Karl-Franzens-Universität Graz & Technische Universität Graz

SPEZIALFORSCHUNGSBEREICH F 003

OPTIMIERUNG

und

KONTROLLE

Projektbereich

DISKRETE OPTIMIERUNG

Oswin Aichholzer

Extremal Properties of 0/1-Polytopes of Dimension 5

Bericht Nr. 132 – July 1998

Extremal Properties of 0/1-Polytopes of Dimension 5

Oswin Aichholzer*
Institute for Theoretical Computer Science
Graz University of Technology
Klosterwiesgasse 32/2, A-8010 Graz, Austria
e-mail: oaich@igi.tu-graz.ac.at

Abstract

In this paper we consider polytopes whose vertex coordinates are 0 or 1, so called 0/1-polytopes. For the first time we give a complete enumeration of all 0/1-polytopes of dimension 5, which enables us to investigate various of their combinatorial extremal properties.

For example we show that the maximum number of facets of a five-dimensional 0/1-polytope is 40, answering an open question of Ziegler [22]. Based on the complete enumeration for dimension 5 we obtain new results for 2-neighbourly 0/1-polytopes for higher dimensions.

1 Introduction

Among the simplest high-dimensional geometric objects is the d-dimensional hypercube (d-cube). It is a convex polytope that, when having unit edge length, may be expressed as $\mathcal{C}^d = [0,1]^d$.

Despite of its simple definition, $\mathcal{C}^d$ has been an object of study from various different points of view. Purely combinatorial properties of $\mathcal{C}^d$, mainly involving certain subgraphs formed by its edges and vertices (the latter are just the various d-tuples of binary digits) have been investigated extensively in coding theory, communication theory, learning theory, and many other fields; see, e.g., [4, 9, 19]. This reveals the fact that the hypercube is the most natural geometric structure combining all binary digits of length d.

The theory of convex polytopes provides classical results concerning sections and projections of hypercubes (see e.g. [8, 10]) as well as for so-called subpolytopes of

*Research supported by the Spezialforschungsbereich F 003, *Optimierung und Kontrolle*.

the d-cube [20]. In this paper we consider the convex hull of a subset $V \subseteq \{0,1\}^d$ of hypercube vertices. A polytope P representing the convex hull of V is called a *0/1-polytope*. Thus the facets of 0/1-polytopes are supported by hyperplanes spanned by d-cube vertices. This set is investigated e.g. in [2].

Motivation for considering 0/1-polytopes comes from Combinatorial Optimization (e.g. the Traveling Salesman Polytope, or the Assignment Polytope) and many other fields, see e.g. Ziegler [21, 22].

A point $p \in P$ is an *extreme point* of P provided $x, y \in P$, $0 < \lambda < 1$, and $p = \lambda x + (1 - \lambda)y$ imply $p = x = y$. In other words, p is an extreme point of P if it does not belong to the relative interior of any segment contained in the closure of P. It is not hard to see that any vertex of V is an extreme point of P: consider the d-dimensional hypersphere S^d with center $(\frac{1}{2}, \ldots, \frac{1}{2})$ and radius $\frac{\sqrt{d}}{2}$. All vertices of the d-cube $\mathcal{C}^d$ lie on S^d and thus any subset V of vertices of $\mathcal{C}^d$ entirely consists of extreme points. Thus a 0/1-polytope P is a so-called subpolytope of the hypercube.

In Section 2 we give for the first time a complete enumeration of all 0/1-polytopes of dimension 5. This enables us to investigate various combinatorial extremal properties, see Section 3. One main result we obtain from this enumeration is to determine the maximum number of facets of a five-dimensional 0/1-polytope. We show that this maximum is 40, answering an open question of Ziegler [22]. We also give extremal results on the edge skeleton of five-dimensional 0/1-polytopes, e.g. we give an example with the maximal number of 112 edges. Moreover we show that the degree of a vertex can exceed 2^{d-1} already for $d \geq 5$.

Based on the complete enumeration for dimension 5 we obtain as a spin-off new results for 2-neighbourly 0/1-polytopes for higher dimensions, see Section 4.1.

2 Complete Enumeration for Dimension 5

Figure 1 shows all types of three-dimensional 0/1-polytopes, along with the number of vertices, edges, facets, and the number of geometrically equivalent copies, respectively. We call two polytopes (geometrically) equivalent if they can be transformed into each other by rotation or reflection, see Section 2.1 for more details. Thus for $d = 3$ there are 12 different types of 0/1-polytopes, each representing an equivalence class of the given cardinality. In total this gives 151 0/1-polytopes in three-space. The remaining 105 possible subsets of vertices of the 3-cube span polytopes of dimension at most two.

Note, however, that we consider geometric equivalence classes as opposed to combinatorially equivalent polytopes as defined in [20]. From Figure 1 it is easy to see that there exist only 8 combinatorially different 0/1-polytopes for dimension three.

For arbitrary dimension d there are $2^{(2^d)}$ possible vertex subsets of the d-cube. Most of them span a d-dimensional 0/1-polytope. In fact, it has been shown recently that there are at least $2^{(2^{d-2})}$ different combinatorial types of d-dimensional 0/1-

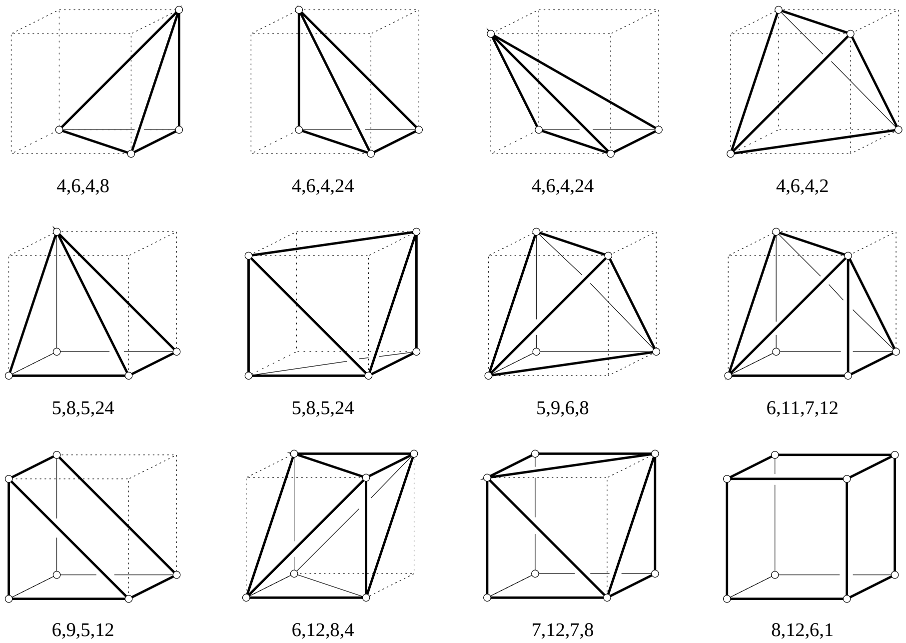

Figure 1: Three-dimensional 0/1-polytopes.

polytopes for $d > 5$, see revised printing of [20]. For $d \leq 4$ a complete enumeration of all sets can simply be done by using standard software. But starting with dimension 5 the number of possible sets increases tremendously. For $d = 6$ there are already about $1.8 \cdot 10^{19}$ possible sets and at least $2^{(2^6)}/(6!\ 2^6) \approx 4.0 \cdot 10^{14}$ symmetry classes, i.e. dimension 6 is even infeasible with use of symmetry. Thus dimension 5 seems to be the first non-trivial and last feasible dimension for enumerating all such sets. In this section we give for the first time a complete enumeration of all non-equivalent 0/1-polytopes for dimension 5. To this end we use some results of [2] and several observations given below.

A straightforward method to enumerate all subsets of vertices of $\mathcal{C}^5$ would be impractical because of the huge number of $2^{(2^5)} \approx 4.3 \cdot 10^9$ such sets. Thus if we could compute about one hundred 5d-convex hulls per second, it would take over one year to enumerate all sets. Fortunately many of these sets are equivalent, i.e. are reflections and rotations of each other. Thus for every equivalence class we need to consider only one representative.

We therefore divide the enumeration into two parts. First we generate exactly one representative vertex set for every equivalence class. We then can easily perform various investigations of these sets in reasonable time, e.g. hunting for the 0/1-polytope with the maximal number of facets.

2.1 Generating Representatives of Equivalence Classes

Let us first consider the equivalence relations. A *reflection* of a vertex set V of the d-cube for an axis i exchanges all zeros and ones on the ith bit position of all vertices of V. Reflections at k axes are thus reflections at a $(d-k)$-subspace. By combining reflections for a certain set of axes we can thus transform a given vertex of V to an arbitrary vertex of the hypercube. For example one can "move" an arbitrary vertex of the set to the origin. Clearly reflections do only change the orientation of the vertex set, but not the properties of their convex hull.

The second operation is called *rotation*. Here we allow arbitrary permutations of the coordinate axes. This operation reflects the fact that we do not weigh the bits of a vertex according to their position, i.e. all directions in d-space have the same significance. Again, rotations might affect the absolute position of the vertices and the orientation of the set, but the structure of their convex hull remains unchanged.

A *class of vertex sets* contains all vertex sets which can be transformed into each other by repeated application of the above two operations. Obviously all vertex sets within a class lead to geometrically equivalent convex hulls and we need only to consider one set per class. In other words the polytopes represented by the vertex sets within one class are affinely isomorphic.

Each vertex of the d-cube can be associated, in a natural way, with its *value*, the decimal value of the binary string corresponding to the vector coordinates. The *vertex vector* $b = (b_0, b_1, \ldots, b_{2^d-1})$ of a set V of vertices from the d-cube is a binary vector of length 2^d with $b_i = 1$ if and only if the vertex with value i is an element of V. For example the vertex vector of the set $\{(0,0,0), (0,1,1), (1,0,1)\}$ is $b = (1,0,0,1,0,1,0,0)$. Clearly, reflections and rotations of a vertex set change its vertex vector.

For any class of vertex sets we can select the set with the lexicographically maximal vertex vector as its representative. In the following we will show that these sets have properties which can be utilized to generate them.

Consider a vertex set V with n vertices of the d-cube and suppose that the vertices are in increasing lexicographical order. We then build a binary $(n \times d)$-matrix $A(V) = (v_1, \ldots, v_n)^T$ with the vertices of V as its rows. A *block* of $A(V)$ is a maximal set of indices of consecutive identical column vectors. This means that permuting the columns within a block does not change the matrix $A(V)$ and thus does not affect the vertices of V.

A vertex $v_i \in V$ has the *block property* if for any block b built by $A(v_1, \ldots, v_{i-1})$ and for any pair $k < l$ of indices within b we have $v_i(k) \leq v_i(l)$, where $v_i(k)$ denotes the kth bit of v_i. In other words, within a block built by the previous vertices, v_i always has the form $(0, 0, \ldots, 0, 1, 1, \ldots, 1)$, i.e. "all ones are shifted to the right".

A set V of vertices satisfies the block property if every vertex of V has the block property. If this is the case it follows by induction that identical column vectors of $A(V)$ are consecutive (recall that the vertices in V have to be in increasing lexicographical order).

Let us give an example for C^9 with $n = 4$:

$$
\text{Œ}\quad
\begin{array}{l}
v_1 = (0,0,0,0,0,0|1,1,1) \\
v_2 = (0,0|1,1,1,1|0,0,0) \\
v_3 = (0|1|0,0,0|1|1,1,1) \\
v_4 = (1|1|0|1,1|0|0|1,1)
\end{array}
$$

$A(v_1, v_2, v_3)$ has blocks of length 1,1,3,1 and 3, respectively. Thus the additional vertex v_4 satisfies the block property. This also holds for v_1, v_2 and v_3, so that the whole vertex set $V = \{v_1, v_2, v_3, v_4\}$ has the block property.

Lemma 1 *In a class of equivalent vertex sets, a lexicographical maximal vertex vector is attained by a vertex set which (a) contains the origin and (b) has the block property.*

Proof. We have to show that any vertex set $V = \{v_1, \ldots, v_n\}$ which does not have properties (a) and (b) can be transformed into an equivalent set V' with a (lexicographically) larger vertex vector, satisfying (a) and (b).

First recall that if the set does not include the origin then by reflection we can move an arbitrary vertex of the set to the origin. This clearly increases the vertex vector. Now consider the vertices in increasing order. Suppose that a vertex v_i, $2 \leq i \leq n$, does not have the block property according to the vertices $v_1, \ldots, v_{i-1}$. By permutation of the positions within the blocks we can rearrange the bits of v_i such that it satisfies the block property. This reduces the value of v_i and clearly affects none of the vertices $v_1, \ldots, v_{i-1}$. Note that although the permutations might change $v_{i+1}, \ldots, v_n$, too, the reduction of the value of v_i still dominates the lexicographic order. Thus v_i does not only have the block property, but we also increased the vertex vector of the set.

By induction we conclude that a vertex set attaining the maximal vertex vector has to satisfy properties (a) and (b). □

Note, however, that in an equivalence class of vertices there might be more than one vertex set with properties (a) and (b). Therefore the algorithm to generate exactly one representative vertex set per equivalence class has two stages.

In the first part we generate only vertices which satisfy properties (a) and (b) of Lemma 1. We use a set of nested for-loops with fixed first element $v_0 = (0, \ldots, 0)$. For every vertex v_i, $0 \leq i \leq 2^5 - 1$, we precompute two bit masks. The first mask has a '1' at every bit position where v_i forces a new block to start, i.e. for the second bit of every '01' or '10' combination of v_i. When adding a new vertex to a set we can therefore update the block information by a simple constant time binary OR operation (assuming constant dimension d). The second mask has a '1' for the second bit of every '10' pair of v_i. In order to ensure that an additional vertex v_i has the block property there must start a new block of the previous vertex set for every '1' in this mask. This means that for every '1' in the second mask of v_i there must be a '1' in the block mask of the previous vertices, which is just the

k	$\binom{2^5}{k}$	generated sets	equivalence classes	class cardinality min. / average / max.		
0	1	1	1	1	1.0	1
1	32	1	1	32	32.0	32
2	496	5	5	16	99.2	160
3	4960	30	10	160	496.0	960
4	35960	230	47	40	765.1	1920
5	201376	1821	131	32	1537.2	3840
6	906192	12789	472	32	1919.9	3840
7	3365856	73880	1326	32	2538.4	3840
8	10518300	344054	3779	20	2783.4	3840
9	28048800	1300574	9013	160	3112.0	3840
10	64512240	4053531	19963	16	3231.6	3840
11	129024480	10582906	38073	32	3388.9	3840
12	225792840	23453731	65664	16	3438.6	3840
13	347373600	44578853	98804	160	3515.8	3840
14	471435600	73233239	133576	80	3529.3	3840
15	565722720	104566543	158658	32	3565.7	3840
16	601080390	130282523	169112	2	3554.3	3840
Σ	2448023843	392484711	698635			

Table 1: Number and cardinality of equivalence classes of vertex sets of the 5-cube.

OR-combination of their first masks. For constant dimension we can thus decide in constant time whether a new vertex satisfies the block property, i.e. whether it has to be considered. An example of a vertex (for dimension 10) and its two bit masks is given below.

$$\begin{aligned} v_i = \quad & (0,0,1,1,0,0,1,0,1,1) \\ mask_1 = \quad & (0,0,1,0,1,0,1,1,1,0) \\ mask_2 = \quad & (0,0,0,0,1,0,0,1,0,0) \end{aligned}$$

With these two masks we can generate all vertex sets with properties (a) and (b) of Lemma 1 very efficiently.

For the second part of our algorithm we apply all possible reflections and rotations to the generated sets. For dimension 5 this gives up to $2^5 \cdot 5! = 3840$ possible copies per set. A vertex set is stored only if the corresponding vertex vector yields the maximum among all resulting vertex vectors. In this way we guarantee that for every equivalence class we store one unique representative.

Table 1 lists the results for $k = 0 \ldots 16$ vertices of $\mathcal{C}^5$. Sets with $k > 16$ vertices can be seen as the complement of sets with $32 - k$ vertices and can easily be obtained from them. The first three columns give the number of all vertex sets, the number of generated sets (part one of the above description) and the number of equivalence classes, respectively. It can be seen that less than $\frac{1}{6}$ of all vertex sets with ≤ 16 vertices satisfy properties (a) and (b) of Lemma 1. Thus we needed to apply the more time consuming rotations and reflections only to this smaller set. The third column shows that there are less than 700000 equivalence classes for $k \leq 16$ and about 525000 for $k > 16$. Therefore the subsequent investigations have to enumerate about 1.2 million sets, which is less than 0.03% of the initial number of sets. This enables us to consider various related questions within a couple of hours instead of month or years.

The number of equivalence classes can also be computed by Pólya's theory of counting [17, 5]. Based on Burnside's lemma [7] the cycle index of the permutation group is built, which then, by Pólya's theorem, gives the number of equivalence classes, see e.g. [12, 16] for more details. The results obtained from this theoretical approach coincide with the output of our program. However, with Pólya's counting theorem it is not possible to obtain a representative vertex set for each equivalence class.

The last three columns of Table 1 show the minimum, average and maximal cardinality of the equivalence classes. There are highly symmetric vertex sets, e.g. for $k = 16$ there is a class with only two sets: The first consists of all vertices with an even number of ones and the second is its complement. On the other hand there are classes with the maximal number of 3840 different sets. On average a class contains over 3000 sets, which results in the comparatively small number of classes.

We used 4 bytes to store the 32-bit vertex vector of every representative vertex set and one additional byte to store the number of vertices, which is clearly redundant but useful for fast access. This results in about 3.5 MB of data, which can easily be handled by any standard computer equipment. In fact we used a simple Personal Computer to compute these results. In a second file we also stored the cardinality of each class (about 1.4 MB). To enable the interested reader to carry out her or his own investigations the files are available upon request from the author.

2.2 Computing the Convex Hull of 0/1-Polytopes

The clear advantage of our approach is that we need to precompute the set of all representative vertex sets only once. Any task which requires a complete enumeration of all subpolytopes of the 5-cube can then be computed easily within a few hours on a standard computer equipment. In this subsection we give a brief description of some convex hull algorithms to derive combinatorial properties of 0/1-polytopes in dimension 5. For further investigations we consider the number of facets and the number of edges as well as properties like 2-neighbourliness, simpliciality and simplicity. In other words we concentrate on the 1-dimensional and $(d-1)$-dimensional faces of these 0/1-polytopes. By complete enumeration of the convex hulls of all representative vertex sets generated in the last subsection we thus get all extremal results on edges and facets for dimension 5.

First we ran a simple implementation of an incremental method to compute higher dimensional convex hulls for point sets in $\mathbb{R}^d$. The algorithms worked well and within several hours we could enumerate all classes. Note that when using a standard convex hull algorithm one has to be careful, since vertices of $\mathcal{C}^d$ are highly degenerate in the sense that there are many linear dependences between them. This may cause numerical troubles in computing the convex hull and in fact many of the existing software packages fail on this task (compare e.g. [6]). For example perturbation methods may result in superpolynomially sized convex hulls for the d-cube [3].

For the second approach we used a tailor-made algorithm for C^5. We utilized the fact that we have exactly 3254 hyperplanes spanned by vertices of the 5-cube, see [2]. This means that for 0/1-polytopes there are 3254 possible ways to support their facets. For every hyperplane we precompute three vertex vectors. The first two contain all vertices of C^5 which are in or above (in or below, respectively) the hyperplane. The third set contains all vertices covered by the hyperplane. Using the first two vertex vectors we can by simple bit operations decide in constant time, whether a hyperplane supports a given set V of vertices or not. Using the third vertex vector we can identify all vertices of V which are covered by the hyperplane. Solving a simple linear system of equations shows us whether these vertices span the hyperplane. If and only if this is the case the hyperplane counts for one facet. Reiterating this for all 3254 possible hyperplanes gives the number of facets of the convex hull of V.

The second approach worked quite well. On a standard Personal Computer (166 MHz Pentium© processor) we needed less than one hour to examine all classes of up to 16 vertices, and an additional hour for the complementary sets.

To compute the number of edges of the convex hull of a vertex set we again used both a standard technique and a tailor-made algorithm. The later version is based on Observation 1 below. We say a subcube $\mathcal{C}^k$, $k \leq d$, is *spanned* by two vertices v_i and v_j of the d-cube, if the edge v_iv_j is a diagonal of $\mathcal{C}^k$. Thus the dimension of $\mathcal{C}^k$ is the Hamming distance between v_i and v_j. Note that $\mathcal{C}^k$ need not include the origin (of $\mathcal{C}^d$) in this case. Let now V be a subset of the vertices of $\mathcal{C}^d$ and $V' \subseteq V$ a subset of $\mathcal{C}^k$. Since the edges of the convex hull of a k-dimensional point set do not change when we add points in higher dimensions only on one side of this set, it follows that all edges of the convex hull of V' are part of the convex hull of V. We thus get the following observation.

Observation 1 *Let V be a vertex set of the d-cube. An edge $e = v_iv_j$, $v_i, v_j \in V$, is part of the convex hull of V iff e is part of the convex hull of the subset induced by the subcube spanned by v_i and v_j.*

Let V be a subset of vertices of the d-cube. From Observation 1 it follows that we can compute the edges of the convex hull of V by inserting all edges spanned by vertices of V in order of non-decreasing length. For every edge e we consider the subcube $\mathcal{C}^k$ spanned by its two endpoints and the subset $V' \subseteq V$ induced by $\mathcal{C}^k$. If the edge skeleton of V' has more than one main diagonal (with respect to $\mathcal{C}^k$) then none of them can belong to the convex hull of V' and thus V. Else we have to check whether the diagonal e is part of it. To this end consider the set E of edges of the (partially) convex hull of V' emanating from one endpoint of e. Note that all these edges are shorter than e and therefore we already know that they are part of the convex hull. Then e belongs to the convex hull iff e is no positive linear combination of edges from E. Thus we have to solve a corresponding linear-programming problem for E and e is part of the convex hull iff the system has no feasible solution. Using this approach we computed the number of edges and the maximal vertex degree of all 0/1-polytopes of dimension 5.

Based on the database obtained by the above investigations we have implemented a small program which enables us to generate the set of all d-dimensional 0/1-polytopes, $2 \leq d \leq 5$, with prescribed properties within a few seconds.* For example one can ask for all five-dimensional 0/1-polytopes with at least 10 vertices and more than 30 facets that are simplicial.† Moreover the program offers the option to generate the output in POLYMAKE-format (see [18]), such that further investigations or the visualization of the resulting polytopes can easily be done by this nice tool.

3 Extremal Properties of 0/1-Polytopes of Dimension 5

In this section we summarize the results obtained from the classification of 0/1-polytopes described in the last section.

3.1 Counting Facets

Motivation for counting the number of facets of 0/1-polytopes is given by Ziegler [21, 22], Henk et.al. [11] and Kortenkamp et.al. [15]. We denote the maximal number of facets of a d-dimensional 0/1-polytope with $f(d)$. It is well known and easy to check that $f(d) = 2^d$ for $d \leq 4$. For dimension 5 a 0/1-polytope with 40 facets is known, i.e. $f(5) \geq 40$, but it was unknown whether this bound is tight. The general question is how fast $f(d)$ grows with d. In particular it is unknown if there exists a constant c such that $f(d) < c^d$ for all d [21, 22]. The latest results in the race for 0/1-polytopes with many facets of up to dimension 13 can be obtained from the homepage of Kortenkamp [14].

*This program can also be accessed via e-mail: write to `cggg@igi.tu-graz.ac.at` with the body "01poly" for further information.

†For the interested reader: There are 7 equivalence classes satisfying these properties, giving together 3008 such 0/1-polytopes, with 32 facets each.

k	full-dim. vertex sets	full-dim. classes	number of facets min. / average / max.		
6	556192	237	6	6.00	6
7	2925056	1062	7	8.35	12
8	10071580	3462	7	11.06	20
9	27678880	8781	7	13.84	26
10	64264048	19767	7	16.41	32
11	128892000	37976	8	18.56	34
12	225738120	65600	7	20.15	40
13	347356800	98786	8	21.16	38
14	471432000	133565	8	21.67	38
15	565722240	158656	8	21.80	36
16	601080360	169110	8	21.64	35
17	565722720	158658	9	21.30	34
18	471435600	133576	8	20.82	31
19	347373600	98804	10	20.24	30
20	225792840	65664	9	19.57	28
21	129024480	38073	10	18.83	27
22	64512240	19963	10	18.03	26
23	28048800	9013	10	17.19	22
24	10518300	3779	9	16.35	20
25	3365856	1326	12	15.52	18
26	906192	472	11	14.74	16
27	201376	131	12	13.99	15
28	35960	47	11	13.28	14
29	4960	10	12	12.58	13
30	496	5	11	11.84	12
31	32	1	11	11.00	11
32	1	1	10	10.00	10
Σ	4292660729	1226525			

Table 2: 5-cube: number of full-dimensional vertex sets, equivalence classes and number of facets of 0/1-polytopes with k vertices.

Table 2 summarizes the results for dimension 5. The first column gives the number k of vertices and the next two columns give the number of vertex sets and the number of classes, respectively, which provide a full-dimensional convex hull. In other words this is the number of sets (classes) where not all vertices lie in a hyperplane. For counting the number of facets or edges we only took these sets into account. Columns 4 to 6 give the minimal, average and maximal number of facets for a fixed number of vertices. Figure 2 shows the corresponding curves. Note that the average is taken over the full-dimensional vertex sets, rather than over the

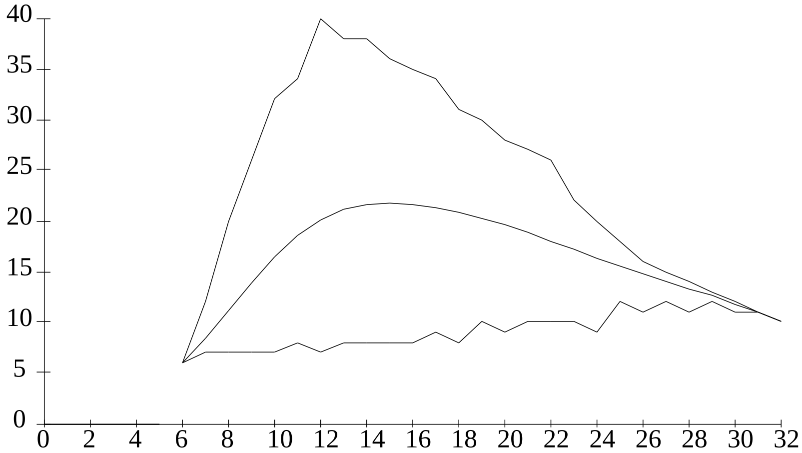

Figure 2: Minimal, average and maximal number of facets of five-dimensional 0/1-polytopes over the number of vertices.

k	full-dim. vertex sets	full-dim. classes	number of facets min. / average / max.		
5	3008	17	5	5.00	5
6	7408	40	6	6.59	9
7	11280	54	6	8.29	13
8	12850	72	6	9.84	16
9	11440	56	6	10.98	15
10	8008	50	7	11.52	14
11	4368	27	8	11.46	13
12	1820	19	7	10.99	12
13	560	6	10	10.37	11
14	120	4	9	9.73	10
15	16	1	9	9.00	9
16	1	1	8	8.00	8
Σ	60879	347			

Table 3: 4-cube: number of full-dimensional vertex sets, equivalence classes and number of facets of 0/1-polytopes with k vertices.

classes. For completeness we give similar results for the 4-cube in Table 3.

Table 2 shows that the average number of facets is maximized for $k = 15$, whereas the "best" single example has fewer vertices, namely $k = 12$. This "shift" can also be observed for $d = 3$ and $d = 4$, cf. Figure 1 and Table 3. Thus it might also be true for higher dimensions and has therefore to be taken into account when looking for "maximizing" sets by investigation of random vertex sets. The most promising vertex sets for maximizing the number of facets might have significantly less vertices than the sets with the maximal average number of vertices.

$v_1 = (0,0,0,0,0)$	$v_5 = (0,1,1,0,1)$	$v_9 = (1,0,1,1,1)$
$v_2 = (0,0,0,0,1)$	$v_6 = (0,1,1,1,1)$	$v_{10} = (1,1,0,0,1)$
$v_3 = (0,0,1,1,0)$	$v_7 = (1,0,0,1,1)$	$v_{11} = (1,1,0,1,0)$
$v_4 = (0,1,0,1,0)$	$v_8 = (1,0,1,0,0)$	$v_{12} = (1,1,1,0,0)$

Table 4: The 12 vertices of the five-dimensional 0/1-polytope with the maximal number of 40 facets.

Our results show that there exists only one unique vertex set of $\mathcal{C}^5$ (up to hypercube symmetries) with 12 vertices and 40 facets and that this is indeed the maximal number of facets for dimension 5.

Lemma 2 *The maximal number of facets of a five-dimensional 0/1-polytope is* $f(5) = 40$. *This number is achieved by the vertex set given in Table 4. It is unique up to hypercube symmetries.*

It is interesting to observe that the equivalence class of the "best" example given in Table 4 contains 192 vertex sets. Its facets are 30 simplices and 10 bipyramids. (All other sets with 12 vertices have ≤ 36 facets.)

Let us close this subsection with a remark on the vertex-facet ratio. Obviously a facet of a d-dimensional 0/1-polytope may contain up to 2^{d-1} vertices, half of the vertices of the d-cube. The other way round it turned out that for $d = 5$ one vertex might be contained in up to 24 facets (achieved e.g. by a set of 14 vertices with 57 edges and 29 facets).

3.2 Counting Edges

Let us now consider the number of edges of 0/1-polytopes. Motivation stems from graph-based algorithms which use the fact that every vertex of a subset of hypercube vertices is extreme, i.e. lies on the convex hull. Thus for many problems local optimization yields a global optimum. Clearly the number of edges and the degrees of the vertices will affect the efficiency of the algorithms.

A trivial lower bound for the maximal number of edges is given by $d2^{d-1}$, the number of edges of the d-cube. Table 5 and Figure 3 show the minimal, average and maximal number of edges of 0/1-polytopes of dimension 5. Table 5 also gives the maximal degree of a vertex.

The maximal number of 112 edges is achieved by a single equivalence class of 60 0/1-polytopes with 24 vertices and 18 facets. The representative set of this class is given in Table 6.

k	number of edges min. / average / max.			max. degree
6	15	15.00	15	5
7	19	19.80	21	6
8	22	25.07	28	7
9	24	30.66	36	8
10	25	36.42	45	9
11	31	42.22	51	10
12	30	47.94	60	11
13	36	53.51	67	12
14	37	58.86	72	13
15	39	63.93	77	14
16	40	68.69	84	15
17	48	73.10	89	16
18	45	77.15	91	17
19	55	80.79	96	17
20	52	84.01	100	17
21	57	86.79	105	17
22	61	89.09	110	17
23	64	90.93	109	16
24	60	92.28	112	16
25	75	93.14	109	16
26	75	93.49	106	15
27	80	93.30	103	14
28	76	92.49	100	13
29	85	90.96	95	12
30	83	88.54	90	10
31	85	85.00	85	8
32	80	80.00	80	5

Table 5: Number of edges and maximal degree of five-dimensional 0/1-polytopes with k vertices.

But also for smaller vertex sets the number of edges might be rather large. For example for 10 vertices there still exists a 2-neighbourly polytope (see Section 4.1), which means that any pair of vertices is adjacent. Thus for small vertex sets the maximal number of edges increases near quadratically with the number of vertices. This can also be seen from Figure 4 where the average number of edges for 10-dimensional 0/1-polytopes is given. Figure 4 also gives the upper and lower bounds attained by 20 random vertex sets for each set size. We thus conclude that if the dimension is very high, e.g. $d \geq 100$, the number of edges of the convex hull of a random vertex set of the d-cube is likely to be quadratic in the number of vertices,

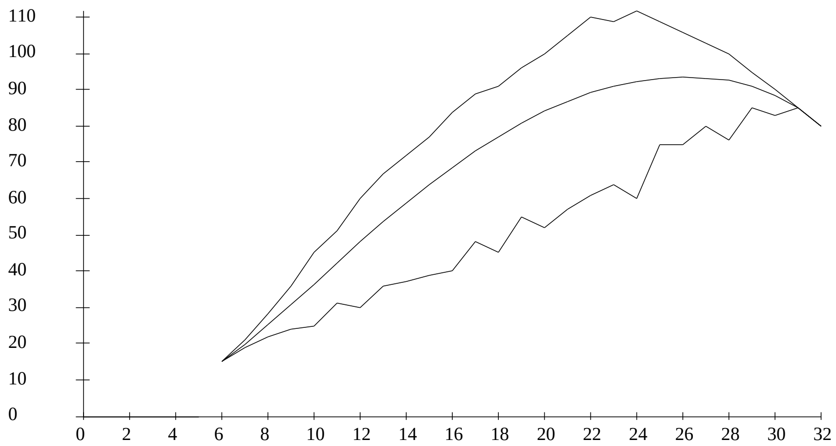

Figure 3: Minimal, average and maximal number of edges of five-dimensional 0/1-polytopes over the number of vertices.

$v_1 = (0,0,0,0,1)$	$v_7 = (0,1,0,0,0)$	$v_{13} = (1,0,0,0,0)$	$v_{19} = (1,1,0,0,0)$
$v_2 = (0,0,0,1,0)$	$v_8 = (0,1,0,0,1)$	$v_{14} = (1,0,0,0,1)$	$v_{20} = (1,1,0,1,1)$
$v_3 = (0,0,1,0,0)$	$v_9 = (0,1,0,1,0)$	$v_{15} = (1,0,0,1,0)$	$v_{21} = (1,1,1,0,0)$
$v_4 = (0,0,1,0,1)$	$v_{10} = (0,1,0,1,1)$	$v_{16} = (1,0,0,1,1)$	$v_{22} = (1,1,1,0,1)$
$v_5 = (0,0,1,1,0)$	$v_{11} = (0,1,1,0,1)$	$v_{17} = (1,0,1,0,0)$	$v_{23} = (1,1,1,1,0)$
$v_6 = (0,0,1,1,1)$	$v_{12} = (0,1,1,1,0)$	$v_{18} = (1,0,1,1,1)$	$v_{24} = (1,1,1,1,1)$

Table 6: The 24 vertices of the five-dimensional 0/1-polytope with the maximal number of 112 edges.

see also Section 4.2.

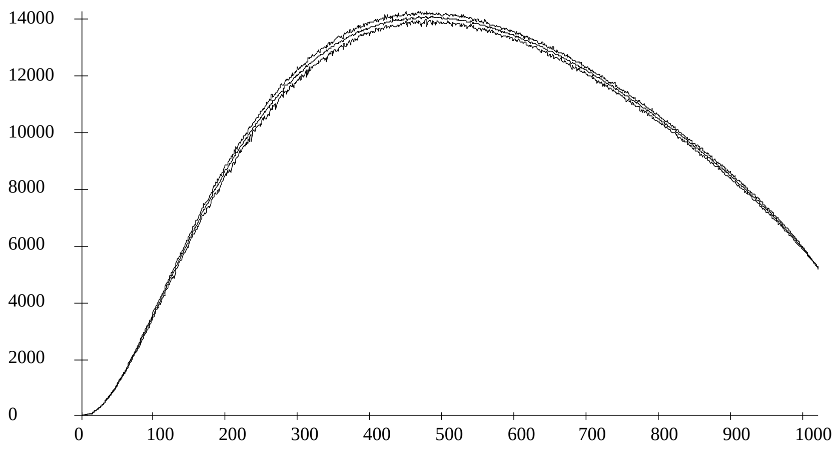

Figure 4: Average number of edges of 10-dimensional random 0/1-polytopes over the number of vertices.

vertices	degree	incident vertices
$v_1 =$ (0,0,0,0,0)	8	$v_2, v_3, v_5, v_8, v_9, v_{10}, v_{11}, v_{12}$
$v_2 =$ (0,0,0,0,1)	7	$v_1, v_4, v_6, v_8, v_9, v_{11}, v_{13}$
$v_3 =$ (0,0,0,1,0)	7	$v_1, v_4, v_7, v_8, v_{10}, v_{11}, v_{14}$
$v_4 =$ (0,0,0,1,1)	7	$v_2, v_3, v_6, v_7, v_8, v_{11}, v_{15}$
$v_5 =$ (0,0,1,0,0)	7	$v_1, v_6, v_7, v_9, v_{10}, v_{11}, v_{16}$
$v_6 =$ (0,0,1,0,1)	7	$v_2, v_4, v_5, v_7, v_9, v_{11}, v_{17}$
$v_7 =$ (0,0,1,1,0)	7	$v_3, v_4, v_5, v_6, v_{10}, v_{11}, v_{18}$
$v_8 =$ (0,1,0,1,1)	11	$v_1, v_2, v_3, v_4, v_9, v_{10}, v_{11}, v_{12}, v_{13}, v_{14}, v_{15}$
$v_9 =$ (0,1,1,0,1)	11	$v_1, v_2, v_5, v_6, v_8, v_{10}, v_{11}, v_{12}, v_{13}, v_{16}, v_{17}$
$v_{10} =$ (0,1,1,1,0)	11	$v_1, v_3, v_5, v_7, v_8, v_9, v_{11}, v_{12}, v_{14}, v_{16}, v_{18}$
$v_{11} =$ (1,0,1,1,1)	17	$v_1, v_2, v_3, v_4, v_5, v_6, v_7, v_8, v_9, v_{10}, v_{12}, v_{13}, v_{14}, v_{15}, v_{16}, v_{17}, v_{18}$
$v_{12} =$ (1,1,0,0,0)	8	$v_1, v_8, v_9, v_{10}, v_{11}, v_{13}, v_{14}, v_{16}$
$v_{13} =$ (1,1,0,0,1)	7	$v_2, v_8, v_9, v_{11}, v_{12}, v_{15}, v_{17}$
$v_{14} =$ (1,1,0,1,0)	7	$v_3, v_8, v_{10}, v_{11}, v_{12}, v_{15}, v_{18}$
$v_{15} =$ (1,1,0,1,1)	7	$v_4, v_8, v_{11}, v_{13}, v_{14}, v_{17}, v_{18}$
$v_{16} =$ (1,1,1,0,0)	7	$v_5, v_9, v_{10}, v_{11}, v_{12}, v_{17}, v_{18}$
$v_{17} =$ (1,1,1,0,1)	7	$v_6, v_9, v_{11}, v_{13}, v_{15}, v_{16}, v_{18}$
$v_{18} =$ (1,1,1,1,0)	7	$v_7, v_{10}, v_{11}, v_{14}, v_{15}, v_{16}, v_{17}$

Table 7: five-dimensional 0/1-polytope with 18 vertices and 75 edges. Vertex v_{11} achieves the maximal degree 17.

Let us now consider the degree of the vertices. Clearly the average degree is just one half of the average number of edges. Thus we ask here only for the maximal degree a vertex can achieve. A lower bound of 2^{d-1} is given by the pyramid over $\mathcal{C}^{d-1}$: Take one half of the cube, say all vertices on the "left" side, and one additional vertex on the "right" side. Then obviously the vertex on the right side is adjacent to all other vertices, i.e. has degree 2^{d-1}.

It suggests itself to conjecture that the above lower bound is tight. By complete enumeration it is easy to verify that this is in fact the case for $d \leq 4$. But surprisingly the conjecture does not hold in general: Table 7 gives an example of 18 vertices of dimension 5, their degree and incident vertices. Here vertex v_{11} is adjacent to all other vertices of the set, i.e. has degree 17.

3.3 Simple and Simplicial 0/1-Polytopes

A d-dimensional polytope is *simplicial* if all its proper faces are simplices, that is, every facet has the minimal number of d vertices. It is *simple* if every vertex is contained in the minimal number of only d facets (see e.g. [20]).

For example the hypercube is a simple 0/1-polytope and the convex hull of any subset of vertices from $\mathcal{C}^d$ in general position gives a simplicial 0/1-polytope.

$$
\begin{array}{ll}
v_1 = (0,0,0,0,0) & v_6 = (1,0,1,1,1) \\
v_2 = (0,0,0,0,1) & v_7 = (1,1,0,1,1) \\
v_3 = (0,0,0,1,0) & v_8 = (1,1,1,0,1) \\
v_4 = (0,0,1,0,0) & v_9 = (1,1,1,1,0) \\
v_5 = (0,1,0,0,0) & v_{10} = (1,1,1,1,1)
\end{array}
$$

Table 8: Vertices of a simplicial five-dimensional 0/1-polytope with the maximal number of 10 vertices, 40 edges and 32 facets.

For dimension 5 there are 506 different classes of simplicial 0/1-polytopes, giving together 1122976 such polytopes. Considering simple 0/1-polytopes we get 265 classes (with 574413 polytopes) of which 237 classes represent 5-simplices. The remaining 28 classes build 6 combinatorial equivalent groups, all of whose are the (combinatorial) product of simplices. This shows that all simple 0/1-polytopes of dimension 5 are a product of simplices. Thus for simple 0/1-polytopes the 5-cube is extremal: There is no other simple 0/1-polytope with more vertices, edges or facets (moreover the 5-cube is the only simple five-dimensional 0/1-polytope with 10 facets). Most recently Kaibel and Wolff showed that in fact all simple 0/1-polytopes are the (combinatorial) product of simplices, see [13].

For simplicial 0/1-polytopes the situation is more interesting, although there exists again an extremal 0/1-polytope maximizing at the same time the number of vertices (10), edges (40) and facets (32), respectively. Table 8 gives the vertex set of one such 0/1-polytope. As already mentioned above, all in all we found 7 equivalence classes of this type, with 3008 0/1-polytopes in total.

If we in addition require a simplicial 0/1-polytope to be 2-neighbourly (see Section 4.1) then we get as extremal values 8 vertices, 28 edges and 20 facets.

Let us close this section with a remark: All the "special" 0/1-polytopes of this paper (Tables 4,6,7,8 and 9) are available in the POLYMAKE library (cf. [18]).

4 Higher Dimensions

In this section we give some results for 0/1-polytopes of dimension $d \geq 6$, obtained as spin-off from the complete enumeration of dimension 5.

4.1 2-Neighbourly 0/1-Polytopes

As mentioned in the last section a 2-neighbourly 0/1-polytope is a polytope where any pair of vertices is adjacent. This means that the convex hull of a 2-neighbourly 0/1-polytope with k vertices has $\frac{k(k-1)}{2}$ edges, or, in other words, it represents a complete graph. Clearly 2-neighbourly 0/1-polytopes are worst case examples for algorithms based on the edge skeleton of their convex hull. Thus for fixed dimension d one may ask for the maximal number $N_2(d)$ of vertices of the d-cube for which a 2-neighbourly 0/1-polytope exists.

Obviously the d-simplex is a 2-neighbourly polytope, i.e. $N_2(d) \geq d+1$. On the other hand "one half" of a 2-neighbourly 0/1-polytope for the d-cube yields a 2-neighbourly 0/1-polytope for the $(d-1)$-cube. And adding one vertex to a 2-neighbourly 0/1-polytope for the $(d-1)$-cube gives a 2-neighbourly 0/1-polytope for the d-cube. Thus $N_2(d-1)+1 \leq N_2(d) \leq 2N_2(d-1)$.

$d=4$	$d=5$	$d=6$
$v_1 =$ (0,0,0,0)	$v_1 =$ (0,0,0,0,0)	$v_1 =$ (0,0,0,0,0,0)
$v_2 =$ (0,0,0,1)	$v_2 =$ (0,0,0,0,1)	$v_2 =$ (0,0,0,0,0,1)
$v_3 =$ (0,0,1,0)	$v_3 =$ (0,0,1,1,0)	$v_3 =$ (0,0,0,1,1,0)
$v_4 =$ (0,1,0,0)	$v_4 =$ (0,1,0,1,1)	$v_4 =$ (0,0,1,0,1,1)
$v_5 =$ (1,0,0,1)	$v_5 =$ (0,1,1,1,0)	$v_5 =$ (0,0,1,1,1,0)
$v_6 =$ (1,1,1,0)	$v_6 =$ (1,0,1,0,1)	$v_6 =$ (0,1,0,1,0,1)
	$v_7 =$ (1,0,1,1,1)	$v_7 =$ (0,1,0,1,1,1)
	$v_8 =$ (1,1,0,0,0)	$v_8 =$ (0,1,1,0,0,0)
	$v_9 =$ (1,1,0,1,1)	$v_9 =$ (0,1,1,0,1,1)
	$v_{10} =$ (1,1,1,0,0)	$v_{10} =$ (0,1,1,1,0,0)
		$v_{11} =$ (1,0,0,0,0,0)
		$v_{12} =$ (1,0,1,1,0,0)
		$v_{13} =$ (1,1,0,0,1,0)

Table 9: Vertices of maximal 2-neighbourly 0/1-polytopes for dimensions 4 to 6.

dimension	1	2	3	4	5	6	7	8	9	10
best example	2	3	4	6	10	13	≥ 18	≥ 25	≥ 33	≥ 44
upper bound	2	3	4	6	10	13	24	48	96	192

Table 10: 2-neighbourly 0/1-polytopes with maximal number of vertices for dimensions 1 to 10.

We have $N_2(d) = d+1$ for $d = 1 \ldots 3$, and it is well known that $N_2(4) = 6$, i.e. there exists a 2-neighbourly 0/1-polytope for dimension 4 that is not a simplex, a counter-intuitive phenomenon which has no analogue for $d \leq 3$.

Complete enumeration gives the maximal value for $d = 5$ and $d = 6$. To this end we utilize a result of the last section: $N_2(5) = 10$, where only one equivalence class provides a 2-neighbourly 0/1-polytope with 10 vertices. For dimension $d = 6$ random vertex sets give a lower bound of $N_2(6) \geq 13$. From the above discussion it follows that any vertex set of $\mathcal{C}^6$ with $N_2(6) \geq 14$ must contain a subset of $\mathcal{C}^5$ with 7 or more vertices. We thus considered all 447 different 2-neighbourly vertex sets of $\mathcal{C}^5$ with at least 7 vertices and completed them with vertices on the "opposite half" of $\mathcal{C}^6$. A complete enumeration of all resulting 6-dimensional 2-neighbourly 0/1-polytopes (about half a million) showed $N_2(6) = 13$.

Table 9 gives the vertex sets for the maximal 2-neighbourly 0/1-polytopes for dimensions 4 to 6. It is interesting to note that the 0/1-polytope for dimension 5 is 'one half' of the 6-dimensional example, but does itself only contain subsets of $\mathcal{C}^4$ with at most 5 vertices. In fact no five-dimensional 2-neighbourly 0/1-polytope that has a subset of 6 vertices from $\mathcal{C}^4$ has more than 9 vertices.

For higher dimensions we made incomplete enumerations. E.g. for dimension $d = 7$ we used a similar method as for dimension 6, getting the lower bound $N_2(7) \geq 18$. The investigations also showed that if there exists a vertex set of $\mathcal{C}^7$ with $N_2(7) \geq 19$ then no 6-dimensional subcube contains more than 12 of its vertices. This yields an upper bound of $N_2(7) \leq 24$. Table 10 gives $N_2(d)$ for dimensions $d = 1 \ldots 10$. For general dimension Kortenkamp et. al. have recently given an exponential lower bound for $N_2(d)$, see [15].

4.2 Edge Skeleton of 0/1-Polytopes

There are several practical applications, such as clustering binary data or $\{0,1\}$-string searching (see e.g. Chapters 7 and 8 in [1]), which are based on the edge skeleton of high-dimensional 0/1-polytopes. Typical input parameters for these tasks might be $d = 100 \ldots 200$ with $n = 1000 \ldots 50000$ vertices. Thus the number of vertices is rather small compared to the number of "corners" of the d-cube. To get some insight of the structure of high-dimensional edge skeletons with few vertices we investigated random vertex sets for dimension $d = 15$ of up to 240 vertices.

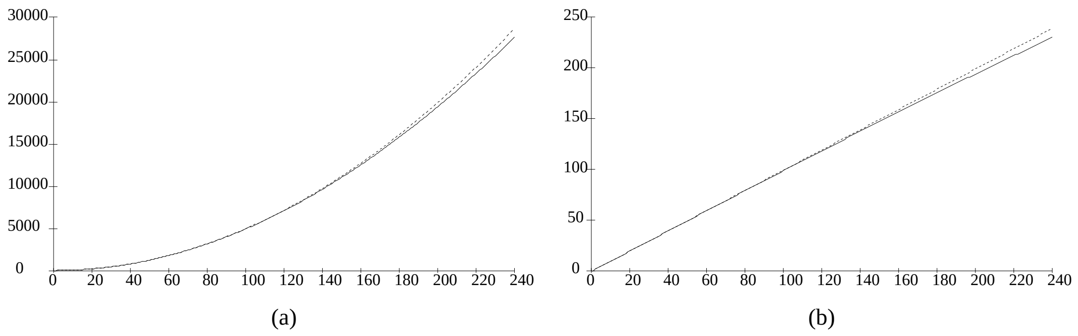

Figure 5: Edge skeleton of 0/1-polytopes for dimension $d = 15$ and $n = 1 \ldots 240$ vertices: (a) average number of edges (solid) and upper bound $n(n-1)/2$ (dotted) (b) average edge degree (solid) and upper bound $n - 1$ (dotted).

For dimension $d = 10$ Figure 4 already shows that for a small number of vertices the maximal number of edges of the convex hull increases quadratically. Figure 5(a) shows the average size of the edge skeleton for dimension $d = 15$ and $n = 1 \ldots 240$ vertices, compared to the upper bound of $n(n-1)/2$. It can be seen that the size of the edge skeleton almost matches the upper bound.

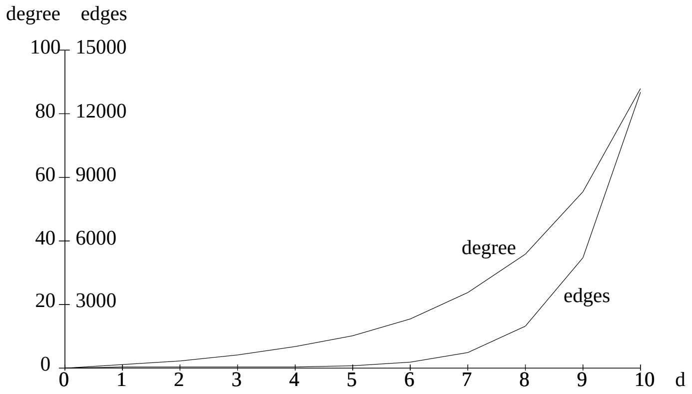

Figure 6: Maximal average edge degree and maximal number of edges of 0/1-polytopes for dimension $d = 1 \ldots 10$.

Figure 5(b) gives the average edge degree and the upper bound $n-1$. Again the curves are very similar, i.e. a random 0/1-polytope with the given parameters is very likely to be a good approximation of a 2-neighbourly 0/1-polytope with the same number of vertices. This indicates that algorithms based on the edge skeleton of the convex hull of high-dimensional 0/1-polytopes are most likely to attain their worst case behavior.

Figure 6 gives the maximal average edge degree and the maximal number of edges of d-dimensional 0/1-polytopes for dimension $d = 1 \ldots 10$. To this end we considered random samples of 100 0/1-polytopes for each dimension and each number of vertices. In correspondence with Figure 5 these curves show that the number of edges and the average edge degree grows significantly with increasing dimensions.

Acknowledgements We would like to thank Franz Aurenhammer, Günter Rote and Günter M. Ziegler for several discussions and helpful comments on the presented topic.

References

[1] O. Aichholzer, *Combinatorial & Computational Properties of the Hypercube*, Ph.D. Thesis, TU-Graz, Austria, April 1997

[2] O. Aichholzer, F. Aurenhammer, *Classifying Hyperplanes in Hypercubes*, SIAM J. Discrete Math, Vol. 9, No.2, pp. 225-232, May 1996

[3] D. Avis, D. Bremner, R. Seidel, *How Good are Convex Hull Algorithms?*, Computational Geometry: Theory and Applications, Vol. 7, pp 265-302, 1997

[4] E.R. Berlekamp, *Algebraic Coding Theory*, McGraw Hill, New York, 1968

[5] N.G. de Bruijn, *Pólya's Theory of Counting*, in E. F. Beckenbach (ed.), Applied Combinatorial Mathematics, Wiley, NY 1964

[6] B. Büeler, A. Enge, K. Fukuda, H.-J. Lüthi, *Exact Volume Computation for Polytopes: A Practical Study*, Abstracts of the 12th European Workshop on Computational Geometry, Münster 1996, pp 57-64

[7] W. Burnside, *Theory of Groups of Finite Order*, Cambridge University Press, 1911

[8] H.S.M. Coxeter, *Regular Polytopes*, Dover Publications, New York, 1963/73

[9] E.N. Gilbert, *Gray Codes and Paths on the n-Cube*, Bell Systems Tech. J. 37, pp 1-12, 1958

[10] B. Grünbaum, *Convex Polytopes*, Interscience, New York, 1967

[11] M. Henk, J. Richter-Gerber, G.M. Ziegler, *Basic Properties of Convex Polytopes*, CRC Handbook on Discrete and Computational Geometry (J.E. Goodman, J.O.'Rourke, eds), pp 243–270, 1997

[12] K. Jacobs, *Einführung in die Kombinatorik*, de Gruyter, Berlin New York, 1983

[13] V. Kaibel, M. Wolff *Simple 0/1-Polytopes*, Preprint

[14] U.H. Kortenkamp, *Small 0/1-Polytopes with Many Facets*, `http://www.math.tu-berlin.de/~hund/01-Olympics.html`

[15] U.H. Kortenkamp, J. Richter-Gerbert, A. Sarangarajan, G. M. Ziegler, *Extremal Properties of 0/1-Polytopes*, Discrete & Computational Geometry Vol. 17, pp 439-448, 1997

[16] J.H. van Lint, R. M. Wilson, *A Course in Combinatorics*, Cambridge University Press, 1992

[17] G. Pólya, *Kombinatorische Anzahlbestimmungen für Gruppen, Graphen und chemische Verbindungen*, Acta Mathematica Vol. 68, pp 145-254, 1937

[18] POLYMAKE, *A versatile tool for the algorithmic treatment of polytopes and polyhedra*, `http://www.math.tu-berlin.de/diskregeom/polymake/doc`

[19] N.J.A. Sloane, *A Short Course on Error Correcting Codes*, CISM Courses and Lectures 188, Springer, Wien, New York, 1975

[20] G.M. Ziegler, *Lectures on Polytopes*, Graduate Texts in Mathematics 152, Springer-Verlag, 1995; Revised printing 1998

[21] G.M. Ziegler, *Recent Progress on Polytopes*, in: "Advances in Discrete and Computational Geometry" (B. Chazelle, J.E. Goodman, R. Pollack, eds.), Contemporary Mathematics, Amer. Math. Soc., Providence, 1998

[22] G.M. Ziegler, *Polytopes and Optimization: Recent Progress and Some Challenges*, GMÖOR Newsletter 3/4, pp 3-12, 1996