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AN ALGORITHM FOR PIECEWISE-LINEAR APPROXIMATION OF AN IMPLICITLY DEFINED MANIFOLD*

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Abstract. A simplicial method is used to approximate the solution manifold to a system of nonlinear equations, $H(x)=\theta$, where $H: \mathbb{R}^{N+K} \to \mathbb{R}^N$. The method begins at a point x_0 in the solution set where the derivative $DH(x_0)$ is of full rank. Given any $\varepsilon > 0$, a piecewise linear manifold is constructed along which $\|H(x)\|_\infty < \varepsilon$. An algorithm is presented to carry out this construction in an efficient fashion.

Key words. simplicial method, continuation method, implicitly defined manifold

1. Introduction. The purpose of this work is to present a simplicial continuation algorithm for approximating a K-dimensional manifold which is implicitly defined as $\{x \in \mathbb{R}^{N+K}: H(x)=\theta\}$ where H is a smooth map from $D \subseteq \mathbb{R}^{N+K}$ with values in $\mathbb{R}^N$.

The algorithm should prove useful in cases where the implicit function theorem has been invoked and where an approximation to the implicitly defined function is desired. A simple example of such an application would be in computer graphics where a surface defined by $\{(x_1, x_2, x_3) \mid H(x_1, x_2, x_3)=0\}$ is to be represented graphically. More sophisticated application of the algorithm could be made to approximating solutions to a discretized operator equation involving several parameters.

Simplicial continuation methods have traditionally been used to zero points of mappings $H: \mathbb{R}^{N+1} \to \mathbb{R}^N$. Usually H is a homotopy between a mapping with easily obtained zeros and a mapping whose zeros are sought. Early work was carried out by Scarf [15], Hansen [8], Kuhn [9], and Eaves [7]. For further reading on the case $K=1$, see e.g. [3], [10], [11] and the further references cited therein.

Recently, Rheinboldt and colleagues (see e.g. [12]–[14]) have explored methods of approximating smooth manifolds $\mathcal{M} \subset H^{-1}(0)$ where $H: \mathbb{R}^{N+K} \to \mathbb{R}^N$ is smooth, by a "gridding" technique. This approach consists of holding $K-1$ of the additional parameters fixed in various combinations and then applying a continuation algorithm to approximate a 1-dimensional solution manifold of the restricted mapping. In contrast to this approach, the algorithm described here yields points approximately on $\mathcal{M}$ which are generated in a sequential ordering which "spirals" outward from $x_0 \in \mathcal{M}$. Thus, no variables are held fixed. The algorithm we describe seems therefore to respond to a need expressed by several researchers (see e.g. [1]).

Our paper is organized as follows. In § 2 a brief amount of notation and terminology concerning triangulations is given, which is sufficient for describing our algorithm. Although this material is relatively standard we include it since it is brief and our article is thereby self-contained. In § 3 a discussion is given of integer labeling and how simplices containing completely labeled N-faces yield "nearly zero points" of H. Section 4 contains the general pattern of a simplicial continuation algorithm for approximating a smooth manifold $\mathcal{M}$ which is implicitly defined by $\mathcal{M} \subset H^{-1}(0)$ where $H: \mathbb{R}^{N+K} \to \mathbb{R}^N$ is a smooth map having a regular zero point $x_0 \in \mathcal{M}$. The reader may obtain an intuitive grasp of the algorithm given here by reading §§ 2–4 with occasional

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reference to the figures presented below. Any specific implementation of the general pattern algorithm requires a specific underlying triangulation. The triangulation used here and some of its crucial properties are discussed in § 5. Section 6 contains material on integer labeling which is used in the implementation. The detailed implementation of the algorithm is presented in § 7. An outlook to future work and extensions is given in § 8.

2. Triangulations. To describe our pattern algorithm, it is necessary to give a brief discussion of triangulations, which is at least adequate to our later needs. The specific triangulation to be used in an implementation of the algorithm is discussed in § 5. For further reading on triangulations arising in the context of simplicial continuation methods we suggest Todd [16] and [17].

DEFINITION 2.1. A set $\{v_k\}_{k=0}^M \subseteq \mathbb{R}^N$ is called *affinely independent* if the set $\{v_k - v_0\}_{k=1}^M$ is linearly independent. The set

$$\sigma = [v_0, \cdots, v_M] := \left\{ v \in \mathbb{R}^N ; v = \sum_{j=0}^{M} \lambda_j v_j \,\middle|\, \sum_{j=0}^{M} \lambda_j = 1, \lambda_j \geqq 0 \right\}$$

is called the *M-simplex* having *vertices* $\{v_j\}_{j=0}^M$. If $\{w_j\}_{j=0}^K$ is a subset of $\{v_j\}_{j=1}^M$, the K-simplex $\tau := [w_0, \cdots, w_K]$ is called a *K-face of* σ. The 0-faces are vertices, the 1-faces are called *edges* and the $(M-1)$-faces are called *facets*. If σ is an M-simplex, the *barycenter of* σ is defined by $b(\sigma) = 1/(M+1) \sum_{j=0}^M v_j$. It is convenient to use a face of σ which is formed from the convex combination of the vertices of σ with one or more specific vertices, $v_{i_1}, \cdots, v_{i_l}$, omitted. We denote such a face as $\tau := [\sigma; \hat{v}_{i_1}, \cdots, \hat{v}_{i_l}]$.

DEFINITION 2.2. A *triangulation* T of a set $D \subseteq \mathbb{R}^N$ is a collection of N-simplices, $\sigma \subseteq \mathbb{R}^N$ such that

i) $\bigcup_{\sigma \in T} \sigma = D$.

ii) If $\sigma_1, \sigma_2 \in T$, then $\sigma_1 \cap \sigma_2$ is either empty or a common face of both σ_1 and σ_2.

iii) Every compact subset of D meets only a finite number of $\sigma \in T$.

The *k-skeleton* of T, T_k, is the set of all k-simplices, τ, $\tau \subseteq \sigma$ for some $\sigma \in T$. The *boundary of* D, ∂D is defined as $\partial D := \{\tau \in T_{N-1}$ such that τ is an $(N-1)$ face of exactly one $\sigma \in T\}$.

It is clear that each $\tau \in T_{N-1}$, $\tau \notin \partial D$, is a face of exactly two distinct N-simplices σ_1 and $\sigma_2 \in T$, so given one simplex σ_1 and a facet of σ_1, $\tau \notin \partial D$, we denote the unique $\sigma_2 \in T$ for which $\sigma_2 \cap \sigma_1 = \tau$ as the simplex obtained by *pivoting from* σ_1 *across* τ; $\sigma_2 = \sigma_1 P(\tau)$. The facet τ is called the *pivot face*.

3. Labelings. Simplicial algorithms provide "nearly zero-points" of a map $H: \mathbb{R}^{N+K} \to \mathbb{R}^N$ via an auxiliary map l_H called a labeling induced by H. The values of l_H at vertices are used in determining whether or not an N-simplex τ is "completely labeled". It is these "completely labeled simplices" which yield "nearly zero points" of H.

There are two basic kinds of labeling used in simplicial algorithms, vector and integer labelings. Because of technical grounds, the discussion in this paper will be confined to integer labeling.

(3.1) For $v \in \mathbb{R}^{N+K}$ *the labeling* of v is defined by $l_H(v) = j$, where $j \in \{0, \cdots, N\}$ is the number of leading nonnegative components of $H(v) \in \mathbb{R}^N$.

Many modifications of labeling are possible and we find it useful to discuss modifications which are needed for initializing simplicial algorithms in § 6.

(3.2) *An N-simplex* $\sigma=[v_0,\cdots,v_N]$ *is completely labeled* if $\{l_H(v_0),\cdots,l_H(v_N)\}=\{0,1,\cdots,N\}$.

The following proposition shows how a completely labeled simplex yields "nearly zero-points" of H. In the sequel the norm which will be used is $\|x\|=\max_i\{|x_i|\}$.

PROPOSITION 3.3. *Let* $H:\mathbb{R}^{N+K}\to\mathbb{R}^N$ *be continuous with modulus of continuity* $\delta(\varepsilon)$, i.e. $\|H(x)-H(y)\|\leqq\varepsilon$ *whenever* $\|x-y\|\leqq\delta(\varepsilon)$. *Given* $\varepsilon>0$, *let* τ *be any N-simplex which is completely labeled and for which* diam $\tau\leqq\delta$. *Then* $\|H(x)\|\leqq\varepsilon$ *for all* $x\in\tau$. (*See Fig.* 1.)

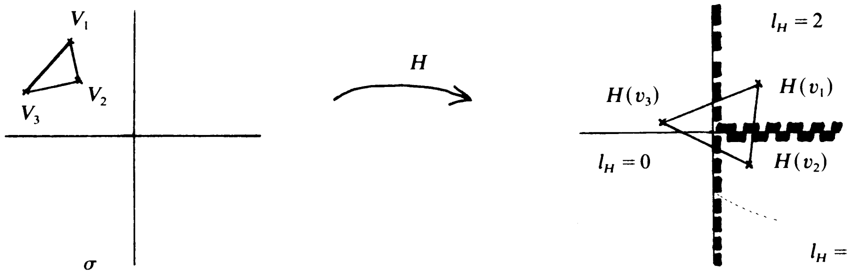

FIG. 1

Proof. Let $\tau=[v_0,\cdots,v_N]$ where, without loss of generality, it can be assumed that $l_H(v_i)=i$. By (3.1), $H_i(v_i)\geqq0$ and $H_i(v_{i-1})<0$, so there exists $\lambda_i\in[0,1]$ so that $H_i(z_i)=0$ where $z_i=(1-\lambda_i)v_{i-1}+\lambda_i v_i$. Since $z_i\in\tau$, then $\|x-z_i\|<\delta$ for all $x\in\tau$, so $|H_i(x)|\leqq\varepsilon$, for $i=1,\cdots,N$. Thus, for any $x\in\tau$, $\|H(x)\|\leqq\varepsilon$.

COROLLARY 3.4. *Let H satisfy the continuity hypothesis of Proposition* 3.3. *Let* σ *be an* $(N+K)$*-simplex having a completely labeled N-face* τ *and* diam $\sigma\leqq\delta$. *Then* $\|H(y)\|\leqq2\varepsilon$ *for all* $y\in\sigma$.

Proof. Let $x\in\tau$. Then $\|H(y)\|\leqq\|H(y)-H(x)\|+\|H(x)\|\leqq2\varepsilon$ by Proposition 3.3.

All completely labeled N-faces of an $(N+K)$-simplex $\sigma=[v_0,\cdots,v_N,v_{N+1},\cdots,v_{N+K}]$ containing a completely labeled N-face $\tau=[v_0,\cdots,v_N]$ are easily found. We observe that the set of labels corresponding to vertices of σ can be written as

(3.5) $$\{0,1,\cdots,N,j_{N+1},j_{N+2},\cdots,j_{N+K}\}\quad\text{where } j_i\in\{0,\cdots,N\}.$$

Any N-face whose vertices assume all labels $\{0,\cdots,N\}$ is completely labeled. Hence, the following result is immediately obtained by inspecting (3.5).

PROPOSITION 3.6. *If the* $(N+K)$*-simplex* σ *contains a completely integer labeled N-face* τ, *then the number of completely labeled N-faces of* σ *is between* $(K+1)$ *and* 2^K.

Let us take as an *approximate zero point* (for H) of a completely labeled N-simplex τ, the barycenter $b(\tau)$. The *approximate zero set* (for H) lying in an $(N+K)$-simplex σ which contains τ is taken to be the convex hull: co $\{b(\tau)$: τ is a completely labeled N-simplex in $\sigma\}$.

The properties of the approximate zero set can be studied with the aid of an affine map L_σ which is defined at the vertices $\{v_i\}_{i=0}^{N+K}$ of σ as follows. If $l_H(v_i)=l\in\{0,\cdots,N\}$, then

$$L_\sigma(v_i)=e_l^N-e_{l+1}^N(\text{mod } N+1)$$

where $e_0^N=\theta\in\mathscr{R}^N$ and $e_j^N\in\mathbb{R}^N$ is the jth standard unit vector.

If an N-simplex $\tau=[v_0,\cdots,v_N]$ is completely labeled, then since L_σ is affine,

$$L_\sigma(b(\tau))=\frac{1}{N+1}\sum_{i=0}^{N}L_\sigma(v_i)=-e_1^N+(e_1^N-e_2^N)+\cdots+(e_{N-1}^N-e_N^N)+e_N^N=\theta.$$

Suppose $\sigma=[v_0,\cdots,v_N,v_{N+1},\cdots,v_{N+k}]$ with

$$l(v_i)=i,\quad i=0,\cdots,N,\qquad l(v_{N+k})=j_{N+k}\in\{0,\cdots,N\},\quad k=1,\cdots,K.$$

Then since L_σ is affine,

$$L_\sigma^{-1}(\theta)\cap\sigma=\sum_{i=0}^{N+K}\lambda_i v_i,\qquad \lambda_i\geqq 0\quad\text{such that}$$

$$(3.7)\quad \begin{pmatrix} 1 & \cdots & 1 & 1 & \cdots & 1 \\ e_0^N-e_1^N & \cdots & e_N^N-e_0^N & e_{j_{N+1}}^N-e_{j_{N+1}+1}^N & \cdots & e_{j_{N+K}}^N-e_{j_{N+K}+1}^N \end{pmatrix}\begin{pmatrix}\lambda_0\\ \vdots\\ \lambda_{N+K}\end{pmatrix}=\begin{pmatrix}1\\0\\ \vdots\\ 0\end{pmatrix}.$$

Since the matrix in (3.7) has full rank $(=N+1)$ and has $N+K+1$ columns, the solution set to (3.7) with all $\lambda_i\geqq 0$ is a convex K-dimensional polytope in $\mathbb{R}_+^{N+K+1}$. Hence, we have

PROPOSITION 3.8. *The approximate zero set for H in σ*: $\operatorname{co}\{b(\tau)\mid\tau$ *is a completely labeled N-face of σ*$\}$ *coincides with $L_\sigma^{-1}(\theta)\cap\sigma$ and is a convex K-dimensional polytope having between $K+1$ and 2^K vertices.*

From Proposition 3.8 we have

COROLLARY 3.9. *The $(K-1)$-dimensional faces of $L_\sigma^{-1}(\theta)\cap\sigma$ lie in the $(N+K+1)$-facets of σ.* (*See Fig.* 2.)

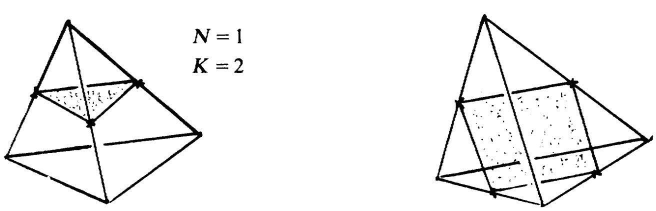

FIG. 2

COROLLARY 3.10. *If σ_1 and σ_2 share an $(N+K-1)$-facet which contains a completely labeled N-face, then the K-polytopes $L_{\sigma_1}^{-1}(\theta)\cap\sigma_1$ and $L_{\sigma_2}^{-1}(\theta)\cap\sigma_2$ share a $(K-1)$-dimensional face.* (*See Fig.* 3.)

The preceding results show that $L_\sigma^{-1}(\theta)$ intersects all faces containing a completely labeled N-face transversally. This motivates

DEFINITION 3.11. An $(N+l)$-simplex ν is *transverse* if ν contains a completely labeled N-face; $l=0,\cdots,K$. Given a transverse $(N+K)$-simplex we will primarily be concerned with the transverse $(N+K-1)$-faces or *transverse facets.* Each transverse facet can be written as $\phi=[\sigma;\hat{v}_i]$ where v_i shares a label with some other vertex in σ. Thus, there are at least $K+1$ transverse facets in a transverse $(N+K)$-simplex and these may be easily found.

4. Pattern algorithm. Before describing the pattern algorithm for approximating the zero set of a mapping $H:\mathbb{R}^{N+K}\to\mathbb{R}^N$, we recall the procedure which has been followed for $K=1$. A triangulation T of $D\subseteq\mathbb{R}^{N+1}$ is given and it is assumed that a completely labeled N-face τ_0 of some $(N+1)$-simplex $\sigma_0\in T$ is known. Proposition 3.6 assures us that σ_0 has exactly two completely labeled N-faces. The N-face $\tau_1\subset\sigma_0$ with $\tau_1\neq\tau_0$ is designated as the pivot facet and an $(N+1)$-simplex σ_1 is obtained by pivoting out of σ_0 across τ_1 to obtain a new $(N+1)$-simplex σ_1 which also contains exactly two completely labeled N-faces, τ_1 and τ_2. This "door-in-door-out" procedure, as it is referred to by Eaves [5], is applied until either an N-face $\tau \in \partial D$ or the N-face τ_0 is encountered. The procedure generates a sequence of completely labeled N-faces from which approximate zero points and a 1-dimensional approximation to the zero set is obtained. The pattern algorithm shares the philosophy of pivoting among transverse $(N+K)$-simplices across transverse facets, although additional procedures must be included because of the increased dimensionality which we handle.

We assume that we are given the compact domain $D \subseteq \mathbb{R}^{N+K}$ which is triangulated by T, the mapping $H: T_0 \to \mathbb{R}^N$, and a transverse $(N+K)$-simplex $\sigma \in T$. The algorithm determines a set of transverse $(N+K)$-simplices Σ and all included completely labeled N-faces.

The procedure for obtaining a triangulation T and the initial transverse $(N+K)$-simplex when given only a point x_0 such that $H(x_0)=\theta$ and such that the derivative $DH(x_0)$ is of full rank is treated separately. It is only at this starting point that any smoothness is required of H.

The choice of which zero data to output is left to the user. The order of approximation of the approximate zero set to the actual zero set depends on this choice as well as on the degree of smoothness of the mapping H. We will not consider this here other than to recall the results of Propositions 3.3 and 3.4. This assures that if H is continuous and if the simplices of T have sufficiently small diameter, then the values of all components of H are uniformly small on the approximate zero set.

The pattern algorithm consists of the following procedures which will be expanded upon in the following sections.

PATTERN ALGORITHM 4.1.

0) Formulate a triangulation T and a transverse $(N+K)$-simplex $\sigma \in T$.
1) Determine
   a) the completely labeled N-faces of σ,
   b) the *transverse facets* of σ, $\Phi(\sigma)=\{\phi \in T_{N+K-1}, \phi \subset \sigma, \phi$ contains a completely labeled N-face and $\phi \notin \partial D\}$. Output or store any zero point data. Set $\Phi=\varnothing$, set $\Sigma=\{\sigma\}$.
2) Select a pivot facet, $\phi^* \in \Phi(\sigma)$ and set $\Phi=\Phi \cup \Phi(\sigma) \setminus \{\phi^*\}$. ($\Phi$ is the set of *expected facets*).
3) Obtain the simplex $\sigma^*=\sigma P(\phi^*)$ by pivoting from σ across ϕ^*; set $\Sigma=\Sigma \cup \{\sigma^*\}$.
4) Determine
   a) the label of the one new vertex of σ^* which does not belong to σ,
   b) the completely labeled N-faces of σ^* and
   c) "new transverse facets", $\Phi(\sigma^*)=\{\phi \in T_{N+K-1} \mid \phi \subset \sigma, \phi$ contains a completely labeled N-face, $\phi \neq \phi^*$, $\phi \notin \partial D\}$.
   Output or store any zero data.
5) Determine $\Psi=\Phi \cap \Phi(\sigma^*)$.

   Set $\Phi=\Phi \setminus \Psi$ and $\Phi(\sigma^*)=\Phi(\sigma^*) \setminus \Psi$.
6) If $\Phi(\sigma^*)=\varnothing$ then perform *restart procedure* else, set $\sigma=\sigma^*$ and go to 2. (See Fig. 3 for an illustration of steps 2), 3), 4) and 6).)

Restart procedure

1) if $\Phi=\varnothing$ then *stop*
   else, continue.
2) Select $\phi^* \in \Phi$, determine $\sigma \in \Sigma$ such that $\phi^* \in \sigma$. Set $\Phi=\Phi \setminus \{\phi^*\}$.
3) Go to step 3) of the pattern algorithm.

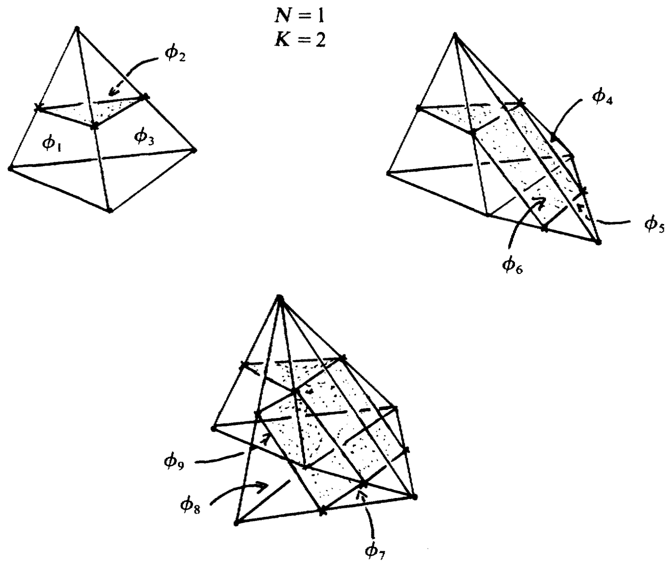

FIG. 3

Remark 4.2. Since D is a compact domain, the algorithm will terminate after a finite number of steps. This is because T contains only a finite number of $(N+K-1)$-facets, and because each transverse facet is encountered exactly twice: once when it is generated and once more when it is "pivoted across", or when "bumped into" as an expected facet.

The set Σ which is constructed is maximal in the sense that any transverse $(N+K)$-simplex of T which is not in Σ either is disjoint from $\bigcup_{\sigma\in\Sigma}\sigma$, or it intersects a transverse $(N+K)$-simplex of Σ in a face which is either not transverse or which lies in the boundary of D. If D is convex, the latter case does not occur.

5. Kuhn triangulation and properties relevant for the pattern algorithm. To simplify the discussion of the several procedures used in the pattern algorithm, we restrict ourselves to a particular triangulation. While most of the ideas we introduce can be generalized to other triangulations, we make the above choices because of ease of computation. In particular, it is shown below (Lemma 5.5) that each $(N+K)$-simplex in the triangulation can be easily recovered from its barycenter. Further, the result in Theorem 5.12 allows us to detect contact between two $(N+K)$-simplices. By use of the contact vector in (5.19) we can check whether the current simplex "bumps into" an earlier simplex. We develop the concepts of gap and adjacency to keep track of the relationship between an $(N+K)$-simplex and neighboring $(N+K)$-simplices. These concepts are used extensively in step 5) of Pattern Algorithm 4.1 to avoid "cycling".

The triangulation which we use is based on the idea of pivoting by reflection. Given an $(N+K)$-simplex $\sigma=[v_0,\cdots,v_j,\cdots,v_{N+K}]$ and a vertex v_j, define the *left and right neighbors* of v_j, respectively, as

$$(5.1)\qquad v_{j-}=\begin{cases} v_{j-1} & \text{if } 0<j\leqq N+K,\\ v_{N+K} & \text{if } j=0;\end{cases}$$
$$v_{j+}=\begin{cases} v_{j+1} & \text{if } 0\leqq j<N+K,\\ v_0 & \text{if } j=N+K.\end{cases}$$

The *reflection of* v_j across the *neighboring edge* $[v_{j-}, v_{j+}]$ is the point

$$r(v_j) = v_{j-} - v_j + v_{j+}.$$

The simplex obtained by replacing v_j in σ by $r(v_j)$ is denoted as $\sigma R_j = [v_0, \cdots, v_{j-} - v_j + v_{j+}, \cdots, v_{N+K}]$. The procedure of obtaining σR_j from σ is called *pivoting by reflection of* v_j (see Fig. 4).

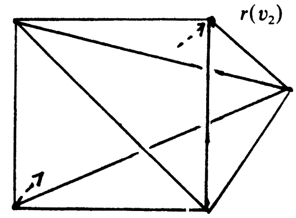

FIG. 4

The action $\sigma \to \sigma R_j$ can be realized as a matrix operation if σ is represented by the $(N-K)\times(N+K+1)$-matrix whose columns are the vertices of σ and if R_j is the $(N+K+1)\times(N+K+1)$-matrix

$$(5.2) \qquad R_j := I^{N+K+1} + (e_{(j+1)-}^{N+K+1} - 2e_{(j+1)}^{N+K+1} + e_{(j+1)+}^{N+K+1})(e_{(j+1)}^{N+K+1})^T$$

where e_i^M is the ith unit vector in $\mathbb{R}^M$ and I^M is the identity on $\mathbb{R}^M$. We abuse notation when convenient by referring to σ as the matrix consisting of the columns of σ in a prespecified order.

An important class of triangulations, the *Freuenthal-Kuhn triangulations*, are generated by the procedure as is indicated in the following theorem.

THEOREM 5.3 (Allgower and Georg [2]). *If* σ_0 *is any* $(N+K)$*-simplex in* $\mathbb{R}^{N+K}$, *then the set* $\mathcal{F}(\sigma_0) = \{\sigma \mid \sigma = \sigma_0 \Pi R_j$ *where finitely many* R_j *are in the product and all are of the form* (5.2)$\}$ *is a triangulation of* $\mathbb{R}^{N+K}$.

A particular example of such a triangulation is that generated by the simplex

$$\sigma_0 = \left[v^0, v^0 + \delta e_1^{N+K}, \cdots, v^0 + \sigma \sum_{i=1}^{j} e_j^{N+K}, \cdots, v^0 + \sigma \sum_{i=1}^{N+K} e_i^{N+K} \right].$$

The reflection triangulation generated by this simplex is called the (translated) *Kuhn triangulation* and is denoted by $\mathcal{K}(v^0, \delta)$ or simply $\mathcal{K}$. (The simplices illustrated in Fig. 4 are such.)

The Kuhn triangulation is a representation of all reflection triangulations as is seen from the following easily proved result.

LEMMA 5.4. *Let* $\mathcal{F}(\sigma_0)$ *be any reflection triangulation. There exists a nonsingular affine mapping*

$$A(X) = Mx + b,$$

where $M = \mathcal{E}[\mathbb{R}^{N+K}]$, *the set of nonsingular linear transformations of* $\mathbb{R}^{N+K} \to \mathbb{R}^{N+K}$ *and where* $b \in \mathbb{R}^{N+K}$, *so that if* $\sigma \in \mathcal{F}(\sigma_0)$, *then* $A(\sigma) \in \mathcal{K}[\theta, 1]$.

Because of this lemma we will refer only to the Kuhn triangulation $\mathcal{K} = \mathcal{K}[v^0, \delta]$ in the sequel.

The Kuhn triangulation is computationally very efficient because of the following facts.

LEMMA 5.5 [2]. *If* $\sigma=[v_0,\cdots,v_{N+K}]\in\mathcal{K}[v^0,\delta]$, *then there exists a unique* $(N+K)$*-vector of integers,* $z(\sigma)$, *and a permutation* $\Pi(\sigma)$ *of the set* $\{1,\cdots,N+K\}$, *so that* $v_0=v^0+\delta z(\sigma)$ *and* $v_j=v_0+\sigma\sum_{i=1}^{j}e_{\pi(i)}^{N+K}$.

Moreover, if σR_j *is obtained by pivoting from* σ *by reflection of* v_j, *then*

$$\pi(\sigma R_j)=\begin{cases}\{\pi(1),\cdots,\pi(j+),\pi(j),\cdots,\pi(N+K)\} & \text{if } 0<j<N+K,\\ \{\pi(2),\cdots,\pi(j+),\cdots,\pi(N+K),\pi(1)\} & \text{if } j=0,\\ \{\pi(N+K),\pi(1),\cdots,\pi(N+K-1)\} & \text{if } j=N+K.\end{cases}$$

LEMMA 5.6. *If* $\sigma\in\mathcal{K}[v^0,\delta]$, *then*

$$b(\sigma)=v^0+\delta\cdot z(\sigma)+\frac{\delta}{N+K+1}\sum_{i=1}^{N+K}(N+K+1-i)\,e_{\pi(i)}^{N+K}.$$

Because of this formula, we see that

$$\text{(5.7) i)}\qquad z(\sigma)=\text{the integer parts of }\frac{b(\sigma)-v^0}{\delta}$$

and π is determined by ordering the components of the

$$\text{(5.7) ii)}\qquad \text{fractional parts of }\frac{b(\sigma)-v^0}{\delta}$$

in decreasing order. Hence $z(\sigma)$ and $\pi(\sigma)$ and thus σ itself can be recovered from $b(\sigma)$. For this reason, we advocate storing $b(\sigma)$ or some easily coded version in place of σ.

Another observation which is based on Lemma 5.6 is that each vertex of σ is assigned a specific index v_j. This index could be thought of as the column location of the vertex in the matrix representation of σ, (5.2). This vertex and any which replace it in subsequent reflections all have the same index.

We next discuss some concepts which are used to carry out the procedure of step 4.1.5) for determining whether a new transverse facet is an expected facet. Since $\mathcal{K}$ is a triangulation, two $(N+K)$-simplices σ_1 and σ_2 either have no intersection or they intersect in a common face. Furthermore, $\mathcal{K}$ is a reflection triangulation, so the simplices σ_1 and σ_2 are related by a sequence of pivotings by reflection, i.e. there exists R_{j_1}, $R_{j_2},\cdots,R_{j_n}$ so that

$$\sigma_2=\sigma_1\prod_{i=1}^{M}R_{j_i}.$$

We concentrate on determining the relation between this product of reflection and the face of contact of σ_1 and σ_2 only in cases where the face is of homogeneous dimension $(N+K-2)$ or more, although analogous results are easily established for lower order contact. An easily proved lemma concerning the reflection matrices R_j defined in (5.2) is

LEMMA 5.8. *If* $R_j=I^{N+K+1}+(e_{(j+1)-}^{N+K+1}-2e_{(j+1)}^{N+K+1}+e_{(j+1)+}^{N+K+1})(e_{(J+1)}^{N+K+1})^T$, *then*
i) $R_jR_j=I^{N+K+1}$,
ii) $R_jR_l=R_lR_j$ iff $j\neq l-$ *and* $j\neq l+$,
iii) $R_jR_{j+}R_j=R_{j+}R_jR_{j+}$
hold for all $l, j=0,\cdots,N+K$.

A corollary result is

LEMMA 5.9. *If $\psi=[\sigma; \hat{v}_{i_1}, \hat{v}_{i_2}](i_1\neq i_2)$ is an $N+K-2$ face of $\sigma\in\mathcal{K}$, then the number of $(N+K)$-simplices containing ψ is exactly*

$$6 \quad \text{if } i_1=i_2+ \text{ or } i_1=i_2-,$$

$$4 \quad \text{if } i_1\neq i_2+ \text{ and } i_1\neq i_2-.$$

Proof. Let σ and $\psi=[\sigma; \hat{v}_{i_1}, \hat{v}_{i_2}]$ be given. The $(N+K)$-simplices which contain ψ can all be obtained by a sequence of pivotings by reflection, alternating the reflected vertex between v_{i_1}, v_{i_2}. That this is so follows because this sequence generates a neighbourhood of any interior point of ψ. The sequence is

$$\sigma, \sigma R_{i_1}, \sigma R_{i_1}R_{i_2}, \sigma R_{i_1}R_{i_2}R_{i_1}, \cdots.$$

In case $i_1=i_2-$ ($i_1=i_2+$ is similar), apply Lemma 5.8i) and iii) using $i_2=i_2+$ to obtain that this sequence is

$$\sigma, \sigma R_{i_1}, \sigma R_{i_1}R_{i_1+}, \sigma R_{i_1}R_{i_1+}R_{i_1}=\sigma R_{i_1+}R_{i_1}R_{i_1+}, \sigma R_{i_1+}R_{i_1}, \sigma R_{i_1+}, \sigma. \tag{5.10}$$

In case $i_1\neq i_2+$ and $i_1\neq i_2-$, apply Lemma 5.8 parts i) and ii) to obtain the sequence

$$\sigma, \sigma R_{i_1}, \sigma R_{i_1}R_{i_2}=\sigma R_{i_2}R_{i_1}, \sigma R_{i_2}, \sigma. \tag{5.11}$$ □

We next consider a means to determine the contact between two simplices in $\mathcal{K}$.

THEOREM 5.12. *Let σ and $\tilde{\sigma}$ be two simplices in $\mathcal{K}$ and let $\sigma=\sigma\prod_{i=1}^{M} R_{j_i}$. Then*

$$TP(\sigma)(b(\tilde{\sigma})-b(\sigma))=\left(\prod_{i=1}^{M} R_{j_i}-I^{N+K+1}\right)e_{\Sigma}^{N+K+1}$$

where T is the $(N+K+1)\times(N+K)$ matrix

$$T=\frac{N+K+1}{\delta}\sum_{j=1}^{N+K}(e_{j+1}^{N+K+1}-e_j^{N+K+1})(e_j^{N+K})^T, \tag{5.13}$$

$P(\sigma)$ is the $(N+K)\times(N+K)$ permutation matrix associated with the permutation $\pi=\pi(\sigma)$

$$P(\sigma)=\sum_{j=1}^{N+K} e_{\pi(j)}^{N+K}(e_j^{N+K})^T \tag{5.14}$$

and

$$e_{\Sigma}^{N+K+1}=\sum_{j=1}^{N+K+1} e_j^{N+K+1}.$$

Proof. Observe that $b(\sigma)=1/(N+K+1)(\sigma)e_{\Sigma}^{N+K+1}$ where (σ) is the matrix representing σ. Thus,

$$\begin{aligned} b(\tilde{\sigma})-b(\sigma)&=\frac{1}{N+K+1}\left(\sigma\prod_{i=1}^{M} R_{j_i}-\sigma\right)e_{\Sigma}^{N+K+1}\\ &=\frac{1}{N+K+1}(\sigma)\left(\prod_{i=1}^{M} R_{j_i}-I^{N+K+1}\right)e_{\Sigma}^{N+K+1}. \end{aligned} \tag{5.15}$$

Now, for any product of reflection matrices and for any $y\in\mathbb{R}^{N+K+1}$, we claim that

$$(e_{\Sigma}^{N+K+1})^T\left(\prod_{i=1}^{M} R_{j_i}-I^{N+K+1}\right)y=0. \tag{5.16}$$

Denoting $z_j:=e_{(j+1)-}^{N+K+1}-2e_{(j+1)}^{N+K+1}+e_{(j+1)+}^{N+K+1}$, we can expand the product using the formula for R_{j_i} in (5.2) to obtain

$$\left(\prod_{i=1}^{M} R_{j_i} - I^{N+K+1}\right) = \left(\prod_{i=1}^{M} (I^{N+K+1} + z_{j_i}(e_{(j_i+1)}^{N+K+1})^T) - I^{N+K+1}\right) \tag{5.17}$$
$$= \sum_{i=1}^{M} z_{j_i}(u_i)^T$$

where u_i is a sum of product terms. Using the fact that

$$(e_{\Sigma}^{N+K+1})^T z_j = (e_{\Sigma}^{N+K+1})^T (e_{(j+1)-}^{N+K+1} - 2e_{(j+1)}^{N+K+1} + e_{(j+1)-}^{N+K+1}) = 0,$$

the result in (5.16) follows.

The proof is completed by showing that $TP(\sigma)(1/N+K+1)(\sigma)$ is the identity on the $(N+K)$-dimensional subspace

$$\mathcal{N} := \{y \in \mathbb{R}^{N+K} (e_{\Sigma}^{N+K+1})^T(y) = 0\}.$$

We first observe that (σ) can be written as

$$(\sigma) = v_0(e_{\Sigma}^{N+K+K1})^T + \delta P(\sigma) \sum_{j=1}^{N+K} \sum_{m=1}^{j} (e_m^{N+K})(e_{j+1}^{N+K+1})^T$$

so that

$$P(\sigma)(\sigma) = P(\sigma)v_0(e_{\Sigma}^{N+K+1})^T + \delta \sum_{j=1}^{N+K} \sum_{m=1}^{j} (e_m^{N+K})(e_{j+1}^{N+K+1})^T. \tag{5.18}$$

Now

$$P(\sigma)(\sigma)|_{\mathcal{N}} = \delta \sum_{j=1}^{N+K} \sum_{m=1}^{j} (e_m)^{N+K}(e_{j+1}^{N+K+1})^T|_{\mathcal{N}}$$

since the first term on the right-hand side of (5.18) vanishes on $\mathcal{N}$. Thus, by (5.13) and the preceding result

$$\frac{1}{N+K+1} TP(\sigma)\sigma|_{\mathcal{N}} = \left(\sum_{j=1}^{N+K} (e_{j+1}^{N+K+1} - e_j^{N+K+1})(e_j^{N+K})^T\right)$$
$$\cdot \sum_{l=1}^{N+K} \left(\sum_{m=1}^{l} (e_m^{N+K})(e_{l+1}^{N+K+1})^T\right)$$
$$= \sum_{j=1}^{N+K} \sum_{l=1}^{N+K} \sum_{m=1}^{l} (e_{j+1}^{N+K+1} - e_j^{N+K+1})(e_j^{N+K})^T(e_m^{N+K})(e_{l+1}^{N+K+1})^T$$
$$= \sum_{j=1}^{N+K} \sum_{m=1}^{N+K} \sum_{l=m}^{N+K} \delta_{jm}(e_{j+1}^{N+K+1} - e_j^{N+K+1})(e_{l+1}^{N+K+1})^T$$
$$= \sum_{j=1}^{N+K} \sum_{l=j}^{N+K} (e_{j+1}^{N+K+1} - e_j^{N+K+1})(e_{l+1}^{N+K+1})^T$$
$$= \sum_{l=1}^{N+K} \left[\sum_{j=1}^{l} (e_{j+1}^{N+K+1} - e_j^{N+K+1})\right](e_{l+1}^{N+K+1})^T$$
$$= \sum_{l=1}^{N+K} (e_{l+1}^{N+K+1} - e_1^{N+K+1})(e_{l+1}^{N+K+1})^T.$$

On the subspace $\mathcal{N}$ where $e_\Sigma^T y = 0$, we can write

$$\frac{1}{N+K+1} TP(\sigma)\sigma y = \left[\sum_{l=2}^{N+K+1} e_l^{N+K+1}(e_l^{N+K+1})^T - (e_1^{N+K+1}) \sum_{l=2}^{N+K+1} (e_l^{N+K+1})^T + e_1^{N+K+1}(e_\Sigma^{N+K+1})^T \right] y = y. \qquad \square$$

By using this theorem, we have a means for checking the order of contact between two simplices. We define the *contact vector* for two $(N+K)$-simplices σ_1 and σ_2 to be

$$c(\sigma_1, \sigma_2) = TP(\sigma_1)(b(\sigma_2) - b(\sigma_1)) \tag{5.19}$$

where T, $p(\sigma_1)$ are as defined in (5.13) and (5.14) and where $b(\sigma)$ is the barycenter of σ. By Theorem 5.12, this vector equals

$$(R - I)e_\Sigma \tag{5.20}$$

where R represents the product of reflection matrices for which

$$\sigma_2 = \sigma_1 R.$$

By comparing the contact vector (5.19) to a catalogue of vectors of the form (5.20), we can determine (at least for low-order contact) exactly how σ_2 is situated relative to σ_1. We can tell whether the two simplices share an $(N+K-1)$-facet or an $(N+K-2)$-face and in this latter case, we can determine exactly how many pivotings would have to be made in pivoting from σ_1 to σ_2.

To aid in organizing our work, we take the point of view that we will attempt to pivot around a transverse $(N+K-2)$-face by successive pivots across transverse facets. According to Lemma 5.9, there are either six or four $(N+K)$-simplices which contain a given $(N+K-2)$-face. By keeping track of the number of simplices out of which we have already pivoted, we know when to expect the earlier facet which shares the $(N+K-2)$-face with the current pivot facet. We formalize this concept in the definition of *gap between two expected facets.*

Let ϕ_1 and ϕ_2 be expected $(N+K+1)$-facets which share an $(N+K-2)$-face, $\phi_1 \cap \phi_2 = \psi$, and let σ_i be the unique $(N+K)$-simplex for which $\phi_i \subseteq \sigma_i$, $i = 1, 2$. If $\phi_1 = [\sigma_1; \hat{v}_{i_1}]$, then setting $\sigma = \sigma_1$ in formulas (5.10) or (5.11) we obtain σ_2 as one of the elements in sequence (5.10) or (5.11). Define the *gap* so that

(5.21) $\text{gap}(\phi_1, \phi_2) :=$ the minimum number of reflection pivots required to obtain the $(N+K)$-simplex σ_2, containing ϕ_2, when starting by reflecting out of σ_1 across ϕ_1.

(See Fig. 5.)

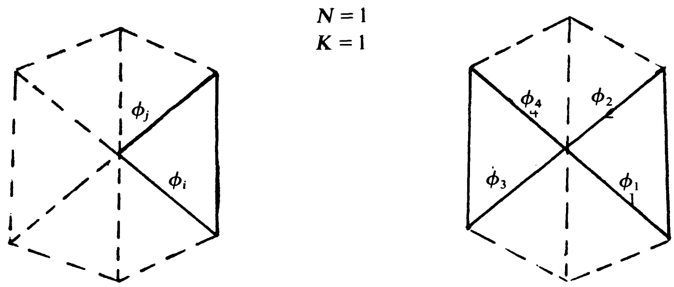

FIG. 5

The following results relate to the gap concept. The first reminds us how the gap is calculated for facets in a new simplex.

LEMMA 5.22. *If* σ *is an* $(N+K)$*-simplex,* v_{i_1}, v_{i_2} *are vertices of* σ, *and* $\phi_j=[\sigma;\hat{v}_{i_j}]$, $j=1,2$. *Then*

$$\operatorname{gap}[\phi_1,\phi_2]=\begin{cases}5 & \text{if } i_1=i_{2^-} \text{ or } i_1=i_{2^+},\\ 3 & \text{if } i_1\neq i_{2^-} \text{ and } i_1\neq i_{2^+}.\end{cases}$$

Proof. This follows from Lemma 5.9 and the definition of gap. □

The next result tells how to detect when distinct simplices contact in an $(N+K-2)$- or $(N+K-1)$-face and how to determine the gap.

LEMMA 5.23. *For* $i=1,2$, *let* σ_i *be distinct* $(N+K)$*-simplices containing* $(N+K-1)$*-facets* ϕ_i *and let* $\psi_i=[\sigma_i;\hat{v}_{i_1},\hat{v}_{i_2}]$ *be* $(N+K-2)$*-facets of the respective* ϕ_i*'s. Information which determines whether or not* σ_1 *and* σ_2 *have an intersection in an* $(N+K-2)$*- or* $(N+K-1)$*-dimensional face and, if so, sets the gap between them is contained in Table 5.24. We assume that* $\phi_1=[\sigma_1;\hat{v}_{i_1}]$ *and that* $\sigma_1\neq\sigma_2$.

TABLE 5.24
All e_j *are unit vectors in* $\mathbb{R}^{N+K+1}$.

(i_1,i_2)	contact vector (5.19)	$c(\sigma_1,\sigma_2)$ order of contact	gap(ϕ_1,ϕ_2)
$i_1=i_2-$	$e_{i_1-}-2e_{i_1}+e_{i_2}$	$\phi_1=\phi_2;\ \sigma_1\cap\sigma_2=\phi_1$	0
	$2e_{i_1-}-3e_{i_1}+e_{i_2+}$	$\phi_1\neq\phi_2;\ \sigma_1\cap\sigma_2=\psi$	1
	$2e_{i_1-}-2e_{i_1}-2e_{i_2}+2e_{i_2+}$	where $\psi=[\sigma_j;\hat{v}_{i_1},\hat{v}_{i_2}]$ $j=1,2$	2
	$e_{i_1-}-3e_{i_2}+2e_{i_2+}$		3
	$e_{i_2-}-2e_{i_2}+e_{i_2+}$	$\sigma_1\cap\sigma_2=(N+K-1)$-face other than ϕ_1 or ϕ_2	4
	any other than above	$\sigma_1\cap\sigma_2=\varnothing$ or a face of lower dimension than $N+K-2$	undefined
$i_1=i_2+$	Change roles of i_1 and i_2 in the preceding since $i_2=i_1-$.		
$i_1\neq i_2-$ and	$e_{i_1-}-2e_{i_1}+e_{i_1+}$	$\phi_1=\phi_2,\ \sigma_1\cap\sigma_2=\phi_1$	0
$i_1\neq i_2+$	$e_{i_1-}-2e_{i_1}+e_{i_1+}$ $+e_{i_2-}-2e_{i_2}+e_{i_2+}$	$\phi_1\neq\sigma_2;\ \sigma_1\cap\sigma_2=\psi$ where $\psi=[\sigma_j;\hat{v}_{i_1},\hat{v}_{i_2}]$	1
	$e_{i_2-}-2e_{i_2}+e_{i_2+}$	$\phi_1\neq\phi_2;\ \sigma_1\cap\sigma_2=(N+K-1)$-face other than ϕ_1 or ϕ_2	2
	any other than above	$\sigma_1\cap\sigma_2=\varnothing$ or a face of lower dimension than $N+K-2$	undefined

Proof. Direct computation of $(\prod_{j=1}^{M}R_{i_j}-I)e_\Sigma$ for all products occurring in sequence (5.10) and (5.11). □

We next observe how the gap changes when a new simplex is obtained by pivoting.

LEMMA 5.25. *Let* $\psi\subseteq\phi_j\subseteq\sigma_j$, $j=1,2$ *where* ψ *is an* $(N+K-2)$*-face.* ϕ_j *are* $(N+K-1)$*-facets and* σ_j *are* $(N+K)$*-simplices. Let* σ *be obtained by pivoting out of* σ_1 *across the face* ϕ_1, *then there exists a unique* $(N+K-1)$*-facet,* $\tilde{\phi}\subseteq\sigma$, *such that* $\tilde{\phi}\cap\phi_1=\psi$. *Furthermore,*

$$\operatorname{gap}(\phi_2,\tilde{\phi})=\operatorname{gap}(\phi_2,\phi_1)-1. \tag{5.26}$$

Proof. By hypothesis, there exist vertices v_{i_1}, v_{i_2} of σ so that $\phi_1=[\sigma;\hat{v}_{i_1}]$ and $\psi=[\sigma;\hat{v}_{i_1},\hat{v}_{i_2}]$. The unique $\tilde{\phi}$ is $\tilde{\phi}=[\sigma;\hat{v}_{i_2}]$. Since σ was obtained by a single pivot, the gap is reduced by one. □

We next introduce the concept of *adjacency* to help decide whether facets obtained by pivoting are expected facets. Let ϕ_i and ϕ_j be expected or new transverse facets as in steps 4.1.2) or 4.1.4) of the pattern algorithm. *ϕ_i is adjacent to ϕ_j if*

i) $\phi_i \cap \phi_j = \psi$ a (transverse) $(N+K-2)$-face,

ii) given any other expected or new transverse facet ϕ such that $\phi_i \cap \phi = \psi$,

$$\text{gap}(\phi_i, \phi_j) < \text{gap}(\phi_i, \phi). \tag{5.27}$$

(In Fig. 5, the facets ϕ_1 and ϕ_3 are adjacent.)

We use the adjacency concept to aid in checking whether new transverse facets obtained by pivoting are expected facets.

LEMMA 5.28. *Let ϕ^* be an expected facet of the transverse $(N+K)$-simplex σ (e.g. the pivot facet as in step 4.1.2) of the pattern algorithm) and let ϕ_i be any expected facet which is adjacent to ϕ^*. Let σ^* be an $(N+K)$-simplex such that $\phi^* = \sigma \cap \sigma^*$. Then σ^* contains exactly one transverse facet $\tilde{\phi}$, for which $\tilde{\phi} \cap \phi^* = \phi_i \cap \phi^*$. Either*

$\text{gap}(\phi^*, \phi_i) = 1$ *in which case $\tilde{\phi} = \phi^*$, or*

$\text{gap}(\phi^*, \phi_i) > 1$ *in which case $\tilde{\phi}$ cannot equal any other expected facet, $\tilde{\phi}$ is adjacent to ϕ_i and* $\text{gap}(\tilde{\phi}, \phi_i) = \text{gap}(\phi^*, \phi_i) - 1$.

Proof. By the definition of adjacency, ϕ_i is the first expected facet which could be encountered on pivoting across ϕ^* around the $(N+K-2)$-face $\phi^* \cap \phi_i$. The conclusion regarding $\tilde{\phi}$ then follows from Lemma 5.25 and the definition of gap, (5.21). □

6. Integer labeling and properties relevant to the pattern algorithm. In this section we develop several results concerning the integer labeling as defined in (3.1) and modified as in (6.1). In the proof of Theorem 6.2 we show how to obtain a completely labeled N-face which contains the given regular zero-point x_0. The discussion from (6.6) through Lemma 6.10 describes how to determine the transverse $(N+K-1)$-facets and $(N+K-2)$-faces of a transverse $(N+K)$-simplex. The discussion from (6.11) through Lemma 6.15 describes how the "new" transverse $(N+K-1)$-facets (referred to in step 4.1.4) are determined after a pivoting has been performed.

We use the following modification of integer labeling for the purpose of obtaining a starting simplex. Given a fixed $(N \times N)$ nonsingular matrix J, the *J-label* assigned to vertex V is

$$l_J(v) = j \in \{0, 1, \cdots, N\} \text{ if exactly the first } j \text{ components of } JH(v) \text{ are nonnegative.} \tag{6.1}$$

The results of § 3 concerning labeling carry over to l_J.

THEOREM 6.2. *Let $H: D(\subseteq \mathbb{R}^{N+K}) \to \mathbb{R}^N$ have a continuous derivative $DH(x)$ near $x_0 \in$ interior of D where $H(x_0) = 0$ and $DH(x_0)$ is of full rank. Then there exists a nonsingular matrix J, a constant $\delta_0 > 0$, and a permutation π of $\{0, \cdots, N+K\}$ so that any simplex*

$$\sigma(\delta) = \left[v_k(\delta) = v_0 + \delta \sum_{j=1}^{k} e_{\pi(j)}^{N+K} \right]_{k=0}^{N+K} \quad \text{with } v_0(\delta) = x_0 - \delta \sum_{j=1}^{N} \frac{N+K-j}{N+1} e_{\pi(j)}^{N+K}$$

and with $\delta < \delta_0$ is a transverse $(N+K)$-simplex with respect to J-labeling as defined in (6.1). (*See Fig.* 6 *for an example where $N = 1$, $K = 2$ and $J = I$ suffices.*)

Proof. Since $DH(x_0)$ is of rank N, there exists some set of N columns of the matrix $DH(x_0)$ which are linearly independent. Set $\pi(1), \cdots, \pi(N)$ equal to the numbers of these columns and assign the remaining column numbers to $\pi(N+1), \cdots, \pi(N+K)$.

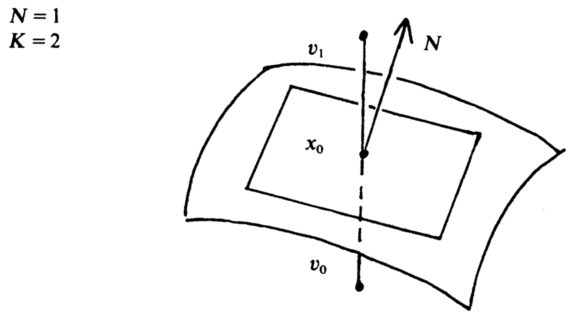

FIG. 6

Let $P=\sum_{i=1}^{N+K} e_{\pi(i)}^{N+K}(e_i^{N+K})^T$ be the permutation matrix representing π and let I^N represent the identity on $\mathbb{R}^N$. We seek an $N\times N$ matrix J for which

$$JDH(x_0)(e_{\pi(i)}^{N+K})=e_i^{N+K} \quad \text{for } i=1,\cdots,N. \tag{6.3}$$

We claim that

$$J=\left[DH(x_0)P\left(\frac{I^N}{\theta}\right)\right]^{-1} \tag{6.4}$$

is such a matrix. First, observe that a projector of $\mathbb{R}^{N+K}$ onto the linear space $\text{span}\{e_{\pi(1)}^{N+K},\cdots,e_{\pi(N)}^{N+K}\}$ is

$$P\left(\frac{I^N}{\theta}\right)(I^N\theta)P^T$$

and that $(I^N|\theta)P^T$ maps $e_{\pi(i)}^{N+K}$ onto e_i^N for $i=1,\cdots,N$. Thus, J in (6.3) has the desired properties.

We next define

$$v_0(\delta)=x_0-\frac{\delta}{N+1}\sum_{j=1}^{N}(N+1-j)e_{\pi(j)}^{N+K} \quad\text{and}\quad v_j(\delta)=v_0(\delta)+\delta\sum_{i=1}^{j}e_{\pi(i)}^{N+K} \tag{6.5}$$

for $j=1,\cdots,N+K$. By using Taylor's theorem valid near x_0, we compute

$$JH(v_i(\delta))=JH(x_0)+JDH(x_0)(v_i(\delta)-x_0)+Jo(\|v_i(\delta)-x_0\|).$$

Since $H(x_0)=0$ and because of the definition of $v_i(\delta)$ (6.5) we see that

$$JH(v_i(\delta))=JDH(x_0)\left(-\delta\sum_{j=1}^{N}\frac{N+1-J}{N+1}e_{\pi(j)}^{N+K}+\delta\sum_{j=1}^{i}e_{\pi(j)}^{N+K}\right)+o(\delta^2)$$

$$=\delta JDH(x_0)\left(\sum_{j=1}^{i}\left(\frac{j}{N+1}\right)e_{\pi(j)}^{N+K}-\sum_{j=i+1}^{N}\left(\frac{N+1-j}{N+1}\right)(e_{\pi(j)}^{N+K})\right)+o(\delta^2).$$

Because of the choice of J to satisfy (6.3) we have

$$JH(v_i(\delta))=\delta\left(\sum_{j=1}^{i}\left(\frac{j}{N+1}\right)e_j^{N+K}-\sum_{j=i+1}^{N}\left(\frac{N+1-j}{N+1}\right)(e_j^{N+K})\right)+o(\delta^2)$$

for $i=0,\cdots,N$. For δ sufficiently small, the signs of the components of $JH(v_i(\delta))$ are determined by the signs of the linear terms. Consequently, $l_J(v_i(\delta))=i$ for $i=0,\cdots,N$ and thus the N-face $[v_0(\delta),\cdots,v_N(\delta)]$ is completely labeled. $\sigma=[v_0(\delta),\cdots,v_{N+K}(\delta)]$ is therefore a transverse $(N+K)$-face. □

Given a transverse $(N+K)$-simplex, it is relatively easy to identify all completely labeled N-faces and all transverse $(N+K-1)$-facets. For any transverse $(N+l)$-simplex τ, one forms the *labeling set for* τ,

(6.6) $$\lambda_j(\tau)=\{v \mid v \text{ is a vertex of } \tau \text{ and } l_J(v)=j\}, j=0, \cdots, N.$$

Since τ is transverse, we know that $\lambda_j \neq \emptyset$ for all j. We call any vertex v *multiply labeled for* τ if for $j=l_J(v)$

(6.7) $$\lambda_j(\tau)\backslash\{v\} \neq \emptyset.$$

We denote the set of multiply labeled vertices of τ as $\mathcal{M}(\tau)$. Two multiply labeled vertices v_1 and v_2 are *compatibly labeled for* τ, if either

(6.8) $$l_J(v_1) \neq l_J(v_2), \quad \text{or if } l_J(v_1)=l_J(v_2), \quad \text{then } \lambda_{l_J(v_1)}\backslash\{v_1, v_2\} \neq \emptyset.$$

The completely labeled N-faces are formed by selecting $(N+1)$-vertices, one from each λ_j. The number of completely labeled N-faces in a transverse $(N+l)$-simplex, denoted as $C_l(\tau)$, is determined by the cardinalities of $\lambda_j(\tau)$,

$$c_j = \text{card } \lambda_j(\tau)$$

according to the formula below.

LEMMA 6.9. *If τ is a transverse $(N+l)$-simplex, then*

$$C_l(\tau)=\prod_{j=0}^{N} c_j.$$

Comment. Since $c_j \geqq 1$ and $\sum_{j=0}^{N} c_j = N+l$ there are only a finite number of possibilities for the product in (6.9). The possibilities are further limited if $N<l$. For example, if $N \geqq l$, then $C_1=2$, $C_2 \in \{3, 4\}$, $C_3 \in \{4, 6, 8\}$, $C_4 \in \{5, 8, 9, 12, 16\}$, but if $N=1$, then $C_3 \in \{4, 6\}$.

It should be observed that the completely labeled N-faces are only used in determining the zero data; they play no direct role in the progress of the algorithm.

The algorithm proceeds on knowledge of transverse $(N+K-1)$-facets and $(N+K-2)$-faces. These are easily determined.

LEMMA 6.10. *If σ is a transverse $(N+k)$-simplex, then*

i) *$\phi=[\sigma; \hat{v}]$ is a transverse $(N+K-1)$-facet if and only if v is multiply labeled for σ.*

ii) *$\psi=[\sigma; \hat{v}_1, \hat{v}_2]$ is a transverse $(N+K-2)$-face if and only if v_1 and v_2 are compatible for σ.*

Proof. σ is assumed to be transverse so we know that all $\lambda_j \neq \emptyset$. $\phi=[\sigma; \hat{v}]$ is transverse if and only if all labels are assumed on the vertices of ϕ. This occurs if and only if v is multiply labeled. The same condition that all labels occur on the vertices of ψ is equivalent to the omitted two multiply labeled vertices either having different labels or, if the same label, then there exists another vertex in σ with the label, thus v_1 and v_2 are compatibly labeled for σ. □

The next result deals with the identification of transverse $(N+K-1)$-facets after pivoting. Assume that the labeling sets, $\lambda_j(\sigma)$, and the multiply labeled vertices $\mathcal{M}(\sigma)=\{v_{i_1}, \cdots, v_{i_M}\}$ are known. Denote by $m(\sigma)=$ *cardinality of* $\mathcal{M}(\sigma)$. The pivoting by reflection of σ across ϕ^* is carried out by replacing the unique $v_{i^*} \in \mathcal{M}(\sigma)$ such that $\phi^*=[\sigma; v_{i^*}]$ by $r(v_{i_*})=v_{i_*-}-v_{i_*}+v_{i_*+}$ and leaving all other vertices of σ unchanged. Notice that $r(v_{i_*})$ is multiply labeled for σ^* as are most of the other vertices in $\mathcal{M}(\sigma)$; in particular, if there were some $\tilde{v}_i \in \mathcal{M}(\sigma)$ which were incompatible with v_{i^*} for σ, then $\tilde{v}_i$ should be provisionally dropped from $\mathcal{M}(\sigma)$. As an intermediate step we determine the multiply labeled vertices of ϕ^* to be

(6.11) $\mathcal{M}(\phi^*) = \mathcal{M}(\sigma)\backslash\{v_{i_*}\}\backslash\{\tilde{v}_i \mid \tilde{v}_i \text{ is incompatible in } \sigma \text{ with } v_{i^*}\}$.

We now determine the label of $r(v_{i^*})$, $l\# = l_J(r(v_{i^*}))$. Two cases are possible:

(6.12)

i) cardinality of $\lambda_{l\#}(\phi^*) > 1$ in which case

$$\mathcal{M}(\sigma^*) = \mathcal{M}(\phi^*) \cup \{r(v_{i^*})\},$$

ii) $\lambda_{l\#}(\sigma^*) = \{v_\#\}$, so $v_\# \notin \mathcal{M}(\phi^*)$, but now $\lambda_{l\#}(\sigma^*) = \{v_\#, r(v_{i^*})\}$ so

$$\mathcal{M}(\sigma^*) = \mathcal{M}(\phi^*) \cup \{r(v_{i^*}), v_\#\}.$$

Observe also that $r(v_{i^*})$ and $v_{i\#}$ are incompatibly labeled for σ^*. We have proved the following.

LEMMA 6.13. *Let σ and σ^* be two transverse $(N+K)$-simplices which share a transverse $(N+K-1)$-facet $\sigma \cap \sigma^* = \phi^* = [\sigma; v_{i^*}]$. Let $\{\phi_{i_j} = [\sigma; v_{i_j}], j = 1, \cdots, m(\sigma)\}$ be the set of transverse facets of σ, then the transverse facets of σ^* are*

$$\{\phi_i^* = [\sigma^*; v_{i_j}], j = 1, \cdots, m(\sigma), i_j \neq i^*, i_j \neq i \text{ for which } \lambda_{l_J(v^{i^*})} = \{v_{i^*}, v_i\}\}$$
$$\cup \{\phi_{i^*}^* = [\sigma^*; r(v_{i^*})]\}$$
$$\cup \{\phi\# = [\sigma^*; v_\#] \mid v_\# \text{ such that } \lambda_{l_J(r(v_{i^*}))}(\sigma^*) = \{r(v_{i^*}), v_\#\}\}.$$

Also,

$$(6.14) \qquad m(\sigma^*) = \begin{cases} m(\sigma) - 1 & \text{if } v_{i^*} \text{ is incompatible with some } \tilde{v}_i \in \mathcal{M}(\sigma) \\ & \text{and } r(v_{i^*}) \text{ is compatible with all } v \in \mathcal{M}(\sigma^*), \\ m(\sigma) + 1 & \text{if } v_{i^*} \text{ is compatible with all } v_i \in \mathcal{M}(\sigma) \text{ and} \\ & r(v_{i^*}) \text{ is incompatible with some } v_\# \in \mathcal{M}(\sigma^*), \\ m(\sigma) & \text{if neither of the above holds.} \end{cases}$$

The problem of finding the completely labeled N-faces of σ^* is addressed in the final remark.

LEMMA 6.15. *If σ and σ^* are as in Lemma* 6.13, *then the completely labeled N-faces of σ^* are those obtained by deleting from the completely labeled N-faces of σ any which include v_{i^*} and by adjoining any completely labeled N-faces of σ^* which include $r(v_{i^*})$.*

7. Implementation of the algorithm. Let us note that the algorithm described here sequentially generates transverse $(N+K)$-simplices by pivoting across transverse facets. The concept of multiply labeled vertices (6.7) permits easy identification of "new" transverse $(N+K-1)$-facets after a pivoting has been performed. The generation of transverse $(N+K)$-simplices proceeds in a manner of "pivoting around" a transverse $(N+K-2)$-face until all of the $(N+K)$-simplices which contain that face have been generated. The gap (defined in (5.21)) is a measure which determines when a "new" facet is actually one into which we expect to be pivoting. (See Lemmas 5.25–5.28.) The contact vector (5.27) affords a means of detecting when a "new" facet is coincident with or adjacent to a transverse $(N+K-1)$-facet of a much earlier $(N+K)$-simplex. This possibility might occur, e.g. when one tries to approximate a manifold such as a torus. The incorporation of these devices allow for an efficient implementation which we describe below.

It is assumed that the domain $D \subseteq \mathbb{R}^{N+K}$ is specified explicitly and that D is bounded. The mapping H from D into $\mathbb{R}^N$ is given and one has a point $x_0 \in D$ such that H is differentiable near x_0, $H(x_0) = 0$, and the derivative $DH(x_0)$ is of full rank. The maximum triangulation diameter δ_0 is also specified.

Step 7.0) determines a transverse $(N+K)$-simplex σ and the matrix J used to determine the J-label of subsequent vertices as in Theorem 6.2. The triangulation $[v_0, \delta]$ as described in (5.3) is used throughout. We denote as $D_{\mathcal{K}} = \bigcup_{\sigma \cap \mathcal{D} = \sigma} \sigma \in \mathcal{K}[v_0, \delta]$.

In step 7.1), we initialize counters which keep track of the simplices, SMP and CSMP and the number of transverse $(N+K-1)$-facets, M. We store the barycenters $b(\sigma)$ of the current simplex to be used for subsequent comparison of $(N+K-2)$-faces and in the construction of σ should a restart be necessary. We determine and output zero information as desired. The multiply labeled vertices $\mathcal{M}(\sigma)$ are found (see 6.7 and Lemma 6.10) and for each corresponding transverse $(N+K-1)$-facet, the adjacency structure is determined and saved. Recall that a facet, say ϕ_j, is determined by a multiply labeled vertex

$$\phi_j = [\sigma; \hat{v}_{i_j}].$$

We record the simplex number to which ϕ_j belongs, $\sigma(j)$, and the index of the omitted vertex opposite ϕ_j, $v_{i(j)}$. $\mathcal{A}(j)$ is defined to be the set of numbers of all facets in σ which are adjacent to ϕ_j. For each facet, $\phi_k \subseteq \sigma$, $k \in \mathcal{A}(j)$ (Lemma 6.10 and 5.27), we record the facet number, $a(k, l)$, the gap, $g(k, l)$, the index of the omitted vertex in the intersection $\phi_j \cap \phi_l$ other than $v_{i(j)}$, $i(j, l)$, and the number $d(j, l)$ assigned to the $(N+K-2)$-face $\phi_j \cap \phi_l$. The index l points to a particular facet which is adjacent to ϕ_j from among the set of facets with numbers in $\mathcal{A}(j)$. The number MNSMP(j) is the minimum simplex number of all simplices in $\mathcal{A}(j)$ which contain facets which are adjacent to ϕ_j. We also store pointers to the facets which intersect in the eth $(N+K-2)$-face, $\tau(e)$, and to the $(N+K-2)$-faces which omit vertices with indices i_1 and i_2, $\tau^{-1}(i_1, i_2)$. These are useful in carrying out comparisons in step 7.5). We construct the list of facets $\phi(\sigma)$ which may be pivoted through or which may be encountered again as the intersection between σ and other transverse $(N+K)$-facets. Notice that we delete from this any facets which lie in the boundary of D. We also save the J-labels in L[CSMP] of all the vertices of σ.

Step 7.2) is the first step in the main loop of the algorithm. Here we select the pivot facet ϕ_{j^*} so that we pivot around that $(N+K-2)$-face which is contained in the earliest simplex available. This strategy attempts to first cover the simplices in a neighborhood of the starting point x_0. The set of expected facets ϕ and the pointers to the $(N+K-2)$-face containing ϕ_{j^*} are now updated.

Step 7.3) involves the computation of the vertex obtained by pivoting, its J-label, the new simplex σ^*, its barycenter and permutation, and the list of labels for the new simplex.

Step 7.4) identifies and reports all the zero data as it is obtained from the completely labeled N-faces. More importantly for driving the algorithm, the "potentially new" transverse $(N+K-1)$-facets are identified. These are determined by first finding all transverse facets which are adjacent to ϕ_{j^*}; these numbers are stored as $\{a(j^*, l)\}$. Corresponding to each of these is an omitted index $i(j^*, l)$ other than $i(j^*)$ such that $[\sigma^*; \hat{v}_{i(j^*)}; \hat{v}_{i(j^*,l)}]$ is a transverse $(N+K-2)$-face. This implies that $v_{i(j^*,l)}$ is a multiply labeled vertex for σ^*. Any other multiply labeled vertex for σ^* must be incompatibly labeled with $r(v_{i(j^*)})$ for σ^*. Otherwise, had a multiply labeled vertex been compatibly labeled with $r(v_{i(j^*)})$, then by Lemma 6.10, it would have been omitted (along with $r(v_{i(j^*)})$) from σ^*. This would have given a transverse $(N+K-2)$-face which would have occurred in the previous simplex. We have accounted previously for all such facets. This then is why we also search for the (necessarily unique, possibly nonexistent) vertex $v_{i_{\#}} \in \sigma^*$ which is incompatibly labeled with $r(v_{i(j^*)})$. We finish step 7.4) by determining the number of potentially new facets, M^*, and by determining, for each, the simplex number and the omitted vertex number. We tentatively set $\Phi(\sigma^*)$ to be all of those facets which do not lie in the boundary of $D_{\mathcal{K}}$.

The purpose of step 7.5) is to identify all facets of $\Phi(\sigma^*)$ which are also in Φ and to remove these from $\Phi(\sigma^*)$ and Φ. This prevents cycling and also provides a criterion for stopping, namely when both Φ and $\Phi(\sigma^*)$ are actually empty. We apply the procedure to all potentially new transverse $(N+K-1)$-facets in σ^* not just to those in $\Phi(\sigma^*)$ since the boundary facets may have adjacency with nonboundary facets. For every new face ϕ_l we determine $\mathscr{A}(l)$ all other new facets which share a transverse $(N+K-2)$-face with ϕ_l. The set $L\#$ describes all new facets ϕ_k which share an $(N+K-2)$-face with the pivot facet ϕ_{j^*} and for which the gap before pivoting, gap(ϕ_{j^*}, ϕ_k) was 1. After pivoting, this gap is zero and thus $\phi_k = \phi_{a(j^*,M-k)}$, the facet which was adjacent to ϕ_{j^*} along the same $(N+K-2)$-face as ϕ_k shares with ϕ_{j^*}. Any facets in $L\#$ are deleted from Φ and $\Phi(\sigma^*)$; however, the adjacency information for facet $\phi_{a(j^*,M-k)}$ is stored as that of ϕ_k to be used later to determine its adjacency to other facets.

In substep iii), if both alternatives hold, then the new facet ϕ_{M+M^*} corresponding to omitted vertex $v_{i\#}$ is known to be adjacent to each $\phi_{M+l} \in L\#$, each of which is itself actually an old facet. Thus, ϕ_{M+M^*} could be equal only to a facet $\in \Phi$ which is adjacent to all of the $\phi_{l+M} \in L\#$. If ϕ_{M+M^*} is equal to one of these, then ϕ_{M+M^*} is placed in $L\#$ and Φ and $\Phi(\sigma)$ are updated. In any event, we continue at substep vi).

If in substep iii), all facets of σ^* which are adjacent to ϕ_{j^*} are actually new, then we proceed to step iv), wherein the $(N+K-2)$-face shared by facets ϕ_{M+M^*} and ϕ_{M+1} (arbitrarily chosen) is checked to see if in fact it is a previously obtained $(N+K-2)$-face. The procedure for checking is described below. After the procedure is applied, we determine in v) whether facet ϕ_{M+M^*} is actually new and if not, we update $L\#$, ϕ, and $\phi(\sigma^*)$. Otherwise, the adjacency information for ϕ_{M+1} and ϕ_{M+M^*} (and any other facets which share the $(N+K-2)$-face $\phi_{M+1} \cap \phi_{M+M^*}$) is updated.

We enter substep vi) with complete information as to $L\#$, the old "new" facets, and use this step to update all adjacency information. This step essentially computes the adjacency information corresponding to ϕ_k and ϕ_l for each $(N+K-2)$-face, $\phi_k \cap \phi_l$, if at least one of ϕ_k or ϕ_l is actually a new face.

The procedure, substep 7.5 viii), for checking adjacency at an $(N+K-2)$-face $[\sigma^*; \hat{v}_{i(l_1)}, \hat{v}_{i(l_2)}]$ involves checking the contact vectors formed from σ^* and $\sigma(n)$, where $\sigma(n)$ contains an $(N+K-1)$-facet which is adjacent to another $(N+K-1)$-facet across an $(N+K-2)$-face whose *omitted vertex indices* are also the pair $(i(l_1), i(l_2))$. This checking in the table continues until a contact vector on Table 5.24 is obtained or the list of candidates is exhaused. If the current simplex, σ^*, has contact with other simplices in at least an $(N+K-2)$-face, then the $(N+K-1)$-facets which share this face are compared to the facet $[\sigma^*; \hat{v}_{i(l_1)}]$ to determine which is adjacent to this facet. If σ has no such contact, then $[\sigma^*, \hat{v}_{i(l_1)}]$ and $[\sigma^*; \hat{v}_{i(l_2)}]$ are adjacent. In any case, the gaps are updated and the adjacency information is output. Relevant $(N+K-2)$-face pointers are also updated.

Step 7.6) checks whether the current simplex has any facets through which we might pivot. If it does, then counters are updated and a return is made to step 7.2). If σ^* contains no pivot facets, then a restart is carried out.

The restart procedure, step 7.7) checks whether each transverse $(N+K-1)$-facet has been encountered twice. If so, then the algorithm stops. If there are still transverse facets in Φ, then one is selected by the same criterion as was used in step 7.2). The transverse $(N+K)$-simplex containing this facet is reconstructed from its barycenter as was described in the discussion following Lemma 5.5. Counters and Φ are updated and a return is made to the main loop at step 7.3).

THE ALGORITHM

7.0) *Obtain a transverse* $(N+K)$*-simplex in* $\mathcal{K}[v^0, \delta]$

i) Determine π and J as in Theorem 6.2, set $\delta = \delta_0$.

ii) Compute $v_i(\delta)$ as in (6.5).

iii) Compute $l_J(v_i(\delta))$ as in (6.1).

iv) If $l_J(v_i(\delta)) \neq i$ for some $i = 0, \cdots, N$ then set $\delta = \frac{1}{2}\delta$ and go to 7.0 ii). Else

v) Set $v_i = v_i(\delta)$, $\sigma = [v_0, \cdots, v_{N+K}]$ and $T = \mathcal{K}[v^0, \delta]$.

7.1) *Determine completely labeled N-faces and transverse* $(N+K-1)$*-facets of* σ *and initialize storage*

i) Set SMP = 1; set CSMP = 1.
Set $b(\text{CSMP}) = (1/(N+K+1))(\sigma)e_\Sigma^{N+K+1}$. Set $\tau(e) = \varnothing$ for all $e \in \mathbb{Z}$
Set $\tau^{-1}(i_1, i_2) = \varnothing$ for all $(i_1, i_2) \in \mathbb{Z}^2$.

ii) Determine the completely labeled N-faces following the procedure preceding Lemma 6.9. Output or store the desired zero data.

iii) Determine $\mathcal{M}(\sigma) = \{v_{i_1}, \cdots, v_{i_{m(\sigma)}}\}$ (i_j increasing). (See Lemma 6.10.) For each $j = 1, \cdots, m(\sigma)$, determine $v_{(i_j)\neq}$, if it exists. (See description of Step 7.4.) Use $\mathcal{A}(j) := \{i_k : v_{i_j}$ and v_{i_k} are compatibly labeled for $\sigma\}$, $m^*(j) := \text{card}\mathcal{A}(j)$, and $m^*(0) := 0$ to define

$$\text{INFO}(j) = \begin{cases} \sigma(j) = \text{CSMP} \\ i(j) = i_j \\ \text{MNSMP}(j) = 1 \\ \text{for } l = 1, \cdots, m^*(j), \text{set} \\ \quad a(j, l) = j_l \text{ if the } l\text{th vertex in } \mathcal{A}(j) \text{ is } v_{j_l} \\ \quad g(j, l) = \begin{cases} 5 \text{ if } i_j = i_{j_l\pm} \\ 3 \text{ if not} \end{cases}, \\ \quad i(j, l) = i_{j_l} \\ \qquad e(j, l) = \left(\sum_{k=0}^{j-1} m^*(k)\right) + l \\ \qquad \tau(e(j, l)) = \{j, j_l\} \\ \qquad \tau^{-1}(i_j, i_{j_l}) = \{e(j, l)\}. \\ \quad \text{for } i_{j_l} < i_j, \text{set} \\ \quad e(j, l) = \left(\sum_{k=0}^{j_l-1} m^*(k)\right) \\ \qquad\qquad + \text{number of vertices of } \mathcal{A}(j) \text{ before or equal to } i_j. \end{cases}$$

iv) Set $\Phi(\sigma) = \{j : \phi_j = [\sigma; v_{i_j}] \not\subset \partial D\}$; set $\Phi = \varnothing$.

v) Set $M = m(\sigma)$, set $j_{\max} = M \times (M-1)/2$.

vi) Set $L[\text{CSMP}] = (l_J(v_0), \cdots, l_J(v_{N+K}))$.

7.2) *Select a pivot pair*

i) Determine any j^* such that

$$\text{MNSMP}(j^*) \leqq \text{MNSMP}(k) \quad \text{for all } k \in \phi(\sigma).$$

ii) Set $\Phi = \Phi \cup \Phi(\sigma) \backslash \{j^*\}$.

iii) Set $\tau(e(j^*, l)) = \tau(e(j^*, l)) \backslash \{j^*, a(j^*, l)\}$ for each l: $i_l \in \mathcal{A}(j^*)$.
If any $\tau(e(j^*, l)) = \varnothing$, set $\tau^{-1}(i(j^*), i(j^*, l))$
$= \tau^{-1}(i(j^*), i(j^*, l)) \backslash \{e(j^*, l)\}$.

7.3) *Pivot* $v_{i_{j^*}}$ *out of* σ *to obtain* σ^*

i) Set $r(v_{i(j^*)}) = v_{i(j^*)-} - v_{i(j^*)} + v_{i(j^*)+}$, compute $l^* = l_J(r(v_{i(j^*)}))$.

ii) Set CSMP = CSMP + 1.

iii) Set $\sigma^* = [v_0, \cdots, r(v_{i(j^*)}), \cdots, v_{N+K}]$ and compute

$$b(\text{CSMP}) = b(\text{SMP}) + \frac{\delta}{N+K+1}[r(v_{i(j^*)}) - v_{i(j^*)}].$$

iv) Determine $\pi(\sigma^*)$ from $\pi(\sigma)$ by Lemma 5.4.

v) Set $L[\text{CSMP}; i(j^*)] = l^*$ and $L[\text{CSMP}; i] = L[\text{SMP}; i]$, $i \neq i(j^*)$.

7.4) *Determine completely labeled N-faces and transverse* $(N+K-1)$*-facets*

i) Identify the completely labeled N-faces of σ^* and output any zero information.

ii) Determine "new" transverse $(N+K-1)$-faces.

a) Recall the adjacency information for the pivot face, ϕ_{j^*}, in particular:

$m^*(j^*)$ = number of expected transverse $(N+K-1)$-facets where are adjacent to ϕ_{j^*} for each $l = 1, \cdots, m^*(j^*)$,

$a(j^*, l)$ = facet number of lth adjacent facet,

$e(j^*, l)$ = face number of the transverse $(N+K-2)$-face $\phi_{j^*} \cap \phi_{a(j^*, l)}$,

$i(j^*, l)$ = vertex number such that $\phi_{j^*} \cap \phi_{a(j^*, l)} = [\sigma(j); \hat{v}_{i(j^*)}, \hat{v}_{i(j^*, l)}]$,

$g(j^*, l) = \text{gap}(\phi_{j^*}, \phi_{a(j^*, l)})$.

b) Determine $v_{i\#} \in \sigma^*$ which is incompatibly labeled for σ^* with $r(v_{i(j^*)})$ if one exists.

c) For each $l = 1, \cdots, m^*(j^*)$ (denote the new transverse facets as $\phi_{M+l} = [\sigma^*; v_{i(j^*, l)}]$). Define some of the adjacency information

$\sigma(M+l) = \text{CSMP}$

$i(M+l) = i(j^*, l)$.

If no $v_{i\#}$ exists as in b) above, then set $M^* = m^*(j^*)$, else, set $M^* = m^*(j^*)+1$

(Define $\phi_{M+M^*} = [\sigma^*; \hat{v}_{i\#}]$)

Set $\sigma(M+M^*) = \text{CSMP}$

Set $i(M+M^*) = i\#$.

iii) Set $\hat{\phi} = \{M+l: l = 1, \cdots, M^*\}$

$\Phi(\sigma^*) = \{M+l: \phi_{M+l} \notin \partial D_k\}$.

7.5) *Determine* $\psi = \Phi \cap \Phi(\sigma^*)$ *and update* Φ *and* $\Phi(\sigma^*)$

i) a) For all $l \in \hat{\phi}$, determine $\mathcal{A}(l) = \{k \in \hat{\phi}: v_{i(l)}$ and $v_{i(k)}$ are compatibly labeled$\}$.

For each $k \in \mathcal{A}(l)$, define $j(l, k) = \text{card}\{j \in \mathcal{A}(l): j \leqq k\}$.

b) Determine $L\# = \{k \in \hat{\phi}: k \leqq M + m^*(j^*);\ g(j^*, M-k) = 1\}$

$(k \in L\#$ iff $\phi_k = \phi_{a(j^*, M-k)})$.

ii) For each $k \in L\#$

Set $\text{INFO}(k) = \text{INFO}(a(j^*, M-k))$.

Set $\Phi = \Phi \backslash \{a(j^*, M-k)\}$.

Set $\Phi(\sigma^*) = \Phi(\sigma^*) \backslash \{k\}$.

iii) If $M^* = m^*(j^*)$ then go to 7.5vi)

else

if $L\# = \varnothing$ then go to 7.5iv)

else

Comment:

Choose each $M+l \in L\#$ ($\phi_{M+l} \cap \phi_{M+M^*}$ is a transverse $(N+K-1)$-face $\forall l = 1, \cdots, M^*-1$)

Determine $\tilde{k}$ such that $i\# = i(l, k)$ — *Comment*: (see step 7.5ii) for definition of INFO(l).)

If $g(l, \tilde{k}) = 1$ then — *Comment*: ($g(l, k) = 1$ iff $\phi_{M+M^*} = \phi_{a(l,\tilde{k})}$)

Set INFO$(M+M^*)$ = INFO$(a(l, \tilde{k}))$.
Set $L^\# = L^\# \cup \{M+M^*\}$.
Set $\Phi = \Phi - \{a(l, \tilde{k})\}$.
Set $\Phi(\sigma^*) = \Phi(\sigma^*)\backslash\{M+M^*\}$.
Set $\tau(e(l, \tilde{k})) = \tau(e(l, \tilde{k}))\backslash\{a(l, \tilde{k})\}$
if $\tau(e(l, \tilde{k})) = \varnothing$ then set
$\tau^{-1}(i\#, i(l)) = \tau^{-1}(i\#, i(l))\backslash\{e(l, \tilde{k})\}$
else, continue.
Go to 7.5vi).

iv) *Comment*:
(All ϕ_{M+l}, $l = 1, \cdots, m^*(j^*)$ are actually new; $M^* = m^*(j^*)+1$; we check ϕ_{M+M^*}.)
Apply procedure *Check* $(N+K-2)$-*face*$[\sigma^*; \hat{v}_{i(M+1)}, \hat{v}_{i\#}]$
input: σ^*; $i(M+1) = i(j^*, 1)$, and $i\#$
output: a) K_1: ϕ_{M+1} is adjacent to ϕ_{K_1}
K_2: ϕ_{M+M^*} is adjacent to ϕ_{K_2}
$g_1 = \text{gap}(\phi_{M+1}, \phi_{K_1})$ $\quad g_2 = \text{gap}(\phi_{M+M^*}, \phi_{K_2})$
$\tilde{e}$: $(N+K-2)$-face $\tau(\tilde{e}) \supseteq \{M+1, M+M^*\}$
b) if $K_1 \neq M+M^*$ then INFO$[K_1]$ and INFO$[K_2]$ are updated.
This procedure is defined in step 7.5) viii).

v) If $K_1 \neq M+M^*$ and $g(M+M^*) = 0$ (*Comment*: occurs iff $\phi_{M+M^*} = \phi_{K_2}$)
then set $L\# = L\# \cup \{M+M^*\}$.
Set INFO$[M+M^*]$ = INFO$[K2]$
Set $\Phi = \Phi\backslash\{K_2\}$
Set $\Phi(\sigma^*) = \Phi(\sigma^*)\backslash\}M+M^*\}$.
For all l: $\phi_{i_l} \in \mathscr{A}(K_2)$, set $\tau[e(K_2, l)] = \tau[e(k, l)\}\backslash\{K_2\}$.
If $\tau[e(K_2, l)] = \varnothing$ then set
$\tau^{-1}(i(K_2), i(k_2, l)) = \tau^{-1}(i(K_2), i(K_2, l))\backslash\{e(K_2, l)\}$.
else
Determine $m^*(M+1)$ = number of facets $\subseteq \sigma^*$ adjacent to ϕ_{M+1}.
Set $a(M+1, m^*(M+1)) = K_1$.
Set $a(M+M^*, 1) = K_2$.
Set $g(M+1, m^*(M+1)) = g_1$.
Set $g(M+M^*, 1) = g_2$.
Set $i(M+1, m^*(M+1)) = i(M+M^*)$.
Set $i(M+M^*, 1) = i(M+1)$.
Set $e(M+1, m^*(M+1)) = e(M+M^*, 1) = \tilde{e}$.
Set $\tau(\tilde{e}) = \tau(\tilde{e}) \cup \{M+1, M+M^*\}$.
Set $\tau^{-1}(i\#, i(M+1)) = \tau^{-1}(i\#, i(M+1)) \cup \{\tilde{e}\}$.

vi) a) For all $l = M+1, \cdots, M+m^*(j^*)$, perform
b) If $l \in L\#$ then go to 7.5) vi) d)
else. (*Comment*: ϕ_l is actually new)
if $l = M+1$ and $M^* = M(j^*)$
and $L\# = \varnothing$ then set $\mathscr{A}(M+1) = \mathscr{A}(M+1)\backslash\{M+M^*\}$
else, continue.

c) For all $k \in \mathscr{A}(l)$: $k > l$
if $k \in L\#$ (*Comment*: $\phi_k = \phi_{a(k^*, k-M)}$))
then determine $\tilde{k}$: $i(l) = i(k, \tilde{k})$
determine $\hat{k}$: $i(k) = i(a(k, \tilde{k}), \hat{k})$.
(*Comment*: Here we are determining the facet $a(k, \tilde{k})$ which is adjacent to ϕ_l over the $(N+K-2)$-face $\phi_l \cap \phi_{k'}$.)
Set $a(l, j(l, k)) = a(a(k, \tilde{k}), \hat{k})$.
Set $i(l, j(l, k)) = i(k)$.
Set $g(l, j(l, k)) = g(k, \tilde{k}) - 1$.
Set $a(a(k, \tilde{k}), \hat{k}) = l$.
Set $g(a(k, \tilde{k}), \hat{k}) = g(k, \tilde{k}) - 1$.
Set $e(l, j(l, k)) = e(a(k, \tilde{k}), \hat{k})$.
Set $\tau(e(l, j(l, k))) = \tau(e(l, j(l, k))) \cup \{l\}$.
Comment:
else ($k \notin L\#$ so both ϕ_l and ϕ_k are actually new.)
Apply procedure: *Check* $(N+K-2)$*-face* $[\sigma^*; \hat{v}_{i(l)}, \hat{v}_{i(k)}]$
Input: σ^*, $i(l)$, $i(k)$
output: a) k_1: ϕ_l is adjacent to ϕ_{k_1}
k_2: ϕ_k is adjacent to ϕ_{k_2}
$g_1 = \text{gap}(\phi_l, \phi_{k_1})$
$g_2 = \text{gap}(\phi_k, \phi_{k_2})$
$\tilde{e} =$ number of $(N+K-2)$-face $\phi_l \cap \phi_k$
b) if $k_1 \neq k$ then INFO$[k_1]$ and INFO$[k_2]$ are updated.
This procedure is undefined in step 7.5) viii)
Set $a(l, j(l, k)) = k_1$.
Set $i(l, j(l, k)) = i(k)$.
Set $e(l, j(l, k)) = \tilde{e}$.
Set $g(l, j(l, k)) = g_1$.
Set $a(k, j(k, l)) = k_2$.
Set $a(k, j(k, l)) = i(l)$.
Set $e(l, j(l, k)) = \tilde{e}$.
Set $g(l, j(l, k)) = g_2$.
Set $\tau(\tilde{e}) = \tau(\tilde{e}) \cup \{l, k\}$.
Set $\tau^{-1}(i(l), i(k)) = \tau^{-1}(i(l), i(k)) \cup \{\tilde{e}\}$.
Return to 7.5) vi) a)

d) (*Comment*: $\phi_l = \phi_{a(j^*, l-M)}$)
For all $k \in \mathscr{A}(l)$, $k > l$, $k \notin L\#$
Determine $\tilde{k}$: $i(k) = i(l, \tilde{k})$.
Determine $\hat{k}$: $i(l) = i(a(l, \tilde{k}), \hat{k})$.
Set $a(k, j(k, l)) = a(a(l, \tilde{k}), \hat{k})$.
Set $i(k, j(k, l)) = i(l)$.
Set $g(l, j(k, l)) = g(l, \tilde{k}) - 1$.
Set $a(a(l, \tilde{k}), \hat{k}) = k$.
Set $g(a(l, \tilde{k}), \hat{k}) = g(l, \tilde{k}) - 1$.
Set $e(k, j(k, l)) = e(a(l, \tilde{k}), \hat{k}) = e^*$.
Set $\tau(e^*) = \tau(e^*) \cup \{k\}$.
Continue procedure 7.5) vi) a).

vii) Set $\Phi = \Phi \cup \Phi(\sigma^*)$.
For each $j \in \Phi(\sigma^*)$, set MNSMP$(j) = \min\{\sigma[a(j, l)]$, all $i_l \in \mathscr{A}(l)\}$.
Go to 7.6)

viii) Procedure: *Check* $(N+K-2)$*-face* $[\sigma; \hat{v}_{i(l_1)}, \hat{v}_{i(l_2)}]$.

input: ϕ_{l_1}, ϕ_{l_2} are new transverse $(N+K-1)$-faces $\subseteq \sigma$ such that $\phi_{l_1} \cap \phi_{l_2} = [\sigma; \hat{v}_{i(l_1)}, \hat{v}_{i(l_2)}]$; σ, $i(l_1)$, $i(l_2)$ are known.

output: k_1: ϕ_{l_1} is adjacent to ϕ_{k_1} and if $k_2 \neq l_2$ then k_2: ϕ_{l_2} is adjacent to ϕ_{k_2}.

$\tilde{e}$: $\phi_{l_1} \cap \phi_{l_2} = \tau_{\tilde{e}}$

INFO$[\phi_{k_1}]$ and INFO$[\phi_{k_2}]$ are updated.

The procedure is defined as follows:

1) If $\tau^{-1}(i(l_1), i(l_2)) = \emptyset$ then go to 5).

2) Else, perform for each $j \in \tau^{-1}(i(l_1), i(l_2))$.

Set $k(j, 1)$ = first number in the set $\tau(j)$

Compute $c_j = c(\sigma, \sigma(k(j, 1)))$ until

$g_1 := \text{gap}(\phi_{l_1}, \phi_{k(j,1)})$ is defined by Table 5.24

For such j, set $\tilde{e} = j$, and for each $k \in \tau(\tilde{e})$ $k \neq k(j, 1)$ compute $g_k = \text{gap}(\phi_{l_1}, \phi_k)$ using Contact table 5.24.

Determine $k_1 \in \tau(\tilde{e})$: $g_{k_1} < g_k$, $k \neq k_1$.

3) If $\text{gap}(\phi_{l_1}, \phi_{k(j,1)})$ is undefined by Contact table 5.24 for all $j \in \tau^{-1}(i(l_1), i(l_2))$ then go to 5).

4) Else, set $g(l_1) = g_{k_1}$.

Determine m_1: $e(k_1, m_1) = \tilde{e}$.

Set $k_2 = a(k_1, m_1)$.

Determine m_2: $a(k_2, m_2) = k_1$.

Set $g(l_2) = g(k_1, m_1) - g(l_2) - 1$.

Set $a(k_1, m_1) = l_1$.

Set $a(k_2, m_2) = l_2$.

Set $g(k_1, m_1) = g(l_1)$.

Set $g(k_2, m_2) = g(l_2)$.

End procedure.

5) Set $\tilde{e} = j_{\max} = j_{\max} + 1$.

6) Set $\tau^{-1}(i(l_1), i(l_2)) = \tau^{-1}(i(l_1), i(l_2))$.

If $(i(l_1) = i(l_2)+)$ or $(i(l_1) = i(l_2)-)$ then set $g(l_1) = g(l_2) = 5$ and end procedure.

Else set $g(l_1) = g(l_2) = 3$ and end procedure.

7.6) If $\Phi(\sigma^*) = \emptyset$ then perform restart procedure 7.7),

else Set $\sigma = \sigma^*$.

Set SMP = CSMP.

Set $M = M + M^*$.

Go to 7.2).

7.7) *Restart procedure*

i) If $\Phi = \emptyset$ then *STOP*

Else continue.

ii) Select $j^* \in \Phi$: MNSMP$(j^*) \leqq$ MNSMP(k), $k \in \Phi$.

iii) Set SMP $= \sigma(j^*)$;

Determine v_0 and π from b(SMP) as was described in 5.5) i) and ii).

Construct σ using Lemma 5.5.

iv) Set $\Phi = \Phi \backslash \{j^*\}$.

Go to 7.3).

8. Outlook for future work. Future work on this subject should proceed in several directions: improving the design of the algorithm, expanding the implementation, exploring applicability, and carrying out analyses of the efficiency and effectiveness of the various implementations. Some of these efforts can be reported upon here.

It is well-known that for $K=1$, the simplicial algorithms function more efficiently and yield better approximations of zero sets if vector labeling is used. Hence, it would seem desirable to develop and implement a version of the present algorithm which utilizes vector labeling. It is shown elsewhere [4] that if an $(N+K)$-simplex has a completely labeled N-face (with respect to vector labeling), then the total number of completely labeled N-faces is no longer independent of N. For example, if $K=2$, there may be between 3 and $N+3$ completely labeled N-faces. The analogue of the approximate zero set described in 3.7 is a convex polygon having between 3 and $N+3$ vertices. Algorithms for determining all of the completely labeled N-faces in an $(N+K)$-simplex have also been formulated in [4].

The present algorithm as described here is currently being programmed. A version will be developed which is designed for a parallel processing computer. This version will perform pivots out of all available transverse $(N+K-1)$-facets concurrently. A version which is specially tailored for computer graphics e.g. $N=1$, $K=2$ is currently being developed.

The present approach to the analysis of implicitly defined manifolds suggests the possibility of obtaining new extensions of the implicit function theorem.

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