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AN ALGORITHM FOR THE EXTREME RAYS OF A POINTED CONVEX POLYHEDRAL CONE*

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Abstract. An algorithm for exhibiting the extreme rays of a pointed convex polyhedral cone is described. The cone is assumed to be initially defined by a system of homogeneous linear inequalities. The method differs from prior procedures in two respects. First, faces of lower dimension than facets for the polar convex cone are used to serially determine the extreme rays; second, the method allows for the possibility of symmetry considerations involving the extreme rays to reduce storage requirements and computation effort.

Key words. extreme ray, polyhedral cone, linear programming

1. Introduction. In this paper an algorithmic procedure is described for exhibiting a complete set of extreme rays for a pointed convex polyhedral cone [1] which is defined by a system of homogeneous linear inequalities. That is, if $\{\bar{e}_i\}_{i=1}^{P}$ is a set of d-dimensional column vectors whose components define normals to a set of d-dimensional hyperplanes, then the inequalities $\bar{e}_i^T\bar{y} \geqq 0$ define the coordinates y of points in the polyhedral cone bounded by these hyperplanes. If the rank of the matrix $\bar{E} = (\bar{e}_1, \bar{e}_2 \cdots)$ is d, the cone is pointed. The problem, then, is to find the extreme rays $\bar{y}$ of the cone (i.e., those $\bar{y}$ which are contained in the intersection of at least $d - 1$ linearly independent hyperplanes and which lie in the surface of the cone).

An example of this type of problem arises in connection with the Slater hull problem, which is a limited version of the N-representability problem ([2]–[5]). In one version of the Slater hull problem, the matrix $\bar{E}$ has $\binom{r}{N}$ columns of dimension $\binom{r}{2}$. Each column i is characterized by a different set of N distinct integers in the range 1 to r. The element $e_{J,i}$ [$J = k + j(j - 1)/2$ for $r \geqq j > k \geqq 1$] is 1 if k and j are both in the set of N integers and 0 otherwise. The extreme rays associated with this particular matrix $\bar{E}$ are far from simplicial. The cone does have a high degree of symmetry, however, since all columns e_i are equivalent under the permutation group on r objects. Even for small integers such as $r = 9$ and $N = 4$, the number of extreme rays for this cone becomes astronomical ($>10^8$).

For very small values of r and N, the double description algorithm as outlined by Koler [6] is an efficient way to generate the extreme rays $\bar{y}$ of $\bar{E}$. For slightly larger dimensions, however, this method fails because it requires simultaneous generation of all extreme rays. On the CDC 6400 computer, this prevents its use when the number of $\bar{y}$ greatly exceeds 10^4.

As will be discussed in more detail later, many of the extreme rays are equivalent under the symmetry operations which send $\bar{E}$ into itself. The double

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description algorithm cannot easily be modified to take account of this simplification because this symmetry is not present during the intermediate stages.

The algorithm outlined in this paper, then, is designed to allow easy use of symmetry and to allow sequential rather than simultaneous generation of extreme rays. It is generally less efficient than the double description method for problems where both will work, but it allows results to be generated for problems too large to handle by the double description procedure.

2. An algorithm for diagonal N-representability.

2.1. Mathematical preliminaries. In the discussion to follow, the symbol $\bar{x}$, unless specified otherwise, will be used to denote either an element x of an abstract Euclidean space or the column matrix representation of x relative to some basis. Moreover, the symbol $\bar{x}^T\bar{y}$ will be used to indicate either the scalar product of two elements x and y of an Euclidean space or their conventional matrix inner product.

The solution set for a finite system of m linear homogeneous inequalities in n unknowns constitutes a convex polyhedral cone [1], called the polar cone of E, which may be symbolized as

$$C(E) = \{\bar{y} | \bar{E}^T\bar{y} \geqq 0\}. \tag{1}$$

Here $\bar{E}^T$ is an $m \times n$ matrix whose rows are the normals at the origin to the hyperplanes bounding the closed half-spaces.

Equation (1), however, is not the only way a convex polyhedral cone may be characterized. A set C in R^n is a convex polyhedral cone if C can be written as the sum of a finite number of half-lines L_i [7, p. 65], i.e., $C = \sum_{i=1} L_i$.

According to this latter definition, there exists a finite set of elements $G = \{\bar{g}_i\}_{i=1}^m$, where $\bar{g}_i$ generates the half-line L_i such that

$$C(G) = \left\{ \bar{\rho} \in R^n | \bar{\rho} = \sum_{i=1}^{m} \omega_i \bar{g}_i, \omega_i \geqq 0 \right\}.$$

If the elements of G are represented as the columns of a matrix $\bar{G}$, then C is given as

$$C(G) = \{\bar{\rho} | \bar{\rho} = \bar{G}\bar{\omega}, \bar{\omega} \geqq 0\}. \tag{2}$$

Now by a theorem stated by Weyl [8], if E is a finite set of vectors in R^n, then there exists a finite set G in R^n such that

$$\bar{C}(E) = C(G) \quad \text{and} \quad \bar{C}(G) = C(E). \tag{3}$$

The explicit characterization of the polar cone $\bar{C}(E)$ is thus given by $C(G)$. The algorithm developed here for computing G for polyhedral cones $\bar{C}(E)$ is based on solving the equation $\bar{C}(G) = C(E)$. In order to exhibit the set G, it is convenient to restrict the discussion to the case where $\bar{C}(E)$ is pointed[1] because a pointed convex polyhedral cone is the convex hull of its extreme rays.

[1] No assumptions are made here concerning the pointedness of the convex cone $C(E)$. In the case, however, that a positive basis for $\bar{C}(E)$ is to be used to characterize the interior of the convex hull of the set E, e.g., in the diagonal N-representability problem, then $C(E)$ must also be pointed.

In order to describe the algorithm for exhibiting these extreme vectors, the facial structure of the convex polyhedral cone must be considered.

The algorithm is based, in part, on two well-known results [9, Chap. 3, Chap. 11].

(I) Each $(n-2)$-face F of a convex polyhedral cone C of dimension n is contained in precisely two facets F_1 and F_2 of C, and $F = F_1 \cap F_2$.

(II) If F_1 is a face of the convex polyhedral cone C and if F_2 is a face of the convex polyhedral cone F_1, then F_2 is a face of C.

In the spirit of (I), two facets are set to be adjacent if they contain in common an $(n-2)$-face.

2.2. The basic algorithm. The basic iterative procedure of the algorithm may be given a geometric interpretation based on (I). If a facet of $C(E)$ is known, then any subfacet within this facet is contained in precisely one adjacent facet. Hence, if the supporting hyperplane containing the initial facet can be "rotated" about this subfacet, it may be brought into coincidence with the adjacent facet.

In order to describe this pivotal procedure more precisely, let E be a finite set of m elements in $R^n (m \geqq n)$ and let $\bar{y}$ be the normal to a facet F of $C(E)$; then $\bar{y}$ satisfies

$$\bar{E}^T\bar{y} = \bar{\eta}, \qquad \bar{\eta} \geqq 0,$$

or

$$\bar{C}^T\bar{y} = 0, \tag{4a}$$

$$\bar{D}^T\bar{y} > 0, \tag{4b}$$

where $\bar{C}^T$ is the matrix of rank $n-1$ whose rows are the rows of $\bar{E}^T$ for which equality with zero holds, and $\bar{D}^T$ is the matrix constructed from the remaining rows of $\bar{E}^T$. If $\bar{z}$ is the element of F normal to the subfacet H of F, then $\bar{z}$ satisfies

$$\begin{vmatrix} \bar{y}^T \\ \bar{C}^T \end{vmatrix} \bar{z} = \begin{vmatrix} 0 \\ \bar{\xi}_c \end{vmatrix}, \qquad \bar{\xi}_c \geqq 0, \tag{5}$$

where the rank of rows of $\bar{C}^T$ on which equality with zero holds is $n-2$. Here $\bar{\xi}_c$ denotes the elements $\bar{E}^T\bar{z} = \bar{\xi}$ formed from the submatrix $\bar{C}$ of $\bar{E}$. To show that such $\bar{z}$ exist, observe that F is the convex polyhedral cone generated as the positive hull of the elements of $\bar{E}$ contained in $\bar{C}$. Moreover, within the $(n-1)$-dimensional linear space determined by the supporting hyperplane normal to $\bar{y}$, F is pointed because the rank of $\bar{C}$ is $n-1$.

The normal to the adjacent facet intersecting F in H may be written as $\bar{v} = \alpha\bar{y} + \beta\bar{z}$. Now since $\bar{v}$ is normal to a facet of $C(E)$, for all columns $\bar{e}_k$ of $\bar{E}$, necessarily

$$\begin{aligned} \bar{e}_k^T\bar{v} &= \alpha\bar{e}_k^T\bar{y} + \beta\bar{e}_k^T\bar{z} \geqq 0, \\ &= \alpha\eta_k + \beta\xi_k \quad\ \geqq 0. \end{aligned} \tag{6}$$

Since an adjacent facet exists, there is at least one $\bar{e}_m$ in $\bar{C}$ for which $\xi_m > 0$.

Since for every $\bar{e}_n$ in $\bar{C}$,

$$\bar{e}_n^T \bar{v} = \beta \xi_n > 0, \tag{7}$$

it follows that $\beta > 0$. Similarly, for at least one $\bar{e}_n$ in $\bar{D}$,

$$\bar{e}_n^T \bar{v} = \alpha \eta_n + \beta \xi_n = 0. \tag{8}$$

As $\eta_j > 0$ for all $\bar{e}_j$ in $\bar{D}$, it follows from (8) that $\xi_n/\eta_n = -\alpha/\beta$ for at least one element of $\bar{D}$. For every $\bar{e}_j$ in $\bar{D}$, necessarily

$$\bar{e}_j^T \bar{v} = \alpha \eta_j + \beta \xi_j \geqq 0 \quad \text{or} \quad -\alpha/\beta \leqq \xi_j/\eta_j. \tag{9}$$

Hence, if $\alpha = -\xi_n$ and $\beta = \eta_n$ are chosen so that

$$\xi_n/\eta_n = \min_{\bar{e} \in \bar{D}} \{\bar{\xi}_j/\bar{\eta}_j\}, \tag{10}$$

then (9) will be satisfied for all $\bar{e}_j$ in $\bar{D}$. Furthermore, because $\eta_j = 0$ and $\xi_j \geqq 0$ for every $\bar{e}_j$ in $\bar{C}$, it follows that $\bar{v} = -\xi_n \bar{y} + \eta_n \bar{z}$ satisfies (6) for every $\bar{e}_k$ in $\bar{E}$, and thus the hyperplane normal to $\bar{v}$ supports $C(E)$. Finally, notice that the intersection of this hyperplane with $C(E)$ is indeed a facet. It obviously contains H and hence at least $n - 2$ linearly independent elements of E. However, the additional element represented by $\bar{e}_n$ that has been included is necessarily linearly independent of these because if it were not, then $\bar{e}_n^T \bar{y}$ would be zero, contrary to the fact that $\bar{e}_n$ was chosen as a row of $\bar{D}$. The intersection thus contains $n - 1$ linearly independent elements of E and is hence a facet. It will frequently happen that n in (10) is not uniquely defined because several elements or D give the same minimum ratio. This is not a problem, however, since every choice of n among this degenerate set leads to the same facet of $C(E)$.

In order to generate every facet of a convex polyhedral cone, it will be necessary to systematically determine each of the subfacets contained in the specified facet. If these subfacets can be found, the rotation procedure described may be used to determine each adjacent facet. In addition, if these adjacent facets are accumulated in a list with the initial facet being the first list item, all facets may be constructed by moving through the list sequentially and repeating the procedure. Of course, only those facets generated which are different from the existing list items will be entered in the list at each iteration. The process of generating all adjacent facets and comparing them with a list to determine those which will be retained may be referred to as *scanning*. The algorithm ends when the last list item is scanned without producing new list entries.

The fact that every facet of $C(E)$ is encountered using this procedure follows because $\bar{C}(E)$ is taken to be pointed. It is possible to identify a convex polytope $\bar{P}(E)$ with $\bar{C}(E)$ by specifying a normalization for the extreme vectors of $\bar{C}(E)$. If the vertices and edges of $\bar{P}(E)$ are viewed as constituting the vertices and edges of a graph to be naturally identified with $\bar{P}(E)$ and hence $\bar{C}(E)$, the resulting graph is $(n - 1)$-connected [9, Chap. 3, Chap. 11].

In the context of this polytopal graph, the process of scanning corresponds to determining all those graph vertices not previously known that are adjacent to (i.e., possess an edge in common with) that graph vertex identified with the facet of $C(E)$ being scanned. Furthermore, rotating about one subfacet in each of a sequence of adjacent facets specifies a sequence of adjacent vertices in the graph known as a *path*. Because the polytopal graph is connected, such a path exists connecting any two vertices. Hence missing a facet of $C(E)$ is impossible because this would require that the associated graph vertex either be isolated or be an element of a component of the graph which is disconnected from that component containing the vertices which have been encountered in scanning.

2.3. Generation of subfaces. The essential feature of the procedure used for exhibiting each of the subfacets in a particular facet may be illustrated by considering the more general problem of determining a complete set of extreme rays for a pointed convex polyhedral cone (in an $(n - p)$-dimensional space) defined as the intersection of p $(p < n)$ orthogonal hyperplanes,

$$H_m = \{\bar{x} \in R^n | \bar{a}_m^T \bar{x} = 0\}, \qquad m = 1, \cdots, p,$$

and q closed half-spaces,

$$\bar{H}_n = \{\bar{x} \in R^n | \bar{b}_n^T \bar{x} \geqq 0\}, \qquad n = 1, \cdots, q,$$

where it is assumed that the vectors a_m, $m = 1, \cdots, p$, are linearly independent of the vectors b_n, $n = 1, \cdots, q$.

In other words, this convex cone is the solution set to the system of equations

$$\begin{vmatrix} \bar{A} \\ \bar{B} \end{vmatrix} \bar{z} = \begin{vmatrix} 0 \\ \bar{\eta} \end{vmatrix}, \qquad \bar{\eta} \geqq 0, \tag{11}$$

where $\bar{B}\bar{z} = \bar{\eta}$, with $\bar{B}$ the $q \times n$ matrix whose rows are the components of the vectors $\bar{b}_n$ and $\bar{A}$ the $p \times n$ matrix whose rows are the components of the vectors $\bar{a}_m$. Let us denote this convex cone by $\bar{C}_A(B)$ and observe that $\bar{C}_A(B)$ is polar to the convex cone $C_A(B)$ generated as the positive hull of the elements in R^n represented by the rows of $\bar{B}$. Moreover, both of these convex cones reside in the $(n - p)$-dimensional linear space determined as the intersection of the specified p orthogonal hyperplanes.

For the purpose of exhibiting a complete set of extreme vectors for $\bar{C}_A(B)$, consider first the case that $p + q = n$. In this case, the matrix $\begin{vmatrix} \bar{A} \\ \bar{B} \end{vmatrix}$ is necessarily nonsingular if $\bar{C}_A(B)$ is pointed. Hence, letting $\bar{U}$ be the inverse matrix and $\bar{z}$ any element of $\bar{C}_A(B)$, observe that

$$U \begin{vmatrix} \bar{A} \\ \bar{B} \end{vmatrix} \bar{z} = \bar{z} = \bar{U} \begin{vmatrix} 0 \\ \bar{\eta} \end{vmatrix} = \sum_{i=1}^{q} \eta_i \bar{u}^{i+p},$$

where $\bar{u}^i$ represents column i of $\bar{U}$. Thus in this simple case, the last q columns of $\bar{U}$ constitute a positive basis for $\bar{C}_A(B)$ and represent a complete set of extreme vectors. In this case, $\bar{C}_A(B)$ and $C_A(B)$ are called *simplicial*.

The other case to consider in this context occurs when $p + q = m$ with $m > n$. The rank of the matrix $\begin{vmatrix} \bar{A} \\ \bar{B} \end{vmatrix}$ is still necessarily n if $\bar{C}_A(B)$ is pointed. Thus let $\bar{U}$ be a generalized inverse, i.e., let $\bar{U}$ be an $m \times m$ nonsingular matrix satisfying

$$\bar{U}\begin{vmatrix}\bar{A}\\ \bar{B}\end{vmatrix} = \begin{vmatrix}I_n\\ 0\end{vmatrix}, \qquad \bar{U}^{-1}\begin{vmatrix}I_n\\ 0\end{vmatrix} = \begin{vmatrix}\bar{A}\\ \bar{B}\end{vmatrix},$$

where I_n is the $n \times n$ identity matrix. If $\bar{z}$ is any element of $\bar{C}_A(B)$, then

$$\bar{U}\begin{vmatrix}\bar{A}\\ \bar{B}\end{vmatrix}\bar{z} = \begin{vmatrix}\bar{z}\\ 0\end{vmatrix} = \bar{U}\begin{vmatrix}0\\ \bar{\eta}\end{vmatrix}, \qquad \bar{\eta} \geqq 0.$$

If $\bar{U}$ is now partitioned as

$$\bar{U} = \begin{vmatrix}\bar{R} & \bar{T}\\ \bar{Q} & \bar{S}\end{vmatrix},$$

where R, T, Q and S are, respectively, $n \times p$, $n \times q$, $(m - n) \times p$ and $(m - n) \times q$ matrices, then clearly

$$\begin{vmatrix}\bar{z}\\ 0\end{vmatrix} = \begin{vmatrix}\bar{T} & \bar{\eta}\\ \bar{S} & \bar{\eta}\end{vmatrix}.$$

Hence for any $\bar{z}$ in $\bar{C}_A(B)$, the associated vector $\bar{\eta}$ must satisfy the homogeneous system of equations

$$\bar{S}\bar{\eta} = 0 \tag{12}$$

in addition to the necessary nonnegative condition

$$\bar{\eta} \geqq 0. \tag{13}$$

Conversely, for any $\bar{\eta}$ satisfying (12) and (13) it is easily demonstrated that if

$$\bar{z} = \bar{T}\bar{\eta}, \tag{14}$$

then $\bar{z}$ satisfies (11). Observe, however, that the solution set to (12) and (13) is the convex polyhedral cone resulting from the intersection of the positive orthant in a q-dimensional Euclidean space and the $m - n$ hyperplanes defined by (12). Denoting this convex cone by $\bar{C}(\eta)$, it is easily verified that the linear transformation in (14) defines a one-to-one correspondence preserving dimension between faces of $\bar{C}(\eta)$ and $\bar{C}_A(B)$. Thus $\bar{C}(\eta)$ is a pointed convex cone of dimension $n - p$. Moreover, an element of $\bar{C}_A(B)$ is an extreme vector if and only if the image of this element is an extreme vector for $\bar{C}(\eta)$. Thus a complete set of extreme vectors for $\bar{C}_A(B)$ may be obtained as the images of a complete set of extreme vectors for $\bar{C}(\eta)$. The task of exhibiting such a set for this latter convex cone is, however, a tractable problem using established procedures if the number of extreme rays is not too large (less than 10,000 for a CDC 6400 computer). Specifically, the algorithm developed by Kohler [6], which is a variant of the double description procedure of Motzkin [10], may be used for this purpose.

2.4. Imbedding sequence for subfaces. Practically, then, a complete set of extreme vectors can be exhibited for a convex polyhedral cone defined according to (11) if the set is not too large. This result may be used to develop the procedure for determining each of the subfacets contained in a specified facet of the convex cone $C(E)$ in R^n.

In general terms, the procedure utilizes the fact that any face of $C(E)$ is a convex polyhedral cone to construct a sequence of faces of $C(E)$ satisfying the imbedding condition,

$$F^k \subset F^{k+1} \subset \cdots F^{n-2} \subset F,$$

where F is any facet and F^k is some k-face. A unique normal at the origin to any face in this sequence may be determined to within a multiplicative constant by requiring that this vector be orthogonal to the normal to each face of greater dimension. It is easily seen that the k-dimensional linear space resulting from the intersection of the orthogonal hyperplanes determined by each of these normals contains F^k. This result is readily cast in the format of (11); and because the polar F^k is pointed in this linear space, either a matrix inversion or the double description method may be used to determine a normal to each facet of F^k where the facets of F^k are just the $(k - 1)$-faces of $C(E)$ contained in F^k. The normals constructed in this manner are then used in conjunction with the rotation procedure described to generate a list of normals to the k-faces adjacent to F^k which still are imbedded in $F^{k+1} \subset \cdots \subset F$. The process then continues by scanning this list to eventually generate the normals to every k-face of F^{k+1}. The normals to the facets of F^{k+1} are then used to generate normals to each $(k + 1)$-face adjacent to F^{k+1}. If this list is then scanned, normals to each $(k + 1)$-face in F^{k+2} may be obtained, and so on, until eventually normals to each subfacet in F are obtained.

At each stage, when the search for faces adjacent to F^d is begun, all faces of lower dimension left from the scan of the previous F^d are invalid and must be discarded. Ideally, at each stage, a program would select the best one of the three possible ways of finding the imbedded F^{d-1} faces. If F^d is simplicial, the F^{d-1} can best be found by inverting a matrix. If F^d has few enough facets, the double description procedure can be used to find them all simultaneously. Finally, if F^d has many facets, a scanning procedure can be initiated to find them sequentially. The algorithm, as actually implemented, applied the double description method to find the faces of F^{n-3}.

A feature of this algorithm which requires emphasis is the fact that the scan of the lists associated with faces of lower dimension need not be completed in order to generate some elements for the lists associated with faces of higher dimension. Admittedly, there will be no assurance that any of the lists are complete if this is done; nonetheless, it is an important capability in view of the symmetry considerations to be discussed in the next section.

2.5. Initial faces. To conclude § 2, a brief description of the method used to find an initial facet is given. This procedure is required not only for the purpose of constructing an initial sequence of imbedded faces, but also in the scanning process whenever it is necessary to find an initial subface of a F^d face.

Several investigators have considered the problem of constructing a solution to a system of inequalities [11], [12], but in general, the treatments given have been within a context where only nonnegative solutions are considered and where the system of inequalities is necessarily presumed to be inhomogeneous. These restrictions present no great difficulty, however, because the homogeneous inequalities encountered in the case of a pointed convex polyhedral cone are easily transformed to meet these conditions.

With reference to the requirements of the algorithm discussed, consider a system of linear inequalities of the form

$$\bar{A}\bar{z} = \begin{vmatrix} \bar{y}_1 \\ \vdots \\ \bar{y}_k \\ \bar{C} \end{vmatrix} = \begin{vmatrix} 0 \\ \vdots \\ 0 \\ \bar{\eta} \end{vmatrix}, \qquad \eta \geqq 0, \tag{15}$$

where $\bar{A}$ is an $m \times n\,(m \geqq n)$ matrix of rank n and where the vectors $\bar{y}_i, i = 1, \cdots, k$, are linearly independent. In order to convert this system to an inhomogeneous one, observe that if $\bar{z}$ is any nonzero solution to (15), and 1_n is a row matrix of 1's, then necessarily

$$\bar{1}_n\bar{A}\bar{z} = \left(\sum_{i=1}^{m} \bar{a}_i\right)\bar{z} = \bar{v}\bar{z} = \sum_{i=1}^{m-k} \eta_i = \alpha > 0,$$

where $\bar{a}_i$ represents row i of $\bar{A}$. This strict inequality for any solution other than zero may be written because the solution set under the given conditions on $\bar{A}$ constitutes a pointed convex polyhedral cone, (i.e., no vector exists which is orthogonal to all the rows of $\bar{A}$, because the rank of $\bar{A}$ is n). It also follows from this fact that for any $\bar{z} \neq 0$, a fixed arbitrary positive value for α may be chosen; hence let $\alpha = 1$ for all $\bar{z} \neq 0$. Finally, notice that for any $\bar{z}$ satisfying (15), obviously

$$\left(\sum_{i=1}^{m} \bar{a}_i\right)\bar{z} = \left(\sum_{i=1}^{m-k} \bar{c}_i\right)\bar{z}.$$

Thus if $\bar{s} = \sum \bar{c}_i$, the following equivalent inhomogeneous inequalities may be considered:

$$\bar{A}'\bar{z} = \begin{vmatrix} \bar{y}_1 \\ \vdots \\ \bar{y}_k \\ \bar{C} \\ \bar{s} \end{vmatrix} \qquad \bar{z} = \begin{vmatrix} 0 \\ \vdots \\ 0 \\ \eta \\ \beta \end{vmatrix}, \qquad \eta \geqq 0, \quad \beta \geqq 1. \tag{16}$$

These inequalities may now be converted to an equivalent system of inhomogeneous inequalities for which a nonnegative solution is sought by utilizing the fact that the rank of $\bar{A}$ is maximal. Thus the vectors $\bar{y}_i$, $i = 1, \cdots, k$, may be augmented with $n - k$ rows of $\bar{C}$ to form a set of n linearly independent vectors. Letting $\bar{V}$ be the nonsingular matrix generated from these vectors, (22) may be written as

$$\begin{vmatrix} \bar{V} \\ \bar{s} \\ \bar{B} \end{vmatrix} \bar{z} = \begin{vmatrix} 0 \\ \vdots \\ \bar{\delta} \\ \beta \\ \bar{\xi} \end{vmatrix}, \qquad \bar{\delta} \geqq 0, \quad \bar{\xi} \geqq 0, \quad \beta \geqq 1,$$

where $\bar{B}$ represents the $m - n + k$ rows of $\bar{C}$ not in $\bar{V}$, and $\bar{\delta}$ corresponds to the rows of $\bar{C}$ in $\bar{V}$. If $\bar{U}$ is the matrix inverse to $\bar{V}$, then

$$\begin{vmatrix} \bar{V} \\ \bar{s} \\ \bar{B} \end{vmatrix} \bar{z} = \begin{vmatrix} \bar{V} \\ \bar{s} \\ \bar{B} \end{vmatrix} \bar{U}\bar{U}^{-1}\bar{z} = \begin{vmatrix} I_n \\ \bar{s}\bar{U} \\ \bar{B}\bar{U} \end{vmatrix} \bar{U}^{-1}\bar{z} = \begin{vmatrix} I_n \\ \bar{D} \end{vmatrix} \bar{x} = \begin{vmatrix} 0 \\ \vdots \\ 0 \\ \bar{\delta} \\ \beta \\ \bar{\xi} \end{vmatrix},$$

where $\bar{x} = \bar{U}^{-1}\bar{z}$ and $\bar{D} = \begin{vmatrix} \bar{s}\bar{U} \\ \bar{B}\bar{U} \end{vmatrix}$. The last matrix equality requires that $\bar{x}$ be nonnegative with the first k components identically zero. Hence the reduced system of inequalities becomes

$$\bar{D}'\bar{x}' = \begin{vmatrix} \beta \\ \bar{\xi} \end{vmatrix}, \qquad \bar{\xi} \geqq 0, \quad \beta \geqq 1, \quad \bar{x}' \geqq 0,$$

where $\bar{D}'$ is the matrix obtained from $\bar{D}$ be deleting the first k columns and $\bar{x}'$ represents the last $n - k$ components of $\bar{x}$.

The inequalities in (17), (or, more accurately, the transpose of this system) are exactly the type of linear inequalities for which the ingenious lexicographic procedure of Gale [12] is designed to construct a basic solution. This is the procedure which has been utilized in the algorithm with only minor modifications in the pivotal steps to eliminate the necessity of divisions.

2.6. Symmetry considerations. The role of permutational symmetry in the diagonal N-representability problem is considerable. In fact it is the presence of this symmetry which makes the algorithm described here (when modified to account for this property) particularly applicable to this problem [13]. For the purpose of this paper, however, the only assumption concerning symmetry which will be made is that there exists a finite group G defined over R^n which is homomorphic to the permutation group of the finite set E which positively spans $C(E)$. As a consequence of this assumption [14, pp. 181–186], the set E may be decomposed exhaustively into equivalence classes with respect to G. Here by an *equivalence class* is meant a subset of E (possibly E itself) consisting of those elements in E which are equivalent under G, where $\bar{e}$ and $\bar{e}'$ in E are said to be *equivalent* (under

G) if there exists some P in G such that $P\bar{e} = \bar{e}'$. Observe that knowledge of one element in an equivalence class is sufficient to obtain all other elements.

The faces of $C(E)$ may also be categorized into equivalence classes, and hence only one representative face of each equivalence class need be retained in order to completely characterize the facial structure of $C(E)$. More important for the purposes of the algorithm, however, is the fact that when scanning a specified k-face, it is only necessary to rotate about one representative for each equivalence class (defined relative to a subgroup $G(F^k)$ of G) of $(k-1)$-faces in this k-face in order to generate one representative for each equivalence class of the adjacent k-faces. This has the obvious consequence of reducing the number of items in the lists associated with the algorithm if the scanning process is modified so that only normals which are not equivalent are retained. This modification, of course, requires a procedure for determining when two normals in a prescribed normalization are not equivalent, and this may be a very difficult problem if the order of the group G is large. For example, in the diagonal N-representability problem, introducing this capability required development of a constructive procedure for determining when two square matrices $\bar{A}$ and $\bar{B}$ were related according to $\bar{A} = \bar{P}^T\bar{B}\bar{P}$, where $\bar{P}$ is a permutation matrix. Because this problem is essentially equivalent to determining when two finite graphs are isomorphic, a detailed account of the procedure will be given in a subsequent paper.

In order to demonstrate that the existence of G does in fact induce equivalence class structure on the faces of $C(E)$, consider first the facets. If $\bar{P}$ is the matrix identified with a member P of G in an orthogonal representation and $\bar{Q}$ is the permutation matrix identified with a corresponding element of the permutation group on E under the aforementioned homomorphism, then $\bar{E}\bar{Q} = \bar{P}\bar{E}$. If $\bar{y}$ is the normal to any facet of $C(E)$, it follows that

$$\begin{aligned}\bar{E}^T\bar{y} &= \bar{E}^T\bar{P}^{-1}\bar{P}\bar{y} = \bar{E}^T\bar{P}^T\bar{P}\bar{y}\\ &= \bar{Q}^T\bar{E}^T\bar{z} = \bar{\eta}, \qquad\qquad \bar{\eta} \geqq 0, \quad \bar{z} = \bar{P}\bar{y},\end{aligned}$$

or

$$\bar{E}^T\bar{z} = \bar{Q}\bar{\eta}, \qquad \bar{Q}\bar{\eta} \geqq 0.$$

If $\bar{C}(\bar{y})$ is the submatrix of $\bar{E}$ for which $\bar{C}^T\bar{y} = 0$, then $\bar{P}\bar{C}$ is the corresponding matrix for $\bar{z}$. The fact that $\bar{z}$ is a basic solution is then easily shown if its is recalled that the rank of matrix is invariant to multiplication by a nonsingular matrix. Hence $\bar{z}$ is normal to a facet of $C(E)$ and the set of solutions $\{\bar{z}|\bar{z} = \bar{P}\bar{y}, P \in G\}$ defines an equivalence class of facets.

A useful definition of the equivalence class structure of the faces of dimension lower than facets within the context of the imbedding sequence may be illustrated by considering the $(n-3)$-faces contained in a given $(n-2)$-face which in turn is contained in a facet of $C(E)$. If $\bar{y}_1$ is a normal to the facet and $\bar{y}_2$ a normal in this facet to the subfacet then, according to the construction in the algorithm, a normal $\bar{y}_3$ to an $(n-3)$-face in the given subfacet satisfies

$$\begin{vmatrix}\bar{y}_1^T\\ \bar{y}_2^T\\ \bar{C}^T\end{vmatrix}\bar{y}_3 = \begin{vmatrix}0\\ 0\\ \bar{\eta}\end{vmatrix}, \qquad \eta \geqq 0.$$

Here it is to be recalled that $\bar{C}^T$ is the matrix whose rows are the representations of the elements of the subset C of E whose positive hull is the specified subfacet, i.e., $\bar{C}^T$ is the submatrix of rows of $\bar{E}^T$ satisfying $\bar{C}^T\bar{y}_1 = \bar{C}^T\bar{y}_2 = 0$.

Analogous to the manner in which an equivalence class was exhibited for the facets of $C(E)$, an equivalence class of $(n - 3)$-faces in this subfacet, characterized by $\bar{y}_3$ as a representative element, may be constructed if a subgroup of G is determined which is homomorphic to the permutation group of the set C. Such a group is the subset G^{n-2} of G consisting of those elements of G which leave $\bar{y}_1$ and $\bar{y}_2$ invariant, i.e., for any P in G^{n-2},

$$\bar{P}\bar{y}_1 = \bar{y}_1 \quad \text{and} \quad \bar{P}\bar{y}_2 = \bar{y}_2.$$

Equivalently, G^{n-2} may be regarded as the subgroup of G^{n-1} which sends F^{n-2} into itself. The fact that the image of any element in C under a member of G^{n-2} is also in C is easily established. Letting $\bar{e}^T$ be any row of $\bar{C}^T$ and $\bar{P}$ the matrix associated with a member of G^{n-2} in an orthogonal representation, then we have

$$0 = \bar{e}^T\bar{y}_1 = \bar{e}^T\bar{P}^T\bar{P}\bar{y}_1 = (\bar{P}\bar{e})^T\bar{y}_1,$$

and similarly,

$$(\bar{P}\bar{e})^T\bar{y}_2 = 0,$$

Hence $(\bar{P}\bar{e})^T$ is a row of $\bar{E}^T$ which is contained in $\bar{C}$. Analogous arguments can be used to define equivalence classes for the $(k - 1)$-faces or their normals in any k-face. Thus for the imbedding sequence, $F^k \subset F^{k+1} \cdots \subset F^{n-1}$, the subgroups are also imbedded as $G^{k+1} \subset \cdots \subset G$. The equivalence class of F^k relative to G^{k+1} is defined as $\{F^k|\bar{C}(F^k) = \bar{P}\bar{C}(F_1^k), P \in G^{k+1}\}$.

Finally, in order to illustrate why one one representative from each equivalence class for the k-faces contained in a specified $(k + 1)$-face need be retained in order to generate at least one representative for each of the equivalence classes characterizing adjacent $(k + 1)$-faces, the preceding example may be used to show that any two normals to $(n - 3)$-faces in the same equivalence class give rise necessarily to equivalent $(n - 2)$-faces.

Assume that $\bar{z}_3$ and $\bar{y}_3$ satisfy (5), where $\bar{z}_3 \neq \bar{y}_3$ and where $\bar{P}\bar{y}_3 = \bar{y}_2$, $\bar{P}\bar{z}_3 = \bar{y}_3$, $P \in G^{n-2}$; then for some α and β determined by the rotation procedure previously described, the vector $\bar{u} = \alpha\bar{y}_2 + \beta\bar{y}_3$ is normal to an $(n - 2)$-face adjacent to that determined by $\bar{y}_2$. Observe, however, that

$$\begin{aligned} \bar{u} &= \alpha\bar{y}_2 + \beta\bar{P}\bar{z}_3 \\ &= \alpha\bar{P}\bar{y}_2 + \beta\bar{P}\bar{z}_3 \\ &= \bar{P}(\alpha\bar{y}_2 + \beta\bar{z}_3) \\ &= \bar{P}\bar{v}. \end{aligned}$$

By construction, for any P in G^{n-2}, necessarily $\bar{P}\bar{y}_1 = \bar{y}_1$, and hence $\bar{y}_1^T\bar{v} = 0$. Moreover, since $P \in G^{n-2} \subset G^{n-1}$, the elements of E in the facet determined by $\bar{y}_1$ are merely permuted by P, and hence $\bar{v}$ is a normal in this facet to an adjacent subfacet. Furthermore, because only two facets intersect in each subfacet, $\bar{v}$ is the only normal which may be obtained from $\bar{y}_2$ and $\bar{z}_3$. Extending this result to faces of general dimension, the conclusion follows that normals to inequivalent $(k+1)$-faces under G^{k+2} adjacent to a specified $(k+1)$-face can arise only from rotations about inequivalent k-faces under G^{k+1} within the given $(k+1)$-face. The converse of this statement does not hold, however, as equivalent $(k+1)$-faces (under G^{k+2}) may arise from inequivalent k-faces (under G^{k+1}).

When rotation has been carried out about one representative element for each equivalence class of k-faces contained in a $(k+1)$-face, there can exist no adjacent $(k+1)$-face which is not equivalent to those adjacent $(k+1)$-faces generated in scanning the specified k-face. To show this, assume such an inequivalent adjacent $(k+1)$-face exists. Necessarily, this adjacent $(k+1)$-face contains a k-face in common with the specified $(k+1)$-face. However this k-face must be an element of one of the characteristic equivalence classes for the k-faces in the original $(k+1)$-face. Thus by the preceding result, the $(k+1)$-face obtained by rotation was carried out about the k-face representing the appropriate equivalence class. Hence by contradiction, the assumed inequivalent adjacent $(k+1)$-face cannot exist.

For the general group G, comparison of the list of known $\bar{y}$ with a new $\bar{y}$ can be facilitated if a standard element of each equivalence class can be defined and kept in the list. One definition of this standard element for small groups might be the lexographically largest element of the equivalence class. That is, for $\{\bar{z}|\bar{z} = \bar{P}\bar{y}, \bar{P} \in G\}$, define $\bar{z}_0 = \max \bar{z}$, where $\bar{z}_1 > \bar{z}_2$ if $z_{i,1} = z_{i,2}$ for all i less than j, and $z_{j,1} > z_{j,2}$ ($\bar{z}_1$ exceeds $\bar{z}_2$ in the first element in which they differ). In general, $\bar{z}_0$ can only be found by generating the whole equivalence class of $\bar{y}$. Clearly two elements are in the same equivalence class if and only if their standard elements are the same.

3. Discussion. A computerized version of this algorithm has been prepared and applied to several elementary fermion and boson diagonal N-representability problems. The results of these calculations have been reported elsewhere [13]. In the most complex case considered ($r = 9$, $N = 5$) the matrix E had dimension 36×126. About 30 hours of CDC 6400 computer time was spent to find the adjacent facets to 195 of the facets. In this way, 1089 equivalence classes were found which contained 2.3×10^8 facets. For the simple cases $(r, N) = (3, 6)$, $(3, 7)$, $(3, 8)$ the dimensions of E are $(15, 20)$, $(21, 35)$, $(28, 56)$. The rotation algorithm required 4.3, 58.5, and 80.9 seconds per equivalence class, respectively, or 0.25, 0.46, and 0.030 seconds per facet. By comparison, the double description algorithm required only 0.04 and 0.17 seconds per facet for the first two cases, but this method was not feasible for the 52,000 facets of the third case.

In any particular application the choice of the minimum dimension for scanning (or, indeed, whether to use the double description method directly for the facets) must be based on expediency. As mentioned previously, the double description method is superior in the absence of symmetry when the expected number of extreme rays is small enough that they can all be kept in a computer at once. With some modifications for using disk storage, the amount of core-storage required can be kept small at the cost of extensive input-output. For the problems for which this new algorithm was designed, the extreme vectors had dimensions in the range of 20–40 and were expected to exceed 10^6 in number. Hence, even disk storage was not large enough to hold all of them at once.

The inefficiency in the scanning procedure described here arises because every facet is generated many times. If there are K facets with an average of L subfacets, then the process of scanning will generate each facet an average of L times. Since L is at least $n - 1$, for high dimensions the process becomes very inefficient.

If high symmetry is present, the situation may be reversed. Suppose each equivalence class contains an average of R facets. Then scanning one element of each equivalence class will produce only KL/R facets. While it is true that only K/R of these are needed, if L/R is much smaller than unity the scanning procedure will become more efficient than the double description algorithm which always generates K facets.

Because of the descent in symmetry and the decrease in the number of adjacent faces as the scanning procedure is carried to lower dimensional faces, beyond some face of minimum dimension the use of the double description method becomes preferred. Ideally this should be dynamically adjusted by the program itself.

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REFERENCES

[1] A. J. GOLDMAN AND A. W. TUCKER, *Polyhedral convex cones*, Ann. Math. Studies, 38 (1956), p. 19.

[2] R. M. ERDAHL AND H. KUMMER, *The N-representability problem*, Report of the Density Matrix Seminar, Queen's University, Kingston, Ontario, June 17–July 12, 1968.

[3] E. R. DAVIDSON, *Linear inequalities for density matrices. I*, J. Math Phys., 10 (1969), p. 725.

[4] M. L. YOSELOFF, *A combinatorial approach to the diagonal N-representability problem*, Ph.D. thesis, Princeton University, Princeton, New Jersey, 1970.

[5] P. O. LÖWDIN, *Quantum theory of many-particle systems. I. Physical interpretation by means of density matrices, natural spin orbitals, and convergence problems in the method of configuration interaction*, Phys. Rev., 97 (1955), p. 97.

[6] D. A. KOHLER, *Projections of convex polyhedral sets*, Ph.D. thesis, University of California, Berkeley, California, 1967.

[7] G. HADLEY, *Linear Programming*, Addison-Wesley, Reading, Mass., 1962, p. 65.

[8] H. WEYL, *The elementary theory of convex polyhedra*, Ann. Math. Studies, 24 (1950), p. 3.

[9] B. GRUNBAUM, *Convex Polytopes*, Interscience Publishers, New York, 1967.

[10] T. S. MOTZKIN, H. RAIFFA, G. L. THOMPSON AND R. M. THRALL, *The double description method*, Ann. Math. Studies, 28 (1953), p. 51.

[11] G. DEBREU, *Nonnegative solutions of linear inequalities*, Internat. Econom. Rev., 5 (1964), p. 178.

[12] D. GALE, *How to solve linear inequalities*, Amer. Math. Monthly, 76 (1969), p. 589.

[13] W. M. MCRAE AND E. R. DAVIDSON, *Linear inequalities for density matrices. II*, J. Math. and Phys., 13 (1972), p. 1527.

[14] M. EISEN, *Elementary Combinatorial Analysis*, Gordon and Breach, New York, 1969.