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Three Cube Packing for All Dimensions

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Abstract: Let $V_n(d)$ denote the least number, such that every collection of n d-cubes with total volume 1 in d-dimensional (Euclidean) space can be packed parallelly into some d-box of volume $V_n(d)$. We show that $V_3(d) = \frac{r^{1-d}}{d}$ if $d \geq 11$ and $V_3(d) = \frac{\frac{1}{r}+1}{r^d+\left(\frac{1}{r}-r\right)^d+1}$ if $2 \leq d \leq 10$, where r is the only solution of the equation $2(d-1)k^d + dk^{d-1} = 1$ on $\left(\frac{\sqrt{2}}{2}, 1\right)$ and $(k+1)^d(1-k)^{d-1}\left(dk^2+d+k-1\right) = k^d\left(dk^{d+1}+dk^d+k^d+1\right)$ on $\left(\frac{\sqrt{2}}{2}, 1\right)$, respectively. The maximum volume is achieved by hypercubes with edges x, y, z, such that $x = \left(2r^d+1\right)^{-1/d}$, $y = z = rx$ if $d \geq 11$, and $x = \left(r^d + (\frac{1}{r}-r)^d + 1\right)^{-1/d}$, $y = rx$, $z = (\frac{1}{r}-r)x$ if $2 \leq d \leq 10$. We also proved that only for dimensions less than 11 are there two different maximum packings, and for all dimensions greater than 10, the maximum packing has the same two smallest cubes.

Keywords: packing of cubes; extreme

1. Introduction

In 1966 (according to [1], in 1963 according to [2]), Leo Moser spread a collection of 50 problems named "Poorly Formulated Unsolved Problems of Combinatorial Geometry". The collection consisted of only mimeographed copies, and was not fully published in its original form until 1991 in [1]. Problem 7 was "What is the smallest number A such that every set of squares of total area 1 can be accommodated in some rectangle of area A?". This problem can also be found in [2–5].

The problem has been extended to higher dimensions, and has been studied for a specific number of squares (cubes). We reformulate the problem, to distinguish between the number of dimensions and cubes and to clarify it.

Packing of a (finite or infinite) collection of d-dimensional cubes (d-cubes, for short) into a d-dimensional rectangular parallelepiped (d-box, for short) means that the union of the d-cubes is a subset of the d-box and the intersection of the interior of any two d-cubes is the empty set. The packing, in which each edge of any packed d-cube is parallel to an edge of d-box, is called parallel packing.

We denote by $V_n(d)$ the least number such that every collection of n d-cubes with the total volume 1 in d-dimensional (Euclidean) space can be packed parallelly into some d-box of volume $V_n(d)$. $V(d)$ denotes the maximum of all $V_n(d)$, $n = 1, 2, 3, \ldots$

Most of the results are for two-dimensional space. In 1967, Moon and Moser [4] proved that $1.2 \leq V(d) \leq 2$. In 1970, Kleitman and Krieger [6] proved that $V(2) \leq \sqrt{3} < 1.733$, and the rectangle with edge lengths 1 and $\sqrt{3}$ is sufficient. Five years later, Kleitman and Krieger [7] again proved that $V(2) \leq \frac{4}{\sqrt{6}} \doteq 1.633$, the rectangle has sides of lengths $\frac{2}{\sqrt{3}}$ and $\sqrt{2}$. After twenty years, Novotný [8] showed that $V_3(2) \doteq 1.228$ and $V(2) \geq \frac{2+\sqrt{3}}{3} > 1.244$. Novotný [9] proved $V_4(2) = V_5(2) = \frac{2+\sqrt{3}}{3}$, and in [10], Novotný proved $V_6(2) = V_7(2) = V_8(2) = \frac{2+\sqrt{3}}{3}$. Platz [11] show up to $V_{11}(2) = \frac{2+\sqrt{3}}{3}$. It is widely believed

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that $V(2) = \frac{2+\sqrt{3}}{3}$. The estimate of $V(2)$ was improved by Novotný [12] $V(2) < 1.53$. Later, this result was improved by Hougardy [13] $V(2) \leq \frac{2867}{2048} < 1.4$ and Ilhan [14] $V(2) < 1.37$.

In 2021, Neuwohner [15] reduced the problem of $V(2)$ to a problem of a finite set of squares, and he limited their number to about 26,000.

The estimate of $V(3)$ was also gradually improved. Meir and Moser [16] proved $V(3) \leq 4$, and later Novotný [17] proved $V(3) \leq 2.26$. The exact results are known for $n = 2, 3, 4, 5$: Novotný [18] $V_2(3) = \frac{4}{3}$, $V_3(3) = 1.44009951$, Novotný [19] $V_4(3) = 1.5196303266$, and in [17], Novotný proved $V_5(3) = V_4(3)$.

Some results for higher dimensions are known too: $V_3(4) = 1.63369662$, by Bálint and Adamko in [20]; $V_3(6) = 1.94449161$, by Bálint and Adamko in [21]; $V_3(8) = 2.14930609$, by Sedliačková in [22]; $V_3(5) \doteq 1.802803792$ and, without a proof, $V_3(7) \doteq 2.05909680$, $V_3(9) \doteq 2.21897778$, $V_3(10) \doteq 2.27220126$, $V_3(11) \doteq 2.31533581$, $V_3(12) \doteq 2.35315527$, $V_3(13) \doteq 2.38661963$, by Sedliačková and Adamko in [23].

Adamko and Bálint proved $\lim_{d\to\infty} V_n(d) = n$ for $n = 5, 6, 7, \ldots$ in [24]. Their proof works for $n \in 2, 3, 4$ as well.

Packing squares into a rectangle is an over half-century-old problem, and even though there are multiple partial results, it remains unresolved. We investigated a modified problem: packing three d-cubes in d-dimensional space. Some results for smaller dimensions are known. We provide the solution for all dimensions $d \geq 2$.

2. Results

Theorem 1.

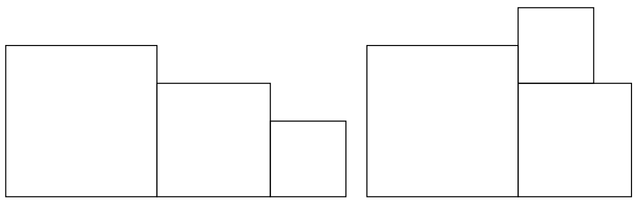
1. $V_3(d) = \frac{r^{1-d}}{d}$ *if* $d \geq 11$, *where* r *is the only solution of the equation* $2(d-1)k^d + dk^{d-1} = 1$ *on* $\left(\frac{\sqrt{2}}{2}, 1\right)$.
2. $V_3(d) = \frac{\frac{1}{r}+1}{r^d + \left(\frac{1}{r}-r\right)^d + 1}$ *if* $2 \leq d \leq 10$, *where* r *is the only solution of the equation* $(k+1)^d(1-k)^{d-1}(dk^2+d+k-1) = k^d\left(dk^{d+1} + dk^d + k^d + 1\right)$ *on* $\left(\frac{\sqrt{2}}{2}, 1\right)$.

The maximum volume is achieved by d-cubes with edges x, y, z, such that:

1. $x = \left(2r^d+1\right)^{-1/d}$, $y = z = rx$ *if* $d \geq 11$.
2. $x = \left(r^d + (\frac{1}{r}-r)^d + 1\right)^{-1/d}$, $y = rx$, $z = (\frac{1}{r}-r)x$ *if* $2 \leq d \leq 10$.

Proof. Let x, y, z be the edge lengths of d-cubes in the d-dimensional Euclidean space ($d \geq 2$), where $1 > x \geq y \geq z > 0$ and the total volume $x^d + y^d + z^d = 1$. Let k and m be real numbers, such that $y = kx$ and $z = mx$. In the proof, we use three constraints:

1. $x^d + (kx)^d + (mx)^d = 1$, i.e., $x^d(k^d + m^d + 1) = 1$, where $d \geq 2$, $d \in \mathbb{N}$.
2. $1 \geq k \geq m > 0$.
3. $kx + mx > x$, i.e., $k + m > 1$. If $k + m \leq 1$, then we pack according to Figure 1b, and the smallest d-cube does not contribute to the total volume.



(**a**) (**b**)

Figure 1. Two cases of packing three d-cubes. (**a**) Packing used by W_1. (**b**) Packing used by W_2.

Three d-cubes can be packed only in two meaningful ways; see Figure 1.

1. Let $W_1 = x^{d-1}(x+y+z) = x^d(k+m+1) = \frac{k+m+1}{k^d+m^d+1}$ be the function of the volume of the packing, as shown in Figure 1a.
2. Let $W_2 = x^{d-2}(x+y)(y+z) = x^d(k+1)(k+m) = \frac{(k+1)(k+m)}{k^d+m^d+1}$ be the function of the volume of the packing, as shown in Figure 1b.

Let $G(k,m) = min(W_1(k,m), W_2(k,m))$. The domain of the function G is bounded by the $1 \geq k \geq m > 0$ and $k+m > 1$. It is shown as the triangle ABC in Figure 2. The domain is the same for each $d \geq 2$.

Our goal is to find the global maximum of G for each dimension ($d \geq 2$) and the edge lengths x, y, z for which it occurs.

If $W_1 = W_2$, then $\frac{k+m+1}{k^d+m^d+1} = \frac{(k+1)(k+m)}{k^d+m^d+1}$ gives the curve PB: $1 = k(k+m)$. PB is continuous and divides the triangle ABC, into two regions (see Figure 2):

1. Region C_1 where $1 \leq k(k+m)$ holds. Therefore, $W_1 \leq W_2$ and, consequently, $G(k,m) = W_1(k,m)$. W_1 is continuous on the region C_1.
2. Region C_2 where $1 \geq k(k+m)$ holds. Therefore, $W_1 \geq W_2$ and, consequently, $G(k,m) = W_2(k,m)$. W_2 is continuous on the region C_2.

The curve PB belongs to both regions. The point $P = (\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2})$ is used in the proofs several times, $G(P) = \frac{\sqrt{2}+1}{2^{1-\frac{d}{2}}+1}$.

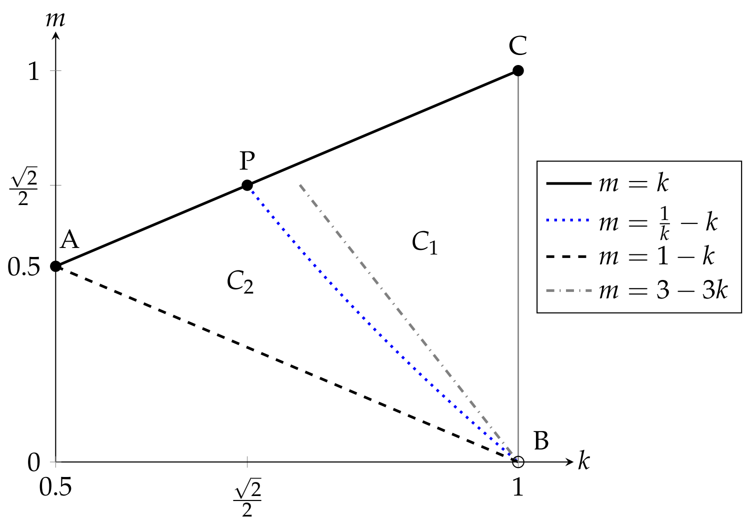


Figure 2. The domain of the function $G(k,m)$.

For the sake of clarity, the rest of the proof is divided into nine claims.

Claim 1. *The global maximum of W_1 must occur on the boundary of the region C_1.*

Proof. $\frac{\partial W_1}{\partial k} = \frac{(k^d+m^d+1)-dk^{d-1}(k+m+1)}{(k^d+m^d+1)^2}$, $\frac{\partial W_1}{\partial m} = \frac{(k^d+m^d+1)-dm^{d-1}(k+m+1)}{(k^d+m^d+1)^2}$. The derivatives are never undefined. The equation $\frac{\partial W_1}{\partial k} = 0 = \frac{\partial W_1}{\partial m}$ gives $k = m$ (line segment PC). So, W_1 has no local extremum inside of the region C_1. The global maximum of W_1 must occur on the boundary of the region C_1. □

Claim 2. *The global maximum of W_2 must occur on the boundary of the region C_2.*

Proof. $\frac{\partial W_2}{\partial m} = \frac{(k+1)(k^d+m^d+1)-dm^{d-1}(k+1)(k+m)}{(k^d+m^d+1)^2}$ is never undefined. The equation $\frac{\partial W_2}{\partial m} = 0$ gives

$$1 = \frac{dm^{d-1}(k+m)}{k^d+m^d+1} \quad (1)$$

Assume, for the sake of contradiction, that if $d \geq 8$, then Equation (1) holds inside of the region C_2. We calculate an upper bound of the right-hand side of Equation (1) using constraints $1 > k(k+m)$, $k+m > 1$, $0.5 \leq k \leq 1$, and $0 < m \leq \sqrt{2}/2$. We maximize the numerator ($k = m = \sqrt{2}/2$) and minimize the denominator ($k = m = 1/2$): $1 \leq \frac{d(\sqrt{2}/2)^{d-1}(\sqrt{2}/2+\sqrt{2}/2)}{(1/2)^d+(1/2)^d+1}$ and we obtain $1 \leq \frac{2^{d/2+1}d}{2^d+2}$. If $d \geq 8$, then we obtain a contradiction. Therefore, if $d \geq 8$, then W_2 has no local extremum inside of the region C_2.

Assume, for the sake of contradiction, that if $2 \leq d \leq 7$, then $\frac{\partial W_2}{\partial k} = \frac{\partial W_2}{\partial m} = 0$ inside of the region C_2.

Step 1: From Equation (1), it follows that

$$m = \left(\frac{k^d + m^d + 1}{d(k+m)} \right)^{\frac{1}{d-1}} \tag{2}$$

We calculate a lower bound of the right-hand side of Equation (2) using $1 > k(k+m)$, $k+m > 1$, $0.5 \leq k \leq 1$, and $0 < m \leq \sqrt{2}/2$. We minimize the numerator ($k = m = 0.5$) and maximize the denominator ($k = m = \sqrt{2}/2$):

For $2 \leq d \leq 7$, the right-hand side of inequality $m \geq \left(\frac{0.5^d+0.5^d+1}{(\sqrt{2}/2+\sqrt{2}/2)d} \right)^{\frac{1}{d-1}}$ is successively greater than $0.530, 0.543, 0.584, 0.623, 0.656, 0.684$. Therefore, m is at least 0.53.

$\frac{\partial W_2}{\partial k} = \frac{(2k+m+1)(k^d+m^d+1) - dk^{d-1}(k+1)(k+m)}{(k^d+m^d+1)^2}$ is never undefined. $\frac{\partial W_2}{\partial k} = 0$ gives

$$k = \left(\frac{(2k+m+1)\left(k^d + m^d + 1\right)}{d(k+1)(k+m)} \right)^{\frac{1}{d-1}} \tag{3}$$

We calculate a lower bound of the right-hand side of Equation (3) using constraints $1 > k(k+m)$, $0.53 \leq m \leq k \leq 1$, and $m \leq \sqrt{2}/2$. We minimize the numerator ($k = m = 0.53$) and maximize the denominator ($k = m = \sqrt{2}/2$).

For $2 \leq d \leq 7$, the right-hand side of inequality $k \geq \left(\frac{(2\cdot 0.53+0.53+1)(0.53^d+0.53^d+1)}{d(\sqrt{2}/2+1)(\sqrt{2}/2+\sqrt{2}/2)} \right)^{\frac{1}{d-1}}$ is successively greater than $0.838, 0.681, 0.677, 0.694, 0.715, 0.734$. Therefore, k is at least 0.67.

Step 2: We repeat the calculations analogously to step 1.

For $2 \leq d \leq 7$, the right-hand side of inequality $m \geq \left(\frac{0.67^d+0.53^d+1}{(\sqrt{2}/2+\sqrt{2}/2)d} \right)^{\frac{1}{d-1}}$ is successively greater than $0.612, 0.585, 0.609, 0.639, 0.666, 0.690$; $m \geq 0.58$.

For $2 \leq d \leq 7$, the right-hand side of inequality $k \geq \left(\frac{(2\cdot 0.67+0.58+1)(0.67^d+0.58^d+1)}{d(\sqrt{2}/2+1)(\sqrt{2}/2+\sqrt{2}/2)} \right)^{\frac{1}{d-1}}$ is successively greater than $1.08, 0.777, 0.735, 0.734, 0.744, 0.756$; $k \geq 0.73$.

Step 3: We repeat the calculations, for the last time.

For $2 \leq d \leq 7$, the right-hand side of inequality $m \geq \left(\frac{0.73^d+0.58^d+1}{(\sqrt{2}/2+\sqrt{2}/2)d} \right)^{\frac{1}{d-1}}$ is successively greater than $0.661, 0.611, 0.627, 0.651, 0.675, 0.697$; $m \geq 0.61$.

For $2 \leq d \leq 7$, the right-hand side of inequality $k \geq \left(\frac{(2\cdot 0.73+0.61+1)(0.73^d+0.61^d+1)}{d(\sqrt{2}/2+1)(\sqrt{2}/2+\sqrt{2}/2)} \right)^{\frac{1}{d-1}}$ is successively greater than $1.21, 0.828, 0.768, 0.757, 0.761, 0.769$; $k \geq 0.75$.

If $\frac{\partial W_2}{\partial k} = \frac{\partial W_2}{\partial m} = 0$ and $2 \leq d \leq 7$, then $k \geq 0.75$ and $m \geq 0.61$, which implies $1 < 0.75(0.75 + 0.61)$. This is a contradiction, since the region C_2 holds $1 \geq k(k+m)$. Hence, if $2 \leq d \leq 7$, then W_2 has no local extremum inside of the region C_2.

So, the global maximum of W_2 must occur on the boundary of the region C_2. $\square$

Claim 3. *The global maximum of W_2 does not occur on AB.*

Proof. AB is a part of a line $m = 1 - k$ if $k \in \left[\frac{1}{2}, 1\right]$. Substituting it into W_2 we obtain $W_2(k, 1-k) = \frac{k+1}{k^d + (1-k)^d + 1}$. Denote it by $W_{AB}(k)$, $k \in \left[\frac{1}{2}, 1\right]$.

If $k \in \left[\frac{1}{2}, 1\right]$, then $W_{AB} < 2$. If $d \geq 7$, then $2 < \frac{\sqrt{2}+1}{2^{1-d/2}+1} = W_2(P)$. Therefore, if $d \geq 7$, then $W_2(P) > W_{AB}$.

Assume, for the sake of contradiction, that if $2 \leq d \leq 6$, then $W_{AB} \geq W_2(P)$ at some $k \in \left[\frac{1}{2}, 1\right]$. From $\frac{k+1}{k^d+(1-k)^d+1} \geq \frac{\sqrt{2}+1}{2^{1-d/2}+1}$ we obtain $k \geq \frac{\left(\sqrt{2}+1\right)\left(k^d+(1-k)^d+1\right)}{2^{1-\frac{d}{2}}+1} - 1$. Let $t(k)$ denote the right-hand side, and $t(k)$ increases on $\left[\frac{1}{2}, 1\right]$. For $2 \leq d \leq 6$, $t\left(\frac{1}{2}\right)$ is successively approximately equal to $0.810, 0.767, 0.810, 0.895, 0.991$, thus $k > 0.76$. We obtain $k > 0.97$ because $t(0.76)$ is successively approximately equal to $0.973, 1.054, 1.151, 1.237, 1.303$. The value of $t(0.97)$ is successively approximately equal to $1.343, 1.704, 2.034, 2.315, 2.540$, which implies $k > 1$, which is a contradiction, since $k \in \left[\frac{1}{2}, 1\right]$. Thus, if $2 \leq d \leq 6$ and $k \in \left[\frac{1}{2}, 1\right]$, then $W_2(P) > W_{AB}$.

$W_2(P) > W_{AB}$ holds for $d \geq 2$, therefore the global maximum of W_2 does not occur on AB. $\square$

Claim 4. *The global maximum of W_2 must occur on PB.*

Proof. AP is a part of a line $m = k$ if $k \in \left[\frac{1}{2}, \frac{\sqrt{2}}{2}\right]$. Substituting it into W_2, we obtain $W_2(k, k) = \frac{2k(k+1)}{2k^d+1}$. We denote it by $W_{AP}(k)$, $k \in \left[\frac{1}{2}, \frac{\sqrt{2}}{2}\right]$.

$W'_{AP} = \frac{(4k+2)\left(2k^d+1\right) - 4d(k+1)k^d}{\left(2k^d+1\right)^2}$ is never undefined. $W'_{AP} = 0$ gives $2(d-2)k^{d+1} + 2(d-1)k^d - 2k - 1 = 0$. We denote the polynomial on the left-hand side by $p(k)$. It has one sign change, as the sequence of signs is $+, +|-, -$ (or $+|-, -$ if $d = 2$). Therefore, according to Descartes' rule of signs, it has exactly one positive real root.

If $d \geq 2$, then $p(2) = 2^{d+1}(3d-5) - 5$ is positive. Setting $2 \leq d \leq 5$ in $p\left(\frac{72}{100}\right) = \frac{1}{25}\left(\left(\frac{18}{25}\right)^d (86d - 122) - 61\right)$, we see that it is negative. If $d \geq 5$, then the exponential term dominates and $p\left(\frac{72}{100}\right)$ is decreasing. So, if $d \geq 2$, then $p\left(\frac{72}{100}\right)$ is negative. Therefore, if $d \geq 2$, then the only positive root of $W'_{AP} = 0$ is greater than 0.72. Since $W'_{AP}\left(\frac{1}{2}\right) = \frac{2^{d+1}\left(-3d+2^{d+1}+4\right)}{\left(2^d+2\right)^2} > 0$ for $d \geq 2$, then W_{AP} is increasing on $\left[\frac{1}{2}, \frac{\sqrt{2}}{2}\right]$. Therefore, the global maximum of W_{AP} occurs at point P, which also belongs to PB. It implies, together with Claims 2 and 3, that the global maximum of W_2 must occur on PB. $\square$

Claim 5. *The global maximum of G does not occur at points P, B, C.*

Proof. $W_1(B) = W_1(1,0) = W_1(C) = W_1(1,1) = 1 < 1.2 < \frac{\sqrt{2}+1}{2^{1-d/2}+1} = W_1(P)$ for $d \geq 2$. Therefore, the global maximum of W_1 does not occur at point B nor C.

The point $(0.76, 0.76) \in PC$. If $d \geq 14$, then the sequence $W_1(0.76, 0.76) = \frac{2\cdot 0.76+1}{2\cdot 0.76^d+1}$ is increasing. $G(P) = \frac{\sqrt{2}+1}{2^{1-\frac{d}{2}}+1} < \sqrt{2}+1 \doteq 2.415$. If $d = 14$, then $2.416 \doteq W_1(0.76, 0.76)$. Hence, if $d \geq 14$, then $G(P) < W_1(0.76, 0.76)$.

The point $(0.72, 0.72) \in PC$. If $11 \leq d \leq 13$, then $G(P)$ is successively less than $2.313, 2.342, 2.363$ and $W_1(0.72, 0.72)$ is successively greater than $2.315, 2.348, 2.373$. Hence, if $11 \geq d \geq 13$, then $G(P) < W_1(0.72, 0.72)$.

Let $k_1 = \frac{\sqrt{2}}{2} + 0.0001$ and $m_1 = \frac{1}{k_1} - k_1$. The point $(k_1, m_1) \in PB$. If $2 \leq d \leq 10$, then $W_1(k_1, m_1)$ is successively greater than
$1.20717, 1.41434, 1.60964, 1.78379, 1.9315, 2.05168, 2.14605, 2.21819, 2.2722011$, and
$G(P)$ is successively less than
$1.20711, 1.41422, 1.60948, 1.78362, 1.9314, 2.05155, 2.14597, 2.21816, 2.2722010$.

Therefore, the global maximum of G does not occur at P. □

Claim 6. *The global maximum of W_1 does not occur on BC.*

Proof. BC is a part of a line $k = 1$ if $m \in (0,1)$. Substituting it into W_1, we obtain $W_1(1,m) = \frac{m+2}{m^d+2}$. We denote it by $W_{BC}(m)$, $m \in (0,1)$. We show that, for each $m_0 \in (0,1)$, there exists k_0, such that point $(k_0, m_0) \in C_1$ and $W_{BC}(m_0) < W_1(k_0, m_0)$ holds.

If $m \in \left[\frac{\sqrt{2}}{2}, 1\right)$ and $d \geq 2$, then $\frac{m-m^d}{(2m^d+1)(m^d+2)} > 0$ holds. It implies $\frac{2m+1}{2m^d+1} > \frac{m+2}{m^d+2}$. Thus, $W_1(m,m) > W_{BC}(m)$ on $m \in \left[\frac{\sqrt{2}}{2}, 1\right)$. Therefore, the global maximum of W_1 does not occur on BC if $m \in \left[\frac{\sqrt{2}}{2}, 1\right)$ and $d \geq 2$.

If $m \in \left(0, \frac{\sqrt{2}}{2}\right)$, then the line $k = 1 - \frac{m}{3}$ is a part of C_1 (see the dash-dotted line in Figure 2). Assume, for the sake of contradiction, that $W_1(1 - \frac{m}{3}, m) \leq W_{BC}(m)$ holds at some $m \in \left(0, \frac{\sqrt{2}}{2}\right)$. From $\frac{2m/3+2}{m^d+(1-m/3)^d+1} \leq \frac{m+2}{m^d+2}$, we obtain $(\frac{2m}{3}+2)\left(m^d+2\right) \leq (m+2)\left(m^d+(1-\frac{m}{3})^d+1\right) < (m+2)\left(m^d+(1-\frac{m}{3})^{\mathbf{1}}+1\right)$ and, finally, $m^2 < m^{d+1}$. This is a contradiction. Therefore, if $m \in \left(0, \frac{\sqrt{2}}{2}\right)$ and $d \geq 2$, then the global maximum of W_1 does not occur on BC.

So, the global maximum of W_1 does not occur on BC. □

The previous claims imply that the global maximum of G must occur on interior of PC or PB.

1. If $m \in \left(\frac{\sqrt{2}}{2}, 1\right)$, then $m = k$. $G(k,k) = \frac{2k+1}{2k^d+1}$. We denote it by $W_{PC}(k)$, $k \in \left(\frac{\sqrt{2}}{2}, 1\right)$.
2. If $m \in \left(0, \frac{\sqrt{2}}{2}\right)$, then $m = \frac{1}{k} - k$. $G(k, \frac{1}{k} - k) = \frac{\frac{1}{k}+1}{k^d+\left(\frac{1}{k}-k\right)^d+1}$. We denote it by $W_{PB}(k)$, $k \in \left(\frac{\sqrt{2}}{2}, 1\right)$.

Claim 7. *If $d \leq 10$, then the global maximum of G must occur on the interior of PB. If $d \geq 11$, then W_{PC} has exactly one critical point on PC.*

Proof. $W'_{PC} = \frac{2\left(2k^d+1\right)-2d(2k+1)k^{d-1}}{\left(2k^d+1\right)^2}$ is never undefined. $W'_{PC} = 0$ gives:

$$2(d-1)k^d + dk^{d-1} = 1 \tag{4}$$

Let $h(k)$ denote the left-hand side of Equation (4). The function $h(k)$ is increasing and continuous if $k > 0$, therefore Equation (4) holds on $\left(\frac{\sqrt{2}}{2}, 1\right)$ if and only if $h(\sqrt{2}/2) \leq 1$ and $h(1) \geq 1$. From the first inequality, we obtain $\left(\sqrt{2}+2\right)d \leq 2^{d/2} + 2$, which only holds for $d \geq 11$, where $h(1) \geq 1$ holds for $d \geq 2$. So, if $2 \leq d \leq 10$, then W_{PC} has no local extremum inside of PC. Therefore, if $2 \leq d \leq 10$, then the global maximum of W_{PC} must occur at P or at C, but G does not attain the global maximum at P or C. Therefore, if $2 \leq d \leq 10$, then the global maximum of G must occur on the interior of PB.

The function $h(k)$ is increasing and continuous if $k > 0$; therefore, if $d \geq 11$, then Equation (4) has exactly one solution on $\left(\frac{\sqrt{2}}{2}, 1\right)$. Therefore, if $d \geq 11$, then W_{PC} has exactly one critical point on PC. □

Claim 8. *If $d \geq 11$, then the global maximum of G must occur on the interior of PC.*

Proof. Assume, for the sake of contradiction, that if $d \geq 11$, then $W_{PB} \geq G(P)$ at some $k \in [0.74, 1)$. Using the endpoints of the interval in W_{PB} we obtain an upper bound of W_{PB} on the interval. The inequality $\frac{\frac{1}{0.74}+1}{0.74^d+\left(\frac{1}{1}-1\right)^d+1} \geq \frac{\sqrt{2}+1}{2^{1-\frac{d}{2}}+1}$ gives $\frac{37}{87}\left(\left(\frac{37}{50}\right)^d+1\right) \leq$

$\left(\sqrt{2}-1\right)\left(2^{1-\frac{d}{2}}+1\right)$. After setting $d=11$ and $d=12$ into the inequality, we see that they do not satisfy it. The left-hand side is always greater than $\frac{37}{87}$, and the right-hand side is decreasing. If $d \geq 13$, then the right-hand side is even smaller than $\frac{37}{87}$.

We obtain a contradiction. Therefore, if $d \geq 11$, then the global maximum of W_{PB} does not occur on $[0.74, 1)$.

$W'_{PB} = \frac{-\frac{1}{k^2}(k^d+\left(\frac{1}{k}-k\right)^d+1)-\left(\frac{1}{k}+1\right)\left(dk^{d-1}+d\left(-\frac{1}{k^2}-1\right)\left(\frac{1}{k}-k\right)^{d-1}\right)}{\left(k^d+\left(\frac{1}{k}-k\right)^d+1\right)^2}$ is continuous on $\left(\frac{\sqrt{2}}{2}, 1\right)$.

Assume, for the sake of contradiction, that if $d \geq 11$, then $W'_{PB} = 0$ at some $k \in \left(\frac{\sqrt{2}}{2}, 0.74\right]$, we obtain:

$$\left(dk^2+d+k-1\right)\left(\frac{1}{k}-k\right)^d = (1-k)\left(dk^{d+1}+dk^d+k^d+1\right) \tag{5}$$

Using the endpoints of the interval in Equation (5), we obtain an upper bound of the left-hand side and a lower bound of the right-hand side.

$(0.74^2 d+d+0.74-1)\left(\frac{1}{\frac{\sqrt{2}}{2}}-\frac{\sqrt{2}}{2}\right)^d \geq (1-0.74)\left(d\left(\frac{\sqrt{2}}{2}\right)^{d+1}+d\left(\frac{\sqrt{2}}{2}\right)^d+\left(\frac{\sqrt{2}}{2}\right)^d+1\right)$

gives $\left(3219-325\sqrt{2}\right)d-650\left(2^{d/2}+2\right) \geq 0$. If $d \doteq 10.95$, then the left-hand side is 0, if $d \geq 7.23$, then the left-hand side is decreasing. Therefore, if $d \geq 11$, then the left-hand side is always negative. This is a contradiction. Hence, if $d \geq 11$, then W_{PB} has no local extremum on $\left(\frac{\sqrt{2}}{2}, 0.74\right)$.

Therefore, if $d \geq 11$, then the global maximum of W_{PB} occurs at P or at B, but G does not attain the global maximum at P or at B. Therefore, if $d \geq 11$, then the global maximum of G must occur on the interior of PC. □

Claim 9. *If* $2 \leq d \leq 10$, *then* W_{PB} *has exactly one critical point inside* PB.

Proof. We remove the fractions from Equation (5) by multiplying it by k^d. The global maximum of G does not occur on BC, so we remove the root $k=1$ by dividing the equation by $(k-1)$, and we obtain:

If d is odd, then we divide the equation additionally by $(k+1)^2$. If $d=2$, then we divide the equation additionally by $(2k+1)$. Removing these roots is not necessary, but we reduce the degree of the polynomial in this way. With the help of Sturm's theorem, we prove that Equation (6) has exactly one solution on $\left(\frac{\sqrt{2}}{2}, 1\right)$. Table 1 shows Sturm chain for $d=5$.

$$(k+1)^d(1-k)^{d-1}\left(dk^2+d+k-1\right)-k^d\left(dk^{d+1}+dk^d+k^d+1\right)=0 \tag{6}$$

Table 1. Sturm chain for $d=5$.

	Sign at $\frac{\sqrt{2}}{2}$	**Sign at 1**
$p_0 = 15k^7-10k^6-5k^5-4k^3+8k^2+3k-4$	−	+
$p_1 = 105k^6-60k^5-25k^4-12k^2+16k+3$	+	+
$p_2 \doteq$ [1] $2.24k^5+0.340k^4+2.29k^3-5.55k^2-2.79k+3.96$	+	+
$p_3 \doteq 120.41k^4-336.93k^3+69.25k^2+263.49k-136.88$	−	−
$p_4 \doteq -19.5k^3+14.3k^2+14.7k-11.5$	−	−
$p_5 \doteq 21.9k^2-4.89k-9.57$	−	+
$p_6 \doteq -8.40k+7.15$	+	−
$p_7 \doteq -2.12$	−	−
The number of sign changes	4	3

[1] The table shows real numbers, but fractions are used in the calculation.

Evaluating $p_i\left(\frac{\sqrt{2}}{2}\right)$, we obtain the pattern: $-|+,+|-,-,-|+|-$, i.e., four sign changes. There are three sign changes at $p_i(1)$. The difference of these values is the number of real roots on $(\frac{\sqrt{2}}{2}, 1]$. For $2 \leq d \leq 10$, we only show the sign patterns and the number of sign changes in Table 2.

Table 2. Summary of Sturm chain for $2 \leq d \leq 10$.

d	Signs	Sign Changes
2	$-+++-$ $++++-$	2 1
3	$-++-$ $+++-$	2 1
4	$-++++--+--$ $+++--+++--$	4 3
5	$-++---+-$ $+++--+--$	4 3
6	$-+++-+++---+--$ $+++--+++-+++--$	6 5
7	$-++++-+---+-$ $+++--+---+--$	6 5
8	$-+++-+++---+---+--$ $+++-+++++-+++-++---$	8 7
9	$-+++--+---+---+-$ $+++-+++--+---+--$	8 7
10	$-+++-+++---+---+---+--$ $+++-+++--+++-+++-++---$	10 9

So, if $2 \leq d \leq 10$, then there is only one solution of Equation (6) on the $\left(\frac{\sqrt{2}}{2}, 1\right)$. Therefore, if $2 \leq d \leq 10$, then W_{PB} has exactly one critical point inside PB. $\square$

Claim 7 guarantees the existence of the global maximum of G on the interior of PB if $2 \leq d \leq 10$. Claim 9 proves the existence of a single critical point of W_{PB} if $2 \leq d \leq 10$. Therefore, if $2 \leq d \leq 10$, then the global maximum of G must occur at the only solution r of Equation (6) on $\left(\frac{\sqrt{2}}{2}, 1\right)$. The global maximum is $W_{PB}(r) = \frac{\frac{1}{r}+1}{r^d+\left(\frac{1}{r}-r\right)^d+1}$ and d-cubes have edges $x = \left(r^d + (\frac{1}{r} - r)^d + 1\right)^{-1/d}$, $y = rx$, $z = (\frac{1}{r} - r)x$.

Claim 8 guarantees the existence of the global maximum of G on the interior of PC if $d \geq 11$. Claim 7 proves the existence of a single critical point of W_{PC} if $d \geq 11$. Therefore, if $d \geq 11$, then the global maximum of G must occur at the only solution r of Equation (4) on $\left(\frac{\sqrt{2}}{2}, 1\right)$. The global maximum is $W_{PC}(r) = \frac{2r+1}{2r^d+1} = \frac{r^{1-d}}{d}$ (from Equation (4)) and d-cubes have edges $x = \left(2r^d + 1\right)^{-1/d}$, $y = z = rx$. $\square$

3. Discussion

There are three d-cubes, that is, three variables. In the previous proofs [20–23], the apparent substitution $z^d = 1 - x^d - y^d$ is used to achieve only two variables. As a result of it, the domain boundaries $x^d + y^d = 1$ and $x^d + 2y^d = 1$ change as the dimension changes. For example, in [23], the shape of the curve $C : x^d y^d + y^{2d} - y^d + (x^2 - y^2)^d = 0$ is analyzed depending on the dimension, concluding: "... the shape of the curve C is similar ...". The word "similar" (but not the same) is essential. The curve C is also dimension dependent. (The curve C in previous proofs has the same role as our curve PB.)

It is difficult, if not impossible, to perform calculations in all dimensions at once when the curve C and the boundaries change with the change in dimension.

Our substitutions $y = kx$, $z = mx$ and $x^d = (k^d + m^d + 1)^{-1}$ lead to the boundaries $m = k$, $k = 1$, $m = 1 - k$, which are simpler than the boundaries in the previous proofs, and do not depend on the dimension (see Figure 2). The curve PB: $1 = k(k + m)$ is also the same for all dimensions, and it is much simpler than the curve C.

Such huge simplifications are not free. For dimensions from 2 to 10, the volume function $x^d + \frac{x^d+1}{y}$ changed to $\frac{(k+1)(k+m)}{k^d+m^d+1}$, but the stable domain more than compensates for this trade-off. The "dimensionless" and simplicity of both the boundaries and the PB curve allowed us to achieve the following:

- The preceding proofs cover only one dimension at a time and only for some dimensions less than 10. We present the results for all dimensions $(d \geq 2)$ in about the same number of pages.
- The previous proofs are based mainly on numerical calculations. There are significantly fewer numerical calculations in our proofs.
- The method of the previous proofs would have a precision problem in higher dimensions. Our proofs are not affected by this problem.
- The presented results are shorter. The final result of the preceding proofs is a system of two equations with two variables. Our result is the single one-variable equation, and it has the same or lesser degree. For example, the final system of equations for the fifth dimension from [23]:
  $7x^6y^5 + 12xy^{10} - 6xy^5 + 5x^5y^6 + 10y^{11} - 5y^6 + (x^2 - y^2)^4(2x^3 - 10y^3 - 12xy^2) = 0,$
  $x^5y^5 + y^{10} - y^5 + (x^2 - y^2)^5 = 0.$
  Our final equation: $15k^7 - 10k^6 - 5k^5 - 4k^3 + 8k^2 + 3k - 4 = 0$.
  Our final equation is even simpler for dimensions greater than 10. For example, if $d = 17$, then $32k^{17} + 17k^{16} = 1$.
  Although the equations are different, we can confirm that the volumes and the lengths of the edges published in [20–23] are the same as ours.
- Compared to the previous results, we guarantee that the final equation has exactly one solution in the interval.
- In [23], it was conjectured that there is only a single maximal packing for each dimension greater than 10, and in these packings, the two smallest d-cubes are the same. We proved this conjecture. The global maximum of G occurs on PB (it means two different maximum packings W_1 and W_2, even though they use the same d-cubes) only if $2 \leq d \leq 10$. If $d \geq 11$, then the global maximum of G occurs only on PC, where $k = m$.
- We present uniform results.

4. Conclusions

These results raise further questions. For example, if we are packing more than three cubes, are there multiple maximal packings and are there some identical cubes in maximal packing for some dimensions? There remains the unanswered question of $V(d)$. We know $V_4(2) = V_5(2) = \ldots = V_{11}(2)$ and $V_5(3) = V_4(3)$. Is it true that for each dimension, the maximal packing volume does not change after a certain number of cubes?

Our method of proof works great for three cubes. It helped that there is only one critical point on the boundary curves for the dimensions that suited us. This is not guaranteed for four or more cubes. It is possible that this method of proof would work for more cubes without some major improvements, but with each additional cube, it gets more complicated.

The concept of maximal packing holds importance in various fields:

- Geometry and packing problems: Maximal packing refers to arranging objects (such as spheres or cubes) within a given space in a way that maximizes their density or minimizes the empty space. In geometry, it is a fundamental question to determine how efficiently we can fill a region with identical objects. The study of maximal packing helps us understand the optimal arrangement of shapes in different dimensions.

- Materials science and crystal structures: In materials science, maximal packing is crucial for understanding the arrangement of atoms or molecules in crystalline structures. Crystals exhibit specific packing arrangements (e.g., face-centered cubic, hexagonal close-packed) that maximize the density of particles while maintaining stability. The efficiency of packing affects material properties such as hardness, conductivity, and optical behavior.
- Optimization and efficiency: Maximal packing problems often arise in optimization scenarios. Solving these problems has practical applications in logistics, manufacturing, and resource utilization.
- Computational complexity: Determining the optimal packing arrangement can be computationally challenging. Researchers use heuristics, algorithms, and mathematical techniques to approximate solutions. The study of maximal packing contributes to our understanding of computational complexity and algorithmic efficiency.
- In historical context: ancient civilizations (such as the Egyptians and Babylonians) were interested in efficient packing for practical reasons (e.g., storing grain, arranging bricks) and Kepler's conjecture about the densest sphere packing in three dimensions dates back to the 17th century.

In summary, maximal packing plays a vital role in understanding spatial arrangements, optimizing resource usage, and solving complex problems across various disciplines.

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