A DEFECT-CORRECTION ALGORITHM FOR MINIMIZING THE VOLUME OF A SIMPLE POLYHEDRON WHICH CIRCUMSCRIBES A SPHERE

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I. INTRODUCTION

Let us define an *n-polyhedron* as a convex polyhedron with n faces, and let us call a polyhedron *simple* if all of its vertices are of degree three. We describe a computer program called LINDELÖF, which first constructs a simple n-polyhedron circumscribing a sphere, and then tilts each face plane, in every iteration, according to a scheme which has been found to reduce the volume of the polyhedron. The initial polyhedron is either randomly generated, or else constructed from specified tangent points. At the λ-th iteration, for each face $f_i(\lambda)$ $(i=1,2,\ldots,n)$ we define

the *defect* $D_i(\lambda) = \tan[\delta_i(\lambda)]$, where $\delta_i(\lambda)$ is the central angle subtended by the face centroid $c_i(\lambda)$ and the face tangent point $r_i(\lambda)$, and

the *correction* $K_i(\lambda) = \tan[\kappa_i(\lambda)]$, where $\kappa_i(\lambda)$ is the angle through which the plane of the face $f_i(\lambda)$ rolls on the sphere.

The relation between correction and defect is illustrated in Fig. 1. For each face $f_i(\lambda)$ in every iteration,

$$\tan[\kappa_i(\lambda)] = w \tan[\delta_i(\lambda)]. \tag{1}$$

The value assigned to the *weight* (or *step length*) w is chosen to maximize the asymptotic rate of decrease of the *rms gap* g, which is a statistical measure - defined in §II.6 - of the overall deviation of face centroids from their associated tangent points. For given n, this optimum value w_0 is found to depend only slightly on the initial configuration of tangent points. For $4 \le n \le 35$, the variation of w_0 with n is described reasonably well by the empirical equation

$$w_0 = .3\ (\overline{m}/3)^{2.75}. \tag{2}$$

$\overline{m}$, which is the average number of edges per face for a simple polyhedron, is given by

$$\overline{m} = 6 - 12/n. \tag{3}$$

In Fig. 2 is shown a graph of Eq. 2, together with values of w_0 obtained for several values of n by averaging the results of calibration runs for a variety of initial configurations of tangent points. So long as $w \approx w_0$, the volume of the n-polyhedron decreases in every iteration, within the limits of precision of the calculation, i.e., until the change in volume per iteration decreases to the noise level.

The set of tangent points in each iteration after the first is related to the set of tangent points from the previous iteration by a non-linear transformation. The expression for this transformation can easily be written in explicit form for the 2-dimensional analog of LINDELÖF, which regularizes any initially irregular plane n-gon circumscribed about the unit circle. Let $T^{(n)}(\lambda) = \{r_j(\lambda) \mid (j=1,2,\ldots,n)\}$ be the set of tangent points of the edges of the n-gon at the λ-th iteration, and let $\Theta_j(\lambda)$ = the polar angle for $r_j(\lambda)$. Then

$$r_j(\lambda+1) = u_j(\lambda)/|u_j(\lambda)|, \tag{4}$$

where

$$\begin{aligned} u_j(\lambda) = {} & (w/4)\sec^2\tfrac{1}{2}(\Theta_j-\Theta_{j-1})\, r_{j-1}(\lambda) \\ & +\{1+(w/4)[\tan^2\tfrac{1}{2}(\Theta_j-\Theta_{j-1})+\tan^2\tfrac{1}{2}(\Theta_j-\Theta_{j+1})]\} r_j(\lambda) \\ & + (w/4)\sec^2\tfrac{1}{2}(\Theta_j-\Theta_{j+1}) r_{j+1}(\lambda). \end{aligned} \tag{5}$$

LINDELÖF is closely related to the question posed by the classical isoperimetric problem for polyhedra:

> Among all n-polyhedra, which has the minimum value of A^3/V^2 ? (A = surface area, and V = volume.)

That such a *best* polyhedron exists was proved by Minkowski [1897]. A theorem by Lindelöf [1869, The i-th face $f_i(\lambda)$ of the simple n-polyhedron $H^{(n)}(\lambda)$ is shown at the beginning of the λ-th iteration. The face $f_i(\lambda)$ is tangent to the unit sphere S at $r_i(\lambda)$; $c_i(\lambda)$ is the centroid of $f_i(\lambda)$, and $\gamma_i(\lambda)$ is the *footpoint* of the centroid.

Let

$$q_i(\lambda) = (1 - w_0)\, r_i(\lambda) + w_0\, c_i(\lambda),$$

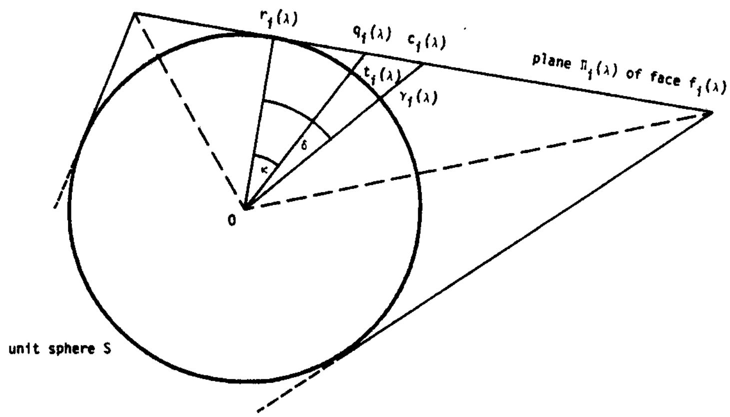
and $t_i(\lambda) = q_i(\lambda) \,/\, |\, q_i(\lambda)\, |$.

At the beginning of the (λ + 1)-th iteration, $r_i(\lambda + 1)$ is set equal to $t_i(\lambda)$, i.e., the face plane $\Pi_i(\lambda)$ is rolled on the surface of S in the direction from $r_i(\lambda)$ to $\gamma_i(\lambda)$, to define $\Pi_i(\lambda + 1)$.

Alternatively, the defect correction may be described by Eq. 1; then

$$\tan[\kappa_i(\lambda)] = |\, q_i(\lambda) - r_i(\lambda)\, |,$$

and $\tan[\delta_i(\lambda)] = |\, c_i(\lambda) - r_i(\lambda)\, |$.



DEFECT CORRECTION BY ROLLING OF FACE PLANE

Fig. 1

1899] states that a necessary condition for a polyhedron H to be best is that
(1) *H circumscribes a sphere,* and
(2) *the inscribed sphere is tangent to all the faces of H at their respective centroids.*
We shall refer to these two conditions as Lindelöf-1 and Lindelöf-2. Since for any polyhedron circumscribed about the unit sphere, $A^3/V^2 = 27V = 9A$, we will hereafter speak of minimizing V (or A) instead of A^3/V^2.

The only values of n for which valid proofs for best polyhedra are recognized are 4, 5, 6, and 12. (Lindelöf completed a 'tentative' proof for n = 7.) The corresponding polyhedra are the regular tetrahedron (n=4), regular trigonal prism (n=5), cube (n=6), regular pentagonal dodecahedron (n=12), and regular pentagonal prism (n=7). Goldberg [1935], in addition to supplying a proof that the regular dodecahedron is best for n=12, also provided plausible arguments to support the conjecture that the best polyhedron is always simple, but this conjecture has never been proved. Goldberg also proved that for an n-polyhedron,

$$A^3/V^2 \geq 54\ (n-2)\ \tan e\ (4 \sin^2 e - 1), \tag{6}$$

where $e = n\pi/[6(n-2)]$; equality holds only for n=4, 6, and 12, i.e., for the three regular polyhedra which are also simple. For all other values of n, Goldberg's lower bound for A^3/V^2 corresponds to a fictitious simple n-polyhedron whose faces are congruent regular $\overline{m}$-gons; $\overline{m}$ is given by Eq. 3.

Steinitz [1928] proved that if a simple polyhedron is the best of its topological type, it must satisfy Lindelöf-1 and Lindelöf-2. (We are unaware of any proof of the converse theorem.) He also found sufficient conditions for a simple polyhedron to be what we shall call *non-inscribable,* i.e., having no metric realization which satisfies Lindelöf-1.

We shall use the terms
inscribable for any polyhedron whose topological type allows it to be metrically realized to satisfy Lindelöf-1,
stabilizable for an inscribable polyhedron whose shape can be adjusted so that it satisfies Lindelöf-2, and
stabilized for a polyhedron which satisfies Lindelöf-2.

It appears that nothing is known about necessary and/or sufficient conditions for a simple polyedron to be stabilizable, aside from Steinitz's criteria for a simple polyhedron to be non-inscribable. Experiments performed with LINDELÖF suggest that it would be quite difficult to find necessary and/or sufficient conditions for a simple polyhedron to be
inscribable, or
inscribable but not stabilizable, or
stabilizable.
Consider, for example, the following conjectures, suggested by these experiments:

The simple 6-polyhedron derived from a trigonal prism by truncating one vertex to produce a triangle face is inscribable but not stabilizable.

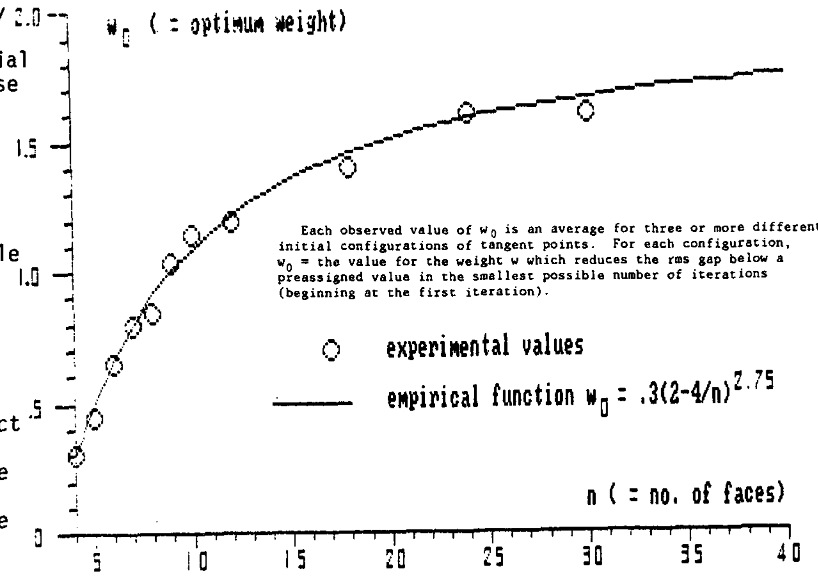
The simple 7-polyhedron derived from the cube by truncating one vertex is stabilizable.

The simple 8-polyhedron derived from the cube by truncating two vertices to produce two triangle faces is inscribable, but it is stabilizable only if the two vertices are incident on the diagonal of a cube face.

The two [unsymmetrical] simple 8-polyhedra whose face inventories are 3(3)4(1)5(2)6(1)7(1) and 3(2)4(3)5(1)6(1)7(1), respectively, are non-inscribable. Steinitz's two sufficient conditions for

non-inscribability are satisfied by neither of these two cases.
It appears that it would not be a trivial matter to confirm or refute any of these conjectures.

If we assume, along with Goldberg, that every best polyhedron is simple, then in order to find the best n-polyhedron (*global* volume minimum), we must adjust every stabilizable simple polyhedron until it satisfies Lindelöf-2, and then compare volumes for all of the stabilized polyhedra (*local* volume minima). Even for relatively small values of n, however, it is not known how to estimate the number S(n) of combinatorially distinct types of stabilizable simple n-polyhedra. Grünbaum [1967] gives the following values for the total number P(n) of combinatorially distinct simple n-polyhedra (whether stabilizable or not):



THE OBSERVED VARIATION WITH n OF THE OPTIMUM WEIGHT w_0, FOR SEVERAL VALUES OF n, COMPARED WITH THE RELATION $w_0 = .3\ (2 - 4/n)^{2.75}$

Fig. 2

n	P(n)	
4	1	
5	1	
6	2	
7	5	
8	14	
9	50	
10	233	
11	1249	(Grace) ("not certain but probably correct")
12	7616	(Brückner) ("probably incorrect")

Goodman and Pollack [1986] have recently shown that for sufficiently large n,

$$c_1\ n \log n < P(n) < 12\ n \log n.$$

One might be inclined to assume that S(n), like P(n), increases rapidly with n. Monte Carlo runs performed with LINDELÖF, however, suggest otherwise. For no value of $n \leq 35$ have more than twelve distinct stabilized solutions been found, in the course of many independent runs. As a result, it appears feasible to perform a virtually exhaustive search for the best simple n-polyhedra for all $n \leq 40$ or so. Of course, this possibility hinges on an assumption which has not been proved, viz., that if the initial configurations of n tangent points on the sphere are randomly distributed[1], then LINDELÖF will eventually generate every possible stabilized simple n-polyhedron, although not all necessarily with the same frequency.

A search has been made for best polyhedra for $4 \leq n \leq 35$ and for n=42. The results, which are discussed in §IV, are summarized in Table 1 and illustrated in Fig. 3. For those cases in which the principal axis of symmetry does not intersect the centroid of a face, an additional *symmetrical* projected view is included in Fig. 3a.

II. DESCRIPTION OF THE ALGORITHM

In the following abbreviated summary of the algorithm for the random mode of LINDELÖF, every occurrence of the subscript i implies that i=1,2,...,n. Refer to Fig. 1 for illustration of some of the definitions in steps 6-8.

1. Set counter $\lambda = 0$. Choose value of $w = w_0$. Assign the set $T^{(n)}(\lambda)$ of n randomly distributed points $r_i(\lambda)$ to the boundary of the unit sphere S, which is centered at the origin O.

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[1] In order to generate the tangent points for an inscribable simple n-polyhedron whose faces are distributed randomly on the sphere, it is not sufficient simply to assign n randomly distributed points to the sphere. To insure that the polyhedron is closed, it is necessary to specify that there exists some 4-point subset of the n points which contains the center of the sphere (Klee [1972]).

CONJECTURE: If d+1 points are randomly distributed on the (d-1)-sphere in R^d (d=1,2,...), then the convex hull of the d+1 points encloses the center of the sphere with probability $1/2^d$.

The proof of this conjecture is trivial for d=1 and d=2. It has been verified within statistical error by 10^7 Monte Carlo runs for d=3 (Schoen [1975], unpublished).

n	A(n) (Area)	A*(n) (Goldberg's lower bound for Area)	A(n)/A*(n)	Symmetry (Schoenflies symbol)	Length distribution for 1-dimensional strings of pentagons	$^{(\nu)}Av$ = average length of 1-dimensional strings of pentagons
4	41.56922	41.56921919	1.000000	T		
5	31.17691	28.90161476	1.078726	D_{3h}		
6	24	24	1.000000	O		
7	21.79627	21.36505014	1.020183	D_{5h}		
8	20.10275	19.71660183	1.019584	D_{2d}		
9	18.78957	18.58770224	1.010860	D_{3h}		
10	17.92357	17.76620682	1.008857	D_{4d}		
11	17.33725	17.14166402	1.011410	C_{2v}		
12	16.65087	16.65087291	1.000000	I		
13	16.35170	16.25505352	1.005945	C_{2v}		
14	15.99389	15.92909072	1.004068	D_{6h}		
15	15.72124	15.65600391	1.004167	C_{2v}		
16	15.47222	15.42390093	1.003133	T		
17	15.28330	15.22420558	1.003882	C_{2v}		
18	15.10339	15.05057731	1.003509	D_3		
19	14.95372	14.89822772	1.003725	C_2		
20	14.80646	14.76347307	1.002912	D_{2d}	12 (closed loop)	12
21	14.68280	14.64343314	1.002688	C_2	12 (open string)	12
22	14.57089	14.53582354	1.002412	D_2	6^2	6
23	14.47430	14.43880948	1.002458	D_3	4^3	4
24	14.38053	14.35089999	1.002065	D_2	3^4	3
25	14.30239	14.27087150	1.002209	C_1	$4, 3^2, 2$	3
26	14.22510	14.19770976	1.001930	C_2	$3^2, 2^3$	2.4
27	14.15108	14.13056787	1.001452	C_{2v}	$2^5, 1^2$	∿1.7
28	14.08949	14.06873237	1.001475	C_3	2^6	2
29	14.03547	14.01159848	1.001704	D_3	2^6	2
30	13.98028	13.95864944	1.001550	C_{2v}	$2^4, 1^4$	1.5
31	13.92713	13.90944189	1.001272	C_{3v}	$2^3, 1^6$	∿1.3
32	13.87325	13.86359307	1.000697	I	1^{12}	1
33	13.83899	13.82077047	1.001318	C_s	$4, 1^9$	∿1.3
34	13.79755	13.78063870	1.001227	D_2	$2^2, 1^8$	1.2
35	13.76104	13.74307996	1.001307	C_{2v}	$2^2, 1^8$	1.2
42	13.54396	13.53343547	1.000778	D_{5h}	1^{12}	1

Table 1

Tentative best n-polyhedra ($4 \leq n \leq 35$; n = 42).

2. If $0 \subset$ the convex hull of some 4-point subset of $T^{(n)}(\lambda)$, then go to step 3 - otherwise choose a new random number seed and return to step 1.

3. Construct the plane $\Pi_i(\lambda)$ tangent to S at $r_i(\lambda)$.

4. From the set $V^{(n)}(\lambda)$ of $\binom{n}{3}$ points $v_{rst}(\lambda) = \Pi_r(\lambda) \cap \Pi_s(\lambda) \cap \Pi_t(\lambda)$ (r,s,t=1,2,...,n), identify the 2n-4 bona fide vertices. They comprise the set $\overline{V}^{(n)}(\lambda) = \{v_{rst}(\lambda) \mid \langle r_i(\lambda), v_{rst}(\lambda)\rangle \leq 1 \text{ for all } i \in [1,n]\}$.

5. Define the face $f_i(\lambda)$ as the convex hull of all vertices $v_{rst}(\lambda) \in \overline{V}^{(n)}(\lambda) \ni r=i$ or $s=i$ or $t=i$, and define the polyhedron $H^{(n)}(\lambda)$ as the convex hull of the 2n-4 vertices $\in \overline{V}^{(n)}(\lambda)$.

6. For each face $f_i(\lambda)$,

   (a) locate both its centroid $c_i(\lambda)$ and also the *footpoint* $\gamma_i(\lambda)$ of $c_i(\lambda)$ ($\gamma_i(\lambda)$ = the intersection of the line through 0 and $c_i(\lambda)$ with the boundary of S);

   (b) compute the local gap $g_i(\lambda) = | c_i(\lambda) - r_i(\lambda) |$.

   If the rms gap $g = [(1/n) \sum_{i=1}^{n} [g_i(\lambda)]^2]^{1/2} \geq$ a preassigned length η ($\eta \cong 10^{-7}$ for single precision calculations), then go to step 7 - otherwise stop.

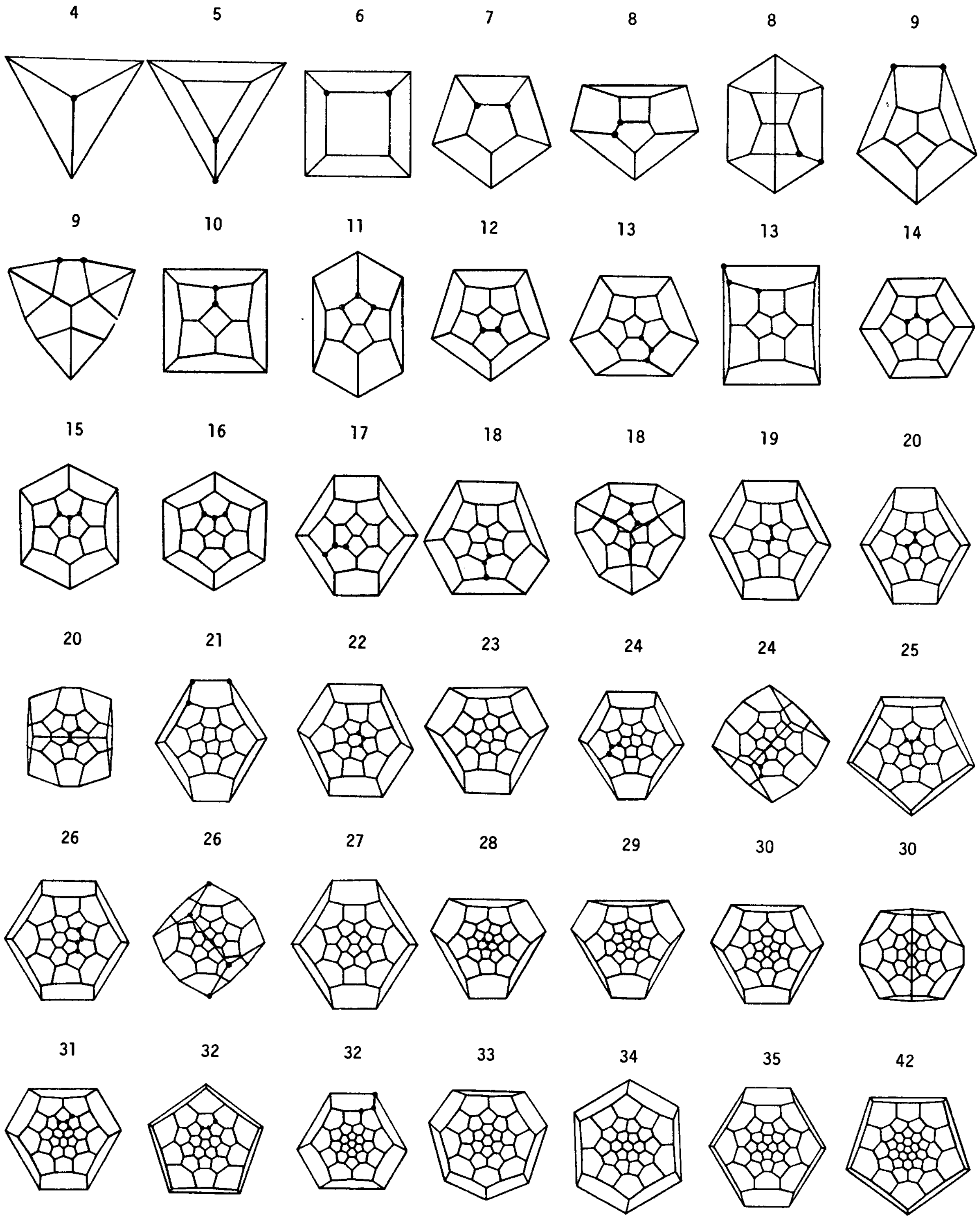


Fig. 3a Schlegel diagrams of tentative best n-polyhedra ($4 \leq n \leq 35$; n=42)

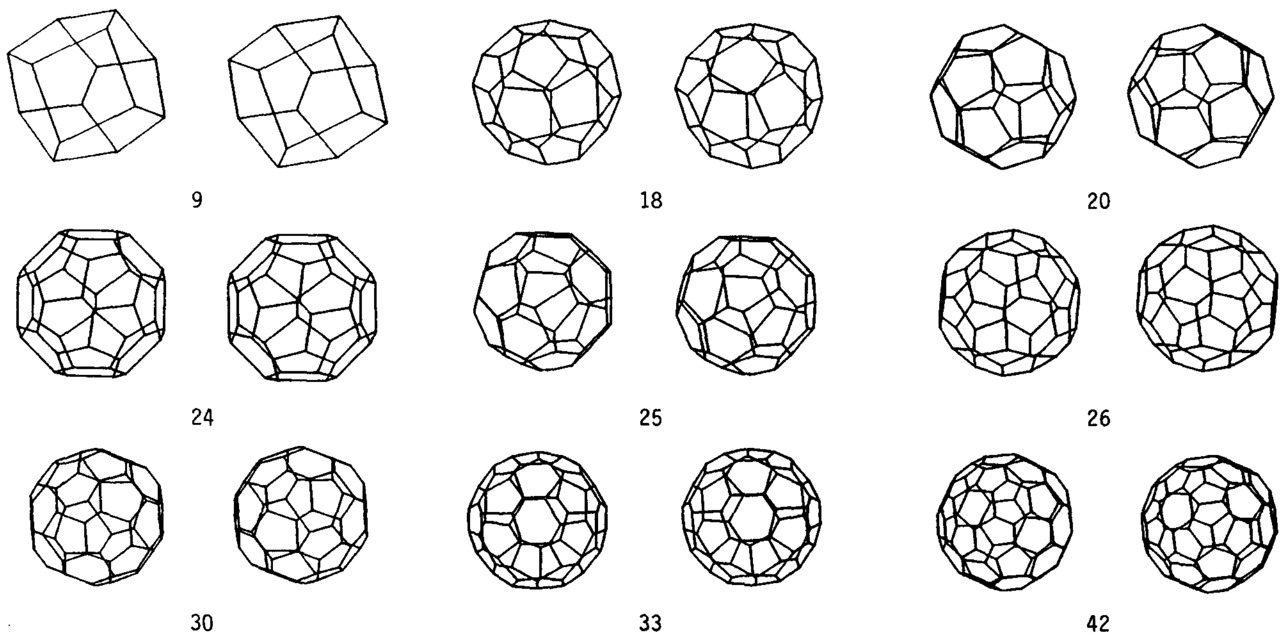


Fig. 3b Stereoscopic projections of selected best n-polyhedra

7. On the face $f_i(\lambda)$, identify the point $q_i(\lambda) = (1 - w_0)\, r_i(\lambda) + w_0\, c_i(\lambda)$,

   and roll the plane $\Pi_i(\lambda)$ on S until it is tangent to S at $t_i(\lambda) = q_i(\lambda) / |q_i(\lambda)|$.

8. Set counter $\lambda = \lambda + 1$. Let $r_i(\lambda) = t_i(\lambda - 1)$. Go to step 3.

In practice, LINDELÖF either (a) calculates the point of intersection for every one of the $\binom{n}{3}$ plane triples in every iteration (*all plane triples* mode), as described above, or else (b) --once it is judged that the topological type will undergo no further changes--calculates points of intersection only for 2n-4 specified plane triples (*fixed vertex set* mode). In mode (a), the run time is somewhat worse than $O(n^3)$, because the average number of type changes which occur before the final transition to a stabilizable type takes place is found to increase with n. In mode (b), run time is O(n).

III. PROGRAM PERFORMANCE

(1) For a given value of n, so long as the topological type remains invariant, the rms gap g shows an asymptotic exponential decrease with iteration number. However, if a change of topological type is about to occur as a result of a single local rearrangement of faces, it is found that the rms gap stops decreasing several iterations before the change and instead increases until after the change has taken place. It then resumes its downward course. During the initial development of LINDELÖF (in compiled PC Basic, single-precision, on an IBM PC AT), it was planned to reduce the run time by exploiting this effect. In a given iteration, the program mode would be *all plane triples* only if the gap value had failed to decrease for one or more faces in the preceding iteration. Otherwise, the program mode would be *fixed vertex set*.

When it was found that a single-precision Fortran version of LINDELÖF ran more than 200 times faster on an IBM 4341 than did the original program on a PC AT, it was decided that even the small effort required for the proposed changes could be justified only if subsequent runs for n >> 30-40 were to be made on a microcomputer, or else if runs for n >> 30 were planned for a mainframe computer. Almost all subsequent runs have in fact been made on the IBM 4341, and no runs for n >> 30 are contemplated. In every run, output data files generated by the program are downloaded to a PC AT or PC XT for graphic display both of separate face polygons and of perspective projections of the polyhedron itself. The symmetry point group for the polyhedron is determined by viewing *stereoscopic* perspective projections directly on the display screen. A program could of course be developed to perform the identification of the symmetry group (cf. Wolter et al. [1985]).

(2) No method has been developed for proving that the n-polyhedron produced in a given iteration is stabilized. Instead, an n-polyhedron at a given iteration is arbitrarily classified as stabilized

only if the rms gap is smaller than some preassigned value (which depends on n) and also has been found to decrease exponentially at an essentially constant rate for a sufficient number of consecutive preceding iterations.

If $w \cong w_0$, then when a transition to what has been classified as a stabilizable type has occurred, continued iteration of plane tilting may either

continue indefinitely - without a change in type - to reduce both volume and rms gap (within the limits of precision of the calculation),

or

induce a transition to another stabilizable type with smaller asymptotic (i.e, stabilized) volume.

No transitions have been observed to occur between two types which have been classified as stabilizable, except when the first of the two types is the (n-2)-prism. It is possible, however, that other such cases have occurred and simply escaped notice. It seems plausible that the probability of a transition from one stabilizable type to another should depend not only on the types and on the current value of the rms gap, but also on the value assigned to the weight w. This question has not been investigated.

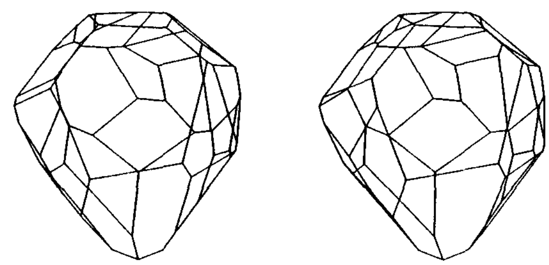


Fig. 3c
Stereoscopic projection of initial state of *random* 33-polyhedron

(3) It is trivial to prove that a right regular (n-2)-prism is a stabilized polyhedron for $n \geq 5$. Runs of LINDELÖF made in random mode have so far yielded the (n-2)-prism as a stabilized solution for all $n < 10$, but not for $n \geq 10$. It is reasonable to assume that in random mode, it becomes more and more unlikely - with increasing n - that precisely n-2 of the initial tangent points will be confined to a narrow equatorial band, while the remaining two points fall into regions in the neighborhood of the north and south poles, respectively. (A configuration of this sort would be required for a polyhedron isomorphic to the (n-2)-prism.) For large n, it is extremely improbable that repeated iterations of plane tilting would produce a change from a type which corresponds to a relatively uniformly dispersed set of tangent points to the quite non-uniform distribution which corresponds to the (n-2)-prism.

IV. DISCUSSION OF RESULTS

1. Goldberg [1935] anticipated the possibility that best polyhedra having *no* symmetry might exist. The tentative best solution for n=25 is just such a case.

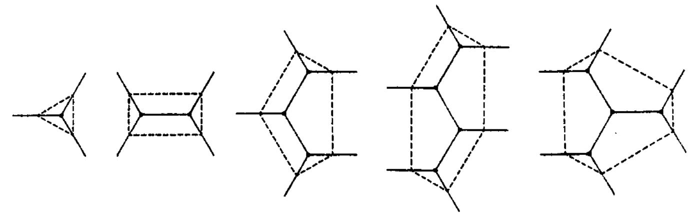
2. The 32 tentative best polyhedra which have been identified display a great variety of types of symmetry (sixteen). It seems likely that a few additional types--e.g., C_i, C_5, C_{5v}, D_{2h} -- will be found if the search is extended to larger values of n.

3. Classifying solutions according to their symmetry is somewhat misleading, since the set of faces of a polyhedron can display a high degree of order in the absence of symmetry. Consider, for example, the broken symmetry in the Schlegel diagram for n=25 shown in Fig. 3. If it were not for the edges which lie inside the boundary of the cluster of four faces near the center of the diagram, the pattern would be isomorphic to an edge skeleton with C_s symmetry (single plane of reflection). Somewhat similar statements may be made about the effect on symmetry of clusters of four or more faces in the diagrams for n=19, 21, 24, 26, and 34.

Goldberg [1935] described candidates for the best 32- and 42-polyhedra, both of which have icosahedral symmetry. He mentioned these cases because - as he stated - they are amenable to hand calculation on account of their high symmetry. The results described here support Goldberg's candidate for n=32 (polyhedron isomorphic to the truncated icosahedron). For n=42, however, the icosahedrally symmetric case described by Goldberg has been found to have slightly larger volume than a polyhedron, illustrated in Fig. 3, which has the symmetry of a right regular pentagonal prism. The contrast between these two examples (n=32 and n=42) illustrates the hazard of attaching special significance to the symmetry of a stabilized solution.

4. If H(n) denotes the tentative best n-polyhedron, then we may say that the topological structures of the edge skeletons for H(n) and H(n+1) exhibit a strong tendency to be related by *vertex truncation:* for 25 of the 31 pairs {H(n), H(n+1)} in the interval $4 \leq n \leq 35$, the Schlegel diagram for H(n+1) can be derived from that of H(n) by one of the vertex truncations illustrated in Fig. 4. (The exceptions

are n=23, 27, 29, 30, 33, and 34). The effect of a truncation is to remove from H(n) the s vertices ($1 \leq s \leq 4$) in the interior of the dashed polygon and to add to H(n) the s+2 edges and s+2 vertices on the boundary of the dashed polygon, yielding H(n+1). (In the Schlegel diagrams of Fig. 3, the vertices in H(n) whose removal by truncation yields H(n+1) are distinguished by large dots.) Alternatively, we may describe H(n+1) as derived from H(n) in these 25 cases by the addition of a new tangent point to the set of n tangent points of H(n). The new point is inserted into the interior of one of the five kinds of dashed polygons of Fig. 4, after which the n original tanget points undergo a general relaxation to stabilize H(n+1).



THE VARIETIES OF VERTEX TRUNCATION WHICH - WHEN APPLIED TO THE BEST n-POLYHEDRON - TEND TO PRODUCE A POLYHEDRON WHICH IS ISOMORPHIC TO THE BEST (n+1)-POLYHEDRON

Fig. 4

5. Goldberg [1935] defined a *medial* polyhedron as a simple polyhedron having no two faces which differ in number of edges by more than one. He conjectured, moreover, that for every n for which a medial polyhedron exists, the best polyhedron is medial. (Medial polyhedra fail to exist only for n=11 and n=13.) Results obtained for n=33 cast doubt on Goldberg's conjecture. The best of the 6 stabilized solutions found in 40 independent runs for n=33 is not medial (cf. Fig. 3). It is comprised of 19 hexagons, 13 pentagons, *and 1 heptagon.*

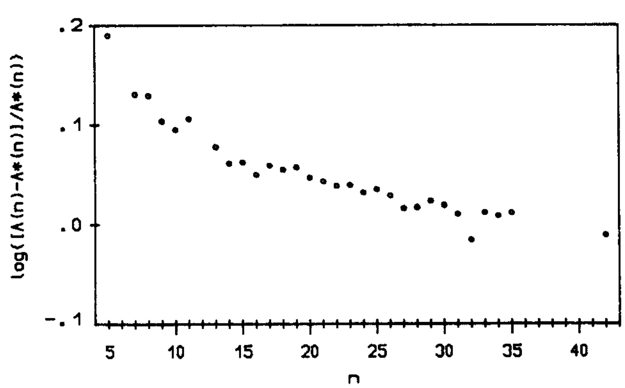
6. Except for the (n-2)-prism, most of the polyhedra found to be stabilizable for $n \geq 24$ can be described roughly as consisting of a quasi-uniform distribution of pentagons in a matrix either of hexagons or else of hexagons plus 1 or 2 quadrangles and/or heptagons. In this regime, pentagons behave as if there is a mutual repulsion between them. If an initial configuration is designed with pentagons assigned principally to one hemisphere, they tend to diffuse into the other hemisphere, against a countercurrent of hexagons.

7. The entries in the sixth column of Table 1, for the interval $20 \leq n \leq 42$, describe the distribution of lengths of *1-dimensional strings* of pentagons. It is hardly surprising that for each best polyhedron in this interval, no vertex is incident on more than two pentagons, and the pentagons form strings whose average length $\langle \nu \rangle_{Av}$ is--roughly speaking--as short as possible. Let A(n) = area of H(n) (tentative best n-polyhedron), and A*(n) = Goldberg's lower bound for A(n) (cf. Eq. 6). For $23 \leq n \leq 35$, the ratio A(n)/A*(n), which is entered in the fourth column of Table 1, is found to decrease with n only when $\langle \nu \rangle_{Av}$ decreases with n. ($\langle \nu \rangle_{Av}$ appears in the seventh column of Table 1.) The variation with n of A(n) - A*(n) is shown in a semi-log plot in Fig. 5.

8. Berman and Hanes [1970] and Klee [1972] mentioned a possible relation between the isoperimetric problem for n-polyhedra (*circumscribed polyhedra*) and the following problem (*inscribed polyhedra):*

> *for what configuration of n points on the sphere is the volume of their convex hull a maximum?*

After Berman and Hanes had obtained the solution for the inscribed 8-polyhedron in closed form, Klee conjectured [1972] that the solutions to these two problems, for every $n \geq 4$, are geometrical duals. In unpublished work in 1975, however, the author found that the case n = 8 provides a counterexample to Klee's conjecture. It was proved that the geometrical dual of the closed form solution for the inscribed polyhedron does not satisfy Lindelöf-2, and therefore cannot be best. (The details will be published elsewhere.)



FRACTIONAL EXCESS AREA, WITH RESPECT TO THE GOLDBERG LOWER BOUND, vs. n

Fig. 5

Since the two polyhedron problems are not always geometrical duals, it seems probable that for some sufficiently large value of n, they are not even topological duals.

For n = 8, in random mode, LINDELÖF has yielded only two solutions: the [tentative best] medial polyhedron, which is the topological dual of the Berman and Hanes figure, and--less often--the right regular hexagonal prism. It was suggested by Goldberg [1935] that the medial polyhedron is probably the best 8-polyhedron. The twice-truncated cube mentioned in the introduction has not been generated in LINDELÖF's random mode.

V. STEP LENGTH TUNING

In the analysis of the 2-dimensional analog of LINDELÖF described by Eqs. 4 and 5, the step length w was assumed to have the same value for all edges of the n-polygon. Similarly, for the 3-dimensional case, the step length was assumed to be the same for all faces of the n-polyhedron. The justification for these assumptions is that they lead to satisfactory asymptotic rates of decrease of the relevant objective function in each case, so long as the value chosen for w is adjusted according to the value of n. The following analysis for the 2-dimensional case suggests the possibility of choosing w, for each edge, to be proportional to the *length* of the edge, for given n.

As in Eqs. 4 and 5, let θ_i be the angle, in plane polar coordinates, of the tangent point for the i-th edge. Let P and A be the perimeter and area of the n-polygon, respectively. We wish to minimize P^2/A, but since for any polygon circumscribed about the unit circle $P^2/A = 4A = 2P$, we may equally well speak of minimizing A (or P). If L_i = the length of the i-th edge,

$$P = \sum_{i=1}^{n} L_i$$

$$= 2\sum_{i=1}^{n} \tan\tfrac{1}{2}(\theta_{i+1}-\theta_i). \tag{7}$$

Then

$$\frac{\partial P}{\partial \theta_i} = \{[\tan\tfrac{1}{2}(\theta_i-\theta_{i-1}) + \tan\tfrac{1}{2}(\theta_{i+1}-\theta_i)]\cdot[\tan\tfrac{1}{2}(\theta_i-\theta_{i-1}) - \tan\tfrac{1}{2}(\theta_{i+1}-\theta_i)]\}$$

$$= 2L_i \tan\delta_i, \tag{8}$$

where δ_i = the central angle subtended by the tangent point r_i and the centroid c_i of the i-th edge. The factor L_i in Eq. 8 suggests that for the λ-th iteration, we might let

$$w_i(\lambda) = \frac{L_i(\lambda)}{\langle L(\lambda)\rangle_{Av}}\, w_0; \tag{9}$$

$w_i(\lambda) = \tan[\kappa_i(\lambda)]/\tan(\delta_i(\lambda)]$, $\langle L(\lambda)\rangle_{Av}$ = average edge length, and w_0 is a constant [average] weight chosen empirically to maximize the asymptotic convergence of the objective function (e.g, perimeter).

Systematic tests have shown that the "tuning" of the step length described by Eq. 9 does not lead to a uniform improvement in the rate of convergence. For n=3 and n=4, in fact, it leads to a significant worsening in program behavior: in the first few iterations, the transformation of the closed polygon into an *open* polygon occurs with increasing frequency. (To prevent this catastrophe, both the 2- and 3-dimensional versions of LINDELÖF replace the assigned fixed value for w_0 by a set of drastically reduced--but increasing--values just for the first five or ten iterations, whenever the initial randomly constructed polygon or polyhedron is excessively large. This strategem, which is required only for $n \lesssim 6$, is completely successful.) For $n \geq 5$, step length tuning usually (but not always!) leads to a somewhat stronger initial rate of decrease of the objective function, but the *net* effect is only to reduce the run time by no more than 2 or 3 iterations, for a given required asymptotic value of the objective function.

Now let us consider the counterpart of this problem in three dimensions. Lindelöf [1869] derived the following expression for the surface area S of a polyhedron whose faces A, B, C, ... lie at the [perpendicular] distances p,q,r,... from a fixed interior point:

$$2S = p\Sigma\,(a\cot\tfrac{\alpha}{2}) + q\Sigma(b\cot\tfrac{\beta}{2}) + \dots\,. \tag{10}$$

If $a_1, a_2, a_3, \dots$ are the lengths of the edges of face A, and $\alpha_1, \alpha_2, \alpha_3, \dots$ are the corresponding *internal* dihedral angles (*IDA's*), then

$$\Sigma(a\cot\tfrac{\alpha}{2}) = a_1\cot\tfrac{\alpha_1}{2} + a_2\cot\tfrac{\alpha_2}{2} + \dots \tag{11}$$

If now we consider only polyhedra circumscribed about the unit sphere, then $|p| = |q| = |r| = \ldots = 1$. Furthermore, if we let $\Theta_j - \Theta_i$ = the *external* dihedral angle (*EDA*) for the edge of length e_{ij} incident on faces i and j, then since *EDA* = π - *IDA*, we may write

$$S = 2 \sum_i \sum_j e_{ij} \tan \tfrac{1}{2}(\Theta_j - \Theta_i) \quad \text{(i and j are adjacent faces).} \tag{12}$$

The formal resemblance between Eqs. 7 and 12 suggests the possibility that the i-th component of the directional derivative of the area S of a circumscribed n-polyhedron might include a factor S_i = the area of the i-th face; the derivative has not been calculated, however. In any case, the results of weighting the step lengths for the *faces* according to their respective *areas* (cf. Eq. 9) are found to be strikingly similar to the corresponding results for 2 dimensions: (a) for n = 4,5, and 6, the transformation of the initial closed polyhedron into an open polyhedron occurs more often (unless the step length is drastically reduced for the first 5 or 10 iterations); (b) for $n \leq 7$, there is usually (but not always!) an increase in the rate of reduction of the objective function for early iterations, but the total run time is rarely reduced by more than the equivalent of 2-3 iterations. One might expect that since the asymptotic values of all of the face areas are identical only when n = 4, 6, or 12, tuning of the step length - if it could be justified theoretically - should, in the general case, lead to a small but detectable improvement in the rate of convergence. The fact that no consistent improvement of this kind has been observed suggests that the foregoing analysis is seriously oversimplified. The effectiveness of the underlying algorithm is already limited, after all, by the following ad hoc approximations:
(a) the correction in each iteration is only first order, and
(b) the step length is empirically derived and is fixed at the same constant value in every iteration, although it is known from experiments performed on modifications of LINDELÖF that convergence can be accelerated if an *optimum* fixed value for step length is determined before every iteration.

VI. ADDENDUM

A recent translation of LINDELÖF into double-precision Fortran accepts as input data the following output from the original single-precision version: (a) the 2n-4 face triples which define vertices, and (b) rectangular coordinates for the n tangent points. Operating in *fixed vertex set* mode (cf. §III(1)), this compiled Fortran program requires only a few seconds of run time on an IBM 4341, even for n = 35, to reduce an rms gap value of 10^{-7} (the standard value for the output of the single-precision program mentioned in III(1)) to $\sim 10^{-12}$ or less. The accuracy of the program is confirmed by noting that for the regular 4-, 6-, and 12-hedra, the values obtained for area are in agreement with the *exact* values to ~12 significant figures.

The author has begun to develop an adaptation of LINDELÖF for producing simple *polytopes* of minimum *hypervolume* in R^4. It is assumed - without proof - that the analogs of Lindelöf's necessary conditions for R^3 hold in R^d for d=2,3,4,... .

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