Convex hulls of finite packs of spheres

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Abstract

This article is the result of 3 months of research for a project undertaken at the University of Luxembourg. It discusses the problem of sphere packing in Euclidean space: which arrangement of non-overlapping n-dimensional balls has smaller volume than the linear packing? All the following results have been calculated in Matlab.

The Sphere Packing Problem

Imagine someone going to the local grocery shop and seeing oranges packed in a net. One could think about all the unnecessary space in the packaging that could be eliminated. What would be the optimal arrangement of the oranges? Would it be lining them up against each other or amassing them in any other form resembling a cluster?

The goal of this project is to find the most profitable arrangements of finite numbers of equally sized balls whose convex hull has less volume than the linear positioning. The convex hull of an arrangement of equally sized balls is the smallest convex set which contains all balls.

Before we proceed with the investigation of the sphere packing in $\mathbb{R}^n$, there is a bit of information one should know to ensure complete comprehension.

Definition 1. *(Finite Sphere Packing) Let B^n be the unit ball in $\mathbb{R}^n$ and $C_N = \{c_1, ..., c_N\}$ be a set consisting of N linear independent vectors in $\mathbb{R}^n$. For each vector $c_i \in C_N$ $(1 \leq i \leq N)$, let $B_i = B^n + c_i$ be the translated copy of B^n. If B_i and B_j $(1 \leq i < j \leq N)$ are disjoint, then the set*

$$P(B^n, C_N) = \{B_i \mid 1 \leq i \leq N\}$$

is a finite sphere packing.

Definition 2. *(Packing Density) Let $P(B^n, C_N)$ be a finite sphere packing, $B^n + C_N$ be the Minkowski sum of $B^n + C_N$ and $conv(S)$ denote the convex hull of a subset $S \subset \mathbb{R}^n$. Then*

$$d(B^n, C_N) = \frac{N \cdot Vol(B^n)}{Vol(conv(B^n + C_N))}$$

is the packing density of the given sphere packing, i.e. the proportion of space occupied by the spheres in their convex hull.

Proposition 1. *Let $B^n(r) = \{(x_1, ..., x_n) \in \mathbb{R}^n \mid \sum_{i=1}^n x_i^2 \leq r^2\}$ be a n-dimensional ball with radius r. Then its volume is given by*

$$Vol(B^n(r)) = \frac{\pi^{\frac{n}{2}} r^n}{\Gamma(\frac{n}{2}+1)}$$

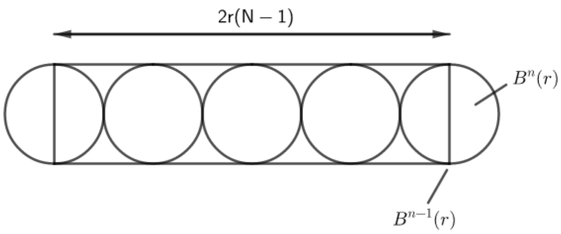
where $\Gamma : \mathbb{R} \to \mathbb{R}$, $z \mapsto \int_0^\infty t^{z-1} e^{-t} dt$ is the Gamma function ([6],p.74-75).

Proof. The proof can be done by induction on n. To find the volume of a disc (i.e. $n = 2$), one takes the function $\sqrt{r^2 - x^2}$ which defines the upper half of the disc on the domain $[-r, r]$. Then: $Vol(B^2(r)) = 4 \int_0^r \sqrt{r^2 - x^2} dx = \pi r^2$. The induction step $n \mapsto n+1$ can be looked up in the literature. $\square$

Proposition 2. *Let $P(B^n(r), C_N)$ be a finite sphere packing with $dim(conv(C_N)) = 1$, so assuming each sphere touches the ones next to it, i.e. $Vol(conv(C_N)) = 2(N-1)r$. In the latter case, we denote C_N by S_N. Moreover, its volume is given by*

$$Vol(P(B^n(r), S_N)) = Vol(B^n(r)) + 2r \cdot (N-1) \cdot Vol(B^{n-1}(r))$$

Proof. The following illustration [1] explains the origin of the formula, which has been established in the literature. $\square$



In $\mathbb{R}^n$ $(2 \leq n \leq 4)$, one has the following:

$$\exists N \in \mathbb{N} \text{ such that } d(B^n(r), S_N) < d(B^n(r), C_N)$$

Such a configuration is called "sausage disaster".

Conjecture 1 (Fejes Tóth). *For $n \geq 5$, the linear packing has maximal density. Hence, there is no other arrangement of hyperspheres whose convex hull has smaller volume ([3],p.126).*

The statement is known as "sausage conjecture", and was proven in dimensions $n \geq 14$ by Betke, Henk and Wills [7]. Hence, the case for $5 \leq n \leq 13$ still remains open. Now we can move on to the investigation of some particular sphere packings.

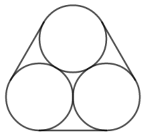
Investigating Sphere Packings

Sphere Packing in $\mathbb{R}^2$

In the 2-dimensional Euclidean space, for every $N \geq 3$, one can find a cluster configuration that satisfies

$$d(B^2, S_3) < d(B^2, C_3)$$

Indeed for $N = 1$ or $N = 2$, one can not distinguish between linear and cluster configuration. For $N = 3$ consider the following configuration [1]:



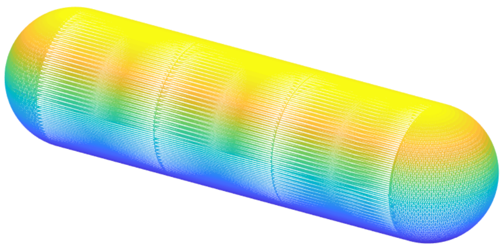
Its volume, computed with Matlab [4], is given by: $Vol(P(B^2(1), C_3)) \approx 10.8708$. Now we want to compare this value with the volume of the linear pack with 3 circles. Using the formula from Proposition 2 with $n = 2$, $r = 1$ and $N = 3$, we get:

$$\begin{aligned} Vol(P(B^2(1), S_3) &= Vol(B^2(1)) + 2 \cdot 1 \cdot (3-1) \cdot Vol(B^1(1)) \\ &= \pi + 2 \cdot 2 \cdot 2 \\ &= 8 + \pi \\ &\approx 11.1316. \end{aligned}$$

Finally, we get: $Vol(P(B^2(1), S_3) > Vol(P(B^2(1), C_3))$.

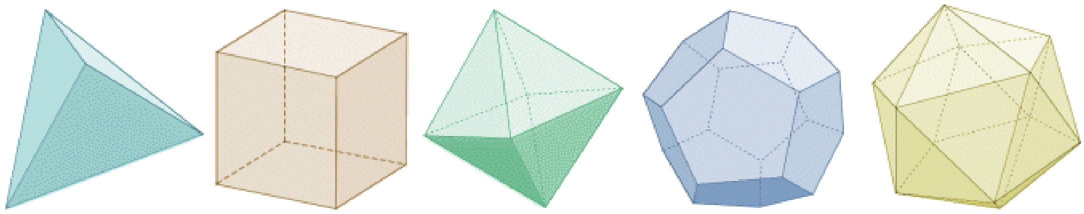
Sphere Packing in $\mathbb{R}^3$

In this section, we aim at finding a packing of equal sized spheres that has smaller volume than the linear packing.

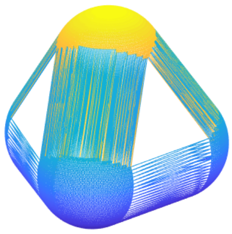


Linear Packing with four 3-spheres in $\mathbb{R}^3$

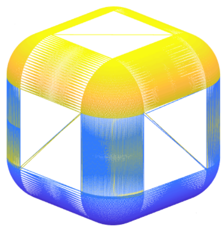
Looking for regular packings in $\mathbb{R}^3$, one first thinks about the platonic solids. To recall: A platonic solid in three-dimensional space is a regular convex polyhedron. It is constructed by using a regular polygon and having the same number of these polygons meeting at each corner. There are exactly five such solids, see for instance [8].



Hence, one can construct a regular sphere packing by placing a sphere at each vertex of a platonic solid. Indeed, we get the following regular packings (drawings made by the author with Matlab):

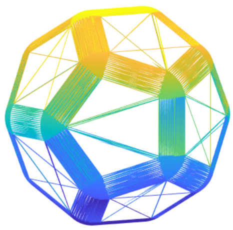


Tetrahedral Packing with four spheres

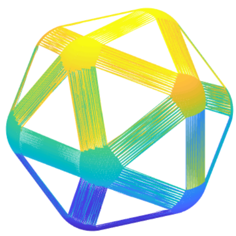


Hexahedral Packing with eight spheres

Octahedral Packing with six spheres



Dodecahedral Packing with twenty-one spheres (twenty vertices and one sphere at the center)



Icosahedral Packing with thirteen spheres (twelve vertices and one sphere at the center)

The following table gives the different volumes of the above depicted packings, computed with Matlab.

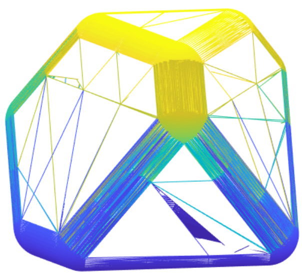
Platonic solids	Volume of our packing	Volume of linear packing
Tetrahedron	23.5096	23.0383
Hexahedron	55.0192	48.1711
Octahedron	63.4380	35.6047
Dodecahedron	181.2516	129.8525
Icosahedron	73.7822	68.4639

One notes that none of these packings has less volume than the linear packing. Indeed, we have the following Proposition:

Proposition. *(Sausage Conjecture in* $\mathbb{R}^3$*, Gandini and Wills* 1992*) A sausage disaster in* 3*-dimensional Euclidean space occurs with* 56 *spheres ([3],p.121).*

To show that this claim is true, we will construct a packing with 56 equally sized spheres whose convex hull has less volume than the linear packing with 56 spheres. The idea of such a construction is to start with a packing consisting of more than 56 spheres and then to remove some spheres until we reach the desired amount.

First one has to note that it is possible to extend the packings above by increasing the length of the edges and then to add enough spheres to get a bigger packing with the same structure. Hence, we can start by constructing a tetrahedral packing with 84 spheres. Let C_{84}^{tetr} be this packing. Then, one cuts off 2 C_4^{tetr} packings from two vertices of the tetrahedron and two C_{10}^{tetr} packings from the other two vertices. The resulting packing consists of 56 spheres and has been drawn as follows by the author with Matlab:



Its volume, computed in Matlab, is given by: $Vol(P(B^3(\frac{1}{2}), C_{56}^{\text{tetr}})) = 39.1940$. The volume of the linear packing with 56 spheres is given by:
$Vol(P(B^3(\frac{1}{2}), S_{56})) = \frac{4}{3}\pi \cdot (\frac{1}{2})^3 + 55\pi \cdot (\frac{1}{2})^2 \approx 43.7204$. Therefore, we have found a sausage disaster in $\mathbb{R}^3$.

Sphere Packing in $\mathbb{R}^4$

Henceforth, any visualisation of a packing is not feasible with the employed tools. Also, up to dimension 3, one can generate spheres with built-in Matlab commands, and let Matlab compute the convex hulls on them. This option breaks down in $\mathbb{R}^n$ for $n \geq 4$, because the convex hull is only implemented for polyhedra with finitely many vertices. Therefore, we have to construct an approximation of an $(n-1)$-sphere with as much precision as possible.

Approximation of Hyperspheres [2]

To recall: An $(n-1)$-sphere with radius r is defined as $S^{n-1}(r) = \{(x_1, ..., x_n) \in \mathbb{R}^n \mid \sum_{i=1}^n x_i^2 = r^2\}$. To get a good approximation of the n-dimensional ball, one has to uniformly distribute points on the surface of an $(n-1)$-sphere and then take the convex hull of these points. For our computations, we first generate n Gaussian random variables $x_1, ..., x_n$. Then the distribution of the vectors

$$\frac{1}{\sqrt{\sum_{i=1}^n x_i^2}} \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}$$

is uniform over the surface S^{n-1}. The amount of generated random variables gives the desired approximation. To get an approximation of a $(n-1)$-sphere with radius r, it suffices to multiply the vectors with r. The following tabular shows the effectiveness of this approximation for the volume of a 4-dimensional ball with radius 1.
Distribution of k^4 points over S^3:

k	3	5	7	10	15	17	20
Volume	2.8175	4.3281	4.6747	4.8327	4.9000	4.9099	4.9187

We recognize a strictly increasing sequence which looks like it's converging to some number.
Proposition 1 gives us a formula to compute the volume of a n-dimensional ball with radius r. Hence for $n = 4$ and $r = 1$, we have:

$$Vol(B^4(1)) = \frac{\pi^{\frac{4}{2}} 1^4}{\Gamma(\frac{4}{2}+1)} = \frac{1}{2}\pi^2 \approx 4.9348$$

Therefore in the probabilistic sense, our sequence converges to the volume of a 4-dimensional ball. Now using this approximation technique, we can construct a sphere packing by defining the center of each sphere and then generating a certain amount of points around it.

Sphere Packing

As in the previous section, one could first try to place the centers of the spheres at the vertices of a regular convex 4-dimensional polytope. This first attempt already fails because of the following claim:

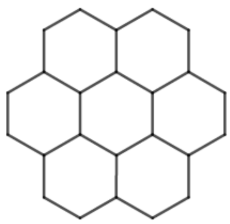
Claim 1 (Gandini and Zucco [5]). *The sausage disaster in $\mathbb{R}^4$ only occurs with around 370000 balls.*

Unlike in three dimensions, the point at which a cluster configuration becomes more dense than a linear configuration has not been exactly determined yet. The next part will give an example of an arrangement of 4-balls which has less volume than the linear pack.

Sausage Disaster

As just mentioned, this part gives an explicit example of an arrangement of 3-spheres which has more density than the linear packing. To understand the arrangement, we first need some definitions. A great deal of the information provided by those definitions is irrelevant for our purposes. It suffices to have a general idea of what follows, but the reader is invited to conduct further studies if needed.

Tessellation
In $\mathbb{R}^n$, a tessellation is a space filling with regular polyhedra, so that there are no gaps. An easy example is given in $\mathbb{R}^2$ [1]:



Tessellation of 2-dimensional space with regular hexagons

One can also fill the 2-dimensional space with squares. Analogously, one can tessellate the 3-dimensional space with cubes and the 4-dimensional space with tesseracts (4-dimensional cubes) and so on. Indeed if we tessellate the space with regular convex polytopes, then every barycenter of a polytope has the same distance to each of its neighbours. Given a tessellation of the n-dimensional space, one can place the centers of the spheres on the barycenters and therefore create a sphere packing. Consequently, the idea is to find the most efficient way to tessellate Euclidean 4-space and then create a sphere packing with maximal density.

24-Cell-Tessellation
The 24-cell is a regular convex 4-polytope. It has 24 vertices and 96 edges. It is self-dual and is the unique regular convex 4-polytope which has no analogue in the 3-dimensional space. It can be constructed by taking the convex hull of its vertices which can be described as the permutations of $(\pm1, \pm1, 0, 0) \in \mathbb{R}^4$.

A regular tessellation of the 4-dimensional space exists with 24-cells. This packing is a good candidate for our sausage disaster because it has the greatest kissing number in $\mathbb{R}^4$, i.e. the highest number of equally sized non-overlapping spheres that can touch another sphere of the same size, and its packing density is $\frac{\pi^2}{16}$, which is the densest arrangement of equally sized spheres.

The regularity of this tessellation gives us an easy way to write our source code. We first start with a 24-cell centered at the origin. As mentioned before, the coordinates are given by the permutations of $(\pm1, \pm1, 0, 0) \in \mathbb{R}^4$. Now we want to build some shells consisting of 24-cells around our first 24-cell. In fact, one can find the center of the nearest 24-cell and then iterate the process to extend the tessellation as much as desired. On the other hand, we recognize that every point has the same distance between each other. Moreover, the sum of the components of each occurring center and vertex is a multiple of 2. Hence, one can identify the centers of each 24-cell with the Hurwitz quaternions with even square norm and their vertices with the Hurwitz quaternions with odd square norm, where the Hurwitz quaternion is defined as a quaternion whose components are either all integers or half integers.

Admitting these criteria, it suffices to find all points in the 4-dimensional space which are of the form $\left\{(x_1, x_2, x_3, x_4) \in \mathbb{R}^4 \mid \sum_{i=1}^{4} x_i \equiv 0 \bmod 2\right\}$. These points are exactly the centers of the 24-cells. Matlab allows us to generate matrices under some conditions. It is then not so difficult to create a matrix consisting of points which meet the criterion above. After finding those points, one can easily create a loop which attributes to each center the 24 vertices, as we already know the coordinates of the vertices for the center $(0, 0, 0, 0)$.

The 24-cell-tessellation is then defined to consist of the Voronoi cells of the set of all created points.

Placing 4-spheres with radius $r = \frac{\sqrt{2}}{2}$ at each point created gives us the desired arrangement. Of course, one has to pay attention that a big amount of spheres decreases the precision of calculation. Nonetheless, this arrangement allows us to claim the following:

Claim 2. *The finite* 4*-balls packing defined above provides an arrangement of* 375769 3*-spheres whose convex hull has less volume than the linear packing with the same amount of* 3*-spheres.*

Indeed, this number fits with Claim 1 of Gandini and Zucco.
One can imagine a giant ball filled with 24-cells. The number 375769 was found by building shell by shell and comparing each time the volume of the arrangement with the linear pack. It took 12 shells in total to build this giant ball, but the result is an arrangement which is stable and more efficient than the linear pack. The following table compares the approximate volume of the linear pack with the volume of our constructed packing.

Number of Spheres	Constructed Packing	Linear Packing	Points on each Sphere
25	62	51	10000
625	1479	1298	10000
7225	16070	14832	9000
21025	45771	43784	8500
70225	149845	145217	8500
177241	373569	370513	6000
297025	622126	620123	4000
375769	785010	786668	3300

The volume of the linear pack was also calculated in Matlab. Indeed, the volume calculated with the formula of Proposition 2 gives $Vol(P(B^4(\frac{\sqrt{2}}{2})), S_{375769}) = 787007.8925$.

Improvement of our Packing

Even though the constructed packing has less volume than the linear packing, one can always try to find an arrangement with less spheres. Hence like in the 3-dimensional case, we will try to remove some spheres in the hope that the resulting packing stays more efficient than the linear packing. We will cut off some spheres by picking a constant c and then removing all points whose x_4-coordinate is less than c. The following table of approximate volumes shows the process:

Constant c	Number of Spheres	Resulting Packing	Linear Pack	Points on each Sphere
-16	371875	776873	777910	3000
-15	367302	767330	768281	1700
-14	361992	756043	756878	1300
-13	355895	743081	743766	1000

We can stop at this point. Indeed, we managed to reduce the amount of points and to get a packing which still has less volume than the linear packing. However, in our implementation, which uses only the outermost shell to construct the convex hull, we need to compute more spheres along the cutting hyperplane the more we are cutting off. So with each augmentation of c, we have to pay the price that we lose precision and the resulting packing loses stability under the varying random positions of the points on each sphere. Actually, the table shows that in the author's experiments, the amount of points generated on each sphere had to be decreased. Therefore, at some stage the values calculated on Matlab lose accuracy. Nonetheless, the precision is enough to conclude that it is possible to remove spheres as indicated above.

Conjecture 2. *With the above described cut-off process, we arrive at a sausage disaster with significantly less* 4*-balls than predicted by Gandini and Zucco.*

Sphere Packing in $\mathbb{R}^n$ $(5 \leq n \leq 8)$

This section is only an outline. The main goal of this project was to construct an explicit example of the sausage disaster in $\mathbb{R}^4$. Moreover, it is conjectured by Fejes Tóth that the sausage disaster does not occur for $n \geq 5$.

We will just give an idea whether a better arrangement may exist or not. To do so, we are going to compare the density of the linear packing with the density of the densest known infinite packings ([3],p.72). We get the following table:

n	densest known infinite packing	density of linear packing with 10^8 n-spheres
2	$\frac{\pi}{2\sqrt{3}} \approx 0.91$	≈ 0.79
3	$\frac{\pi}{3\sqrt{2}} \approx 0.74$	≈ 0.67
4	$\frac{\pi^2}{16} \approx 0.62$	≈ 0.59
5	$\frac{\pi^2}{15\sqrt{2}} \approx 0.47$	≈ 0.53
6	$\frac{\pi^3}{48\sqrt{3}} \approx 0.37$	≈ 0.49
7	$\frac{\pi^3}{105} \approx 0.30$	≈ 0.46
8	$\frac{\pi^4}{374} \approx 0.25$	≈ 0.43

The densities of the different linear packings were calculated with the formula from Definition 2. This comparison shows again that there must be a better arrangement than the linear packing for $n \leq 4$. For $n \in [5, 8]$, this comparison does not give a guarantee that there exists a better arrangement. This question remains open.

Conclusion

In this report, we have investigated sphere packings in up to 4 dimensions. In $\mathbb{R}^2$ and $\mathbb{R}^3$, we gave the most profitable arrangement with a minimal amount of spheres as it was already known in the literature. In $\mathbb{R}^4$, we gave an explicit example of an arrangement which has more density than the linear packing. However, our packing does not have the minimal amount of spheres. The lack of precision makes it impossible to find out how many spheres we could remove. Indeed there could be a completely different optimal packing with less spheres. What we can conjecture for sure, is that there are packings which reach the sausage disaster with significantly less points than claimed by Gandini and Zucco. There is still a lot more to be investigated, including the sausage conjecture in $\mathbb{R}^n$ for $n \geq 5$.

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