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SIMPLICES RARELY CONTAIN THEIR CIRCUMCENTER IN HIGH DIMENSIONS

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Abstract. Acute triangles are defined by having all angles less than $\pi/2$, and are characterized as the triangles containing their circumcenter in the interior. For simplices of dimension $n \geqslant 3$, acuteness is defined by demanding that all dihedral angles between $(n-1)$-dimensional faces are smaller than $\pi/2$. However, there are, in a practical sense, too few acute simplices in general. This is unfortunate, since the acuteness property provides good qualitative features for finite element methods. The property of acuteness is logically independent of the property of containing the circumcenter when the dimension is greater than two. In this article, we show that the latter property is also quite rare in higher dimensions. In a natural probability measure on the set of n-dimensional simplices, we show that the probability that a uniformly random n-simplex contains its circumcenter is $1/2^n$.

Keywords: simplex; circumcenter; finite element method

MSC 2010: 65M60, 52A05

1. Introduction

A triangle is classified as obtuse, right or acute if its maximum angle is greater than, equal to or smaller than $\pi/2$, respectively. The circumcircle is the circle containing all three vertices of the triangle. Using the circumcenter, which is the center of the circumcircle, a triangle is obtuse, right or acute if its circumcenter is outside the triangle, on one of its edges, or in its interior, respectively.

For tetrahedra and higher dimensional simplices, acuteness is defined by demanding that all dihedral angles are less than $\pi/2$.

Definition 1.1. A simplex of dimension $n \geqslant 1$ is called *acute* if all its dihedral angles between facets ($(n-1)$-dimensional faces) are smaller than $\pi/2$.

If $n = 1$ this is an empty condition, and if $n = 2$ it is the usual acuteness condition for triangles. In general, the dihedral angle between two facets can be computed

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using their outward normals $\mathbf{n}_1$ and $\mathbf{n_2}$ as $\arccos(-\mathbf{n_1}\cdot\mathbf{n_2}/|\mathbf{n_1}||\mathbf{n_2}|)$, where $\cdot$ in the numerator signifies the Euclidean scalar product. Already in dimension three, the acuteness property is more difficult to work with than its two-dimensional counterpart is, see e.g. VanderZee et al. [15]. In higher dimensions, there are surprising restrictions on what is possible to achieve with acute simplices. One striking result is that a point in $\mathbb{R}^n$, $n \geqslant 5$, cannot be surrounded by acute simplices that are face-to-face (see Křížek [12], Kalai [7] or Kopczyński et al. [8]).

Acute triangles and simplices are useful for the finite element methods. For instance, acute simplicial meshes guarantee the validity of discrete maximum principles, see e.g. Ciarlet [4]. Acute simplicial meshes satisfy the maximum angle condition, which provides convergence of the finite element approximations, see Křížek [11], and also Korotov and Křížek [9] for further information.

Another generalization of acuteness to higher dimensions uses the property of containing the circumcenter. Any set of $n+1$ points in $\mathbb{R}^n$ not contained in an affine hyperplane lies on a unique sphere, the circumsphere. The center of this sphere is called the *circumcenter*. Following e.g. VanderZee et al. [14], we give the following definition:

Definition 1.2. A simplex of dimension $n \geqslant 1$ is called *well-centered* if it contains its circumcenter in the interior.

If $n = 1$ this definition is automatically satisfied, as the circumcenter of an interval is its midpoint. If $n = 2$, being well-centered is equivalent to acuteness.

Being well-centered is a good property for finite element methods, as it allows for a good mesh refinement technique, the so-called *yellow* refinement, particularly if the faces are acute. This procedure is interesting from a geometrical point of view also, as the constructed smaller simplices are *path* simplices. See for instance Korotov and Stańdo [10], and Brandts et al. [2]. Another interesting geometric result is Hošek's result that 3D space can be tiled by identical well-centered tetrahedra [6].

Lemma 1.3. *For simplices of dimension $n \geqslant 3$, the properties of being acute and of being well-centered are logically independent.*

Proof. Note that the regular simplex is both acute and well-centered. We will provide examples of acute, but not-well-centered simplices in Example 1.6 and nonacute, but well-centered simplices in Example 1.7. Example 1.6 also includes an example of a simplex with neither property. $\square$

This is discussed in VanderZee et al. [14], which also includes more refined independency results relating properties of faces with different dimensions.

R e m a r k 1.4. Note that we only claim *logical* independence of the properties of being acute and being well-centered. It seems likely that the properties are not independent in the *probabilistic* sense, as both conditions are satisfied for simplices close to the regular simplex. This is strongly supported by computer experiments in Example 1.8. It would be interesting to pursue this direction, and to determine the precise probabilistic relationship between the two conditions. Also, other geometric versions of centers could be considered as in Hajja and Walker [5].

E x a m p l e 1.5. The difference between the situations in two and three dimensions is illustrated in Figures 1 and 2.

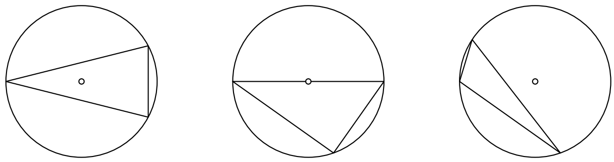
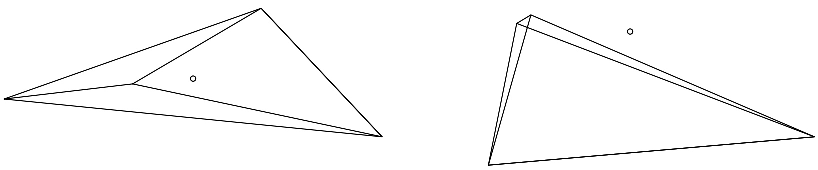


Figure 1. A triangle is acute if and only if the circumcenter is in the interior (it is well-centered). The borderline case is that a right triangle has its circumcenter on an edge.



(A) Well-centered but not acute (B) Acute but not well-centered

Figure 2. Acuteness is logically independent from well-centeredness for tetrahedra, as indicated by this figure (cf. [14]). The circumcenter, marked by a small circle, is in the interior of a nonacute tetrahedron on the left and in the exterior of an acute tetrahedron on the right. For explicit coordinates, see Examples 1.6 and 1.7.

In Figure 1, the two cases with the well-centered acute triangle on the left and the obtuse triangle, not well-centered, on the right are shown. If the largest angle is right, the circumcenter will lie on the edge opposite the right angle, as in the middle. In Figure 2, we show examples of tetrahedra satisfying one but not the other of the conditions in Lemma 1.3. On the left, an obtuse, well-centered tetrahedron is shown. On the right, an acute tetrahedron that is not well-centered is shown. In dimensions higher than three, the situation is similar to the situation in dimension three.

E x a m p l e 1.6 (Acute, not well-centered simplices). We consider $n+1$ points in $\mathbb{R}^n$. The first n points are simply the points in the standard basis $\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_n$. The last point is $P = -\varepsilon \sum\limits_{i=1}^{n} \mathbf{e}_i$. When $\varepsilon = 0$, these points form a *corner* at the origin, a simplex with many right dihedral angles. When $\varepsilon > 0$ this becomes an acute simplex. The circumcenter lies on the line where all coordinates are equal, so it is of the form $S = x \sum_{i=1}^{n} \mathbf{e}_i$. We can compute the exact point by solving the equation $|\mathbf{e}_i S| = |PS|$. This gives

$$S = \frac{1 - n\varepsilon^2}{2 + 2n\varepsilon} \sum_{i=1}^{n} \mathbf{e}_i.$$

As long as

$$\frac{1 - n\varepsilon^2}{2 + 2n\varepsilon} > \frac{1}{n} \quad \text{or} \quad \varepsilon < \frac{\sqrt{n-1} - 1}{n}$$

the simplex is not well-centered. For $\varepsilon = 0.1$ and $n = 3$, this is shown in Figure 2 on the right. Note that for ε negative but close to zero, the simplex will be neither acute nor well-centered.

Example 1.7 (Well-centered, not acute simplices). We consider $n + 1$ points in S^{n-1} in a special position, and then move them slightly. Informally, we take two antipodal points and move them slightly upwards. Then we take $n - 1$ points forming a regular simplex and move this collection slightly downwards. The resulting simplex will be well-centered with dihedral angles arbitrarily close to π. Formally, let $\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_n$ be the standard basis for $\mathbb{R}^n$. Let $P = \mathbf{e}_1 + \varepsilon\mathbf{e}_n$ and $Q = -\mathbf{e}_1 + \varepsilon\mathbf{e}_n$. Let then $\{R_i\}_{i=1}^{n-1}$ be the vertices of a regular simplex on the unit sphere in the span of $\mathbf{e}_2, \ldots, \mathbf{e}_{n-1}$ and let $\overline{R}_i = R_i - \varepsilon\mathbf{e}_n$. The points $P, Q, \overline{R}_1, \ldots, \overline{R}_{n-1}$ lie on a sphere with radius $\sqrt{1 + \varepsilon^2}$ centered at the origin. Since $\sum_{i=1}^{n-1} R_i = 0$, we see that

$$(n-1)(P+Q) + 2\sum_{i=1}^{n-1} \overline{R}_i = (n-1)2\varepsilon\mathbf{e}_n + 2(n-1)\cdot(-\varepsilon\mathbf{e}_n) = 0.$$

So the circumcenter is a positive linear combination of the vertices of the simplex, which thus is well-centered. We will compute the dihedral angle between the facet $\hat{\imath}$ omitting $\overline{R}_i$ and the facet $\hat{\jmath}$ omitting $\overline{R}_j$. Note that the scalar product $p = R_i \cdot R_j < 0$ is independent of the choice of $i \neq j$, since the simplex formed by the R_i is regular. An outward normal to $\hat{\imath}$ is $\mathbf{n}_i = R_i + \frac{p}{2\varepsilon}\mathbf{e}_n$. Indeed, there are three types of edges in $\hat{\imath}$, and we will demonstrate the scalar product with $\mathbf{n}_i$ is zero for each of the three types. First, $\mathbf{n}_i \cdot \overrightarrow{PQ} = \mathbf{n}_i \cdot 2\mathbf{e}_1 = 0$, since $\mathbf{n}_i$ is in the span of $\mathbf{e}_2, \ldots, \mathbf{e}_n$. Second, $\mathbf{n}_i \cdot \overrightarrow{\overline{R}_j\overline{R}_k} = R_i \cdot \overrightarrow{R_j R_k} = p - p = 0$. Finally,

$$\mathbf{n}_i \cdot \overrightarrow{P\overline{R}_j} = \left(R_i + \frac{p}{2\varepsilon}\mathbf{e}_n\right) \cdot (R_j - \mathbf{e}_1 - 2\varepsilon\mathbf{e}_n) = p - p = 0.$$

The case $\overrightarrow{Q\overline{R}_j}$ is similar.

We can then compute the dihedral angle as

$$\arccos\Bigl(-\frac{\mathbf{n}_i\cdot\mathbf{n}_j}{|\mathbf{n}_i|\cdot|\mathbf{n}_j|}\Bigr)=\arccos\Bigl(-\frac{p+p^2/4\varepsilon^2}{1+p^2/4\varepsilon^2}\Bigr)=\arccos\Bigl(-\frac{4p\varepsilon^2+p^2}{4\varepsilon^2+p^2}\Bigr).$$

In the degenerate limit, when $\varepsilon=0$, this is $\arccos(-1)=\pi$. When $\varepsilon>0$, the numerator gets smaller (since $p<0$) and the denominator gets larger. This shows that the angle is arbitrarily close to π as $\varepsilon\to 0$. For $\varepsilon=0.1$ and $n=3$, this is shown in Figure 2 on the left.

In the literature about degenerations of simplices, this shape for tetrahedra is known as a *sliver*, see for instance Brandts et al. [3].

Example 1.8. It is not clear how the notions of acuteness and well-centeredness compare in the probabilistic setting. Here are some results from computer experiments, using MATLAB. The set-up for the experiments was as follows: For $s=3,4,5$ and 6, one million randomly produced s-simplices were tested for being acute and for being well-centered. The results are summarized in a table of the form

acute and well-centered	acute and not well-centered
not acute and well-centered	not acute and not well-centered

$s=3$:

21699	8645
103001	866655

$s=4$:

472	393
61955	937180

$s=5$:

2	10
31038	968950

For $s=6$, there were no acute simplices among the one million randomly produced simplices.

Even if well-centeredness is relatively rare, being acute is a lot rarer. Also, it seems that there is a strong dependence between acuteness and well-centeredness. For instance, among the 12 acute 5-simplices, 2 were well-centered (a much higher proportion than $1/32$). Since the number of acute simplices is so small, we should be careful about drawing too strong conclusions in dimension 5. For $s=4$, more than half of the acute simplices were well-centered, as compared to $1/16$ in the whole set. For $s=3$ there is an even stronger connection. It would be interesting to see how these notions compare in general, including what the probability is for choosing an acute simplex by our methods.

Since the number of acute simplices is so small in these experiments, it is difficult to formulate a sensible conjecture about the probability that a random n-simplex is acute.

In what follows, we will consider the set, or space, of simplicial shapes. On this set (actually on a closely related set, see Definition 2.1) we will choose a probability measure, and we will prove the following

Main result: *The probability that an n-dimensional simplex contains its circumcenter is* $1/2^n$.

The statement will be more precise in Theorem 3.1.

2. Measuring probability on the set of simplices

There is no canonical choice for a probability measure on the set (or space) of simplicial shapes. The choice of representation leads to differences in probability, even in very simple-looking examples. The classical Bertrand paradox [1], about probability on the set of pairs of points on a circle (or equivalently, a chord), exemplifies this. Searching the web for Bertrand's paradox will provide many interesting illustrations and variants. We choose a probability measure that is well suited to the problem at hand, namely to consider the center of the circumsphere. A given nondegenerate simplex has a circumsphere. We can scale the simplex, and thus the sphere, so that it has radius equal to one. We can then translate the simplex so that the circumcenter lies at the origin of $\mathbb{R}^n$. In other words, we normalize our situation so that the simplices considered have vertices on the standard unit sphere $S^{n-1} = \{P \in \mathbb{R}^n \colon |P| = 1\}$. This sphere has a natural measure as a subset of the Euclidean space $\mathbb{R}^n$.

Definition 2.1. The parameter space for shapes of n-simplices, $n \geqslant 2$, is $(S^{n-1})^{n+1}$, the Cartesian product of $n+1$ copies of S^{n-1}. This space has a natural measure as a subset of the Euclidean space $(\mathbb{R}^n)^{n+1}$. We choose this measure, scaled so that the total measure is one, to obtain a probability space for n-simplices.

Each copy of S^{n-1} corresponds to choosing one vertex of the simplex. Almost surely (with probability 1), the simplex produced will be nondegenerate, i.e. the $n+1$ points are not contained in an affine hyperplane. Note that a given simplicial shape can be represented in this space in many ways, since we can permute the vertices and rotate the whole sphere. Note also that we explicitly remove the case $n = 1$. Choosing two points randomly from the 0-sphere $S^0 = \{\pm 1\}$ will only give a nondegenerate 1-simplex with probability $1/2$. See Remark 3.2 for an explanation of how the case $n = 1$ fits in with the main theorem.

We can easily sample from this probability distribution, using a procedure described for instance by Muller [13]. To choose uniformly a random point on S^{n-1}, we can form a vector where each of the n coordinates is a normal stochastic variable with expectation zero and variance one. Then normalize it to have unit length. When $n+1$ points are chosen in this manner, we get our randomly defined simplex.

It should also be mentioned that our way of constructing a space of simplicial shapes could be less suitable for studying other phenomena, for instance degenerations. Almost surely, $n+1$ points chosen by our procedure will form a nondegenerate simplex. However, if we restrict to degenerate cases, we will usually get $n+1$ points that lie on a sphere in a hyperplane, which is a special case.

As in three-space, we say that an ordered set of n points in $\mathbb{R}^n$ forms a right-handed set if the matrix with the coordinates of the points as columns has positive determinant, and left-handed if the determinant is negative. In particular, this can be applied to any facet of an n-simplex, which is given by choosing n of the $n+1$ vertices. With our choice of probability measure, we can prove the following independence result:

Lemma 2.2. *Let a random simplex be given by its ordered set of vertices* $(P_0, \dots, P_n) \in (S^{n-1})^{n+1}$. *The handedness of each facet, i.e. each n-subset of vertices, is independent of the handedness of the other facets.*

To facilitate the proof of this lemma, we introduce some notation that will only be used here. Define the antipodal map ι_i of the ith sphere:

$$\begin{gathered}\iota_i\colon (S^{n-1})^{n+1} \to (S^{n-1})^{n+1},\\ (P_0, \dots, P_i, \dots P_n) \mapsto (P_0, \dots, -P_i, \dots P_n).\end{gathered}$$

The facet defined by $(P_0, \dots, P_{i-1}, P_{i+1}, \dots P_n)$ will be denoted by $\widehat{P}_i$. For a subset $I \subset \{0, 1, \dots, n\}$, $|I|$ denotes its cardinality and $\overline{I}$ its complement. Composition of the antipodal maps will be denoted as

$$\iota_I = \iota_i \circ \iota_j \circ \iota_k \dots \quad \text{if } I = \{i, j, k, \dots\}.$$

Finally, we choose some (linear) hyperplane H and let π_H be the reflection in this hyperplane: Decompose a vector as a sum of one vector contained in H and one vector orthogonal to H. The reflection changes the sign of the orthogonal part:

$$\begin{gathered}\pi_H\colon (S^{n-1})^{n+1} \to (S^{n-1})^{n+1},\\ (P_0, \dots, P_n) \mapsto (\pi_H(P_0), \dots, \pi_H(P_n)),\\ \pi_H(P_i) = P_i - (2 \text{ times the part of } P_i \text{ orthogonal to } H).\end{gathered}$$

P r o o f. We are only interested in probabilities. Therefore, there are some considerations involving subsets of measure zero that we will not be explicit about. For instance, the maps ι_i defined above do not preserve the property of being nondegenerate exactly, and the reflection π_H only works as stated below for facets not contained in H.

The ι_i are independent, commuting maps. This is true, since they act on different copies of S^{n-1}.

The ι_i are measure preserving involutions. This is obviously true, since ι_i is the antipodal map. As a consequence, ι_I also preserves measure for any subset $I \subset \{0, 1, \ldots, n\}$.

Using ι_i changes the handedness of the facets $\widehat{P_j}$ for $j \neq i$, and preserves the handedness of $\widehat{P_i}$. As a consequence, using ι_I changes handedness based on the parity of $|I|$. If $|I|$ is odd, ι_I changes the handedness of the facets $\widehat{P_j}$ for $j \in \overline{I}$, and preserves the handedness of the facets $\widehat{P_j}$ for $j \in I$. If $|I|$ is even, ι_I changes the handedness of the facets $\widehat{P_j}$ for $j \in I$, and preserves the handedness of the facets $\widehat{P_j}$ for $j \in \overline{I}$.

If n is odd, we can now finish the proof. Decompose $(S^{n-1})^{n+1}$ into 2^{n+1} disjoint subsets according to the handedness of the facets. Each part in the decomposition has the same size, since the maps ι_I interchange the parts and preserve measure. This proves the independence in the statement of the lemma.

If n is even, there is still one ingredient missing. Since $|I|$ and $|\overline{I}|$ in this case have opposite parities ($|I| + |\overline{I}| = n + 1$), ι_I and $\iota_{\overline{I}}$ will change the handedness of the same set of facets. The effect of this is that we can only change parities of an even number of facets using ι_Is. To conclude the proof, we can use the additional reflection map π_H, which changes the handedness of all facets. We can then conclude using the collection of maps ι_I and the composed maps $\pi_H \circ \iota_I$ as in the case of odd n. The only difference is that we have a decomposition into 2^{n+2} parts of equal size, where pairs of these parts correspond to handedness of the facets. $\square$

3. Proof of the main result

This section is devoted to proving Theorem 3.1.

Theorem 3.1. *Consider the space of n-simplices, $n \geqslant 2$, endowed with the probability measure from Definition* 2.1. *The probability that an n-simplex is well-centered is* $1/2^n$.

P r o o f. We start with $n+1$ vertices $\{P_i\}$ chosen randomly on the standard unit sphere S^{n-1}. We want to determine the probability that the simplex contains its circumcenter, which is, due to our choices, the origin O. To express O in terms of the vertices $\{P_i\}$ of the simplex, we can solve the equation

$$a_0P_0 + a_1P_1 + \ldots + a_nP_n = O. \tag{3.1}$$

If there is a solution with all a_i positive, the simplex is well-centered. Since the right hand side is zero, we can scale any solution to obtain another. For instance, if the a_i are scaled so that the sum is equal to one, these are the barycentric coordinates of the simplex. In matrix form,

$$\begin{pmatrix} P_0 & P_1 & \ldots & P_n \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_n \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}.$$

We can now simplify slightly, since we are only interested in probabilities. Almost surely, the simplex is nondegenerate, and $a_n \neq 0$. We can then divide equation (3.1) by a_n and look for a solution of the form $(a_0, a_1, \ldots, a_{n-1}, 1)$. This translates the problem into

$$\begin{pmatrix} P_0 & P_1 & \ldots & P_{n-1} \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_{n-1} \end{pmatrix} = -P_n.$$

Cramer's rule now states that

$$a_i = \frac{\det\begin{pmatrix} P_0 & \ldots & P_i \text{ replaced by } -P_n & \ldots & P_{n-1} \end{pmatrix}}{\det\begin{pmatrix} P_0 & P_1 & \ldots & P_{n-1} \end{pmatrix}}. \tag{3.2}$$

To conclude the proof, we need to know if the two signs of the coefficients a_i are equally likely. But this can be seen from Cramer's rule: a_i is the ratio of two determinants. Hence $a_i > 0$ if these two determinants have the same signs. For each of the two determinants, the n columns are randomly chosen vectors on the n-sphere, and the sign of the determinant only tells us if the vectors form a left-handed or a right-handed system. These are equally likely, and therefore the probability that $a_i > 0$ is $1/2$.

Furthermore, the set of signs of the $n + 1$ n-determinants involved in the computation describe the handedness of the facets of the simplex. By the independence result Lemma 2.2, we conclude that the probability that all the a_i are positive is the product of the probability that each is greater than zero. Therefore, the probability that the simplex is well-centered is 2^{-n}. □

R e m a r k 3.2. The statement of the theorem for $n = 1$ would be that a 1-simplex, i.e. an interval, is well-centered with probability $1/2$. But the center of an interval is always inside it, so the probability is actually 1! The argument presented in the theorem fails for the following reason. Our procedure for creating a random simplex will produce a nondegenerate simplex with probability 1 if $n \geqslant 2$, but only with probability $1/2$ if $n = 1$. For $n = 1$, $S^{n-1} = S^0$ consists of only two points. Therefore, there is a probability of $1/2$ that the same point is chosen twice, so that the equation (3.1) takes the form $a_0P_0 + a_1P_0 = O$, and there is no positive solution. A statement that also includes $n = 1$ would be that the probability that $n+1$ randomly chosen points on S^{n-1} form a nondegenerate, well-centered simplex is $1/2^n$.

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