ON GENERALIZED BISECTION OF *n*-SIMPLICES

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ABSTRACT. A generalized procedure of bisection of *n*-simplices is introduced, where the bisection point can be an (almost) arbitrary point at one of the longest edges. It is shown that nested sequences of simplices generated by successive generalized bisection converge to a singleton, and an exact bound of the convergence speed in terms of diameter reduction is given. For regular simplices, which mark the worst case, the edge lengths of each worst and best simplex generated by successive bisection are given up to depth *n*. For n = 2 and 3, the sequence of worst case diameters is provided until it is halved.

1. INTRODUCTION

The convex hull $S = [v_1, \ldots, v_{n+1}]$ of n+1 affinely independent vectors v_1, \ldots, v_{n+1} in \mathbb{R}^n is called an *n*-simplex with vertices v_1, \ldots, v_{n+1} (more exactly "the vertex representation of an *n*-simplex"). A family $\{S_i : i \in I\}$, I finite set of indices, of *n*-simplices satisfying

(1)
$$S = \bigcup_{i \in I} S_i$$
 and $\operatorname{int} S_i \cap \operatorname{int} S_j = \emptyset \quad \forall i, j \in I, i \neq j,$

is said to be a (full-dimensional) simplicial partition of S.

Nested sequences of n-simplices, where each element of the sequence is a member of a simplicial partition of its predecessor, are of crucial interest in several fields of computational applied mathematics, where—to a certain extent—the research in each field has been developed independently of the other fields. Usually, one seeks partitioning rules which ensure convergence of each such sequence to a singleton at a fast convergence rate which is often measured by means of the corresponding sequence of diameters in the Euclidean norm. However, the speed in which the diameters converge to zero is not always the determining factor, since often we are interested in the behavior of a certain sequence of functions associated to the sequence of simplices.

One of these fields comprises triangulation methods, in particular piecewise– linear homotopy methods, for finding roots of mappings and related problems, where, however, variable dimension simplicial partitions seem to be even more important than the full–dimensional ones we are interested in here. Among the many excellent books and surveys of this field, see, e.g. [4, 2, 3] and references therein.

A second field, where in particular, the case n = 2 is of interest (triangulation in the literal sense with some generalizations for n = 3 (meshes of tetrahedra)), deals

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with adaptive and multilevel finite element methods for elliptic boundary value problems (e.g., [2, 12, 13, 14] and references therein).

A third field which has recently received much attention comprises branch and bound methods and related techniques for certain broad classes of multiextremal global optimization problems such as minimization of a concave function over a compact convex set, and even the more general problem of minimizing differences of convex functions (for recent books which include abundant relevant references, see [8, 9]). Here, one is usually interested in the case of dimensions n considerably larger than three.

In [6] (see also [7]) it was shown that the following "radial" subdivision of an *n*-simplex $S = [v_1, \ldots, v_{n+1}]$ generates a simplicial partition: let $w \in S \setminus \{v_1, \ldots, v_{n+1}\}$, which is uniquely represented by

(2)
$$w = \sum_{i=1}^{n+1} \lambda_i v_i, \qquad \lambda_i \ge 0, \ i = 1, \dots, n+1, \ \sum_{i=1}^{n+1} \lambda_i = 1,$$

and, for each *i* such that $\lambda_i > 0$, form the simplex S(i, w) obtained from *S* by replacing the vertex v_i by w, i.e., $S(i, w) = [v_1, \ldots, v_{i-1}, w, v_{i+1}, \ldots, v_{n+1}]$.

When w is the midpoint of one of the longest edges of S, we obtain the important *bisection* of simplices which was independently introduced in [6, 7, 10, 17]; see also [5, 16]. Consider a sequence of n-simplices $S_k = [v_{k,1}, \ldots, v_{k,n+1}], k = 1, 2, \ldots$, with longest edges $[v_{k,1}, v_{k,2}]$, where S_{k+1} is constructed from S_k by bisection at $w_k = (v_{k,1} + v_{k,2})/2$. Let $\delta(S_k) = \max\{||x - y|| : x, y \in S_k\} = ||v_{k,1} - v_{k,2}||$ be the diameter of S_k , $k = 1, 2, \ldots$. Then it was shown in [7, 10, 17] that $\delta(S_k) \to 0$ as $k \to \infty$. Kearfort [10] proved that

(3)
$$\delta(S_{k+p}) \le (\sqrt{3}/2)^{\lfloor p/n \rfloor} \, \delta(S_k) \quad \forall \, k, p \in \mathbb{N},$$

where |p/n| is the largest integer less than or equal to p/n. This is equivalent to

(4)
$$\delta(S_{k+n}) \le \sqrt{3/2} \, \delta(S_k) \quad \forall \ k \in \mathbb{N},$$

which has been reproved by somewhat different arguments in [12] and [9, Proposition IV.2]. Sharper bounds and a number of additional results regarding conformal triangular meshes and similarity classes are known for the two-dimensional case of triangles [1, 15, 17, 18] and for some special three-dimensional simplices [5, 11, 16].

In the next section we introduce a new kind of generalized bisection of nsimplices, $n \geq 2$, where now bisection at an arbitrary point $w_k \in [(v_{k,1} + v_{k,2})/2, v_{k,2})$ is admitted provided that there is some $0 < c \leq \frac{1}{2}$ such that $0 < c < ||w_k - v_{k,2}||/||v_{k,2} - v_{k,1}||$ holds for all simplices S_k in a nested sequence. An exact bound for the radius of the smallest ball centered at w_k and containing S_{k+1} is given, from which $\delta(S_k) \to 0$ and a bound which generalizes (4) is derived. For the special case of midpoint bisection we obtain a new proof of (4).

The bound (4) and its generalization to nonmidpoint bisection are exact for regular initial simplices. Therefore, Section 3 presents a closer look at successive bisection of regular simplices. For depths $k, 1 \leq k \leq n$, the lengths of all edges of each "worst" simplex will be given, and it will be shown that at depth n, the "best" simplex will be regular with edge lengths one half of the edge lengths of the initial simplex. For n = 2 (triangles) and n = 3 (tetrahedra) it is shown how many further bisections are necessary to reduce the diameter of each simplex to one half of the initial one.

2. Nonmidpoint bisection

Theorem 1. For a sequence of *n*-simplices $S_k = [v_{k,1}, \ldots, v_{k,n+1}]$, $n \ge 2, k = 1, 2, \ldots$, with longest edges $[v_{k,1}, v_{k,2}]$, where each simplex S_{k+1} is constructed from its predecessor S_k by (generalized) bisection at a point

(5)
$$w_k = \lambda_k v_{k,1} + (1 - \lambda_k) v_{k,2}, \quad 0 < c \le \lambda_k \le \frac{1}{2},$$

for some fixed number $0 < c < \frac{1}{2}$, there holds

- (i) $\delta(w_k, S_k) := \max\{||w_k v_{k,i}|| : i = 1, \dots, n+1\} \le \delta(S_k)\sqrt{1 + \lambda_k^2 \lambda_k},$
- (ii) $\lim \delta(S_k) = 0$ as $k \to \infty$,
- (iii) if, for all k, $\lambda_k = c$, $0 < c \le \frac{1}{2}$, then

$$\delta(S_{k+n}) \le \sqrt{1 + c^2 - c \,\delta(S_k)} \quad \forall k \in \mathbb{N}.$$

Proof. (i): Let $||w_k - v_{k,j}|| = \max\{||w_k - v_{k,i}|| : i = 3, ..., n+1\}$ and consider the triangle $[v_{k,1}, v_{k,2}, v_{k,j}]$ with vertices $v_{k,1}, v_{k,2}, v_{k,j}$. From the definition of $\delta(S_k)$ it follows that

(6)
$$||v_{k,i} - v_{k,j}|| \le \delta(S_k), \quad i = 1, 2, \dots$$

Geometrically, the inequality (6) states that $v_{k,j}$ can neither lie outside the circle C_1 centered at $v_{k,1}$ with radius $\delta(S_k)$, nor outside the circle C_2 centered at $v_{k,2}$ with radius $\delta(S_k)$ (Fig. 1).



FIGURE 1

Since in (5) we consider $\lambda_k \leq \frac{1}{2}$, i.e., $w_k \in [(v_{k,2} + v_{k,1})/2, v_{k,2}]$, it is easy to see that the largest allowed $\delta(w_k, S_k)$ occurs when $v_{k,j}$ lies on the boundary of C_2 . Consider the triangle $[w_k, v_{k,2}, v_{k,j}]$ and let, in this triangle, α_k be the angle at $v_{k,2}$ (Fig. 1). We must have $0 \leq \alpha_k \leq \pi/3$ because $\alpha_k > \pi/3$ and $v_{k,j}$ on the boundary of C_2 would imply that $v_{k,j}$ lies outside C_1 (the two circles intersect at $\alpha_k = \pi/3$). We know from elementary geometry (law of cosine) that

$$\begin{aligned} ||w_k - v_{k,j}||^2 &= ||v_{k,2} - v_{k,j}||^2 + ||v_{k,2} - w_k||^2 \\ &- 2||v_{k,2} - v_{k,j}|| \cdot ||v_{k,2} - w_k||\cos\alpha_k. \end{aligned}$$

Inserting (5) at the right-hand side, we obtain

$$\begin{aligned} ||w_{k} - v_{k,j}||^{2} &= ||v_{k,2} - v_{k,j}||^{2} + \lambda_{k}^{2} ||v_{k,2} - v_{k,1}||^{2} \\ &- 2\lambda_{k} ||v_{k,2} - v_{k,j}|| ||v_{k,2} - v_{k,1}|| \cos \alpha_{k} \\ &\leq \delta^{2}(S_{k})(1 + \lambda_{k}^{2} - \lambda_{k}), \end{aligned}$$

where the last inequality follows from (6) and $\cos \alpha_k \ge \cos \pi/3 = 1/2$. Taking into account the distance from w_k to $v_{k,2}$ and to $v_{k,1}$, respectively, we see that

(7)

$$\delta(w_k, S_k) \le \max\{\lambda_k; \ 1 - \lambda_k; \ \sqrt{1 + \lambda_k^2 - \lambda_k}\} \ \delta(S_k) = \delta(S_k)\sqrt{1 + \lambda_k^2 - \lambda_k}$$

since $\lambda_k \leq \frac{1}{2}$.

(ii), (iii): The smallest value in (7) is $\sqrt{3}/2$ (attained at $\lambda_k = \frac{1}{2}$), the largest one is attained at $\lambda_k = c$. Therefore, we have

(8)
$$1/2 < \sqrt{3}/2 \le \sqrt{1 + \lambda_k^2 - \lambda_k} \le \sqrt{1 + c^2 - c} < 1.$$

To prove (iii) it suffices to consider the case k = 1. Assign to each vertex and each edge of the initial simplex S_1 the label "old", and assign to each vertex and each edge of any S_i , i > 1, which is not labelled "old" the label "new". When for some i > 1 an "old" edge is bisected, the simplex S_{i+1} has one "new" vertex more than S_i . Since an *n*-simplex has n + 1 vertices, we see that a "new" edge must be bisected (i.e., be a longest edge) at some step $i \le n + 1$. This ensures (iii) because of (7), (8).

Property (ii) follows from (iii), (7), (8) and $\delta(S_{k+1}) \leq \delta(S_k) \quad \forall k$.

Remark 1. Clearly, the bound in (i) is exact whenever the simplex S_k contains an equilateral triangle with sidelength $\delta(S_k)$ and vertices in the vertex set of S_k ; the bound (iii) is exact for regular simplices.

3. Bisection of regular simplices

Returning to classical bisection (c = 1/2 in Theorem 1 (iii)), we next will have a closer look at regular simplices which mark the worst case in Theorem 1.

In order to compare simplices with respect to their edge lengths we associate with each simplex the $\binom{n+1}{2}$ -vector x of its edge lengths in decreasing order such that, for the components x_i of x, we have $x_i \ge x_{i+1}$, $i = 1, \ldots, \binom{n+1}{2}$. A simplex S will be called "worse" than a simplex S' when its edge lengths vector x is lexicographically greater than the edge lengths vector x' of S'. (S' will be said to be "better" than S in this case). A lexicographically greatest (smallest) of such vectors will define a "worst" (resp. "best") simplex in a finite set of simplices.

Proposition 1. In the process of successive bisections up to depth n of a regular n-simplex with edge lengths 1

- (i) only edge lengths $1, \sqrt{3}/2, \sqrt{2}/2, 1/2$ can occur.
- (ii) At depth 1 ≤ k ≤ n, each worst simplex has (^{n+1-k}) edges of length 1, k(n k + 1) 1 edges of length √3/2, k edges of length 1/2. The remaining of its (ⁿ⁺¹) edges have length √2/2 (where the number is 0 for k = 1, 2, and (^{k-1}) for k ≥ 3).

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In particular, for k = n, each worst simplex has (n-1) edges of length $\sqrt{3}/2$, $\binom{n-1}{2}$ edges of length $\sqrt{2}/2$ and n edges of length 1/2. (iii) The best simplex at depth n is regular with edge lengths 1/2 and occurs exactly

iii) The best simplex at depth n is regular with edge lengths 1/2 and occurs exactly $2\binom{n+1}{2}\prod_{k=1}^{n-1} (n-k)$ times in the set of all possible simplices generated at depth n.

Proof. Edges and vertices of the initial simplex S_0 will be labelled "old". All edges and vertices appearing in the process which are not labelled "old" will be labelled "new". At level (depth) 1, all possible immediate descendants of S_0 are considered, at level 2, all possible immediate descendants of all simplices of level 1, and so forth.

Bisection of a certain simplex S at the midpoint w of an edge \overline{AB} with length c, gives rise to two immediate descendants, in each of which n new edges are generated. One of these has length c/2, and the length m of each of the remaining (n-1) of these new edges can be determined from the well-known elementary formula

(9)
$$m^2 = 1/2 \left(a^2 + b^2 - c^2/2\right)$$

in each of the n-1 triangles ABC with $a = \overline{AC}$, $b = \overline{BC}$, where C ranges over all vertices of S different from A, B. Notice that formula (9) holds for arbitrary triangles.

Clearly, in each of the first n levels, an old edge is bisected, and we have seen in the preceding section that at level n, no old edge is left in any simplex. At level 1 we have the situation of Fig. 2, all possible $2 \cdot \binom{n+1}{2}$ immediate descendants have one new edge of length 1/2, n-1 new edges of length $\sqrt{3}/2$ and $\binom{n}{2}$ old edges. Because of this similarity we start our investigation at one of these simplices of level 1 so that subsequently detected numbers of simplices of a certain similarity type have to be multiplied by $2 \cdot \binom{n+1}{2}$.



Figure 2

From the proof of Theorem 1, we know that the situation of Fig. 2 can occur only until levels $k \leq n-2$. In levels $1 < k \leq n$, in addition to Fig. 2, we can only have the triangles depicted in Figs. 3 and 4, so that only new lengths of 1/2 and $\sqrt{2}/2$ can occur.

Fig. 3 occurs when the currently bisected edge is adjacent to (i.e., has a common vertex with) a previously bisected edge.



Figure 3

FIGURE 4

	1	$\sqrt{3}/2$	$\sqrt{2}/2$	2 1/2
k = 1	-n	+(n-1)	0	+1
k = 2	-(n-1)	+(n-2)	0	+1
k > 2	-(n-k+1)	+(n-k) - (k-2)	+k-2	+1

Since in every bisection at least one new edge of length 1/2 is generated, each simplex at level n must have at least n edges of length 1/2. Since, moreover, in level 2 we can choose the simplex corresponding to the left triangle in Fig. 3 (with lengths $2 \times 1/2$, $(2n-3) \times \sqrt{3}/2$, $\binom{n-1}{2} \times 1$); and in subsequent levels $3 \le k \le n$ we can always choose the situation of Fig. 4, the simplex of level n with the least number of edges of length 1/2 must have exactly n edges of length 1/2. Likewise, we see, that in this way we do indeed find a worst simplex at any level $2 \le k \le n$: the number of edges of length 1 is $\binom{n+1-k}{2}$ in each simplex at level k, and in each transition from k to k + 1, the increase in the number of edges of length $\sqrt{3}/2$ is maximal in this strategy. Table 1 shows the changes in the number of edges of the occurring lengths for each worst simplex in every level k, where, of course, for each $n \ge 2$, the table is valid only for $1 \le k \le n$.

Summing up, we see that a worst simplex at level $1 \le k \le n$ has $\binom{n+1-k}{2}$ edges of length 1, k(n-k+1)-1 edges of length $\sqrt{3}/2$, k edges of length 1/2, and the remaining of its $\binom{n+1}{2}$ edges of length $\sqrt{2}/2$ (the number is 0 for k = 1, 2, and $\binom{k-1}{2}$ for $k \ge 3$). If in the number k(n-k+1)-1, $1 \le k \le n$, we replace k by n-k+1, $1 \le k \le n$, we obtain the same number, i.e., for n even, the sequence $\{k(n-k+1)-1\}, 1 \le k \le n$, is monotonically increasing until k = n/2, and decreasing in reverse order until k = n; for n odd, it increases until $k = \lfloor n/2 \rfloor + 1$ and repeats its first $\lfloor n/2 \rfloor$ values in reverse order from $k = \lfloor n/2 \rfloor + 2$ to k = n. At level n, a worst simplex has (n-1) edges of length $\sqrt{3}/2$, $\binom{n-1}{2}$ edges of length $\sqrt{2}/2$ and n edges of length 1/2.

Finally, the regular simplices of edge length 1/2 are generated by choosing at each level the simplex corresponding to the right-hand simplex in Fig. 3 (which

amounts to a successive bisection of all n old edges incident to one of the vertices of the first bisected old edge).

Continuation of the above analysis for k > n is cumbersome, in particular for $n \ge 4$. We confine ourselves to the sequence of diameters of the worst simplex until it is halved.

Corollary 1. Let S_0 be a regular *n*-simplex of diameter $\delta(S_0) = 1$. Then, for each nested sequence of simplices $\{S_k\}$ generated from S_0 by successive bisection, we have

 $\delta(S_1) = 1, \quad \delta(S_2) \le \sqrt{3}/2, \quad \delta(S_3) \le 1/2 \quad if \ n = 2;$ $\delta(S_1) = \delta(S_2) = 1, \quad \delta(S_3) \le \sqrt{3}/2, \quad \delta(S_4) \le \sqrt{3}/2, \quad \delta(S_5) \le \sqrt{2}/2,$ $\delta(S_6) \le \sqrt{5}/4, \quad \delta(S_7) \le 1/2 \quad if \ n = 3.$

Proof. For $k \leq n$, the assertion follows from Proposition 1. If n = 2, all simplices generated after two bisections have either edge lengths $\sqrt{3}/2, 1/2, 1/2$ or 1/2, 1/2, 1/2, i.e., after the next bisection the diameter is brought down to 1/2. For n = 3, the worst simplex S_3 has edge lengths $\sqrt{3}/2, \sqrt{3}/2, \sqrt{2}/2, 1/2, 1/2, 1/2$. From the proof of Proposition 1 it is easy to see that in S_3 two edges of length $\sqrt{3}/2$ can be adjacent, but S_3 cannot have a facet of edge lengths $\sqrt{3}/2, \sqrt{3}/2, \sqrt{3}/2, \sqrt{3}/2, \sqrt{2}/2$. It follows from (9) that the 4th bisection generates only one new edge of length greater 1/2, namely the edge of length $\sqrt{5}/4$ resulting from the triangle of edge lengths $\sqrt{3}/2, \sqrt{3}/2, \sqrt{3}/2, 1/2$.

Therefore, the three longest edges of the worst simplex S_4 have lengths $\sqrt{3}/2$, $\sqrt{2}/2$, $\sqrt{5}/4$, whereas the remaining edges have lengths less than or equal to 1/2. Formula (9) shows that further bisections cannot give rise to new edge lengths greater than or equal to 1/2, which proves the last part of Corollary 1.

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