a small cube is* ..." instead of "the sum of weights of points in a small cube is ...".

Lemma 3. *If three points are permissibly packed in a small cube then the weight of this small cube is at most* $1 + 1/8$. *If four points are permissibly packed in a small cube then the weight of this small cube is at most* $1+3/16$.

Proof. Without loss of generality we can suppose that the small cube is $[0, 1/2]^6$. By Lemma 2 we know that all co-ordinates of three (resp. four) points belong into $\{0, 1/2\}$.

If the weight of some point is 1, then it must be the point $(0, \dots, 0)$. In this case every remaining point has at least four coordinates $1/2$, hence its weight is at most $1/16$. So the sum of weights of points is at most $1+2\cdot(1/16)$ for three points and $1 + 3 \cdot (1/16)$ for four points.

Further we suppose that there is no point with the weight 1. If there is a point with the weight $1/2$, then one of its coordinates is $1/2$ and the remaining coordinates are 0. Therefore every remaining point has at least three coordinates $1/2$. So the sum of weights of points is at most $1/2+2\cdot(1/8)$ for three points and $1/2 + 3 \cdot (1/8)$ for four points.

Finally, we suppose that there is no point with the weight 1 or $1/2$. Now the sum of weights of three points is at most $3\cdot(1/4)$ and the sum of weights of four points is at most $4 \cdot (1/4)$. □

From Lemma 3 we get that the weight of a small cube C_i is at most two, $w(C_i) \leq 2$, where equality holds if and only if the small cube contains two points with weight 1. So $f(6) = \sum w(C_i) \leqq 64 \cdot 2$.

Corollary 4. $f(6) \leq 128$.

The conjectured value for $f(6)$ is 76, see [3]. To verify that $f(6) \geq 76$ let us consider 64 vertices of 6-dimensional unit cube and the following 12 points:

$$\left(0,0,\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2}\right) \quad \left(0,1,\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2}\right) \quad \left(1,0,\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2}\right)$$
$$\left(1,1,\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2}\right) \quad \left(\frac{1}{2},\frac{1}{2},0,0,\frac{1}{2},\frac{1}{2}\right) \quad \left(\frac{1}{2},\frac{1}{2},0,1,\frac{1}{2},\frac{1}{2}\right)$$
$$\left(\frac{1}{2},\frac{1}{2},1,0,\frac{1}{2},\frac{1}{2}\right) \quad \left(\frac{1}{2},\frac{1}{2},1,1,\frac{1}{2},\frac{1}{2}\right) \quad \left(\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2},0,0\right)$$
$$\left(\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2},0,1\right) \quad \left(\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2},1,0\right) \quad \left(\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2},1,1\right).$$

We see that for these 76 points every small cube contains four points and the weight of every small cube is exactly $1+3/16$ (recall Lemma 3). The gap between conjectured value $f(6) = 76$ and proved $f(6) \leq 128$ (Corollary 4) is due to small cubes with the weight 2. In the following we show an upper bound for the number of small cubes with the weight 2 and consequently we get a better upper estimate for $f(6)$.

Lemma 5. *At most* 15 *points can be permissibly packed into a box of edge-length* $1, 1, 1, 1/2, 1/2, 1/2$ *and this bound cannot be improved.*

Before we prove this lemma we define a new weight function w_P that is associated with some box P instead of a unit cube. *The weight* w_P *of the point* $X = (x_1, \ldots, x_6) \in P = [0,1]^3 \times [0,1/2]^3$ is $w_P(X) = 1/2^k$ if exactly k of the first three co-ordinates of the point X are equal to $1/2$. For example the weight of point $X = (0, 1/2, 0, 1/2, 0, 1/2)$ is $w_P(X) = 1/2$. Recall that $w(X) = 1/8$, but the weight w_P depends on the first three coordinates only. Obviously the sum $\sum w_P(C_i)$ of weights of small cubes is equal to the number of points in box P. Note that box P contains 8 small cubes, denote the vertices of 6-dimensional unit cube associated with these small cubes by V, so

$$V = \{(0,0,0,0,0,0), (1,0,0,0,0,0), \ldots, (1,1,1,0,0,0)\}.$$

Proof. Using the notion of weight w_P we want to prove that $\sum w_P(C_i) < 16$. Let us suppose that $\sum w_P(C_i) \geq 16$.

As a straightforward modification of the proof of Lemma 3 we get that a small cube C_i with three or four points has the weight at most

$$w_P(C_i) \leq 1 + \frac{1}{2} + \frac{1}{4} = 1 + \frac{3}{4}$$

or

$$w_P(C_i) \leq 1 + \frac{1}{2} + \frac{1}{4} + \frac{1}{8} = 1 + \frac{7}{8},$$

respectively. Now it is clear that $\sum w_P(C_i) \geq 16$ if and only if every small cube contains exactly two points with the weight $w_P = 1$.

For a vertex $v \in V$ of P denote by $SB_q(v)$ the box contained in P with edges of lengths $q, q, q, 1/2, 1/2, 1/2$ parallel to the coordinate axes, and with one of its vertices being v; see Figure 1.

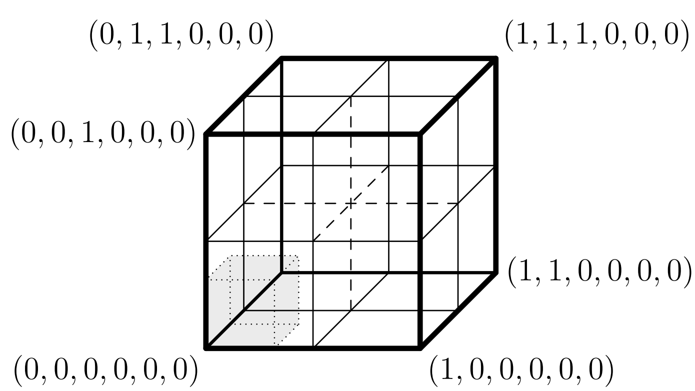

FIGURE 1. $SB_{q=0.3}(0,0,0,0,0,0)$ is depicted as the gray cube. Note that the lenght of sides for remaining three coordinates are $1/2$.

Since the weight of every point is 1 (it means that none of the first three coordinates is 1/2), there exists a number $0 < q_1 < 1/2$ such that every point lies in $SB_{q_1}(v)$ for some $v \in V$. As every small cube contains exactly two points, we get that for every vertex v the box $SB_{q_1}(v)$ contains two points. The idea of the proof is that there is a decreasing sequence $\{q_k\}_{k=1}^{\infty}$ such that points belong into $SB_{q_k}(v)$ for every k. On the other hand there is k such that $SB_{q_k}(v)$ is to small to contain two points with distance 1.

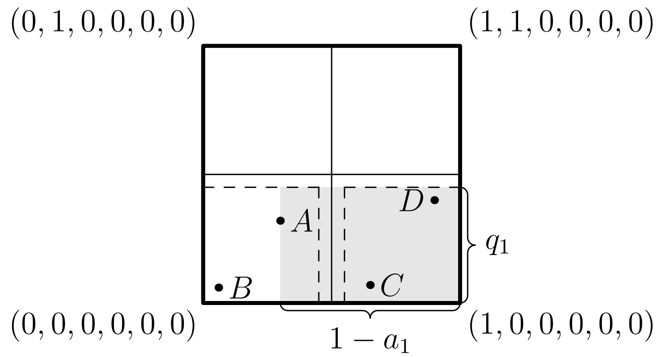

FIGURE 2. Points with the weight $w_P = 1$. Squares with two dashed sides represent $SB_{q_1}(0,0,0,0,0,0)$ and $SB_{q_1}(1,0,0,0,0,0)$. The gray rectangle is a box enclosing points A, B, C with the edge lengths $1 - a_1, q_1, q_1, 1/2, 1/2, 1/2$.

Now consider points $A = (a_1, a_2, a_3, a_4, a_5, a_6) \in SB_{q_1}(0,0,0,0,0,0)$ and $C, D \in SB_{q_1}(1,0,0,0,0,0)$; see Figure 2. These three points are permissibly packed in a box with the edge lengths $1-a_1, q_1, q_1, 1/2, 1/2, 1/2$. By Lemma 1 we have

$$\frac{3}{2} \leq (1-a_1)^2 + 2q_1^2 + 3\left(\frac{1}{2}\right)^2,$$

hence

$$a_1 \leq 1 - \sqrt{\frac{3}{4} - 2q_1^2}.$$

As, by assumption, $SB_{q_1}(0,1,0,0,0,0)$ and $SB_{q_1}(0,0,1,0,0,0)$ also contain two points, it follows that

$$a_2 \leq 1 - \sqrt{\frac{3}{4} - 2q_1^2} \quad \text{and} \quad a_3 \leq 1 - \sqrt{\frac{3}{4} - 2q_1^2}.$$

So point A, and with regard to the symmetry all points lie in some box $SB_{q_2}(v)$ for some v, where $q_2 = 1 - \sqrt{3/4 - 2q_1^2}$. This argument can be repeated and we get a sequence $\{q_k\}_{k=1}^{\infty}$, where

$$0 < q_1 < \frac{1}{2} \quad \text{and} \quad q_{k+1} = 1 - \sqrt{3/4 - 2q_k^2}$$

such that for all k every point lies in $SB_{q_k}(v)$ for some v.

If there is k such that $q_k \le 1/6$, then there are two points in a box $SB_{q_k \le 1/6}(v)$, but $3\cdot(1/6)^2+3\cdot(1/2)^2 = 30/36 < 1$, a contradiction. Therefore $1/6 < q_k < 1/2$ for every k and it is easily seen that the difference

$$q_k - q_{k+1} = q_k + \sqrt{3/4 - 2q_k^2} - 1$$

is positive. So, the sequence $\{q_k\}$ is decreasing and from $q_k > 1/6$ we get that there is $\lim_{k\to\infty} q_k = L$. Nevertheless, also $\lim_{k\to\infty} q_{k+1} = L$ and it follows that $L = 1 - \sqrt{3/4 - 2L^2}$. As a consequence of $L < 1/2$ we get $L = 1/6$. Hence, there is an index j such that $q_j < 1/4$. Now two points lie in the box $s_{1/4}(0,0,0,0,0,0)$ and we have a contradiction

$$3 \cdot \left(\frac{1}{4}\right)^2 + 3 \cdot \left(\frac{1}{2}\right)^2 = \frac{15}{16} < 1.$$

Note that the box $[0,1]^3 \times [0,1/2]^3$ contains 15 points from the 76 points described above, so the bound 15 cannot be improved. $\square$

Simple consequence of this Lemma is Theorem 6, stating that $f(6) \le 8 \cdot 15 = 120$.

Theorem 6. $f(6) \le 120$.

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