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EXTREME COPOSITIVE QUADRATIC FORMS, II

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A real quadratic form $Q = Q(x_1, \cdots, x_n)$ is called copositive if $Q(x_1, \cdots, x_n) \geqq 0$ whenever $x_1, \cdots, x_n \geqq 0$. If we associate each quadratic form $Q = \sum q_{ij}x_ix_j$ $q_{ij} = q_{ji}$ $(i, j = 1, \cdots, n)$ with a point

$$(q_{11}, \cdots, q_{nn}, \sqrt{2}\, q_{12}, \cdots, \sqrt{2}\, q_{n-1,n})$$

of Euclidean $n(n+1)/2$ space, then the copositive forms constitute a closed convex cone in this space. We are concerned with the extreme points of this cone. That is, with those copositive quadratic forms Q for which $Q = Q_1 + Q_2$ (with Q_1, Q_2 copositive) implies $Q_1 = aQ, Q_2 = (1-a)Q, 0 \leqq a \leqq 1$. In this paper we limit ourselves almost entirely to 5-variable forms and announce the discovery of an hitherto unknown class of extreme copositive quadratic forms in 5 variables. In view of the known extension process whereby extreme copositive quadratic forms in n variables may be used to generate extreme forms in n' variables for any $n' > n > 2$, this new class of forms thus provides new extreme copositive forms in any number of variables $n' \geqq 5$.

Copositive quadratic forms arise in the theory of inequalities and also in the study of block designs. The paper of Diananda [2] provides the connection with inequalities while the paper of Hall and Newman [3] outlines the application of copositive quadratic forms to block designs.

2. Preliminaries. As indicated above, a real quadratic form $Q = Q(x_1, \cdots, x_n)$ is called copositive if $Q(x_1, \cdots, x_n) \geqq 0$ whenever $x_1, \cdots, x_n \geqq 0$. Thus any positive semi-definite quadratic form is copositive. Further, any quadratic form all of whose coefficients are nonnegative in clearly copositive. Denoting these classes of forms by S and P respectively, we see that any quadratic form expressible as a sum of elements of P and S is necessarily copositive. In fact, Diananda [2, Th. 2] has shown that all copositive quadratic forms in $n \leqq 4$ variables are of this type (i.e., $Q \in P + S$ if Q is copositive and $n \leqq 4$). On the other hand, A. Horn [3] has constructed an extreme copositive quadratic form in 5 variables which does *not* belong to $P + S$. The extreme copositive quadratic forms belonging to $P + S$ have been determined by Hall and Newman [3, Th. 3.2]; thus we can restrict our attention to those outside of $P + S$ whenever it is desirable to do so. (Complete details of this theorem of Hall and Newman are given in the first paragraph of § 4 below.)

If $Q(x_1, \cdots, x_n)$ is an extreme copositive form so is $Q(p_1x_1, \cdots, p_nx_n)$

for any choice of $p_i > 0$ $(i = 1, \cdots, n)$. Hence, in dealing with forms having $q_{ii} > 0$ $(i = 1, \cdots, n)$ we may assume $q_{ii} = 1$ $(i = 1, \cdots, n)$ without loss of generality. Furthermore, note that relabeling of the variables has no effect on extremity or copositivity either.

We state here two results which we shall use later, whose statement at the time of their usage would interrupt the flow of thought.

(LEMMA 1 *of Diananda*). *If a quadratic form is nonnegative in some neighborhood of one of its zeros, it is positive semi-definite.*

(THEOREM 4.1 *of Hall and Newman*). *Let $Q = Q(x_1, \cdots, x_n)$ be an extreme copositive quadratic form, not of the type bx_ix_j. Let x_r, x_s be any two of the variables $x_1, \cdots, x_n$. Then upon replacing some of $x_1, \cdots, x_n$ by zero but neither x_r nor x_s, Q becomes a positive semi-definite form in the remaining variables.*

3. **Extremes with $q_{ij} = \pm 1$.** Diananda has shown [2, Lemma 2] that a copositive quadratic form Q has $q_{ii} \geqq 0$ $(i = 1, \cdots, n)$ and that if $q_{ii} = 0$ for some i, then for that i, $q_{ij} \geqq 0$ $(j = 1, \cdots, n)$. This implies that an extreme copositive quadratic form in $n \geqq 3$ variables will have positive diagonal coefficients. Thus they may be scaled so that $q_{ii} = 1$ $(i = 1, \cdots, n)$. If we so scale the extremes belonging to $P + S$ (see the first paragraph of § 4 for a listing of these), we see that $q_{ij} = \pm 1$ $(i, j = 1, \cdots, n)$, with the exception of the extremes of the type bx_ix_j, $b > 0$. Similarly the extreme form found by A. Horn [3], $Q = (x_1 - x_2 + x_3 + x_4 - x_5)^2 + 4x_2x_4 + 4x_3(x_5 - x_4)$, also has this property. In fact, Theorem 4.1 of Hall and Newman [3] guarantees that a so-scaled extreme copositive form (not of the type bx_ix_j, $b > 0$) will satisfy $-1 \leqq q_{ij} \leqq 1$ $(i, j = 1, \cdots, n)$. Hence the extremes mentioned above have all off-diagonal coefficients at the limits of their range. This explains our interest in:

LEMMA 3.1. *If Q is an extreme copositive quadratic form in* 5, 6 *or* 7 *variables which has $q_{ij} = \pm 1$ $(i, j = 1, \cdots, n)$, then Q is either positive semi-definite or Q can be derived from the Horn form by adding variables judiciously.*

Proof. Our method is simply to consider all quadratic forms having $q_{ij} = \pm 1$ $(i, j = 1, \cdots, n)$, $n = 5, 6$, and 7, and discard those which are not copositive or not extreme.

We start with $n = 5$. Copositivity obviously implies $q_{ii} \neq -1$, hence $q_{ii} = 1$ $(i = 1, \cdots, 5)$. We relabel the variables so that the first row of the matrix has at least as many -1's as any other row and so that $q_{12} = \cdots = q_{1r} = -1$, while $q_{1,r+1} = \cdots = q_{15} = 1$. Suppose $q_{12} = q_{13} = q_{14} = q_{15} = -1$, then all the remaining q_{ij}'s must be $+1$ in order to preserve copositivity. Thus $Q = (x_1 - x_2 - x_3 - x_4 - x_5)^2$ which is extreme and positive semi-definite. Suppose $q_{12} = q_{13} = q_{14} = -1$, $q_{15} = 1$ then copositivity implies that $q_{23} = q_{24} = q_{34} = 1$ and as $(x_1 - x_2 - x_3 - x_4 + x_5)^2$ is extreme no other extremes will result from the choices $q_{25}, q_{35}, q_{45} = \pm 1$. Suppose $q_{12} = q_{13} = -1$ and $q_{14} = q_{15} = 1$ then copositivity requires $q_{23} = 1$. At most one of $q_{24}, q_{25} = -1$, for otherwise row 2 would have 3 entries of -1 which violates our assumption. Thus by relabeling the variables, if necessary, we can insure that $q_{24} = 1$. So if $q_{34} = 1$ we get a form

$$(x_1 - x_2 - x_3 - x_4 + x_5)^2 \\ + 4x_1x_4 + 2(q_{25} + 1)\, x_2x_5 + 2(q_{35} + 1)\, x_3x_5 + 2(q_{45} + 1)\, x_4x_5$$

which is obviously not extreme for any choice of q_{25}, q_{35}, q_{45}. Hence $q_{34} = -1$ and counting -1's in row 3 yields $q_{35} = 1$. If we now assume $q_{25} = q_{45} = -1$ we get a form which is equivalent under a relabeling of the variables to the Horn form, see above. Hence any other choice of q_{25}, q_{45} yields a nonextreme form. Suppose $q_{12} = -1$, $q_{13} = q_{14} = q_{15} = 1$ then $q_{23} = q_{24} = q_{25} = 1$ by the -1 assumption. If any other row contains a -1 we relabel the variables to make it row 3 and to make $q_{34} = -1$. Thus $q_{35} = q_{45} = 1$ and so

$$Q(x_1, \cdots, x_5) = Q(x_1, \cdots, x_4, 0) + x_5^2 + 2 \sum_{i=1}^{4} x_i x_5$$

is not extreme, as $Q(x_1, \cdots, x_4, 0) \in P + S$. From which it follows that the remaining cases (1) $q_{12} = -1, q_{34} = +1$ and (2) $q_{12} = q_{34} = +1$ are not extreme either. Thus the only 5-variable extremes having $q_{ij} = \pm 1$ are equivalent to one of

$$(x_1 - x_2 - x_3 - x_4 - x_5)^2,\ (x_1 - x_2 - x_3 - x_4 + x_5)^2$$

or the Horn form, as was to be proved.

For $n = 6$, let $q_{12} = q_{13} = q_{14} = q_{15} = q_{16} = -1$, then in order to be copositive all others are $+1$, which is a positive semi-definite extreme. Changing q_{16} to $+1$ gives an extreme with $q_{26} = q_{36} = q_{46} = q_{56} = -1$, hence, any other values for these variables is nonextreme. Let $q_{12} = q_{13} = q_{14} = -1, q_{15} = q_{16} = 1$ thus $q_{23} = q_{24} = q_{34} = 1$ and q_{25}, q_{26} can be $-1, -1$; $-1, 1$; $1, -1$; $1, 1$ the second and third of which are equivalent. If $q_{25} = q_{26} = -1$ then $q_{56} = +1$ for copositivity and since $q_{35} = q_{36} = q_{.5} = q_{46} = -1$ is a positive semi-definite extreme, all other choices of $q_{35}, q_{36}, q_{45}, q_{46}$ are not extreme. In the remaining cases we may assume $q_{56} = -1$ for $q_{56} = +1$ yields a nonextreme form depending on the previous one. If $q_{25} = q_{26} = 1$ then we may assume $q_{35} = q_{36} = q_{\ 5} = q_{\ 6} = 1$ for otherwise a change of variable would put us into one of the other cases. But if this is true the form is not extreme. Thus only $q_{25}, q_{26} = -1, 1$ remains. Here there are six essentially distinct choices for $q_{35}, q_{36}, q_{45}, q_{46}$, these are:

$$\begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix}, \begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix}, \begin{bmatrix} -1 & 1 \\ 1 & 1 \end{bmatrix}, \begin{bmatrix} 1 & -1 \\ 1 & -1 \end{bmatrix}, \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}, \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}.$$

The first of these yields four -1's in row 5 and thus was considered previously. The permutation (56) (24) takes the fourth case into the second. Cases 3, 5, 6 depend on Case 2 (that is, they are copositive and not extreme if Case 2 is copositive). Thus, if we show that Case 2 is copositive we need not consider them further. But we can generate this matrix from the Horn form by the mapping $x_2 \to x_2 + x_6$ and a renumbering of the variables. Now Theorem 3.8 of [1] states that this kind of mapping preserves both copositivity and extremity. Hence it is a copositive extreme. Thus at this point we have the extremes of Figure 1 (where $-$ stands for -1).

$$\begin{bmatrix} 1&-&-&-&-&- \\ -&1&1&1&1&1 \\ -&1&1&1&1&1 \\ -&1&1&1&1&1 \\ -&1&1&1&1&1 \\ -&1&1&1&1&1 \end{bmatrix} \quad \begin{bmatrix} 1&-&-&-&-&1 \\ -&1&1&1&1&- \\ -&1&1&1&1&- \\ -&1&1&1&1&- \\ -&1&1&1&1&- \\ 1&-&-&-&-&1 \end{bmatrix} \quad \begin{bmatrix} 1&-&-&-&1&1 \\ -&1&1&1&-&- \\ -&1&1&1&-&- \\ -&1&1&1&-&- \\ 1&-&-&-&1&1 \\ 1&-&-&-&1&1 \end{bmatrix} \quad \begin{bmatrix} 1&-&-&-&1&1 \\ -&1&1&1&-&1 \\ -&1&1&1&-&1 \\ -&1&1&1&1&- \\ 1&-&-&1&1&- \\ 1&1&1&-&-&1 \end{bmatrix}$$

FIGURE 1. Extreme Copositive Quadratic Forms in 6 Variables.

If $q_{12} = q_{13} = -1$, $q_{14} = q_{15} = q_{16} = 1$, then $q_{23} = 1$. Either $q_{24} = -1$ or by a change of variable we may assume $q_{24} = q_{25} = q_{26} = q_{34} = q_{35} = q_{36} = +1$. In this latter case, every copositive completion of the matrix yields a nonextreme form. Thus we may assume $q_{24} = -1$, and hence, $q_{25} = q_{26} = 1$ (for otherwise we would have three -1's in row 2, a previous case). For the triple q_{34}, q_{35}, q_{36} we could have $-1, 1, 1$; $1, -1, 1$; $1, 1, -1$; or $1, 1, 1$. Of these, the third is equivalent to the second under $x_5 \leftrightarrow x_6$. Suppose q_{34}, q_{35}, q_{36} are $-1, 1, 1$, then (by the -1 count in row 4) $q_{45} = q_{\,6} = +1$. So the form is nonextreme regardless of the choice of q_{56}. Let q_{34}, q_{35}, q_{36} be $1, -1, 1$ then q_{45}, q_{46} can be $-1, 1$; $1, -1$; or $1, 1$. For $-1, 1$ we have $q_{56} = +1$ (-1 count) and the form is a copositive nonextreme. If q_{45}, q_{46} is $1, -1$, then $q_{56} = 1$ is nonextreme as $q_{56} = -1$ is copositive. To see this we use the permutation (643) and note that the resulting form is dependent on $(x_1 - x_2 + x_3 - x_4 + x_5 - x_6)^2$. Thus, neither $q_{56} = \pm 1$ is extreme. If $q_{45}, q_{46} = 1, 1$ we again get a form dependent on the last one. This leaves $q_{34} = q_{35} = q_{36} = 1$, hence $q_{45}, q_{46} = -1, 1$

or 1, -1 as 1, 1 is not extreme. As these two are equivalent, we may assume $q_{45}, q_{46} = 1, -1$, which is nonextreme and dependent upon $(x_1 - x_2 + x_3 - x_4 + x_5 - x_6)^2$, after a change of variable.

If at most one entry per row is -1 the form is not extreme for the worst case has $q_{12} = q_{34} = q_{56} = -1$ and the rest $+1$, obviously a copositive nonextreme. Thus, there are just the 4 extremes of Figure 1. Three positive semi-definite and the other derived from the Horn form.

For $n = 7$, we have the positive semi-definite extremes

$$(x_1 - x_2 - x_3 - x_4 - x_5 - x_6 - x_7)^2 ,$$
$$(x_1 - x_2 - x_3 - x_4 - x_5 - x_6 + x_7)^2$$

and

$$(x_1 - x_2 - x_3 - x_4 - x_5 + x_6 + x_7)^2$$

as before and we can start with

$$q_{12} = q_{13} = q_{14} = q_{15} = q_{67} = -1 ,$$
$$q_{16} = q_{17} = q_{23} = q_{24} = q_{25} = q_{34} = q_{35} = q_{45} = +1 .$$

If the remaining positions are all $+1$, then the form is not extreme, hence, we may assume that $q_{26} = -1$. If $q_{27} = -1$, then copositivity is violated, hence $q_{27} = 1$. Thus we have the 3 cases

$$\begin{bmatrix} q_{36}, q_{37} \\ q_{46}, q_{47} \\ q_{56}, q_{57} \end{bmatrix} = \begin{bmatrix} -1 & 1 \\ -1 & 1 \\ -1 & 1 \end{bmatrix}, \begin{bmatrix} -1 & 1 \\ -1 & 1 \\ 1 & -1 \end{bmatrix}, \begin{bmatrix} -1 & 1 \\ 1 & -1 \\ 1 & -1 \end{bmatrix}$$

and those derived from these by replacing some -1's by $+1$'s. The first of these is nonextreme depending upon $(x_1 - x_2 - x_3 - x_4 - x_5 + x_6 - x_7)^2$. The second and third are extreme as they arise from the last 6-variable extreme by adjoining a variable properly [1, Th. 3.8]. As these are all copositive, the remaining cases cannot be extreme. Let $q_{12} = q_{13} = q_{14} = -1$, $q_{15} = q_{16} = q_{17} = +1$, thus $q_{23} = q_{24} = q_{34} = +1$. Here q_{25}, q_{26}, q_{27} can be $-1, -1, 1$; $-1, 1, 1$; or $1, 1, 1$. In this last case we may assume by change of variable that $q_{35} = q_{36} = q_{37} = q_{45} = q_{46} = q_{47} = 1$ which yields a nonextreme form as long as the remainder is filled out copositively. If q_{25}, q_{26}, q_{27} is $-1, -1, 1$, then $q_{56} = +1$, and we have a number of choices for the block

$$q_{35}, q_{36}, q_{37}$$
$$q_{45}, q_{46}, q_{47} .$$

Note that this number can be significantly reduced by use of the permutations (56) and (34). If $q_{35} = q_{36} = q_{37} = -1$ then there are too many -1's in row 3. Similarly at least one of q_{45}, q_{46}, q_{47} must be

$+1$. If this block contains two -1's and one $+1$ per row, it is equivalent to one of

$$\begin{bmatrix}-1, -1, 1\\ -1, -1, 1\end{bmatrix}, \begin{bmatrix}-1, & -1, & 1\\ -1, & 1, & -1\end{bmatrix}, \begin{bmatrix}-1, 1, -1\\ -1, 1, -1\end{bmatrix}, \begin{bmatrix}-1, & 1, & -1\\ 1, & -1, & -1\end{bmatrix}.$$

The first of these implies (by -1 count) that $q_{57} = q_{67} = +1$, whence it is a copositive nonextreme. In the second case $q_{57} = +1$ necessarily, and if $q_{67} = -1$ we have an extreme copositive form (call it A) which is related to the Horn form. One way to see this is to take the last 6-variable extreme above and put $x_1 + x_7$ for x_1 then relabel the variables using the permutation (567). So by [1, Th. 3.8] we have a copositive extreme, hence the other choice $q_{67} = +1$ is not extreme. In the third case $q_{57} = +1$ as before and if $q_{67} = -1$ we get extreme A if we apply (67)(243). Thus the alternate $q_{67} = +1$ is nonextreme. In the last case copositivity requires that $q_{57} = q_{67} = +1$ and we get a nonextreme depending on the form $(x_1 - x_2 - x_3 - x_4 + x_5 + x_6 + x_7)^2$.

If two of q_{35}, q_{36}, q_{37} are -1's and only one of q_{45}, q_{46}, q_{47} is -1, then the form is equivalent to one with block

$$\begin{bmatrix}-1, & -1, & 1\\ -1, & 1, & 1\end{bmatrix}, \begin{bmatrix}-1, & -1, & 1\\ 1, & 1, & -1\end{bmatrix}, \begin{bmatrix}-1, & 1, & -1\\ -1, & 1, & 1\end{bmatrix}, \begin{bmatrix}-1, & 1, & -1\\ 1, & -1, & 1\end{bmatrix}, \begin{bmatrix}-1, 1, -1\\ 1, 1, -1\end{bmatrix}.$$

In the first case $q_{57} = +1$ (-1 count) and the form is a copositive nonextreme depending on extreme A above regardless of the choice of q_{67}. In the second case $q_{57} = q_{67} = -1$ yields a copositive extreme (call it B) related to the Horn form. (Take the last 6-variable extreme above and replace x_5 by $x_5 + x_7$, then use the permutation (67) and [1, Th. 3.8].) Hence the other choices for q_{57}, q_{67} yield nonextreme forms. In the remaining cases, copositivity requires $q_{57} = +1$ and we get nonextreme forms related to extreme A after suitable permutation of the subscripts.

If two of q_{35}, q_{36}, q_{37} are -1's and $q_{45} = q_{46} = q_{47} = +1$ then q_{35}, q_{36}, q_{37} can take only two inequivalent values, i.e., $-1, -1, 1$ or $-1, 1, -1$. The first of these is nonextreme depending on B. In the second case copositivity requires $q_{57} = +1$ and we have a nonextreme depending on A.

The cases where q_{35}, q_{36}, q_{37} have at most one -1 and q_{45}, q_{46}, q_{47} have at most one -1 are all equivalent to one of

$$\begin{bmatrix}1, 1, -1\\ 1, 1, -1\end{bmatrix}, \begin{bmatrix}1, -1, 1\\ 1, -1, 1\end{bmatrix}, \begin{bmatrix}-1, & 1, & 1\\ 1, & -1, & 1\end{bmatrix},$$

$$\begin{bmatrix}-1, & 1, & 1\\ 1, & 1, & -1\end{bmatrix}, \begin{bmatrix}-1, 1, 1\\ 1, 1, 1\end{bmatrix}, \begin{bmatrix}1, & 1, & -1\\ 1, & 1, & 1\end{bmatrix}, \begin{bmatrix}1, 1, 1\\ 1, 1, 1\end{bmatrix}.$$

In the first of these we may assume that at worst (by -1 count) one of q_{57}, q_{67} is -1 and we may take it to be q_{67} without loss of generality. Here the permutation (24)(67) shows nonextremity depending on the extreme A. In the second case $q_{67} = +1$ necessarily (-1 count) and the permutation (56) shows the form is nonextreme depending on A. In the third case, we have $q_{57} = q_{67} = -1$ as the worst possibility and this is nonextreme depending on

$$(x_1 - x_2 - x_3 - x_4 + x_5 + x_6 - x_7)^2 ,$$

thus the other choices for q_{57}, q_{67} are nonextreme also. The remaining cases are all nonextreme depending on B.

If q_{25}, q_{26}, q_{27} is $-1, 1, 1$ then we may assume that q_{35}, q_{36}, q_{37} has at most one -1 as does q_{45}, q_{46}, q_{47} thus our blocks are

$$\begin{bmatrix} -1, 1, 1 \\ -1, 1, 1 \end{bmatrix}, \begin{bmatrix} -1, & 1, 1 \\ 1, -1, & 1 \end{bmatrix}, \begin{bmatrix} 1, -1, & 1 \\ 1, & 1, -1 \end{bmatrix}, \begin{bmatrix} -1, 1, 1 \\ 1, 1, 1 \end{bmatrix}, \begin{bmatrix} 1, -1, 1 \\ 1, & 1, 1 \end{bmatrix}, \begin{bmatrix} 1, 1, 1 \\ 1, 1, 1 \end{bmatrix}$$

all others being equivalent to one of these. The first of these has $q_{56} = q_{57} = +1$ (-1 count) and is thus obviously nonextreme depending on $(x_1 - x_2 - x_3 - x_4 + x_5)^2 + (x_6 - x_7)^2$ regardless of the choice of q_{67}. In the second case at least one of $q_{56}, q_{57} = +1$ (-1 count). If $q_{56} = 1$ the form is nonextreme depending on

$$(x_1 - x_2 - x_3 - x_4 + x_5 + x_6 - x_7)^2 .$$

If $q_{57} = 1$ the form depends on B as the permutation (67) shows. In the third case at least one of q_{56}, q_{57}, q_{67} is $+1$ to insure copositivity and in each of these events the form is nonextreme dependent on B after suitable permutation. The fourth, fifth and sixth cases are nonextreme dependent on the second, third and third respectively.

If $q_{12} = q_{13} = -1$ and $q_{14} = q_{15} = q_{16} = q_{17} = q_{23} = 1$ then

$$\begin{bmatrix} q_{24}, q_{25}, q_{26}, q_{27} \\ q_{34}, q_{35}, q_{36}, q_{37} \end{bmatrix} = \begin{bmatrix} -1 & 1 & 1 & 1 \\ -1 & 1 & 1 & 1 \end{bmatrix}, \begin{bmatrix} -1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 \end{bmatrix}, \begin{bmatrix} -1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix}, \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix}$$

the last of which is not extreme for any copositive choice in the remaining positions. In the first case $q_{45} = q_{46} = q_{47} = +1$ (-1 count) and nonextremity follows. In the second case q_{45}, q_{46}, q_{47} can be $-1, 1, 1$ or $1, -1, 1$ or $1, 1, 1$. If $-1, 1, 1$ then $q_{56} = q_{57} = +1$ and the form is nonextreme. If $1, -1, 1$ then at least one of q_{56}, q_{57} is $+1$. If $q_{57} = 1$ then the permutation (34) show that the form is nonextreme dependent on $(x_1 - x_2 + x_3 - x_4 + x_5 - x_6 + x_7)^2$. If $q_{56} = 1$ we apply the permutation (472) which yields nonextremity dependent on B above. If $q_{45} = q_{46} = q_{47} = +1$ the form is nonextreme and depends on the case $1, -1, 1$ for these coefficients. In the third case above there are two choices for q_{45}, q_{46}, q_{47} either $1, -1, 1$ or $1, 1, 1$ the last of which is obviously nonextreme for any copositive completion. If q_{45}, q_{46}, q_{47} are $1, -1, 1$ the form is again nonextreme depending on that part of the second case above having these same values for q_{45}, q_{46}, q_{47}.

Since there are no extreme forms in 7 variables with at most one -1 in a row we have exhausted all possibilities. Thus we have determined 6 extreme copositive forms in 7 variables having $q_{ij} = \pm 1$ (the extremes A, B are equivalent as the permutation (165)(45) shows). These are the three positive semi-definite extremes

$$(x_1 - x_2 - x_3 - x_4 - x_5 - x_6 - x_7)^2 ,$$
$$(x_1 - x_2 - x_3 - x_4 - x_5 - x_6 + x_7)^2 ,$$
$$(x_1 - x_2 - x_3 - x_4 - x_5 + x_6 + x_7)^2$$

together with the three derived from the Horn form by the use of [1, Th. 3.8] (see Figure 2). The only equivalences which could exist between these would have to be between the last 3 (i.e., certainly the positive semi-definite extremes are not equivalent to each other or to any form which is not positive semi-definite). But there are no equivalences between the last 3 as a tally of the -1's in each row clearly shows. Thus there are exactly 6 inequivalent extreme copositive quadratic forms in 7 variables having the property $q_{ij} = \pm 1$ $(i, j = 1, \cdots, 7)$ and each of them can be derived from such a 6-variable extreme by the use of [1, Th. 3.8]

$$\begin{bmatrix} 1 & - & - & - & - & 1 & 1 \\ - & 1 & 1 & 1 & 1 & - & 1 \\ - & 1 & 1 & 1 & 1 & - & 1 \\ - & 1 & 1 & 1 & 1 & - & 1 \\ - & 1 & 1 & 1 & 1 & 1 & - \\ 1 & - & - & - & 1 & 1 & - \\ 1 & 1 & 1 & 1 & - & - & 1 \end{bmatrix} \quad \begin{bmatrix} 1 & - & - & - & - & 1 & 1 \\ - & 1 & 1 & 1 & 1 & - & 1 \\ - & 1 & 1 & 1 & 1 & - & 1 \\ - & 1 & 1 & 1 & 1 & 1 & - \\ - & 1 & 1 & 1 & 1 & 1 & - \\ 1 & - & - & 1 & 1 & 1 & - \\ 1 & 1 & 1 & - & - & - & 1 \end{bmatrix} \quad \begin{bmatrix} 1 & - & - & - & 1 & 1 & 1 \\ - & 1 & 1 & 1 & - & - & 1 \\ - & 1 & 1 & 1 & - & - & 1 \\ - & 1 & 1 & 1 & - & 1 & - \\ 1 & - & - & - & 1 & 1 & 1 \\ 1 & - & - & 1 & 1 & 1 & - \\ 1 & 1 & 1 & - & 1 & - & 1 \end{bmatrix}$$

FIGURE 2. Extreme Copositive Quadratic Forms in 7 Variables.

4. A new class of extreme forms. A conjecture. According to Hall and Newman [3, Th. 3.2] the extreme copositive quadratic forms in n variables which belong to $P + S$ are of three types:

(i) $ax_i^2, a > 0$ $\quad (i = 1, \cdots, n)$

(ii) $bx_ix_j, b > 0$ $\quad (i \neq j; i, j = 1, \cdots, n)$

(iii) $(U - V)^2$ with $U = \sum_{i=1}^{r} a_iu_i$, $V = \sum_{i=1}^{s} b_iv_i$,

where the u's and v's are disjoint subsets of $x_1, \cdots, x_n$ and $a_i > 0$,

$b_i > 0$, $r \geqq 1$, $s \geqq 1$. Thus, if we only consider extremes in 3 or more variables, we note that for every index pair i, j $(1 \leqq i, j \leqq n)$ the extremes have zeros u $(u_i > 0; i = 1, \cdots, n)$ where $u_i u_j > 0$. The Horn form (see first part of § 3) also has this property. We conjecture that this is always true, i.e.:

CONJECTURE 4.1. If $Q(x_1, \cdots, x_n)$, $n \geqq 3$ is an extreme copositive quadratic form, then for every index pair i, j $(1 \leqq i, j \leqq n)$, Q has a nonnegative component zero u with $u_i u_j > 0$.

Note that the special case $i = j$ has been established [1, Th. 3.4].

If we consider only those extreme copositive forms in 5 variables for which the conjecture is valid, and scale them so that $q_{ii} = 1$ $(i = 1, \cdots, 5)$, we can say quite a bit about their *nonnegative* component zeros. In fact, assuming these forms are *not* positive semi-definite, we have:

(i) Each zero has at least two nonzero components (since $q_{ii} = 1$, $i = 1, \cdots, 5$).

(ii) Each zero has at least two *zero* components. (Lemma 1, Diananda, and [1, Corollary 3.7].)

(iii) For every index pair i, j $(1 \leqq i, j \leqq 5)$, Q has a zero u with $u_i u_j > 0$. (Conjecture 4.1).

(iv) Q has at *most* six 2-variable zeros.

This follows because each 2-variable zero implies that a different off-diagonal coefficient is -1 (since $q_{ii} = 1, i = 1, \cdots, 5$) and because $-1 \leqq q_{ij} \leqq 1$ (Theorem 4.1, Hall and Newman); thus, if Q had more than 6 such zeros, then $Q(1, 1, 1, 1, 1) < 0$, which contradicts copositivity. Since all 10 pairs $(i \neq j)$ appear together in some zero (by iii), we have

(v) Q has at *least* two 3-variable zeros.

Note that by relabeling the variables we can insure that the required 3-variable zeros are $(u_1, u_2, u_3, 0, 0)$ and one of $(v_1, 0, 0, v_4, v_5)$, $(w_1, w_2, 0, w_4, 0)$.

This information on their nonnegative component zeros allows us to specify the structure of these zeros completely, if we remember that we are considering only extreme copositive forms in 5 variables which are *not* positive semi-definite, which have $q_{ii} = 1$ $(i = 1, \cdots, 5)$ and for which Conjecture 4.1 is valid. In order to do this we introduce some terminology.

DEFINITION 4.2. A quadratic form $Q(x_1, \cdots, x_n)$ has $A^*(n)$ or $Q \in A^*(n)$, if (1) Q is copositive and (2) if for all i, j $(i, j = 1, \cdots, n)$ the form $Q - \varepsilon x_i x_j$ is *not* copositive for any $\varepsilon > 0$.

We note that every extreme copositive quadratic form in $n \geqq 3$

variables has $A^*(n)$. Further, if Q is any copositive quadratic form and if Q has a nonnegative component zero u with $u_1, u_2 > 0$, then $Q - \varepsilon x_1 x_2$ is not copositive for any $\varepsilon > 0$. Thus, one way of establishing $Q \in A^*(n)$ is by examining its nonnegative component zeros. We use this extensively below.

DEFINITION 4.3. The *pattern* of an n-dimensional vector $v = (v_1, \cdots, v_n)$ is the vector obtained by replacing its *nonzero* components with 1's. Thus $(3, -2, 0, 4, -971)$ has pattern $(1, 1, 0, 1, 1)$.

Our principle tool in determining the zero structure is the following lemma:

LEMMA 4.4. *If Q has $A^*(5)$ and some 4-variable sub-form Q_4 has $A^*(4)$, then Q is positive semi-definite.*

Proof. Q_4 has $A^*(4)$ implies that Q is positive semi-definite (Theorem 2, Diananda). But Theorem 4 of Diananda states that if Q_n is a positive semi-definite quadratic form having $A^*(n)$, then Q_n has a zero with all components positive. Thus Q_4 has a zero with 4 positive components. Hence, so does Q, and thus [1, Corollary 3.7] Q is positive semi-definite.

In what follows we shall only be interested in nonnegative component zeros and then for the most part only in their patterns. Thus any zero pattern mentioned will be the pattern of a nonnegative component zero. We prove:

LEMMA 4.5. *If Q is an extreme copositive quadratic form in 5 variables which is not positive semi-definite and which satisfies Conjecture 4.1., then Q has 5 nonnegative component zeros which have the patterns* (11100), (01110), (00111), (10011) *and* (11001). *Further if Q is not the Horn form (see § 3), then Q has no further nonnegative component zeros.*

Proof. Lemma 2 of Diananda insures $q_{ii} > 0$ $(i = 1, \cdots, 5)$, whence without loss of generality we may assume $q_{ii} = 1$ $(i = 1, \cdots, 5)$. According to (i), $\cdots$, (v) above, there are two main cases depending on the 3-variable zeros which occur. Case a has zeros (11100), (10011) and Case b has zeros (11100), (11010). We shall often use Lemma 4.4 to show that the form we are considering is positive semi-definite. One should be careful to realize that more explicitly this means the form is positive semi-definite if it is copositive at all.

CASE a. The zero $u_2 u_4 \neq 0$ can appear with patterns (01010), (11010), (01110), (01011) and calling these a.1, a.2, a.3, a.4 respectively, we see that a.4 is equivalent to a.3 under a relabeling of the variables. Hence we need not consider it further. The zero $u_2u_5 \neq 0$ may be added to case a.1 as (01001), (11001), (01101), (01011) which we call a.1.a, a.1.b, a.1.c, a.1.d. Here a.1.b is positive semi-definite by Lemma 4.4 above, since $Q_4 = Q(x_1, x_2, 0, x_3, x_4)$ has zero patterns (1011), (0110), (1101) and thus clearly has $A^*(4)$. So we need not consider a.1.b further. Adding the zero $u_3u_4 \neq 0$ to case a.1.a in all possible ways yields cases a.1.a.1, a.1.a.2, a.1.a.3, a.1.a.4 with additional patterns (00110), (10110), (01110), (00111). In case a.1.a.2, $Q_4 = Q(x_1, x_2, x_3, x_4, 0)$ and Lemma 4.4 make Q positive semi-definite, so we delete that case. The zero $u_3u_5 \neq 0$ adjoined to case a.1.a.1 yields a.1.a.1.a. (00101), a.1.a.1.b (10101), a.1.a.1.c (01101) and a.1.a.1.d (00111). In case a.1.a.1.a, $q_{24} = q_{25} = q_{34} = q_{35} = -1$ and hence $Q(0, x_2, x_3, x_4, 0)$ copositive implies $q_{23} = 1$. Similarly $Q(0, 0, x_3, x_4, x_5)$ copositive implies $q_{45} = 1$, thus $Q(0, 1, 1, 1, 1) = 0$ and so Q is positive semi-definite [1, Corollary 3.7]. Case a.1.a.1.b yields Q positive semi-definite also, since $Q_4 = Q(x_1, x_2, x_3, 0, x_5)$ has $A^*(4)$. Cases a.1.a.1.c and a.1.a.1.d are contained in a.1.a.4. At this point, all of a.1.a.1 has been either eliminated or assumed under another case, and as a.1.a.2 was previously eliminated we consider a.1.a.3. Adding $u_3u_5 \neq 0$ yields a.1.a.3.a (00101), a.1.a.3.b (10101), a.1.a.3.c (01101) and finally a.1.a.3.d (00111). Now a.1.a.3.b and a.1.a.3.d are positive semi-definite by the lemma, so we discard them. Further a.1.a.3.a is equivalent to a.1.a.1.c and thus contained in a.1.a.4 as was that case. Thus we are left for the moment with a.1.a.3.c and a.1.a.4 both of which are contained in future cases as we shall see.

Having thus accounted for all of a.1.a, and eliminated a.1.b, we turn to a.1.c. Adding $u_3u_4 \neq 0$ yields a.1.c.1 (00110), a.1.c.2. (10110), a.1.c.3 (01110) and a.1.c.4 (00111). Here a.1.c.1 is equivalent to a.1.a.4; a.1.c.2 and a.1.c.4 are positive semi-definite by the lemma and a.1.c.3 remains—actually it is contained in a future case. We note that a.1.a.3.c is a sub-case of a.1.c.3, hence we discard a.1.a.3.c. Adding $u_3u_4 \neq 0$ to a.1.d yields a.1.d.1 (00110), a.1.d.2 (10110), a.1.d.3 (01110) and a.1.d.4 (00111). Now a.1.d.2 is positive semi-definite by the lemma and a.1.d.4 is equivalent to a.1.c.3. We now add $u_3u_5 \neq 0$ to a.1.d.1 giving a.1.d.1.a (00101), a.1.d.1.b (10101), a.1.d.1.c (01101) and a.1.d.1.d (00111). Of these a.1.d.1.b and a.1.d.1.c are positive semi-definite by the lemma, and a.1.d.1.a is included in a.1.a.4 while a.1.d.1.d is a sub-case of a.1.c.3. Adding $u_3u_5 \neq 0$ to the remaining case a.1.d.3 yields a.1.d.3.a (00101), a.1.d.3.b (10101), a.1.d.3.c (01101) and a.1.d.3.d (00111). Here a.1.d.3.b is included in a future case and the others are positive semi-definite. Thus we have a.1.a.4, a.1.c.3 and a.1.d.3.b as the only patterns remaining from a.1 (and these all will appear as sub-cases of others).

Turning to a.2 we add $u_2u_5 \neq 0$ getting a.2.a (01001), a.2.b (11001), a.2.c (01101) and a.2.d (01011). The other three being positive semi-definite we consider only a.2.c. Adding $u_3u_4 \neq 0$ gives a.2.c.1 (00110), a.2.c.2 (10110), a.2.c.3 (01110) and a.2.c.4 (00111), with a.2.c.4 providing the only solution as the three other cases are positive semi-definite. Note that a.1.d.3.b is contained in a.2.c.4. As for a.3, we add $u_2u_5 \neq 0$ to get a.3.a (01001), a.3.b (11001), a.3.c (01101) and a.3.d (01011). Note that a.3.c includes a.1.c.3. It also includes a.1.a.4 for in this case $q_{24} = q_{25} = -1$ and so $q_{45} = 1$ to insure copositivity. Hence $Q(0, x_2, 0, x_4, x_5) = (x_2 - x_4 - x_5)^2$ and thus a.1.a.4 has the additional zero pattern (01011) from which we see that a.1.a.4 is indeed included in a.3.c. Now adding $u_3u_5 \neq 0$ to a.3.a yields a.3.a.1 (00101), a.3.a.2 (10101), a.3.a.3 (01101) and a.3.a.4 (00111). Of these a.3.a.2 and a.3.a.4 are positive semi-definite and the others are included in a.3.c. To a.3.b we adjoin $u_3u_5 \neq 0$ and get a.3.b.1 (00101), a.3.b.2 (10101), a.3.b.3 (01101) and a.3.b.4 (00111). Here a.3.b.4 is a sub-case of a.2.c.4 and the others are positive semi-definite. Turning to a.3.d we add $u_3u_5 \neq 0$ yielding a.3.d.1 (00101), a.3.d.2 (10101), a.3.d.3 (01101) and a.3.d.4 (00111) of which the second is a sub-case of a.2.c.4 and the others are positive semi-definite.

Since a.4 was equivalent to a.3 we have exhausted Case a and discovered only two possible zero patterns a.2.c.4 and a.3.c; relabeling the variables gives

a.2.c.4 (11100), (01110), (00111), (10011), (11001)
a.3.c (11100), (11010), (11001), (00111) .

CASE b. Here we have (11100) and (11010) as the basic patterns and we add $u_1u_5 \neq 0$ yielding b.1 (10001), b.2 (11001), b.3 (10101) and b.4 (10011). Now b.3 and b.4 were considered under Case a, thus only b.1 and b.2 need be investigated. Adding $u_2u_5 \neq 0$ to b.1 gives b.1.a (01001), b.1.b (11001), b.1.c (01101) and b.1.d (01011) of which b.1.c and b.1.d are sub-cases of a. Adjoining $u_3u_4 \neq 0$ to b.1.a yields b.1.a.1 (00110), b.1.a.2 (10110), b.1.a.3 (01110) and b.1.a.4 (00111). This last is a sub-case of a and the others are positive semi-definite. Adding $u_3u_4 \neq 0$ to b.1.b gives b.1.b.1 (00110), b.1.b.2 (10110), b.1.b.3 (01110) and b.1.b.4 (00111). Here again the last case belongs to a and the others are positive semi-definite. Considering b.2 now, we add $u_3u_4 \neq 0$ and get b.2.a (00110), b.2.b (10110), b.2.c (01110) and b.2.d (00111). Of these, the first is positive semi-definite and the others are sub-cases of a. Hence case b adds no new solutions.

In dealing with our two solutions, a.2.c.4 and a.3.c, we shall continuously use the facts that $q_{ii} = 1$ $(i = 1, \cdots, 5)$ and hence that

$-1 \leqq q_{ii} \leqq 1$ (Theorem 4.1, Hall and Newman). Let us label the known zeros of a.3.c as follows

$$u = (u_1, u_2, u_3, 0, 0) ,$$
$$v = (v_1, v_2, 0, v_4, 0) ,$$
$$w = (w_1, w_2, 0, 0, w_5) ,$$

and

$$z = (0, 0, z_3, z_4, z_5) .$$

Applying [2, Th. 2] to $Q_4 = Q(x_1, x_2 x_3, x_4, 0)$ we see that it is contained in $P + S$, hence zeros u, v of Q imply that $Q_4 = Q' + bx_3x_4$ where Q' has $A^*(4)$ for $b \geqq 0$ large enough. Thus Q' is positive semi-definite and [2, Th. 4] has a zero with all components positive. So [1, Corollary 3.7] implies that Q is positive semi-definite if $b = 0$. Thus we may assume $b > 0$; but with Q' positive semi-definite this yields $q_{34} > -1$. Similarly $q_{35}, q_{45} > -1$. Since $q_{34}, q_{35}, q_{45} > -1$, Q has no zeros with patterns 00110, 00101, 00011 and any further zero patterns that Q might have are equivalent to one of $A(11000)$, $B(10100)$ or $C(10110)$ by a relabeling of the variables. In Case C, $Q_4 = Q(x_1, x_2, x_3, x_4, 0)$ and the lemma prove that Q is positive semi-definite. In Case B, $q_{13} = -1$ and $Q(x_1, x_2, x_3, 0, 0)$ being positive semi-definite (Lemma 1, Diananda) we see that $Q(u) = 0$ implies that (q_{12}, q_{23}) is $(1, -1)$ or $(-1, 1)$. Using the facts that $Q(x_1, x_2, 0, x_4, 0)$ and $Q(x_1, x_2, 0, 0, x_5)$ are similarly positive semi-definite with zeros v and w yields five cases.

(B1) $\quad q_{12} = 1, q_{14} = q_{15} = q_{23} = q_{24} = q_{25} = -1$

(B2) $\quad q_{14} = q_{15} = q_{23} = 1, q_{12} = q_{24} = q_{25} = -1$

(B3) $\quad q_{14} = q_{23} = q_{25} = 1, q_{12} = q_{15} = q_{24} = -1$

(B4) $\quad q_{15} = q_{23} = q_{24} = 1, q_{12} = q_{14} = q_{25} = -1$

(B5) $\quad q_{23} = q_{24} = q_{25} = 1, q_{12} = q_{14} = q_{15} = -1$

For B1 we have $Q(x_1, 0, x_3, x_4, 0)$ copositive, thus $q_{34} \geqq 1$. But since $Q(x_1, \cdots, x_5)$ is extreme, Theorem 4.1 of Hall and Newman yields $-1 \leqq q_{ij} \leqq 1$ $(i, j = 1, \cdots, 5)$. Thus $q_{34} = 1$ and similarly $q_{35} = q_{45} = 1$ but this contradicts the existence of the zero z. In case B2, $Q(0, x_2, 0, x_4, x_5)$ copositive implies that $q_{45} = 1$, hence $Q(0, 0, x_3, x_4, x_5)$ positive semi-definite with $Q(z) = 0$ and $q_{ii} = 1$ $(i = 1, \cdots, 5)$ yields $q_{34} = q_{35} = -1$, contradicting $q_{34} > -1$ as assumed above. Case B3 proceeds similarly using $Q(x_1, 0, x_3, 0, x_5)$ copositive to establish that $q_{35} = 1$ and hence [using $Q(0, 0, x_3, x_4, x_5)$] that $q_{34} = q_{45} = -1$, which violates our assumption. In case B4, we establish $q_{34} = 1$ and hence that $q_{35} = q_{45} = -1$ similarly, arriving at the same contradiction. For B5, $Q(x\ , 0, x_3, x_4, 0)$ copositive yields $q_{34} = 1$ and proceeding similarly we establish that $q_{25} = q_{45} = 1$ which contradicts $Q(z) = 0$. Only Case A remains, here $q_{12} = -1$ whence one of $q_{13}, q_{23} = -1$ and thus by relabeling x_1, x_2 if necessary we have a sub-case of B. So we conclude that a.3.c cannot have any further zero patterns, which implies $q_{ij} > -1$ $(i, j = 1, \cdots, 5)$. Further if $q_{ij} = 1$ for some $i \neq j$ $(i, j = 1, \cdots, 5)$ then at least one of

$$Q(x_1, x_2, x_3, 0, 0),\ Q(x_1, x_2, 0, x_4, 0),\ Q(x_1, x_2, 0, 0, x_5),\ Q(0, 0, x_3, x_4, x_5)$$

would be of the form $(x_i + x_j - x_k)^2$ which would produce an additional zero $x_i = x_k = 1$, contradiction. Hence for a.3.c we know that $-1 < q_{ij} < 1$ $i \neq j$ $(i, j = 1, \cdots, 5)$. Note further that if Q has two distinct zeros in $S(5)$ with the same pattern, say for example the pattern u, then $Q(x_1, x_2, x_3, 0, 0)$ is $(x_1 \pm x_2 \pm x_3)^2$ where the signs are not both plus. That is, this also introduces a new zero pattern. But we have ruled out such happenings, thus in the case a.3.c the only nonnegative component zeros of Q are u, v, w, z and these are unique.

Since u is a unique zero of Q we know that

$$Q(x_1, x_2, x_3, 0, 0) = (x_1 + q_{12}x_2 + q_{13}x_3)^2 + k\left(\frac{x_2}{u_2} - \frac{x_3}{u_3}\right)^2 \qquad k, u_2, u_3 > 0$$

and hence that

$$\begin{aligned} Q = {} & (x_1 + q_{12}x_2 + q_{13}x_3 + q_{14}x_4 + q_{15}x_5)^2 && (=L_1^2) \\ & + k\left(\frac{x_2}{u_2} - \frac{x_3}{u_3} + ex_4 + fx_5\right)^2 && k, u_2, u_3 > 0 \ (=kL_2^2) \\ & + bx_3x_4 + cx_3x_5 && b > 0, c \geqq 0 \\ & + Ax_4^2 + Bx_4x_5 + Cx_5^2 \end{aligned}$$

where $b \geqq 0, c \geqq 0$ because $\partial Q(u)/\partial x_4 = bu_3$ and $\partial Q(u)/\partial x_5 = cu_3$ and copositivity requires these slopes to be nonnegative. But [1, Corollary 3.3] states that if Q is extreme and *not* positive semi-definite, then at least one of these slopes must be positive. By relabeling the variables if necessary we may assume $b > 0$. (Note that if this relabeling is done, it produces no change in the zero patterns.) $A, C \leqq 0$ follow from $Q(v) = Q(w) = 0$. Now $Q(x_1, x_2, 0, x_4, 0)$ is positive semi-definite (Lemma 1, Diananda), whence $Q(v) = 0$ implies $A = 0$. Similarly $C = 0$. So $Q(z) = 0$ implies $B < 0$ since $b > 0, c \geqq 0$. Now let $r = v + w$, then $Q(r) = L_1^2(r) + kL_2^2(r) + Br_4r_5 < 0$ since $L_1(w) = L_1(v) =$

$L_2(w) = L_2(v) = 0$ which contradicts the copositivity of Q, and thus rules out pattern a.3.c.

Case a.2.c.4 remains and it certainly has solutions, since the Horn form clearly belongs to this category. Let the known zeros of Q be

$$\begin{aligned} u &= (u_1, u_2, u_3, 0, 0) , \\ v &= (0, v_2, v_3, v_4, 0) , \\ w &= (0, 0, w_3, w_4, w_5) , \\ y &= (y_1, 0, 0, y_4, y_5) , \end{aligned}$$

and

$$z = (z_1, z_2, 0, 0, z_5) .$$

Applying Theorem 2 (Diananda) to $Q_4 = Q(x_1, x_2, x_3, x_4, 0)$ we see that it is contained in $P + S$, hence zeros u, v of Q imply that $Q_4 = Q' + bx_1x_4$ where Q' has $A^*(4)$ for $b \geqq 0$ large enough. Thus Q' is positive semi-definite and [2, Th. 4] has a zero with all components positive. So [1, Corollary 3.7] implies that Q is positive semi-definite if $b = 0$. Thus we may assume $b > 0$; hence as Q' is positive semi-definite $q_{14} > -1$. Similarly, we see $q_{25}, q_{13}, q_{24}, q_{35} > -1$. Thus Q has no zeros with patterns (10010), (01001), (10100), (01010), (00101). Hence if Q has any 2-variable zeros they must involve x_i, x_{i+1}; so without loss of generality we may assume that $q_{12} = -1$. Then $q_{13} > -1$ implies $Q(x_1, x_2, x_3, 0, 0) = (x_1 - x_2 + x_3)^2$, whence $q_{23} = -1$. So

$$Q(0, x_2, x_3, x_4, 0) = (x_2 - x_3 + x_4)^2 ,$$

and similarly

$$\begin{aligned} Q(0, 0, x_3, x_4, x_5) &= (x_3 - x_4 + x_5)^2 , \\ Q(x_1, 0, 0, x_4, x_5) &= (x_4 - x_5 + x_1)^2 \end{aligned}$$

and

$$Q(x_1, x_2, 0, 0, x_5) = (x_5 - x_1 + x_2)^2 .$$

That is Q is the Horn form. Thus we may assume that Q has no 2-variable zeros. If Q has an additional 3-variable zero pattern we have a sub-case of a.3.c, which was already eliminated. Suppose Q has two distinct nonnegative component zeros with the same pattern, say the pattern u. Then $Q(x_1, x_2, x_3, 0, 0) = (x_1 \pm x_2 \pm x_3)^2$ where the signs are not both plus, hence Q has a 2-variable zero which contradicts our assumption. Hence the only nonnegative component zeros of Q are u, v, w, y, z, and these are unique. Thus we have completed the proof of Lemma 4.5.

THEOREM 4.6. *There exist extreme copositive quadratic forms in 5 variables with $q_{ii} = 1$ $(i = 1, \cdots, 5)$, which do not have $q_{ij} = \pm 1$ for all i, j $(1 \leqq i, j \leqq 5)$.*

Proof. The proof is in three parts. First we exhibit a quadratic form in 5 variables which has the zero patterns of Lemma 4.5 and which has $q_{12} = -7/8$. Secondly we demonstrate that this form is indeed copositive and finally we establish its extremity.

Note that if a copositive quadratic form $Q(x_1, \cdots, x_5)$ has the zeros u, v, w, y, z then (Lemma 1, Diananda)

$$Q(x_1, x_2, x_3, 0, 0), Q(0, x_2, x_3, x_4, 0), \cdots, Q(x_1, x_2, 0, 0, x_5)$$

are all positive semi-definite. As homogeneity allows us to assume $u_3 = v_4 = w_5 = y_1 = z_2 = 1$, this implies

$$\begin{aligned} u_1 + u_2 q_{12} + q_{13} &= 0 \\ u_1 q_{12} + u_2 + q_{23} &= 0 \\ u_1 q_{13} + u_2 q_{23} + 1 &= 0 \end{aligned} \tag{4.1}$$

with similar equations involving the v_i's, $\cdots$, z_i's. The determinant of the system 4.1 being $-2u_1u_2 < 0$ we can solve for q_{12}, q_{13}, q_{23} in terms of the zero u. Solving the other equations also we may express all q_{ij} in terms of the zeros $u, \cdots, z$. If we specify $q_{12}, u_1, v_2, w_3, y_4$ the form is determined from these equations. Whence letting $q_{12} = -7/8$, $u_1 = v_2 = w_3 = y_4 = 1/8$, we determine a solution to these equations which happens to be a new extreme copositive form. There is nothing sacred about the values we picked for these parameters, however they are not completely free either, as we shall see.

Being a solution to the indicated equations does not of itself guarantee either copositivity or extremity. Thus we must establish these properties for our solution. It will be clear however, from the way these properties are established, that any suitably small perturbation of our initial parameters will likewise yield an extreme copositive quadratic form. Hence there exists a whole class of such extreme copositive quadratic forms. The particular form of interest now is:

$$\begin{aligned} q_{11} = q_{22} = q_{33} = q_{44} = q_{55} &= 1 \\ 8q_{12} = -7,\ 8^3 q_{13} &= 7(8^4 - 15)^{1/2} - 15 \\ 8^9 q_{14} &= (8^8 - 15)^{1/2}(8^{10} - 15)^{1/2} - 15 \\ 8^5 q_{15} &= -(8^{10} - 15)^{1/2} \\ 8^2 q_{23} &= -(8^4 - 15)^{1/2} \\ 8^5 q_{24} &= (8^4 - 15)^{1/2}(8^6 - 15)^{1/2} - 15 \\ 8^6 q_{25} &= 7(8^{10} - 15)^{1/2} - 15 \end{aligned}$$

$$8^3 q_{34} = -(8^6 - 15)^{1/2}$$
$$8^7 q_{35} = (8^6 - 15)^{1/2}(8^8 - 15)^{1/2} - 15$$
$$8^4 q_{45} = -(8^8 - 15)^{1/2}$$

This form has zeros u, v, w, y, z where

$$8^2 u = \{8, 7 + (8^4 - 15)^{1/2}, 8^2, 0, 0\}$$
$$8^3 v = \{0, 8^2, (8^4 - 15)^{1/2} + (8^6 - 15)^{1/2}, 8^3, 0\}$$
$$8^4 w = \{0, 0, 8^3, (8^6 - 15)^{1/2} + (8^8 - 15)^{1/2}, 8^4\}$$
$$8^5 y = \{8^5, 0, 0, 8^4, (8^8 - 15)^{1/2} + (8^{10} - 15)^{1/2}\}$$
$$8z = \{7 + (8^{10} - 15)^{1/2}, 8, 0, 0, 8^5\}$$

Note that $u_1 v_2 w_3 y_4 z_5 = 1$, which is characteristic of extremes of this type. It follows from Equations 4.1, etc.

Letting Q_i be the 4-variable sub-form obtained by deleting the i^{th} variable, we see that

$$Q_5 = t_5 x_1 x_4 + [x_1 + q_{12}x_2 + q_{13}x_3 + (q_{14} - (1/2)t_5)x_4]^2$$
$$+ g_5[x_2 - u_2 x_3 + (-v_2 + u_2 v_3)x_4]^2$$

where $g_5 = 1 - q_{12}^2$ and t_5 is selected so that

$$q_{12}v_2 + q_{13}v_3 + (q_{14} - (1/2)t_5)v_4 = 0 .$$

$Q_1, \cdots, Q_4$ have similar representations and as $t_1, \cdots, t_5 > 0$ we see that $Q_i \in P + S$ $(i = 1, \cdots, 5)$. Hence we only need establish copositivity for those vectors with $x_i > 0$ $(i = 1, \cdots, 5)$. Using homogeneity, we can ascertain this from the values of $Q(x)$ restricted to $x_5 = 1$. To do this we first note that $Q(x) \geqq 0$ for all x on the boundary of $J = \{x : x_5 = 1, x_i \geqq 0\ (i = 1, \cdots, 4)\}$. For those portions having $x_i = 0$ for some i $(i = 1, \cdots, 4)$ this follows from $t_1, \cdots, t_4 > 0$. A typical point on the other part of the boundary might be $\lim\,(951, M, 3, M, 1)$ as $M \to \infty$. Now let y_j be a sequence of points converging to this part of the boundary of J. For each y_j let $N_j = y_{j1} + \cdots + y_{j4} + 1$, then by homogeneity

$$Q(y_j) = N_j^2 Q(y_j/N_j)$$

and thus in particular $Q(y_j)$ and $Q(y_j/N_j)$ have the same sign for all j. Hence in the limit they have the same sign also. But $\lim Q(y_j/N_j) \geqq 0$ since $y_{j5}/N_j \to 0$ and $t_5 > 0$. If this limit is positive we are done, otherwise it could happen that $\lim Q(y_j) < 0$. We shall show that this doesn't occur.

In the case we are considering we have $\lim y_j/N_j$ as a nonnegative component zero of our form with $x_5 = 0$. We shall show that it thus must be a scalar multiple of our zeros u or v, as Q has no other such zeros with $x_5 = 0$. Since $q_{ij} \neq -1$ $(i, j = 1, \cdots, 5)$ and $q_{ii} = +1$ $(i = 1, \cdots, 5)$, Q has no zeros with only one or two positive components. If Q had a zero $(\neq au, a > 0)$ with the same three positive components as in u then g_5 would be zero (see above), a contradiction as it implies $q_{12} = \pm 1$. Similarly for v the analogous term g_1 would be zero and hence $q_{23} = \pm 1$. If Q had a different three component zero with $x_5 = 0$ it would have to be $(s_1, s_2, 0, s_4, 0)$ or $(s_1, 0, s_3, s_4, 0)$ but then Q_5 would have $A^*(4)$ and thus [2, Th. 2] be positive semi-definite. This contradicts $t_5 > 0$. If Q had a zero $(s_1, s_2, s_3, s_4, 0)$, $s_i > 0$, then (as Q_5 is copositive) Lemma 1 of Diananda shows that Q_5 is positive semi-definite, i.e., $t_5 = 0$, a contradiction. Thus $\lim y_j/N_j$ is a scalar multiple of u or v. As these two cases can be handled in the same way, we assume it to be au, $a > 0$. Computing $\partial Q(au)/\partial x_5$ we see that it is greater than zero for all $a > 0$. Let N_ε be that part of a ε-neighborhood of au which contains the nonnegative component vectors having $x_1 + \cdots + x_5 = 1$. If we can establish that $Q \geqq 0$ in N_ε and that $Q > 0$ in those parts of N_ε where $x_5 > 0$, then it will follow that $\lim Q(y_j) \geqq 0$ if $y_j/N_j \to au$. As Q_5 is copositive we need only consider $x \in N_\varepsilon$ with $x_5 > 0$. Write $x = au + r$, where $r_5 > 0$. Then

$$Q(x) = Q(x_1, \cdots, x_4, 0) + r_5(\partial Q(au)/\partial x_5 + 2q_{15}r_1 + \cdots + 2q_{45}r_4 + r_5)$$

where $Q(x_1, \cdots, x_4, 0) \geqq 0$ and $\partial Q(au)/\partial x_5 > 0$ as previously determined. Hence for sufficiently small $\varepsilon > 0$ we have $Q(x) > 0$ (for $x \in N_\varepsilon$ and $x_5 > 0$). Thus we have shown that $Q \geqq 0$ on the boundary of J.

Let us suppose that there exists a point s in J for which $Q(s) = d < 0$. (We wish to show that this implies that Q has a stationary point in J.) Consider the set $T = \{x \text{ in } J: Q(x) \leqq (1/2)d\}$, clearly $s \in T$ and T is closed. If T were not bounded there would exist a sequence of points of T approaching a boundary point of J. But T is closed, thus this boundary point must have function value $\leqq (1/2)d$, contradiction. Thus T is bounded. So there exists an R such that all of T lies inside the intersection of the sphere of radius R with the set J. This is a closed and bounded region outside of which $Q > (1/2)d$, thus Q has a minimum $\leqq d$ in this region. As Q is continuous Q has a stationary point in the interior of $R \cap J$ at which the minimum is taken.

In our case we apply Lagrange's method to $Q(x) + \lambda x_5$ yielding a system of linear equations involving the matrix of our form Q. As this matrix has determinant ~ 11.925 we solve for the vector $x \sim (-0.1272, -513.6, -521.6, -8.017, 1)$ with associated value $Q(x) \sim -961.8$. But as $x \notin R \cap J$ there is no stationary point in $R \cap J$ and hence Q is copositive.

Finally we show that our form Q is extreme. Suppose not, then $Q = R + T$ where R, T are copositive and hence have the zeros u, v, w, y, z of Q. We shall show that these zeros determine Q up to a scalar multiple and hence that $R = aQ$, $T = (1 - a)Q$, $0 \leqq a \leqq 1$.

Since R has the zeros u, v, w, y, z and is copositive, we see that $R \in A^*(5)$ and thus $r_{ii} > 0$ $(i = 1, \cdots, 5)$. Thus multiplying R by a suitable scalar we may assume $r_{11} = 1$. The zero u plus copositivity imply that $R(x_1, x_2, x_3, 0, 0)$ is positive semi-definite (Lemma 1, Diananda) and hence

$$\begin{aligned} u_1 + r_{12}u_2 + r_{13} &= 0 \\ r_{12}u_1 + r_{22}u_2 + r_{23} &= 0 \\ r_{13}u_1 + r_{23}u_2 + r_{33} &= 0 . \end{aligned}$$

Thus, letting $r_{12} = b$, $r_{22} = e$ we can solve for r_{13}, r_{23} and r_{33} in turn, getting in each case a linear equation in b and e. Using these values and the analogous equations for the zero v we determine r_{24}, r_{34} and r_{44}. Ultimately we establish all the r_{ij} as linear expressions in b and e. Explicitly we have

$$\begin{aligned}
r_{11} &= 1 , \\
r_{12} &= b , \\
r_{13} &= -u_1 - bu_2 , \\
r_{14} &= (by_5 + z_1y_5 - z_5)/y_4z_5 , \\
r_{15} &= (-b - z_1)/z_5 , \\
r_{22} &= e , \\
r_{23} &= -bu_1 - eu_2 , \\
r_{24} &= -v_2e + (bu_1 + eu_2)v_3 , \\
r_{25} &= (-e - bz_1)/z_5 , \\
r_{33} &= u_1^2 + 2bu_1u_2 + eu_2^2 , \\
r_{34} &= v_2(bu_1 + eu_2) - v_3(u_1^2 + 2bu_1u_2 + eu_2^2) , \\
r_{35} &= (v_3w_4 - w_3)(u_1^2 + 2bu_1u_2 + eu_2^2) - v_2w_4(bu_1 + eu_2) , \\
r_{44} &= v_2^2e - 2v_2v_3(bu_1 + eu_2) + v_3^2(u_1^2 + 2bu_1u_2 + eu_2^2) , \\
r_{45} &= (bz_5 + z_1z_5 - z_1^2y_5 - 2bz_1y_5 - ey_5)/y_4z_5^2 , \\
r_{55} &= (z_1^2 + 2bz_1 + e)/z_5^2 .
\end{aligned}$$

An examination of these equations would show that they were obtained without the use of relations

$$r_{35}w_3 + r_{45}w_4 + r_{55} = 0 \quad \text{and} \quad r_{34}w_3 + r_{44}w_4 + r_{45} = 0 .$$

Using these and $u_1v_2w_3y_4z_5 = 1$ yields

$$
\begin{aligned}
&(u_1^2 v_3 w_3 w_4 y_4 z_5^2 - u_1^2 w_3^2 y_4 z_5^2 + w_4 z_5 z_1 - w_4 y_5 z_1^2 + y_4 z_1^2) \\
&\quad + (2u_1 u_2 v_3 w_3 w_4 y_4 z_5^2 - 2u_1 u_2 w_3^2 y_4 z_5^2 - 2w_4 y_5 z_1 + 2y_4 z_1)b \\
&\quad + (u_2^2 v_3 w_3 w_4 y_4 z_5^2 - u_2^2 w_3^2 y_4 z_5^2 - u_2 v_2 w_3 w_4 y_4 z_5^2 - w_4 y_5 + y_4)e = 0 \\
&(-u_1^2 v_3 w_3 y_4 z_5^2 + u_1^2 v_3^2 w_4 y_4 z_5^2 + z_1 z_5 - y_5 z_1^2) \\
&\quad + (-2u_1 u_2 v_3 w_3 y_4 z_5^2 - 2u_1 v_2 v_3 w_4 y_4 z_5^2 + 2u_1 u_2 v_3^2 w_4 y_4 z_5^2 + 2z_5)b \\
&\quad + (u_2 v_2 w_3 y_4 z_5^2 - u_2^2 v_3 w_3 y_4 z_5^2 + v_2^2 w_4 y_4 z_5^2 - 2u_2 v_2 v_3 w_4 y_4 z_5^2)e \\
&\quad + (-2z_1 y_5)b + (u_2^2 v_3^2 w_4 y_4 z_5^2 - y_5)e = 0 \,.
\end{aligned}
$$

For our particular values of $u_i, \cdots, z_i$ these two equations have the unique solution $b = -7/8, e = 1$. Hence R is unique and thus Q is extreme. Thus we have established that our particular example is an extreme copositive quadratic form, which completes the proof of Theorem 4.6.

The existence of a large class of similar forms follows from continuity considerations applied to our argument above. Now each member of this class of extreme copositive quadratic forms in 5 variables may be extended to an extreme form in 6, 7, $\cdots$ variables [**1**, Th. 3.8]. Hence we have new extremes $Q(x_1, \cdots, x_n)$ for all $n \geqq 5$.

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