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FROM BINARY CUBE TRIANGULATIONS TO ACUTE BINARY SIMPLICES

Jan Brandts, Jelle van den Hooff, Carlo Kuiper, Rik Steenkamp

Korteweg-de Vries Institute for Mathematics, Faculty of Science
University of Amsterdam, Amsterdam, Netherlands
janbrandts@gmail.com

Abstract

Cottle's proof that the minimal number of 0/1-simplices needed to triangulate the unit 4-cube equals 16 uses a modest amount of computer generated results. In this paper we remove the need for computer aid, using some lemmas that may be useful also in a broader context. One of the 0/1-simplices involved, the so-called antipodal simplex, has acute dihedral angles. We continue with the study of such acute binary simplices and point out their possible relation to the Hadamard determinant problem.

1. On a personal note

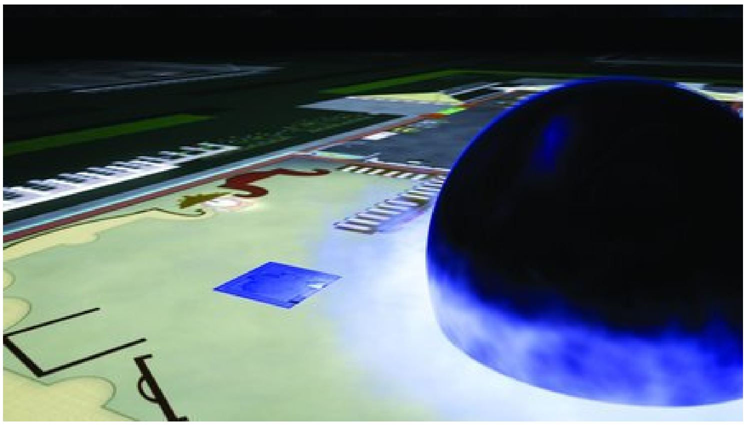
Until 1997, I lived in the two-dimensional world created by Edwin A. Abbott in 1884: Flatland. This is meant, of course, metaphorically, or maybe better mathematically. My mathematical output, mostly in the context of superconvergence in finite element methods, dealt with partial differential equations formulated on a two-dimensional domain Ω. When people asked me if I could generalize my theorems to three space dimensions, I shrugged and gave an answer along the lines of: "I suppose so. What's different in three than in two dimensions?"

A square from Flatland is introduced to the third dimension in *Flatland the Movie*.

My PhD supervisors did not push the matter, but things became differently when I arrived at the Mathematical Institute of the Academy of Sciences in Prague on October 1, 1997.

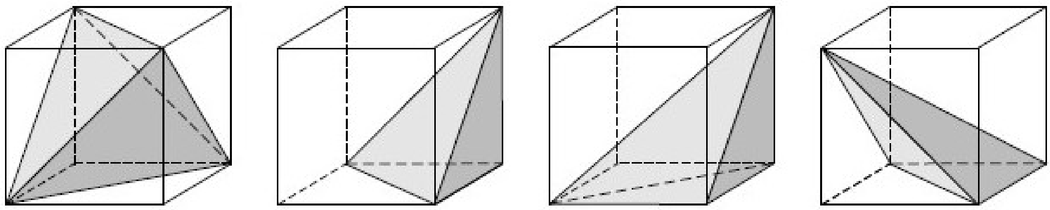
1.1. From two via three to arbitrary dimension

Michal Křížek, who had encouraged me to apply for the position that I was going to hold for a year, investigated not only superconvergence in finite element methods, but also discrete maximum principles. Both topics include certain demands to be placed on the triangulation of the domain Ω. Also the convergence of the method involves conditions on the triangulation. From his publications [1, 2, 3] around that time, it is clear that Michal Křížek was not afraid to look beyond dimension two. At that moment, if I remember it well, he was already involved with research together with Sergey Korotov and Pekka Neittaanmäki that led to the two papers [4, 5] in the influential journals *Mathematics of Computation* and *SIAM Journal on Numerical Analysis*. And, as most of the readers of these proceedings dedicated to Michal's 60th birthday will have experienced themselves as well, Michal's enthusiasm for the geometrical aspects of finite element methods is difficult to ignore. More positively formulated, it is contagious. Thus, not unlike the Flatland character of Spherius, the three-dimensional visitor of Flatland, who teaches the ignorant Flatlanders about higher dimensions, Michal started to motivate me to do mathematics in three dimensions.



Spherius reveils himself by intersecting with Flatland.

At first, this went slow. We studied superconvergence of quadratic tetrahedral finite element methods already quite soon, but proved it only in [6]. In the mean time, I, the pupil, had even surprised the master, Michal, by suggesting to prove superconvergence for linear finite elements in dimensions higher than three, resulting in the dimension independent superconvergence proof in [7]. This paper seemed to have started, at least for me, a new chapter in my mathematical life. From that point onwards, I always tried to think dimension independently, and was, of course, enthusiastically encouraged by Michal in doing so. This led even to geometric results that were a bit further away from the numerical analysis background of finite element meshes. For instance, a right triangle can trivially be subdivided into two right triangles, and with a bit of effort, a path-tetrahedron, which is a tetrahedron having a path of three mutually orthogonal edges, can be subdivided into three of such path-tetrahedra. This was already known, but we managed to prove the corresponding result for path-simplices of arbitrary dimension in [8]. Even though remotely related to local nonobtuse refinement of higher dimensional finite element meshes, the trend was now that we did geometry for the sake of geometry. The last developments in this direction are that we study nonobtuse and acute binary simplices, which are simplices whose vertices are vertices of the unit n-cube. With these simplices one can try to triangulate the n-cube, which led to the result [9] that, using nonobtuse binary simplices, this can be done in only two ways, modulo the action of the cube symmetries, the elements of the hyperoctahedral group.



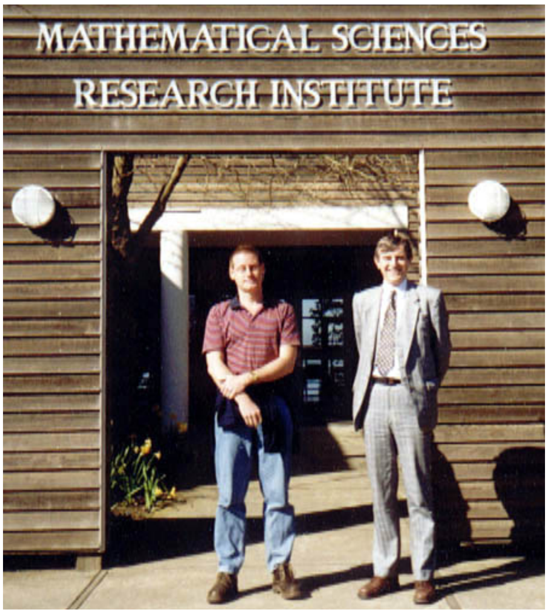
Binary simplices in the three-cube.

This paper, in fact, started another chapter in my research. From this point onwards, I got my own students who work with me, and with Michal on the background in Prague, on topics like this. Starting January 2012, even a first PhD student will work on the abstract geometrical questions that all originated from Michal's enthusiasm, dating back to the final years of the previous millennium. I am looking forward to the coming four years of this PhD project.

1.2. Other dimensions and facets

Apart from mathematical influence, Michal Křížek has had a big impact on my career and personal development. He was involved in many of the invitations that I got to speak at conferences, to visit institutions, and even in the jobs that I got. We traveled together to many places, among which Berkeley and Beijing, and he was the only visitor that I got during the position that I held at the University of New South Wales in Sydney. As a result, Michal Křížek is a member of the select group of people that I have met on four different continents. The group is so select that it has no other members (as far as I know).

For completeness of this account, I will also mention a less positive experience that I had with Michal. During our visit to MSRI in Berkeley, we decided to travel to the Arizona Impact Crater and to the Grand Canyon, by car. Well, Michal decided to travel there, much against the wishes of conference organizer Ivo Babuška who rather had us prove theorems also during that weekend. I went along, while



not making myself more useful than to read the map – I have no driver's license. All went well, until the Sunday morning. We had slept in the car on a parking somewhere in the Arizona desert. You may be aware of the fact that temperatures can be quite low during desert nights, so we hardly slept due to the clattering of our teeth. At sunrise, a bit past four, we decided to move on again, completely frozen, very sleepy, hungry, not feeling well at all. I do not know how long it took, but it felt like a long time before, finally, a gasoline station with restaurant was announced, and I was counting the miles. When finally I told Michal to take the exit to the gasoline station, his answer was one of surprise: "Go here? Why? Our tank is still three quarters full. We do not need gasoline for hours and hours!". While the exit appeared out of sight behind us, and after I had recovered my speech after a moment of being completely stupefied, all I could do was shout two words, and to repeat them to make a statement: "Gasoline?? Gasoline?? Coffee!! Coffee!!".

With this, I think I have mentioned Michal's single greatest flaw: he does not drink coffee. I'm sure that Paul Erdös would agree. In spite of that, he is a great person and a true friend.

2. Minimal cube triangulation with binary simplices

As mentioned in the previous section, one topic of recent interest was the triangulation of the unit cube using binary simplices, which are simplices whose vertices are vertices of the unit cube. Although the three- and four-dimensional cases have been well-understood already for a few decades, I would like to add some minor observations. In all that follows, we only consider triangulations with binary simplices, also called 0/1-simplices, as special cases of 0/1-polytopes.

2.1. Triangulating the unit three-cube

One of the first questions that we asked ourselves when confronted with the question *what is the minimal number of* 0/1*-simplices needed to triangulate the unit* n*-cube* I^n was the following: of course, we knew that the answer for $n = 3$ is five, but how does one actually *prove* such a statement?

The classical proof by Mara [10] is based on the inequality $P_n \geq 2P_{n-1}$, where P_j denotes the minimal number of 0/1-simplices that is needed to triangulate I^j. This inequality is derived from the fact that I^n has $2n$ facets, which each show at least P_{n-1} 0/1-simplices of dimension $n-1$. Since each binary n-simplex in a triangulation of I^n has at most n facets that lie on the boundary ∂I^n of I^n, this immediately gives the statement. Together with the simple fact that $P_2 = 2$ this gives that $P_3 \geq 4$. Mara [10] continues with the rather complicated argument that the interior facet of a 0/1-simplex having n exterior facets can not be met by another 0/1-simplex having n exterior facets. Apply this to the case $n = 3$. Then ∂I^3 shows 12 triangular facets. If these are the exterior facets of four 0/1-tetrahedra, their four interior facets cannot meet one another, and a fifth 0/1-tetrahedron is necessary to complete the triangulation.

We can now adapt the argument by Mara as follows. It will result in a stronger version of the inequality $P_n \geq 2P_{n-1}$ that will also be sufficient to prove minimality of a triangulation of I^4 in 16 binary simplices.

Theorem 2.1. *For* $n \geq 2$ *we have that*

$$P_n \geq 2P_{n-1} + \frac{(n-2)(n-1)!}{\mathcal{H}_n},$$

where $\mathcal{H}_n$ *is the maximum absolute value of the determinant of a* 0/1*-matrix of size* $n \times n$*.*

Proof. Let I^n be triangulated into binary n-simplices. This induces triangulations of each of the facets of I^n. The crucial observation is that the $(n-1)$-simplicial facets that are visible in two opposite facets of I^n must be facets of distinct binary

n-simplices in I^n. Indeed, a binary n-simplex in I^n with $n \geq 2$ cannot have two facets in opposite facets of I^n, or it would have $2n$ vertices. This proves Mara's inequality $P_n \geq 2P_{n-1}$. However, the total Euclidean volume of all the 0/1-simplices that are visible in the two opposite cube facets equals only $2/n$. This can be seen using the formula that the volume of a binary n-simplex equals $1/n$ times the volume of a facet, times the height of the vertex opposite this facet. The sum of the $(n-1)$-volumes of the exterior facets equals two (the added volume of the two triangulated facets of the n-cube) and their heights are all equal to one. The remaining volume of $1 - 2/n = (n-2)/n$ needs to be filled by other 0/1-simplices. The volume $|S|$ of a 0/1-simplex S in I^n that has the origin as one of its vertices equals

$$|S| = \left| \frac{\det(P)}{n!} \right|$$

where the 0/1-matrix P has the remaining n vertices of S as columns. Dividing $(n-2)/n$ by the largest possible value of this volume results in the statement. □

Corollary 2.2. $P_3 \geq 5$.

Proof. One easily verifies that the largest determinant of a 0/1-matrix of size 3×3 equals two. One can also use the Hadamard bound, valid for 0/1-matrices of size $n \times n$,

$$\mathcal{H}_n \leq 2 \left(\frac{\sqrt{n+1}}{2} \right)^{n+1}. \tag{1}$$

In both cases we find, using Theorem 2.1 above, that $P_3 \geq 2P_2 + 1 = 5$. □

The 1893 Hadamard maximal determinant conjecture is contained in the question what is the value of $\mathcal{H}_n$ in terms of n. This is still an open problem.

Jaques Hadamard (1865–1963)

See Sloan's *Online Dictionary of Integer Sequences*, item *A*003432, for the rather small number of known values for $\mathcal{H}_n$, the first of which are given below.

n	2	3	4	5	6	7	8	9	10	11	12	13
$\mathcal{H}_n$	1	2	3	5	9	32	56	144	320	1458	3645	9477

We will get back to this problem further on.

For now, note that of course, the lower bound of five 0/1-tetrahedra is attained by the triangulation of I^3 consisting of an interior regular 0/1-tetrahedron with edge length $\sqrt{2}$ and four 0/1-tetrahedra having each three exterior facets, so-called cube corners. The regular 0/1-tetrahedron is depicted in the most left picture in the figure in Section 1.1, a typical cube corner is displayed directly on its right.

2.2. Triangulating the unit four-cube with binary 4-simplices

Theorem 2.1 provides an immediate lower bound for the number P_4 of binary 4-simplices that are needed to triangulate the unit four-cube, I^4.

Corollary 2.3. $P_4 \geq 14$.

Proof. The Hadamard bound (1) shows that $\mathcal{H}_4 \leq 3$. Moreover, there exist binary 4-simplices whose matrix representation P indeed have determinant 3 (see also Section 3). Thus, by Theorem 2.1,

$$P_4 \geq 2P_3 + \frac{2 \cdot 6}{3} = 2 \cdot 5 + 4 = 14.$$

Note that even though the Hadamard bound is not an integer, $\mathcal{H}_n$ always is. □

Now, this lower bound is not sharp, and the reason for this is that all 0/1-simplices in I^4 of maximum volume 3/24 intersect one another. Hence, at most one of them can be used in a triangulation. In the following we will prove this. Note that the original result is by Cottle [11] but he used computer generated information. The proofs below do not.

First we define the *antipodal* 0/1*-simplices.* An example is the convex hull of the standard unit basis vectors and the all-ones vector. As such, it shares an interior facet (spanned by the standard unit basis vectors) with a cube corner, and this also explains its name. Of course, there are 2^n distinct cube corners in I^n, and thus as many 0/1-antipodal simplices. It is easy to see that the midpoint of the cube is interior to each antipodal 0/1-simplex, and thus, that a triangulation of I^n into 0/1-simplices contains at most one of them. In the case $n = 4$, to prove that all 0/1-simplices of maximum volume 3/24 intersect, it is therefore sufficient to prove that all 0/1-simplices of volume 3/24 are antipodal 0/1-simplices.

Lemma 2.4. *Let S be a binary n-simplex with an edge of length one. Then there exists a binary n-simplex $\hat{S}$ with an exterior facet such that $|S| = |\hat{S}|$.*

Proof. Without loss of generality, assume that the edge of length one of S sprouts from the origin. Then the matrix P whose columns are the vertices of S other than the origin has a column equal to a standard basis vector. As a result, the 0/1-simplex $\hat{S}$ represented by the origin and the columns of P^t has an exterior facet because P^t has a row with only one nonzero entry. Obviously $\det(P) = \det(P^t)$ and thus the volumes of S and $\hat{S}$ coincide. □

Definition 2.5. Write e for the all-ones vector in $\mathbb{R}^n$. Given a vertex x of I^n, the point $e - x$ is called the antipodal vertex of x.

Lemma 2.6. *Let S be a binary n-simplex with two antipodal vertices. Then there exists a binary n-simplex $\hat{S}$ with an exterior facet such that $|S| = |\hat{S}|$.*

Proof. Without loss of generality, we assume that the antipodal vertices of S are the origin and the all-ones vector e. Then the matrix P whose columns are the vertices of S other than the origin has a column equal to e. As a result, the 0/1-simplex $\hat{S}$ represented by the origin and the columns of P^t has an exterior facet because P^t has a row with no zero entries. Obviously $\det(P) = \det(P^t)$ and thus the volumes of S and $\hat{S}$ coincide.

The purpose of the above two lemmas is to conclude the following.

Corollary 2.7. *A binary 4-simplex S with maximal volume has no exterior facet and does not contain two vertices x and y that are antipodals, or joined by a cube egde.*

Proof. The volume of any binary 0/1-simplex with an exterior facet is at most 1/4 times the volume of that facet (which is at most 1/3), and thus at most 2/24. Thus, S has no exterior facet, and hence by the above lemmas the rest of the statement follows as well. □

Lemma 2.8. *Each binary 4-simplex S of volume 3/24 is an antipodal 0/1-simplex.*

Proof. By Corollary 2.7., S has no exterior facet. Thus, no cube facet of I^4 contains 4 vertices of S. Hence, we may suppose without loss of generality that the facet C_0 of I^4 with $x_4 = 0$ contains the vertices p_1, p_2 and p_3 of S, and that the facet C_1 of I^4 parallel to C_0 contains the remaining vertices p_4 and p_5. Since by Corollary 2.7. no cube edge is an edge of S, the vertices of S in C_0 are the regular triangular facet of a three-dimensional cube corner. Again without loss of generality we choose the origin such that $p_1 = e_1, p_2 = e_2$ and $p_3 = e_3$. The remaining two vertices of S lie in the facet C_1 parallel to C_0. Again by Corollary 2.7., they are not connected by a cube edge to p_1, p_2, p_3, nor are they antipodal to them. This disqualifies six of the eight vertices of C_1. Thus, only one choice for the pair p_4, p_5 remains. One easily verifies that one of them is e_4, and that the other is the all-ones vertex e. In particular, this shows that S is an antipodal 0/1-simplex. □

Theorem 2.9. *Each triangulation $\mathcal{T}$ of I^4 into 0/1-simplices contains at least 16 binary simplices.*

Proof. Using Theorem 2.1, we need at least ten 0/1-simplices of total volume 1/2 plus some additional 0/1-simplices that are needed to fill the remaining volume of 1/2. These additional 0/1-simplices can only have volumes 1/24, 2/24 or 3/24 due to the Hadamard bound (1). Due to Lemma 2.8., together with the fact that each antipodal 0/1-simplex contains the midpoint of I^4 in its interior, there is at most one 0/1-simplex S of volume 3/24 in a triangulation $\mathcal{T}$ of I^4. If there is none, then at least six 0/1-simplices of volume 2/24 are needed to complete the triangulation. If there is one, then at least five more 0/1-simplices are needed to complete $\mathcal{T}$. In both cases, the total number $|\mathcal{T}|$ of 0/1-simplices in $\mathcal{T}$ is at least 16. □

A triangulation of I^4 into 16 binary simplices exists and was given already by Mara [10].

3. Acute simplices

In dimensions $2, 3$, and 4, the antipodal 0/1-simplices are the ones with the largest volume in I^n. The antipodal 0/1-simplex that is opposite the cube corner at the all ones vector e has the origin as vertex together with $e - e_1, \ldots, e - e_n$, where $e_1, \ldots e_n$ are the standard unit basis vectors. Thus, the matrix having those vectors as columns is

$$P = ee^t - I,$$

where I is the $n \times n$ identity matrix. Since the rank-one matrix ee^t obviously has $n-1$ eigenvalues equal to zero, and one equal to n due to $ee^te = en$, subtracting the identity results in P having $n-1$ eigenvalues equal to -1 and one equal to $n-1$. This shows that the antipodal 0/1-simplex has volume $(n-1)/n!$ in dimension n.

Moreover, each antipodal 0/1-simplex is an *acute* simplex, meaning that all its dihedral angles are acute. Recall that a dihedral angle between two facets equals π minus the angle between two exterior normals to those facets. For triangles, this reduces to the usual angle. Even though it is intuitively clear that an antipodal 0/1-simplex is acute, it can also be prove rigorously by showing that the inverse of the matrix P^tP has negative upper triangular entries and positive row sums.

Proposition 3.1. ([8]) *The simplex with as vertices the origin and the columns of the matrix P is acute if and only if $(P^tP)^{-1}$ has all upper triangular entries negative and all row sums positive.*

Remark 3.2. *Note that Q, where $Q^tP = I$, has normals to the facets of S as columns, because the j-th column of Q is orthogonal to all columns of P but the j-th. Thus, $Q^tQ = (P^tP)^{-1}$ contains dihedral angle information in its upper triangular part, but not for the facet opposite the origin, whose corresponding normal equals $-Qe$, where e is the all-ones vector. Thus, the remaining dihedral angle information is in the row sums of $(P^tP)^{-1}$. For details, see [8].*

Acute binary simplices are extremely rare compared to all binary simplices, in fact, even relative to all nonobtuse binary simplices. The total numbers of acute binary simplices in the n-cube, modulo the action of the hyperoctahedral group of cube symmetries, are

n	3	4	5	6	7	8	9	10	11
#	1	1	2	6	13	29	67	162	392

Note that in dimensions 3 and 4, the single acute binary simplex is, in fact, the antipodal 0/1-simplex.

We computed the above numbers by a nontrivial computer program. Nontrivial, because it is impossible to generate all binary simplices, to verify which are acute, and then to put them into equivalence classes generated by the cube symmetries. For this, the total amount of 0/1-simplices is simply too large. Thus, the trick is to generate representatives of all equivalence classes of binary simplices directly. It is beyond the scope of this paper to explain the method in detail.

Our computational results so far show, that for $3 \leq n \leq 13$, apart from dimensions $9, 10$ and 13, the maximal determinant over all acute binary simplices is the same as when taken over all binary simplices, as can be seen by comparing with the table in Section 2.1. This leads to a conjecture, although based on little evidence.

n	2	3	4	5	6	7	8	9	10	11	12	13
det	1	2	3	5	9	32	56	96	224	1458	3645	7290

Conjecture: For dimensions $n \geq 3$ and $n = 0 \,(\text{mod } 4)$ and $n = 3 \,(\text{mod } 4)$ there exists a 0/1-matrix representing an acute binary simplex that has maximal determinant.

Before trying to prove this conjecture, we would like to collect more computational data. This is not a trivial task, since the structure of acute binary simplices is not yet understood. Some simple properties can, however, be easily proved.

Proposition 3.3. *A nondegenerate acute binary simplex S has the following properties:*

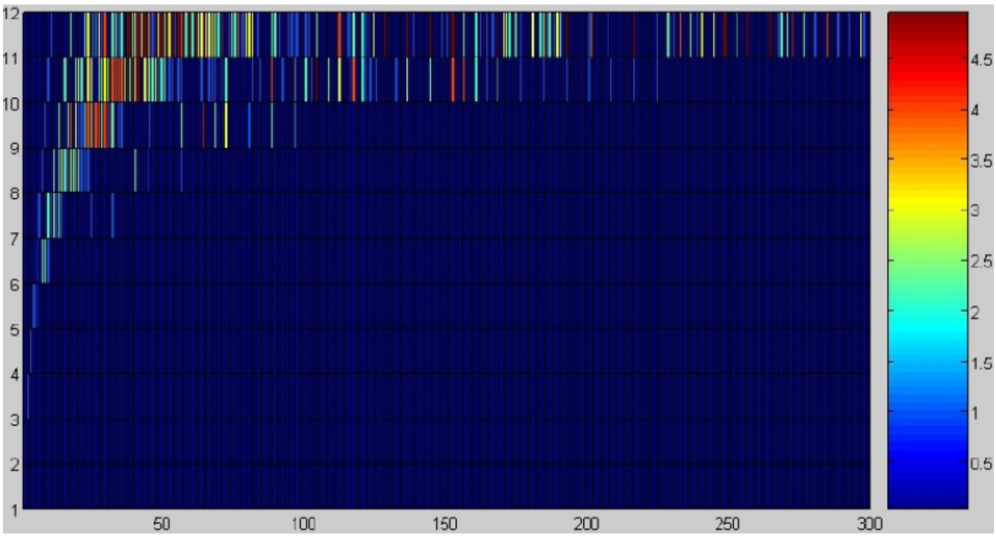
- *S has no pair of antipodal points as vertices;*
- *S has no edge of the cube as edge;*
- *S has no external facet.*

Proof. Without loss of generality, we give the proof for an acute binary simplex having the origin as a vertex. Let x be a vertex of S other than e or the origin. Then $x, e-x$ and the origin form a right triangular facet of S because $x^t(e-x) = 0$. Indeed, x and $e-x$ differ in all coordinates thus the sum of their products vanishes. This contradicts the well known fact that acute simplices have acute facets. Next, let x, y be vertices of S other than the origin with $x - y = e_k$, a standard basis vector of $\mathbb{R}^n$. Then $x^t e_k = 1$ and $y^t e_k = 0$ but $e_k = x - y$ hence $y^t(x-y) = 0$. Thus, $y, x-y$ and the origin form a right triangle, again contradicting that S is acute. Finally, if

S has an external facet F, it is by definition a subset of a facet of I^n. The vertex v of S opposite F is connected via an edge of I^n with a vertex of F, see also [9]. We already proved above that this cannot happen in an acute binary simplex. □

While generating the acute binary simplices, we also investigated which values their determinant can actually have, instead of only looking at their maximum value. The set of determinant values of 0/1-matrices in general is known as the *determinant spectrum*, and thus we investigate the subset that we will call the *acute determinant spectrum*.

Below we present a global illustration of this acute binary determinant spectrum. For values of n up to 11, we indicate by brightness how many distinct acute 0/1-simplices have a certain determinant value. For instance, the slightly brighter line between the vertical values 3 and 4 indicates the 3-antipodal. Slightly to its right and between values 4 and 5 on the vertical axis, we see the 4-antipodal. In fact, the antipodal 0/1-simplices are the left-most acute 0/1-simplices in the spectrum for each value of n. There do not seem to exist acute 0/1-simplices with a smaller volume.



On the other hand, the values of the determinant rapidly increase with the dimension, as the Hadamard bound suggests. Moreover, and this is not really well visible in the above diagram, we can distinguish several families, parametrized by n, whose determinant is linear in n, similar as the determinant of the antipodal equals $n-1$.

One of the tasks of my new PhD student will be to study these structures, from 2012 to 2016, and we hope that Michal Křížek is going to play a part in this project.

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