The largest small Polytopes

Andreas Klein and Markus Wessler

29th March 2022

Abstract

The aim of this paper is the determination of the largest \( n \)-dimensional polytope with \( n + 3 \) vertices of unit diameter. This is a special case of a more general problem Graham proposes in [2].

1 Introduction

We know that among the geometric objects in Euclidean \( n \)-space with given diameter the sphere has maximal volume. A natural question arises if we consider polytopes instead, and in fact this problem has been considered several times. In this paper we deal with the following question: Given natural numbers \( k \) and \( n \), which polytope with \( k \) vertices of unit diameter in Euclidean \( n \)-space has the largest volume? To this end we define the following volume function:

**Definition 1.1** Let \( n \geq 2 \) and \( k \geq n + 1 \) be positive integers. Then we define \( V(n, k) \) to be the maximum volume of a polytope with \( k \) vertices of unit diameter in Euclidean \( n \)-space.

Let us briefly recall the following well-known results. For \( k \) odd, Reinhardt showed [4] that \( V(2, k) \) is achieved by the plain regular \( k \)-gon. In this case we have

\[
V(2, k) = \frac{k}{2} \cdot \cos\left(\frac{\pi}{k}\right) \cdot \tan\left(\frac{\pi}{2k}\right).
\]

It is also known that \( V(2, 4) \) is achieved by the square (though not in a unique way, see [3]).

However, for even \( k > 4 \), it is definitely not the plain regular \( k \)-gon which has maximal area. In fact, Graham showed [4] that for \( k = 6 \) the largest area is not obtained by the regular hexagon. The latter one is approximately equal to 0.6495, whereas \( V(2, 6) = 0.6749 \ldots \).

Considering an \( n \)-simplex, we observe:
Remark 1.2 For every $n \geq 2$, $V(n, n + 1)$ is achieved by the regular $n$-simplex, and we have

$$V(n, n + 1) = \frac{1}{n!} \sqrt{\frac{n + 1}{2^n}}.$$  

We proceed as follows. For $k = n + 2$ the optimal configuration is obtained in a similar way, as we shall see in the next section. In order to determine $V(n, n + 3)$ we first consider the special case $V(3, 6)$ which in fact gives rise to a more general procedure leading to the main result of this paper, Theorem \[.3\]. We end with an outlook over open problems and some concluding remarks.

2 The calculation of $V(n, n + 2)$

Each configuration of $n + 2$ points in $n$-dimensional space is topologically equivalent to a double pyramid, which we obtain in the following way. Let us choose $n$ points in a hyperplane $H$ forming an $(n - 1)$-simplex $S$ and two points $P_1$ and $P_2$ lying on opposite sides of $S$. Then we have

$$V(\text{double pyramid}) = \frac{1}{n} \cdot \text{height} \cdot \text{base},$$

where the height is, of course, bounded by $d(P_1, P_2)$, hence by 1, and the base is bounded by $V(n - 1, n)$. On the other hand, this maximum is really achieved (though not in unique way). Thus we obtain the following

Theorem 2.1 For $n \geq 2$ we have

$$V(n, n + 2) = \frac{1}{n} \cdot V(n - 1, n)$$

(where $V(1, 2) = 1$). Hence, by [1.3],

$$V(n, n + 2) = \frac{1}{n!} \sqrt{\frac{n}{2^{n-1}}}.$$  

3 The calculation of $V(3, 6)$

The construction of the maximal $n$-dimensional polytopes with $n + 3$ vertices is best understood if we look at the special case $n = 3$ first.

Without loss of generality, we may restrict our investigation to polyhedra with triangular faces. By Euler’s polyhedra formula we obtain that each
A polyhedron with 6 vertices must have 8 faces and 12 edges. There are two topologically distinct cases:

1. No vertex has a valence greater than 4. In this case the polyhedron is topologically equivalent to the regular octahedron. (We shall call this the octahedral case.)

2. At least one vertex has valence 5. In this case the polyhedron is topologically equivalent to a pyramid over a pentagon which is partitioned into three triangles. In particular, there are two vertices with valence 5. (We shall call this the pyramidal case.)

Figure 1: The octahedral and the pyramidal case

The next step is to determine the maximal volume in each of these cases. It will turn out that the volume achieved in the octahedral case is much smaller than the volume achieved in the pyramidal case.

3.1 The octahedral case

We fix two opposite vertices $P$ and $Q$. Since each vertex has valence 4, we know that for all the other vertices $P_1, P_2, P_3, P_4$ the line segments $P_iP$ and $P_iQ$ are edges of the polyhedron.

Let $P'_1, P'_2, P'_3, P'_4$ be the projections of $P_1, P_2, P_3, P_4$ to the plane $p$ that is perpendicular to $PQ$ and that intersects $PQ$ in its center. It is obvious that $d(P'_i, P'_j) \leq d(P_i, P_j)$ and $\max(d(P'_i, P), d(P'_i, Q)) \leq \max(d(P_i, P), d(P_i, Q))$. Thus the polyhedron with vertices $Q, P, P'_1, P'_2, P'_3$ and $P'_4$ has diameter less than 1.

Since the volume of $PQP'_1P'_k$ equals the volume of $PQP'_1P'_k$ (the height and the area of the base is the same in both pyramids), the volume of $QPP'_1P'_2P'_3P'_4$ equals the volume of $QPP'_1P'_2P'_3P'_4$. Thus we can restrict ourselves to the case that the vertices $P_1, P_2, P_3$ and $P_4$ lie in the plane $p$. 

3
But in this case we know that the volume of the polytope is bounded by \(\frac{1}{3} V(2, 4) = \frac{1}{3}\). (In case of the regular octahedron we can achieve equality.)

### 3.2 The pyramidal case

Now we investigate the pyramidal case. Let \(P\) and \(Q\) be the vertices with valence 5 and \(P_1, P_2, P_3\) and \(P_4\) the other vertices of the polyhedron. Let \(p\) be the plane perpendicular to \(PQ\) intersecting \(PQ\) in its center. As in the octahedral case we conclude that the volume of the polyhedron does not change if we project the points \(P_1, P_2, P_3\) and \(P_4\) into the plane \(p\). Thus we may again assume that the vertices \(P_1, P_2, P_3\) and \(P_4\) lie in \(p\).

Let \(P_5 = PQ \cap p\) and \(h = d(P, Q)\). Since \(d(P, P_i) \leq 1\) \((i = 1, \ldots, 4)\) we obtain \(d(P_5, P_i)^2 + \frac{h^2}{4} \leq 1\), i.e. \(d(P_5, P_i) \leq r = \sqrt{1 - \frac{h^2}{4}}\). Since \(h \in [0, 1]\), we obtain \(r \in [\frac{\sqrt{3}}{2}, 1]\).

The volume of the polytope is \(\frac{1}{3} h S\) where \(S\) is the area of the pentagon \(P_1 P_2 P_3 P_4 P_5\). Thus we must solve the planar problem to maximize the area of \(P_1 P_2 P_3 P_4 P_5\) depending on \(r\).

The pentagon \(P_1 P_2 P_3 P_4 P_5\) satisfies \(d(P_5, P_i) \leq r\) for \(i = 1, \ldots, 4\) and \(d(P_i, P_j) \leq 1\) for \(1 \leq i < j \leq 4\). We define the diameter graph \(D\) of the pentagon by:

- The vertices of \(D\) are the points \(P_1, \ldots, P_5\).
- \(\{P_i, P_5\}\) \((1 \leq i \leq 4)\) is an edge of \(D\) if and only if \(d(P_i, P_5) = r\).
- \(\{P_i, P_j\}\) \((1 \leq i < j \leq 4)\) is an edge of \(D\) if and only if \(d(P_i, P_j) = 1\).

In the following we identify an edge \(\{P_i, P_j\}\) of \(D\) with the line segment \(P_i P_j\).

As in [2] (Fact 2) we conclude that the diameter graph of the pentagon with maximal area is connected.

Suppose \(P_i P_j\) and \(P_k P_l\) have no point in common, then the triangle inequality yields \(d(P_i, P_j) + d(P_k, P_l) < d(P_i, P_k) + d(P_l, P_j)\) (see Figure 3). Thus \(\{P_i, P_j\}\) or \(\{P_k, P_l\}\) is not an edge of \(D\).

Graphs with this property are said (by Conway) to have a linear track-ation. By a result of Woodall [6] the graph \(D\) must be one of the following:

The problem of determining the area of the pentagon is now reduced to an examination of each of the six cases.

An easy calculation reveals that in the cases (a)-(d) the pentagon has an area less than 0.567 for each possible value of \(r\) in \([\frac{\sqrt{3}}{2}, 1]\). (For example, in case (b) the pentagon lies in a sixth part of a circle with radius 1 and...
therefore the polygon has an area less than 0.53.) As we shall see later, the maximal area in case (f) is always larger than 0.58.

Thus the only remaining cases are (e) and (f). We shall prove that in case (e) there is no local maximum and therefore the maximal area of the pentagon is obtained in case (f).

In case (e) we have the situation shown in Figure 4.

We must maximize the area of pentagon $P_1P_2P_3P_4P_5$ depending on $\alpha_1, \alpha_2$ and $\beta$. By elementary geometry it follows immediately that a local maximum can only be achieved for $\alpha_1 = \alpha_2 = \frac{\pi}{2}$. But then it is clear that the maximal area is achieved for the case $\beta = 0$. This means that there is no local maximum in case (e).

Thus we are left with the last case (f). This is shown in Figure 3a.

A simple but tedious calculation shows that in order to maximize the area of the pentagon, it is necessary that $\angle P_4P_2P_3 = \angle P_2P_3P_1$. Thus we are left
with the symmetric case shown in Figure 5 b. We obtain $y = \sqrt{1 - \left(\frac{1}{2} + x\right)^2}$ and $z = \sqrt{r^2 - x^2}$. The area of the pentagon is

$$A(r, x) = \frac{1}{2}x\sqrt{3 - 4x - 4x^2} + \frac{1}{2}\sqrt{r^2 - x^2}.$$ 

This expression has a unique local maximum for $x \in [0, \frac{1}{2}]$ which can be found by setting the first derivative equal to zero. The resulting optimal value $x_0(r)$ is a solution of a sixth order algebraic equation. Since $r \geq \frac{\sqrt{3}}{2}$ we obtain that $A(r, x_0(r)) > A\left(\frac{\sqrt{3}}{2}, x_0\left(\frac{\sqrt{3}}{2}\right)\right) = 0.5862\ldots$. This proves that the maximal area of the pentagon is obtained in case (f) and not in any of the cases (a)-(e).

Finally, the maximal volume of the polyhedron can be found by maximizing the expression $\frac{1}{3}hA\left(\sqrt{1 - \frac{h^2}{4}}, x_0\left(\sqrt{1 - \frac{h^2}{4}}\right)\right)$ for $h \in [0, 1]$. Some more calculations reveal that the maximum is obtained for $h = 1$. In this case the volume is

$$V(3, 6) = 0.1954\ldots$$

and there exists a unique polyhedron that archive this maximum.
4 The calculation of $V(n, n + 3)$

Now we are ready to generalize the arguments of the previous section to higher dimensions.

As in the 3-dimensional case we have two topologically distinct possibilities:

In the octahedral case we have 6 vertices with valence $n + 1$ and $n - 3$ vertices of valence $n + 2$. Let $P$ and $Q$ be two vertices of valence $n + 1$ and $R_1, \ldots, R_{n-3}$ the vertices with valence $n + 2$. Let $p$ be the plane orthogonal to $PQR_1 \ldots R_{n-3}$ intersecting the $(n - 2)$-simplex $PQR_1 \ldots R_{n-3}$ in the center of its surrounding sphere. We can generalize the projection argument of section 3.1 to see that in this case the volume of the polytope is less than $\frac{1}{n} V(2, 4)V(n - 2, n - 1)$.

In the pyramidal case we find $n - 1$ vertices $P_1, \ldots, P_{n-1}$ with valence $n - 2$. Let $p$ be the plane orthogonal to $P_1 \ldots P_{n-1}$ intersecting the $(n - 2)$-simplex $P_1 \ldots P_{n-1}$ in the center of the surrounding sphere. If we project the remaining four points to $p$ we obtain the planar optimization problem of section 3.2. In the $n$-dimensional case, $r \in \left[ \sqrt{1 - \frac{(n-2)}{2(n-1)}}, 1 \right]$. (The distance of the center of $P_1 \ldots P_{n-1}$ to the vertices is at most $\frac{n-2}{n-1} \sqrt{\frac{n-1}{2(n-2)}}$.) Since now $r$ can be smaller than in section 3.2, we must improve the bounds in the cases (a)-(d), but nevertheless, we find that the area of the pentagon is still maximal in case (f). Thus we can proceed in the same way as in the 3-dimensional case and conclude that the maximal volume is achieved if the $(n - 2)$-simplex $P_1 \ldots P_{n-1}$ has maximal volume.

Theorem 4.1 For $n \geq 3$ let $r = \sqrt{1 - \frac{(n-2)}{2(n-1)}}$. Then we have

$$V(n, n + 3) = \frac{A(r, x_0(r))}{n} V(n - 2, n - 1),$$

where $A$ is the function defined in section 3.2 with local maximum at $x_0(r)$.

In particular, for $n \to \infty$ we have $r \to \frac{1}{\sqrt{2}}$ and $A(r, x_0(r)) \to 0.5002\ldots$, hence

$$\lim_{n \to \infty} n \cdot \frac{V(n, n + 3)}{V(n - 2, n - 1)} = 0.5002\ldots$$

(1)

We remark that

$$\lim_{n \to \infty} n \cdot \frac{V(n, n + 2)}{V(n - 1, n)} = 1$$

(2)

(see Theorem 2.1).
5 Concluding Remarks

In principle, the preceding techniques (consideration of the topologically distinct cases, projection, linear trackleation) may be applied to the determination of $V(n, n+k)$ for $k > 3$. However, Bender and Wormald \(^{[1]}\) showed that

$$\frac{1}{972(k-1)(2k-5)(3k-6)} \binom{4k-10}{k+2}$$

is a good approximation for the number of topologically distinct cases in three dimensions. The number of possible linear trackleations of the $(2n)$-gon is

$$\frac{1}{8m} \sum_{\substack{d|m \\text{odd} \atop d|m}} \phi(d)4^{m/d} + 4^{m-2} + 2^{m-1} - 1.$$ 

Thus the number of topologically distinct cases and the number of possible linear trackleations in each case, grows exponentially.

However, one could ask if, corresponding to the limit formulae \(^{[1]}\) and \(^{[2]}\), we can determine

$$\lim_{n \to \infty} n \frac{V(n, n+k)}{V(n-k+1, n-k+2)}$$

for $k > 3$.

We remark that the maximal polytopes with $n+1$, $n+2$ or $n+3$ vertices have an axis of symmetry. The problem whether each maximal polytope has at least one axis of symmetry (see \(^{[2]}\)) is still open.

The calculations in section 3.2 suggest the following generalized problem. Given a symmetric $(k \times k)$-matrix $D$, determine the largest $k$-gon $P_1 \ldots P_k$ with $d(P_i, P_j) \leq D_{i,j}$.

References

[1] E.A. Bender and N.C. Wormald, *The number of rooted convex polyhedra*, J. Can. Math. Bull. 31 (1988), 99-102.

[2] R.L. Graham, *The largest small Hexagon*, J. Comb. Theory 18 (1975), 165-170.

[3] H.Lenz, *Ungelöste Probleme 12*, Elemente der Math. 11 (1956), 99-102.
[4] K. Reinhardt, *Extremale Polygone gegeben Durchmessers*, Jber. dt. Math.-Ver. **31** (1922), 251-270.

[5] J.J. Schäfer, *Nachtrag zu Ungelöste Probleme 12*, Elemente der Math. **13** (1958), 85-86.

[6] D.R. Woodall, *Thrackles and Deadlock*, in Combinatorial Mathematics and Its Applications (D.J.A. Welsh, ed.), Academic Press (1971), 335-347, Proceedings of a Conference held at the Mathematical Institute, Oxford, from 7-10 July, 1969.

Andreas Klein
Universität Kassel
Fachbereich 17 (Mathematik und Informatik)
D-34109 Kassel
klein@mathematik.uni-kassel.de

Markus Wessler
Universität Kassel
Fachbereich 17 (Mathematik und Informatik)
D-34109 Kassel
wessler@mathematik.uni-kassel.de