EXTREME COPOSITIVE QUADRATIC FORMS

Thesis by

Leonard Daniel Baumert

In Partial Fulfillment of the Requirements

For the Degree of

Doctor of Philosophy

California Institute of Technology

Pasadena, California

1965

(Submitted October 20, 1964)

ACKNOWLEDGEMENTS

I wish to express my appreciation to Professor Marshall Hall, Jr. for his guidance and encouragement during the preparation of this thesis. I also wish to thank the California Institute of Technology for providing tuition scholarships during this period of study.

ABSTRACT

A real quadratic form $Q = Q(x_1, \ldots, x_n)$ is called copositive if $Q(x_1, \ldots, x_n) \geq 0$ whenever $x_1, \ldots, x_n \geq 0$. If we associate each quadratic form $Q = \sum q_{ij} x_i x_j$ $q_{ij} = q_{ji}$ $(i, j = 1, \ldots, n)$ with a point $(q_{11}, \ldots, q_{nn}, \sqrt{2} q_{12}, \ldots, \sqrt{2} q_{n-1, n})$ 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 $Q_1 = aQ$, $Q_2 = (1 - a) Q$, $0 \leq a \leq 1$. We show that

(1) If $Q(x_1, \ldots, x_n)$ $n \geq 3$ is an extreme copositive quadratic form then for any index pair i, j ($i = j$ included) Q has a zero u with $u_1, \ldots, u_n \geq 0$ where $u_i, u_j > 0$.

(2) If Q_n is an extreme copositive quadratic form in $n \geq 3$ variables $x_1, \ldots, x_n$ then replacing x_i by $x_i + x_{n+1}$ in Q_n yields a new copositive form Q_{n+1} which is also extreme.

(3) If $Q(x_1, \ldots, x_5)$ is an extreme copositive quadratic form then either (i) Q is positive semi-definite, or (ii) Q is related to an extreme form discovered by A. Horn, or (iii) Q possesses exactly five zeros having non-negative components. In this later case the zeros can be assumed to be $u = (u_1, u_2, 1, 0, 0)$, $v = (0, v_2, v_3, 1, 0)$, $w = (0, 0, w_3, w_4, 1)$, $y = (1, 0, 0, y_4, y_5)$ and $z = (z_1, 1, 0, 0, z_5)$ where $u_1 v_2 w_3 y_4 z_5 = 1$ and $u_1, u_2, v_2, v_3, \ldots, z_5, z_1 > 0$.

EXTREME COPOSITIVE QUADRATIC FORMS

1. Introduction. A real quadratic form $Q = Q(x_1, \ldots, x_n)$ is called copositive if $Q(x_1, \ldots, x_n) \geq 0$ whenever $x_1, \ldots, x_n \geq 0$. If we associate each quadratic form $Q = \Sigma\, q_{ij} x_i x_j \;\; q_{ij} = q_{ji}$ $(i, j = 1, \ldots, n)$ with a point $(q_{11}, \ldots, q_{nn}, \sqrt{2}q_{12}, \ldots, \sqrt{2}q_{n-1,n})$ of Euclidean $n(n+1)/2$ space then (Ref. 2) the copositive forms constitute a closed convex cone in this space. We shall be 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 $Q_1 = aQ$, $Q_2 = (1-a)Q$, $0 \leq a \leq 1$.

Let P denote the class of quadratic forms all of whose coefficients are non-negative, let S be the class of positive semi-definite quadratic forms and let P + S be the set of all forms expressible as a sum of elements of P and S. Clearly, every form in P + S is copositive; in fact there are no other copositive quadratic forms for $n \leq 4$ variables (Thm. 2, Diananda Ref. 1). The extreme copositive forms which belong to P + S have been determined (Thm. 3.2, Hall and Newman Ref. 2). Thus our main interest lies with those extreme copositive forms which do not belong to P + S. In section 2 we list the known extreme copositive quadratic forms. These forms have many interesting properties and we state a series of conjectures based on these properties (indicating which are proved or disproved subsequently). Section 3 contains general results on copositive quadratic forms, i.e., results which are independent of the number of variables n. The most important of these are:

Corollary 3.5. If $Q(x_1, \ldots, x_n)$ $n \geq 3$ is an extreme copositive quadratic form then for any index pair i, j ($i = j$ included) Q has a zero u with $u_1, \ldots, u_n \geq 0$ where u_i and $u_j > 0$.

Theorem 3.12. If Q_n is an extreme copositive quadratic form in $n \geq 3$ variables $x_1, \ldots, x_n$ then replacing x_i by $x_i + x_{n+1}$ in Q_n yields a new copositive form Q_{n+1}, which is also extreme.

In section 4 we concern ourselves wholly with the problem for $n = 5$ variables, but in so doing we establish the existence of a previously unknown class of extreme copositive quadratic forms, which can then be extended (Theorem 3.12) to any number of variables $n' \geq 5$.

Before proceeding further, let us say why we are interested in extreme copositive quadratic forms. To do this we need the concept of a dual set in E_m (Euclidean m space). If H is a subset of points of E_m, the dual set of H is $H* = \{x:(x, h) \geq 0 \text{ for all } h \text{ in } H\}$. Now (Ref. 2) the dual set of the cone of copositive quadratic forms is a closed convex cone. The quadratic forms associated with the points of this dual cone are called completely positive and they constitute all forms Q which are expressible as a sum of squares of non-negative linear forms. That is, a quadratic form Q is completely positive, if

$$Q = L_1^2 + \ldots + L_t^2$$

where $L_k = c_{1k}x_1 + \ldots + c_{nk}x_n$ ($c_{ik} \geq 0$, $k = 1, \ldots, t$). An important subset of the cone of completely positive quadratic forms arises in the theory of block designs. A balanced incomplete block design is an arrangement of v objects into b sets (called blocks) in such a manner that (1) each block contains exactly k different objects, (2) each object occurs in exactly r different blocks and (3) each unordered pair of objects occurs in exactly λ different blocks. If the j^{th} block is associated with the linear form $L_j = a_{1j}x_1 + \ldots + a_{vj}x_v$ where $a_{ij} = 1$ if the i^{th} object appears in the j^{th} block and $a_{ij} = 0$ otherwise, then

$$Q = L_1^2 + \ldots + L_b^2 = (r - \lambda)(x_1^2 + \ldots + x_v^2) + \lambda(x_1 + \ldots + x_v)^2.$$

Thus a completely positive quadratic form Q is associated with each block design.

Let us assume that we are attempting to decide whether a block design exists for a particular set of values of b, v, r, k and λ. Further, suppose (as is often the case) that the first t blocks of the hypothetical design have been specified, then

$$\overline{Q} = Q - L_1^2 - \ldots - L_t^2 = L_{t+1}^2 + \ldots + L_b^2$$

must be completely positive. As $\overline{Q}$ is known at this point, it can be tested for complete positivity; thus such a test would be useful for early rejection of otherwise plausible sets of initial blocks. Hence, we are interested in a test for complete positivity of a quadratic form. Duality tells us that a form is completely positive if and only if its inner product with every copositive quadratic form is ≥ 0. This is certainly the case if the form has non-negative inner product with all the extreme copositive quadratic forms. Hence a tabulation of the extreme copositive quadratic forms would provide us with a text for complete positivity.

2. Known extreme copositive quadratic forms. Conjectures. We shall often be concerned with the values taken by a quadratic form for $x_i \geq 0$ $(i = 1, \ldots, n)$, to which end homogeneity will usually permit us to restrict attention to those x for which $x_1 + \ldots + x_n = 1$. We call this subset $S(n)$, that is $S(n) = \{x \text{ in } E_n\colon\ x_1 + \ldots + x_n = 1,\ x_i \geq 0$ $(i = 1, \ldots, n)\}$.

Note that $Q(x_1, \ldots, x_n)$ is an extreme form if and only if $Q(r_1x_1, \ldots, r_nx_n)$ is extreme for $r_i > 0$ $(i = 1, \ldots, n)$; hence in questions of extremity whenever $q_{ii} > 0$ $(i = 1, \ldots, n)$ there is no loss of generality in assuming that $q_{ii} = 1$ $(i = 1, \ldots, n)$.

The extreme copositive quadratic forms belonging to $P + S$ were given by Hall and Newman (Thm. 3.2, Ref. 2). Considering only forms with n variables or less these are: ax_i^2, $a \geq 0$ $(i = 1, \ldots, n)$; bx_ix_j, $b \geq 0$ $(i \neq j;\ i, j = 1, \ldots, n)$ and $(U - V)^2$, where $U = \sum_{i=1}^{r} a_iu_i$, $V = \sum_{i=1}^{s} b_iv_i$ $(a_i > 0,\ b_i > 0,\ r \geq 1,\ s \geq 1)$ and the u's, v's are disjoint subsets of $x_1, \ldots, x_n$. In many ways the extremes $(U - V)^2$ are typical, while the others (ax_i^2, $a \geq 0$ and bx_ix_j, $b \geq 0$) are not. Hence most of our general results are subject to the qualification $Q \neq ax_i^2$, $a \geq 0$ and $Q \neq bx_ix_j$, $b \geq 0$, which will usually be enforced by limiting ourselves to $n \geq 3$ variables. This restriction also excludes the extremes $(ax_i - bx_j)^2$ $a, b > 0$ $i \neq j$ for which the results are generally true. But since the extreme copositive forms are completely determined for $n \leq 4$ variables (by the results quoted above) not much is lost by this exclusion.

In addition to the extremes belonging to $P + S$, A. Horn (Ref. 2) has discovered another extreme copositive quadratic form in 5 variables:

$$Q = (x_1 + x_2 + x_3 + x_4 + x_5)^2 - 4x_1x_2 - 4x_2x_3 - 4x_3x_4 - 4x_4x_5 - 4x_5x_1.$$

Note that the matrix associated with Q takes the form

$$\begin{vmatrix} 1 & -1 & 1 & 1 & -1 \\ -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 & 1 \end{vmatrix}$$

and that Q has a continuum of zeros u in $S(5)$ which are of 5 types

	$\partial Q(u)/\partial x_i$, $i =$ 1	2	3	4	5
1. $(z, \frac{1}{2}, \frac{1}{2}-z, 0, 0)$	0	0	0	$4z$	$2-4z$
2. $(0, z, \frac{1}{2}, \frac{1}{2}-z, 0)$	$2-4z$	0	0	0	$4z$
3. $(0, 0, z, \frac{1}{2}, \frac{1}{2}-z)$	$4z$	$2-4z$	0	0	0
4. $(\frac{1}{2}-z, 0, 0, z, \frac{1}{2})$	0	$4z$	$2-4z$	0	0
5. $(\frac{1}{2}, \frac{1}{2}-z, 0, 0, z)$	0	0	$4z$	$2-4z$	0

for $0 \leq z \leq \frac{1}{2}$.

Hall and Newman (Thm. 4.1, Ref. 2) have shown that if $Q(x_1, \ldots, x_n)$ is an extreme copositive quadratic form ($Q \neq bx_ix_j$, $b \geq 0$) and if $i \neq j$ $(1 \leq i, j \leq n)$ then upon replacing some of $x_1, \ldots, x_n$

by zero (but neither x_i nor x_j) Q becomes a positive semi-definite quadratic form in the remaining variables. Hence, if $q_{kk} = 1$ $(k = 1, \ldots, n)$ then $-1 \le q_{rs} \le 1$ for $r, s = 1, \ldots, n$.

Based on this information, with an eye toward the Horn form and the extreme copositive quadratic forms of P + S, we make the following conjectures:

Conjecture 2.1. If an extreme copositive quadratic form Q has $q_{ii} = 1$ $(i = 1, \ldots, n)$ then $q_{ij} = \pm 1$ $(i, j = 1, \ldots, n)$. (False for $n \ge 5$, see Corollary 4.4.)

Note that if this conjecture had been true, the search for extreme copositive quadratic forms with $q_{ii} = 1$ would have been simplified, in fact reduced to a combinatorial matter.

Conjecture 2.2. For each i, j $(1 \le i, j \le n;\ n \ge 3)$ an extreme copositive quadratic form has a zero u in S(n) with $u_i, u_j > 0$. (True, see Corollary 3.5.)

Conjecture 2.3. Each zero u in S(n) of an extreme copositive quadratic form, not belonging to P + S, has at least two zero components. (True, see Corollary 3.11.)

Conjecture 2.4. For each i $(1 \le i \le n)$ an extreme copositive quadratic form, not belonging to P + S, has a zero u in S(n) with $u_i = 0$. (True for $n \le 5$ variables, see Theorem 4.3; for $n > 5$?)

Conjecture 2.5. Each zero in S(n) of an extreme copositive quadratic form in $n \ge 3$ variables has at least two non-zero components. (True, proof of Corollary 3.7 applies.)

Conjecture 2.6. For each zero u in S(n) of an extreme copositive quadratic form, not in P + S, there exists an i ($1 \le i \le n$) such that $\partial Q(u)/\partial x_i > 0$. (True, see Corollary 3.2.)

Call a zero u in S(n) of a quadratic form Q, a maximal zero of Q if there does not exist another zero y of Q in S(n) for which (1) $y_i = 0$ implies $u_i = 0$ ($i = 1, \ldots, n$) and (2) there is a j ($1 \le j \le n$) for which $u_j = 0$ and $y_j > 0$. For example, $(\frac{1}{4}, \frac{1}{2}, \frac{1}{4}, 0, 0)$ is a maximal zero of the Horn form whereas the zero $(\frac{1}{2}, \frac{1}{2}, 0, 0, 0)$ is not.

Conjecture 2.7. Let u be a maximal zero in S(n) of an extreme copositive quadratic form, then $u_i = 0$ implies $\partial Q(u)/\partial x_i > 0$ for any $i = 1, \ldots, n$. (True for $n \le 5$, see Corollary 4.5; for $n > 5$?)

Note that for $n \ge 3$ the extreme copositive quadratic forms in P + S have a continuum of zeros in S(n) and so does the Horn form. In fact since Conjecture 2.6 is valid, the Implicit Function Theorem guarantees that no zero of an extreme copositive quadratic form (for $n \ge 3$) is isolated in $X(n) = \{x \text{ in } E_n : x_1 + \ldots + x_n = 1\}$. This leads us to

Conjecture 2.8. No zero of an extreme copositive quadratic form in $n \ge 3$ variables is isolated in S(n). (False, see Theorem 4.3.)

The Horn form has the property that $\sum_i \partial Q(u)/\partial x_i = 2$ for all zeros u in S(5). This is not generally true. That is, an extreme copositive quadratic form, not belonging to P + S, does not necessarily have $\sum_i \partial Q(u)/\partial x_i = c$ for some constant c and all zeros u in S(n). For example, consider the form Q which arises when x_2 is replaced by $x_2 + x_6$ in the Horn form. This is an extreme copositive quadratic form (see Theorem 3.12). Among its zeros in S(6) are $(0, 0, 0, \frac{1}{2}, \frac{1}{2}, 0)$

for which $\sum_i \partial Q(u)/\partial x_i = 4$ and $(\frac{1}{2}, \frac{1}{2}, 0, 0, 0, 0)$ for which $\sum_i \partial Q(u)/\partial x_i = 2$.

Conjecture 2.9. If R and Q are two extreme copositive quadratic forms in n variables having the same zeros in S(n), then $R = aQ$, $a > 0$. (True, if either Q or R is the Horn form or if either Q or R belongs to $P + S$, otherwise?)

If Q belongs to $P + S$, this follows from the determination of those extremes by Hall and Newman (Ref. 2). Validity for the Horn form follows from Theorem 4.3. Note that the validity of this conjecture would imply that the extreme copositive quadratic forms are characterized by their zeros in S(n).

3. General results. In many instances the concept of extremity for a copositive quadratic form is hard to handle — and it often suffices to replace it with the weaker property which (following Diananda) we call $A^*(n)$. We say that a quadratic form $Q(x_1, \ldots, x_n)$ has $\underline{A^*(n)}$, or $Q \in A^*(n)$, if (1) Q is copositive and (2) if for all i, j (i, j = 1, ..., n) $Q - \epsilon x_i x_j$ is not copositive for any $\epsilon > 0$. (That is, if Q is a copositive quadratic form which is "reduced" with respect to the extremes of P.)

We prove first a lemma which will be required later. It has an immediate corollary which validates one of our conjectures.

Lemma 3.1. If $Q(x_1, \ldots, x_n)$ is a copositive quadratic form having a zero u on S(n), at which $u_1, \ldots, u_m > 0 = u_{m+1} = \ldots = u_n$ and $\partial Q(u)/\partial x_i = 0$ $(i = 1, \ldots, n)$, then

$$Q(x_1, \ldots, x_n) = L_1^2 + \ldots + L_s^2 + Q_1(x_{m+1}, \ldots, x_n),$$

where Q_1 is copositive and by renumbering the x_i $(i = 1, \ldots, m)$ we may assume that L_i is a linear form in $x_i, \ldots, x_n$ $(i = 1, \ldots, s)$.

Proof. Since $\partial Q(u)/\partial x_i = 0$ $(i = 1, \ldots, n)$, letting $x_i^* = x_i - u_i$ we have

$$Q(x_1, \ldots, x_n) = Q^*(x_1^*, \ldots, x_n^*) = Q^*(x_1^*, \ldots, x_m^*, x_{m+1}, \ldots, x_n). \qquad (3.1)$$

Further Q copositive implies that $Q^* \geq 0$ for $x_i^* \geq -u_i$ $(i = 1, \ldots, n)$. Since $Q^*(x_1^*, \ldots, x_m^*, 0, \ldots, 0)$ is non-negative in a neighborhood of the origin it is positive semi-definite and we collect squares with respect to $x_1^*, \ldots, x_m^*$ in $Q^*(x_1^*, \ldots, x_n^*)$ yielding

$$Q^* = L_1^{*2} + \ldots + L_s^{*2} + 2 \sum_{i=s+1}^{m} \sum_{j=m+1}^{n} a_{ij} x_i^* x_j + Q_1(x_{m+1}, \ldots, x_n) \qquad (3.2)$$

where by renumbering the x_i^* $(i = 1, \ldots, m)$ we may assume that L_i^* is a linear form in $x_i^*, \ldots, x_n^*$ $(i = 1, \ldots, s)$.

For any set of $x_i^* \geq 0$ $(i = s+1, \ldots, n)$ provided they are sufficiently small the values of $x_i^* \geq -u_i$ $(i = 1, \ldots, s)$ may be chosen so that $L_1^* = \ldots = L_s^* = 0$. But $Q^* \geq 0$ for these values of x_i^* $(i = 1,\ldots,n)$ and thus so is

$$2 \sum_{i=s+1}^{m} \sum_{j=m+1}^{n} a_{ij} x_i^* x_j + Q_1(x_{m+1}, \ldots, x_n) \equiv Q_2(x_{s+1}^*, \ldots, x_m^*, x_{m+1}, \ldots, x_n).$$

Thus by homogeneity Q_2 is copositive, and so, by Lemma 2 of Diananda (Ref. 1), $a_{ij} \geq 0$ $(i = s+1, \ldots, m;\ j = m+1, \ldots, n)$. By (3.1),

$Q^*(u) = 0$ and $\partial Q^*(u)/\partial x_j^* = 0$ $(j = 1, \ldots, n)$. Let $m + 1 \leq j \leq n$, then by (3.2)

$$\partial Q^*(u)/\partial x_j^* = 2g_1 L_1^*(u) + \ldots + 2g_s L_s^*(u) + 2 \sum_{i=s+1}^{m} a_{ij} u_i + \partial Q_1(u)/\partial x_j^* = 0$$

where g_k is the coefficient of x_j^* in L_k^* $(k = 1, \ldots, s)$. Now $Q^*(u) = 0$ and Q_2 copositive imply by (3.2) that $L_k^*(u) = 0$ $(k = 1, \ldots, s)$; further $\partial Q_1(u)/\partial x_j^* = 0$ since $u_{m+1} = \ldots = u_n = 0$. Thus since $u_i > 0$ $(i = s + 1, \ldots, m)$ we have $a_{ij} = 0$ $(i = s + 1, \ldots, m;\ j = m + 1, \ldots, n)$. Hence

$$Q^* = L_1^{*2} + \ldots + L_s^{*2} + Q_1(x_{m+1}, \ldots, x_n)$$

where Q_1 is copositive.

Recalling that $x_i^* = x_i - u_i$, we see that $L_i^* = L_i + c_i$, where the c_i's are constants, thus

$$Q = (L_1 + c_1)^2 + \ldots + (L_s + c_s)^2 + Q_1(x_{m+1}, \ldots, x_n).$$

Letting $x_i = 0$ $(i = 1, \ldots, n)$ we find $c_i = 0$ $(i = 1, \ldots, s)$, so

$$Q = L_1^2 + \ldots + L_s^2 + Q_1(x_{m+1}, \ldots, x_n)$$

with Q_1 copositive, and the L_i's constituted as desired, which completes the proof.

Corollary 3.2. If $Q(x_1, \ldots, x_n)$ is an extreme copositive quadratic form which has, among its zeros on $S(n)$, a zero u at which $\partial Q(u)/\partial x_i = 0$ $(i = 1, \ldots, n)$ then Q is positive semi-definite.

Proof. By relabeling the variables we may assume that $u_1, \ldots, u_m > 0 = u_{m+1} = \ldots = u_n$, where $1 \leq m \leq n$. Thus by the lemma

$$Q(x_1, \ldots, x_n) = L_1^2 + \ldots + L_s^2 + Q_1(x_{m+1}, \ldots, x_n)$$

with Q_1 copositive. Since Q is extreme we must have $L_2^2 + \ldots + L_s^2 + Q_1(x_{m+1}, \ldots, x_m) \equiv aL_1^2$ for some $a \geq 0$, but this is impossible for $a > 0$ (as x_1 appears in L_1^2 but not in $L_2^2 + \ldots + L_s^2 + Q_1$). Hence $a = 0$ which implies that Q is positive semi-definite.

Since the slopes at a zero u in S(n) of a copositive quadratic form are necessarily ≥ 0 (otherwise, copositivity would be violated), we conclude that any extreme copositive quadratic form which does not belong to P + S must have a positive slope at each of its zeros in S(n), i.e., Conjecture 2.6 is valid. As we shall presently use this information, we note further that copositivity requires $\partial Q(u)/\partial x_i = 0$ whenever $u_i > 0$, if u in S(n) is a zero of the copositive quadratic form Q.

Our next result is the most important of this paper; almost everything that is new here depends upon it in one way or another. In many respects it is an extension of Theorem 4.1 (Hall and Newman, Ref. 2).

Theorem 3.3. A copositive quadratic form $Q(x_1, \ldots, x_n)$ has a zero u on S(n) with $u_i, u_j > 0$ if and only if $Q - \epsilon x_i x_j$ is not copositive for any $\epsilon > 0$, $(1 \leq i, j \leq n)$.

Proof. If Q has such a zero u then $Q(u) - \epsilon u_i u_j = -\epsilon u_i u_j < 0$ for any $\epsilon > 0$. On the other hand, proceeding by induction on n, let

$n = 1$, then $Q = qx_1^2$ $(q \geq 0)$, but $Q - \epsilon x_1^2$ not copositive for all $\epsilon > 0$ implies that $q = 0$, whence Q has the zero $x_1 = 1$ of $S(1)$. For $n = 2$, there are only 3 essentially distinct copositive Q's, these are (1) qx_1x_2 $(q \geq 0)$, (2) $q_{11}x_1^2 + 2q_{12}x_1x_2$ $(q_{11}, q_{12} > 0)$, (3) $q_{11}x_1^2 + 2q_{12}x_1x_2 + q_{22}x_2^2$ $(q_{11}, q_{22} > 0)$.

Case 1. Q has zeros $x_1 = 1$, $x_2 = 0$ and $x_1 = 0$, $x_2 = 1$ and $(q - \epsilon)x_1x_2$ not copositive for all $\epsilon > 0$ implies that $q = 0$, so $x_1 = x_2 = \frac{1}{2}$ is our zero on $S(2)$.

Case 2. $Q - \epsilon x_ix_j$ not copositive for all $\epsilon > 0$ implies that $i = j = 2$, and Q has the zero $x_1 = 0$, $x_2 = 1$ on $S(2)$.

Case 3. Since $q_{ii} > 0$ we can assume without loss of generality that $q_{11} = q_{22} = 1$, thus $Q = x_1^2 + 2q_{12}x_1x_2 + x_2^2 = (x_1 - x_2)^2 + kx_1x_2$ where $k \geq 0$ since Q is copositive. Now $Q - \epsilon x_ix_j$ not copositive for all $\epsilon > 0$ implies (Lemma 4 Diananda, Ref. 1) that $Q = (x_1 - x_2)^2 + kx_1x_2$, $k \geq 0$ has a zero on $S(2)$ which can only be $x_1 = x_2 = \frac{1}{2}$, thus $k = 0$. So $x_1 = x_2 = \frac{1}{2}$ is the desired zero on $S(2)$.

More generally, since $Q - \epsilon x_ix_j$ is not copositive for $\epsilon > 0$, there exists a non-negative n-tuple z [which may be assumed to be on $S(n)$] for which $Q(z) < \epsilon z_iz_j$. By taking successively smaller positive ϵ's we construct a sequence of non-negative n-tuples, of which a subsequence converges to an n-tuple u of $S(n)$. We denote the generic member of this subsequence by v, and note that continuity implies $Q(u) = 0$. There are 6 cases to consider, which are (1) $i \neq j$, $u_iu_j \neq 0$, (2) $i \neq j$, $u_i \neq 0 = u_j$, (3) $i \neq j$, $u_i = 0 \neq u_j$, (4) $i \neq j$, $u_i = u_j = 0$, (5) $i = j$, $u_i = 0$, and (6) $i = j$, $u_i \neq 0$. In cases 1 and 6 we are done and case 2 is equivalent to case 3; thus only cases 3, 4, and 5 remain. Let us renumber the variables so that $i = j = 1$, $u_2 > 0$ in case 5 and otherwise $i = 1$, $j = 2$; and further $u_3, \ldots, u_m > 0 = u_{m+1} = \ldots = u_n$, where $\partial Q(u)/\partial x_i = 0$ $(i = m+1, \ldots, k)$ and $\partial Q(u)/\partial x_i > 0$ $(i = k+1, \ldots, n)$.

In the sequence of points $v = (v_1, \ldots, v_n)$ approaching $u = (0, u_2, \ldots, u_m, 0, \ldots, 0)$ put $v_i = u_i + w_i$ $(i = 1, \ldots, n)$ so that the w_i all approach zero as v approaches u. Since $\partial Q(u)/\partial x_n = 2q_{n1}u_1 + \ldots + 2q_{nn}u_n > 0$ and $u_n = 0$ we have

$$Q(v) = Q(v_1, \ldots, v_{n-1}, 0) + w_n\left(\frac{\partial Q(u)}{\partial x_n} + 2q_{n1}w_1 + \ldots + 2q_{nn-1}w_{n-1} + q_{nn}w_n\right)$$

Here if $v_n = w_n > 0$, then for sufficiently small w's [since $\partial Q(u)/\partial x_n > 0$] we have

$$0 \leq Q(v_1, \ldots, v_{n-1}, 0) < Q(v) < \epsilon v_1 v_2 \tag{3.3}$$

Thus there exists a subsequence of the v's in which we may replace $v = (v_1, \ldots, v_n)$ by $v' = (v_1, \ldots, v_{n-1}, 0)$ to yield a sequence which approaches u and has the property $Q(v') < \epsilon v_1 v_2$. Repeating this process we replace all the non-zero $v_{k+1}, \ldots, v_n$ in some suitable subsequence of the v's by zero. This yields a form $Q_1(x_1, \ldots, x_k) = Q(x_1, \ldots, x_k, 0, \ldots, 0)$ and a sequence of k-tuples (in which we again designate the generic member by v) $v = (v_1, \ldots, v_k)$ approaching $u = (u_1, \ldots, u_k)$ for which $Q_1(v_1, \ldots, v_k) < \epsilon v_1 v_2$ and for which $\partial Q_1(u)/\partial x_i = 0$ for $i = 3, \ldots, k$ (copositivity implies $\partial Q_1(u)/\partial x_i = 0$ if $u_i > 0$). Since $u_1 = 0$ we have

$$Q_1(v_1, \ldots, v_k) = w_1(q_{11}w_1 + \frac{\partial Q_1(u)}{\partial x_1} + 2q_{12}w_2 + \ldots + 2q_{1k}w_k)$$

$$+ Q_1(0, v_2, \ldots, v_k)$$

with $w_1 = v_1 > 0$ (follows from 3.3). Since $Q_1(0, v_2, \ldots, v_k) \geq 0$ the inequality $Q_1(v_1, \ldots, v_k) < \epsilon v_1 v_2$ can only hold for sufficiently small w's if $\partial Q_1(u)/\partial x_1 = 0$. If $u_2 \neq 0$ then $\partial Q_1(u)/\partial x_2 = 0$ by copositivity, whereas $u_2 = 0$ yields $\partial Q_1(u)/\partial x_2 = 0$ by the process used for $u_1 = 0$. Hence for $Q_1(x_1, \ldots, x_k)$ we have $Q_1(u) = 0$ and $\partial Q_1(u)/\partial x_i = 0$ $(i = 1, \ldots, k)$.

Cases 3 and 5. Here $u_2 > 0$ and we apply Lemma 3.1 getting

$$Q_1(x_1, \ldots, x_k) = L_2^2 + \ldots + L_s^2 + Q_2(x_1, x_{m+1}, \ldots, x_k) \qquad (3.4)$$

with Q_2 copositive and we may assume that L_i is a linear form in $x_1, x_i, \ldots, x_k$ $(i = 2, \ldots, s)$.

If $(v_1, \ldots, v_k) = v$ is one of our k-tuples for which $Q_1(v) < \epsilon v_1 v_2$ then (3.4) shows that $Q_2(v_1, v_{m+1}, \ldots, v_k) < \epsilon v_1 v_2$. Note that in what follows it is immaterial whether Q_2 actually contains x_1, the proof goes through even when $Q_2 \equiv 0$. Now $0 < k - m + 1 < n$ so by the induction hypothesis Q_2 has a zero $z = (z_1, z_{m+1}, \ldots, z_k)$ on $S(k - m + 1)$ with $z_1 \neq 0$. Now $Q_1(u) = 0$, hence (by 3.4) $L_2(u) = \ldots = L_s(u) = 0$ where $u_1 = 0 = u_{m+1} = \ldots = u_k$ and $u_i > 0$ $(i = 2, \ldots, m)$. Due to the structure of the L_i's, the equations

$$L_2 = \ldots = L_s = x_{s+1} = \ldots = x_m = 0,$$

$$x_1 = z_1, \; x_{m+1} = z_{m+1}, \ldots, x_k = z_k$$

have a unique solution $(z_1, \ldots, z_k)$ where the z_i $(i = 2, \ldots, s)$ may be negative. Taking $t > 0$ large enough we can insure that $w_i \equiv tu_i + z_i \geq 0$ $(i = 1, \ldots, k)$ and $w_i > 0$ for $(i = 1, \ldots, m)$. Since $w_1 = z_1$ and $w_i = z_i$ $(i > m)$ we have $Q_2(w) = 0$; further $L_2(w) = \ldots = L_s(w) = 0$. Hence (3.4) implies that $Q_1(w) = 0$ with $w_1, w_2 > 0$, thus there is a zero of Q_1 on $S(k)$ with $x_1, x_2 > 0$. Since $Q_1(x_1, \ldots, x_k) = Q(x_1, \ldots, x_k, 0, \ldots, 0)$ the theorem is proved in these cases.

Case 4. Here $u_2 = 0$ and we apply the lemma to get

$$Q_1(x_1, \ldots, x_k) = L_3^2 + \ldots + L_s^2 + Q_2(x_1, x_2, x_{m+1}, \ldots, x_k)$$

with Q_2 copositive and the L_i's linear forms in $x_1, x_2, x_i, \ldots, x_k$ $(i = 3, \ldots, s)$. This yields $Q_2(v) < \epsilon v_1 v_2$ and using the induction hypothesis we find a zero z of Q_2 on $S(k - m + 2)$, for which $z_1, z_2 > 0$. As before $L_3(u) = \ldots = L_s(u) = 0$ where $u_1 = u_2 = 0 = u_{m+1} = \ldots = u_k$, $u_i > 0$ $(i = 3, \ldots, m)$ and the equations

$$L_3 = \ldots = L_s = x_{s+1} = \ldots = x_m = 0, \; x_1 = z_1$$

$$x_2 = z_2, \; x_{m+1} = z_{m+1}, \ldots, x_k = z_k$$

possess a unique solution $(z_1, \ldots, z_k)$ with z_i $(i = 3, \ldots, s)$ possibly negative. Similarly, $w_i \equiv tu_i + z_i$ provides a solution for $t > 0$ large enough with $w_1, w_2 > 0$, and thus $Q(x_1, \ldots, x_k, 0, \ldots, 0)$ has a zero on $S(n)$ with $x_1, x_2 > 0$ in this case also. So the theorem is proved.

In the following we state the equivalent results for extreme forms and for forms possessing $A^*(n)$. We shall often do this, because while our main concern is extreme copositive forms the proofs have a unique solution $(z_1, \ldots, z_k)$ where the z_i $(i = 2, \ldots, s)$ may be negative. Taking $t > 0$ large enough we can insure that $w_i \equiv tu_i + z_i \geq 0$ $(i = 1, \ldots, k)$ and $w_i > 0$ for $(i = 1, \ldots, m)$. Since $w_1 = z_1$ and $w_i = z_i$ $(i > m)$ we have $Q_2(w) = 0$; further $L_2(w) = \ldots = L_s(w) = 0$. Hence (3.4) implies that $Q_1(w) = 0$ with $w_1, w_2 > 0$, thus there is a zero of Q_1 on $S(k)$ with $x_1, x_2 > 0$. Since $Q_1(x_1, \ldots, x_k) = Q(x_1, \ldots, x_k, 0, \ldots, 0)$ the theorem is proved in these cases.

Case 4. Here $u_2 = 0$ and we apply the lemma to get

$$Q_1(x_1, \ldots, x_k) = L_3^2 + \ldots + L_s^2 + Q_2(x_1, x_2, x_{m+1}, \ldots, x_k)$$

with Q_2 copositive and the L_i's linear forms in $x_1, x_2, x_i, \ldots, x_k$ $(i = 3, \ldots, s)$. This yields $Q_2(v) < \epsilon v_1 v_2$ and using the induction hypothesis we find a zero z of Q_2 on $S(k - m + 2)$, for which $z_1, z_2 > 0$. As before $L_3(u) = \ldots = L_s(u) = 0$ where $u_1 = u_2 = 0 = u_{m+1} = \ldots = u_k$, $u_i > 0$ $(i = 3, \ldots, m)$ and the equations

$$L_3 = \ldots = L_s = x_{s+1} = \ldots = x_m = 0, \; x_1 = z_1$$

$$x_2 = z_2, \; x_{m+1} = z_{m+1}, \ldots, x_k = z_k$$

possess a unique solution $(z_1, \ldots, z_k)$ with z_i $(i = 3, \ldots, s)$ possibly negative. Similarly, $w_i \equiv tu_i + z_i$ provides a solution for $t > 0$ large enough with $w_1, w_2 > 0$, and thus $Q(x_1, \ldots, x_k, 0, \ldots, 0)$ has a zero on $S(n)$ with $x_1, x_2 > 0$ in this case also. So the theorem is proved.

In the following we state the equivalent results for extreme forms and for forms possessing $A^*(n)$. We shall often do this, because while our main concern is extreme copositive forms the proofs often require knowledge of the $A^*(n)$ case. Hence Theorem 3.3 has the immediate corollaries:

Corollary 3.4. $Q(x_1, \ldots, x_n)$ is a quadratic form having $A^*(n)$ if and only if for every index pair i, j ($i = j$ included), Q has a zero u on $S(n)$ with u_i, $u_j > 0$.

Corollary 3.5. If $Q(x_1, \ldots, x_n)$ $n \geq 3$ is an extreme copositive quadratic form then for any index pair i, j ($i = j$ included) Q has a zero u on $S(n)$ with u_i, $u_j > 0$.

Thus we have established Conjecture 2.2. From these facts we may deduce slightly more than Theorem 4.1 (Hall and Newman, Ref. 2), that is:

Corollary 3.6. Let $Q(x_1, \ldots, x_n)$ be a copositive quadratic form such that, for some fixed index pair i, j ($i = j$ allowed), $Q - \epsilon x_i x_j$ is not copositive whenever $\epsilon > 0$. Then upon replacing some of the x_k ($k = 1, \ldots, n$) by zero, but neither x_i nor x_j, Q becomes a positive semi-definite quadratic form in the remaining m variables which has $A^*(m)$.

Proof. Let $i = 1$ and if $j \neq i$ let $j = 2$. Let u be a zero of Q on $S(n)$ with u_i, $u_j > 0$, where the remaining non-zero components of u have indices $2, \ldots, m$ or $3, \ldots, m$ respectively. Then Lemma 1 of Diananda (Ref. 1) says that $Q_1(x_1, \ldots, x_m) = Q(x_1, \ldots, x_m, 0, \ldots, 0)$ is a positive semi-definite quadratic form. Clearly Q_1 has $A^*(m)$.

Note that if a copositive form $Q(x_1, \ldots, x_n)$ has $A^*(n)$ then $q_{ii} > 0$ ($i = 1, \ldots, n$), for otherwise $q_{ii} = 0$ for some i, and then (Lemma 2 Diananda, Ref. 1) $q_{ij} \geq 0$ ($j = 1, \ldots, n$), whence

$Q = Q_1(x_1, \ldots, x_{i-1}, 0, x_{i+1}, \ldots, x_n) + 2 \sum_j q_{ij}x_ix_j$ where Q_1 is copositive, which contradicts $A^*(n)$. Thus if Q is an extreme copositive quadratic form, not of the type qx_ix_j, then $q_{ii} > 0$ $(i = 1, \ldots, n)$.

Corollary 3.7. Let $Q(x_1, \ldots, x_n)$ be a quadratic form having $A^*(n)$ and let i, j be any indices (not necessarily distinct). Then upon replacing some of $x_1, \ldots, x_n$ by zero, but neither x_i nor x_j, Q becomes a positive semi-definite quadratic form in the remaining m variables and has $A^*(m)$. Further, even if $i = j$, the residual form contains at least two variables.

Proof. The only question is that of the number of residual variables. But the method of proof (Thm. 3.3) indicates that the residual form has a zero in $S(m)$ and since $q_{ii} > 0$ $(i = 1, \ldots, n)$ this can only happen if at least two variables are > 0.

Corollary 3.8. Let $Q(x_1, \ldots, x_n)$ $n \geq 3$ be an extreme copositive quadratic form and let i, j be any two of the indices ($i = j$ included), then upon replacing some of $x_1, \ldots, x_n$ by zero, but neither x_i nor x_j, Q becomes a positive semi-definite quadratic form in the remaining m variables which has $A^*(m)$. Further, even if $i = j$, the residual form contains at least two variables.

Note that Corollary 3.7 yields $-1 \leq q_{ij} \leq 1$ if $q_{ii} = 1$ $(i = 1, \ldots, n)$ for copositive quadratic forms having $A^*(n)$ in the same way that Theorem 4.1 (Hall and Newman, Ref. 2) yielded it for extreme copositive forms (see section 2). As we shall need this result under this less stringent condition, we state it separately.

Corollary 3.9. If $Q(x_1, \ldots, x_n)$ has $A^*(n)$ and has $q_{ii} = 1$ $(i = 1, \ldots, n)$ then $-1 \leq q_{ij} \leq 1$.

Another immediate result of Theorem 3.3, which we make extensive use of in the next section is:

Corollary 3.10. If $Q(x_1, \ldots, x_n)$ is a quadratic form having $A^*(n)$, and if, among its zeros on $S(n)$, Q has a zero u with $u_1, \ldots, u_{k-1}, u_{k+1}, \ldots, u_n > 0 = u_k$, then Q is positive semi-definite.

Proof. By Lemma 11 Diananda (Ref. 1), we are done if we can show that Q has a zero with $u_k > 0$, but this follows from Corollary 3.4.

Corollary 3.11. If $Q(x_1, \ldots, x_n)$ $n \geq 3$ is an extreme copositive quadratic form which has a zero u on $S(n)$ with $u_1, \ldots, u_{k-1}, u_{k+1}, \ldots, u_n > 0 = u_k$, then Q is positive semi-definite.

Thus Corollary 3.11 vindicates Conjecture 2.3. Our final result of this section allows us to construct extreme copositive forms in n variables from those in $n' < n$ variables.

Theorem 3.12. If Q_n is an extreme copositive quadratic form in $n \geq 3$ variables $x_1, \ldots, x_n$ then replacing x_i by $x_i + x_{n+1}$ in Q_n yields a new copositive form Q_{n+1}, which is extreme.

Proof. We may assume that $i = n$ and that $q_{jj} = 1$ for all j (since $n \geq 3$ and Q_n is extreme). Q_{n+1} is obviously copositive. Now suppose that

$$Q_{n+1} = Q' + Q'' \tag{3.5}$$

with Q', Q'' copositive, then by setting $x_{n+1} = 0$ and $x_n = 0$ in turn, we get

$$Q_n = aQ_n + (1-a)Q_n, \qquad Q_n^* = bQ_n^* + (1-b)Q_n^* \qquad (0 \leq a, b \leq 1)$$

by the extremity of Q_n, Q_n^*. By (3.5) the coefficients of x_{11}^2 in aQ_n and bQ_n^* are the same and as $q_{11} = 1 \neq 0$ we have $a = b$. So we see that

$$Q' = a(Q_n + x_{n+1}^2 + 2\sum_{i=1}^{n-1} q_{in}x_ix_{n+1}) + kx_nx_{n+1}$$

$$Q'' = (1-a)(Q_n + x_{n+1}^2 + 2\sum_{i=1}^{n-1} q_{in}x_ix_{n+1}) + tx_nx_{n+1}$$

with $k + t = 2$. Thus

$$Q' = aQ_{n+1} + (k-2a)x_nx_{n+1},$$

$$Q'' = (1-a)Q_{n+1} + (t + 2a - 2)x_nx_{n+1}$$

Since Q_n is extreme it has a zero u in $S(n)$ with $u_n > 0$ (Corollary 3.5), thus $(u_1, \ldots, u_{n-1}, u_n/2, u_n/2)$ is a zero of Q_{n+1} in $S(n+1)$ with $x_nx_{n+1} > 0$. At this zero $Q' = \frac{1}{4}(k-2a)u_n^2$ and $Q'' = \frac{1}{4}(t+2a-2)u_n^2$, thus the copositivity of Q', Q'' insures that $(k-2a) \geq 0$ and $(t+2a-2) \geq 0$ respectively. But $Q_{n+1} = 0$ here so $k-2a = t+2a-2 = 0$. Thus $Q' = aQ_{n+1}$, $Q'' = (1-a)Q_{n+1}$ and so Q_{n+1} is extreme.

4. Extreme Copositive Quadratic Forms in Five Variables.

In this section we show (Lemma 4.1) that the only extreme copositive quadratic forms in 5 variables which satisfy Conjecture 2.1 (i.e. have $q_{ij} = \pm 1$ $i, j = 1, \ldots, 5$) are the Horn form (see section 2) and the positive semi-definite extremes. Further we exhibit a copositive quadratic form which does not belong to the convex hull generated by the previously known extremes (i.e. the extremes of P + S taken together with the Horn form). Thus we establish the existence of a new class of 5-variable extremes (Thm. 4.3) and hence (Thm. 3.12) of n-variable extremes for $n \geq 5$. In fact we are able to show that our specifically exhibited form is itself a new extreme of this type. As Conjecture 2.1 implies (Lemma 4.1) the non-existence of these new 5-variable extremes, we see that Conjecture 2.1 is not valid. Further our method of proof shows that any 5-variable extreme which does not belong to P + S and is not the Horn form must belong to this new class.

In the determination of the extreme 5-variable forms we need only concern ourselves with forms for which $q_{ii} > 0$ $(i = 1, \ldots, 5)$; for $q_{ii} = 0$ (some i) implies that Q does not have A*(5) (by the remarks immediately preceding Corollary 3.7) and hence cannot be extreme or that Q does not contain all the variables explicitly. In the latter case the form can be considered to be a four variable form and thus the extremes have been previously determined. So Q has $q_{ii} > 0$ $(i = 1, \ldots, 5)$ whence we may assume $q_{ii} = 1$ $(i = 1, \ldots, 5)$ without loss of generality. Further we already know the Horn form and those positive semi-definite forms which are also copositive extremes (Thm. 3.2 Hall and Newman), so we will summarily reject any line of reasoning which leads to these. In particular we shall often discard cases saying that they are positive semi-definite, more precisely this means that if the form is copositive then it is positive semi-definite. Since most of our conclusions depend on Q having $A^*(5)$, we shall specifically point out where extremity is required.

Lemma 4.1. If Q is an extreme copositive quadratic form in 5 variables which has $q_{ij} = \pm 1$ $(i, j = 1, \ldots, 5)$, then Q is either positive semi-definite or by a relabeling of the variables we can make Q into the Horn form.

Proof. Our method of proof is simply to consider all quadratic forms having $q_{ij} = \pm 1$ $(i, j = 1, \ldots, 5)$ and discard those which belong to $P + S$ or are not copositive or are not extreme.

Copositivity obviously implies $q_{ii} \neq -1$ hence $q_{ii} = 1$ $(i = 1, \ldots, 5)$. 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 $q_{12} = \ldots = q_{1r} = -1$, while $q_{1,r+1} = \ldots = q_{15} = 1$. 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 $(x_1 - x_2 - x_3 - x_4 + x_5)^2 + 4x_1x_4 + 2(q_{25} + 1) + 2(q_{35} + 1) + 2(q_{45} + 1)$ 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. Hence any other choice of q_{25}, q_{45} yields a non-extreme 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 $Q(x_1, \ldots, x_5) = Q(x_1, \ldots, x_4, 0) + x_5^2 + 2 \sum_{i=1}^{4} x_i x_5$ is not extreme. 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.

Similar searches have been performed for 6 and 7 variables, the results of which are that the only 6(7)-variable extremes having $q_{ij} = \pm 1$ can be derived from the 5 variable ones through the use of Theorem 3.12.

Thus we have Lemma 4.1 which will prove to be vital to the existence of our new class of extreme forms. Before turning to that proof we give a summary of its stages. First we establish (by exhaustive search) that any new extreme copositive forms in 5 variables will have one of two classes of zeros in S(5). Secondly, we show for forms with the first class of zeros that they cannot have any further zeros in S(5) and from this it follows that they are not copositive. The Horn form has zeros of the second class and we establish that any extreme copositive quadratic form, not belonging to P + S, which has the zeros of the second class and any additional zeros in S(5) is necessarily the Horn form. Thus we are left with quadratic forms having a particular class of zeros and no others in S(5). The structure of these zeros is such that the coefficients q_{ij} $i \neq j$ of the form can be expressed in terms of the zeros. We do this and the resulting equations together with other restrictions are noted. Further we give a solution of these equations, which is then tested and shown to be copositive and to be outside the convex hull of the previously known extremes. Thus we are able to conclude (using Lemma 4.1) that there exists a new class of extreme quadratic forms in 5 variables, and hence (Thm. 3.12) in n variables for $n \geq 5$.

We shall require the following lemma:

Lemma 4.2. 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_4 is positive semi-definite (Thm. 2, Diananda), whence Q_4 has a zero u with 4 positive components (Thm. 4, Diananda). Hence so does Q, and thus by Corollary 3.10, Q is positive semi-definite.

Definition. The <u>pattern</u> of an n-dimensional vector v = $(v_1, \ldots, v_n)$ is the vector obtained by replacing those $v_i \neq 0$ by 1. Thus (3, -2, 0, 4, -971) has pattern (1, 1, 0, 1, 1).

We shall see that the 5-variable extreme forms can be classified by the patterns of their zeros. Let us summarize what we know about the zeros in S(5) of a quadratic form Q in A*(5) which has $q_{ii} = 1$ $(i = 1, \ldots, 5)$ and is not positive semi-definite.

1. Each zero has at least two <u>non-zero</u> components (since $q_{ii} = 1$; $i = 1, \ldots, 5$).

2. Each zero has at least two zero components. (Lemma 1, Diananda and Corollary 3.10.)

3. Q has a zero with $u_i u_j \neq 0$ $(i, j = 1, \ldots, 5)$ (Corollary 3.4).

4. Q has at most six 2-variable zeros.

This last follows because each 2-variable zero implies that a different off-diagonal coefficient is -1 (since $q_{ii} = 1, i = 1, \ldots, 5$) and (Corollary 3.9) because $1 \le q_{ij} \le 1$ $(i \neq j; i, j = 1, \ldots, 5)$; thus if Q had more than 6 such zeros then $Q(1, 1, 1, 1, 1) < 0$, contradiction. Since all $\binom{5}{2} = 10$ pairs $(i \neq j)$ appear together in some zero (by 3) we have

5. Q has at least two 3-variable zeros.

The required 3-variable zeros may be assumed to be $(u_1, u_2, u_3, 0, 0)$ and one of $(v_1, 0, 0, v_4, v_5)$, $(w_1, w_2, 0, w_4, 0)$. We shall call these case a and b respectively and refer only to their zero patterns. Thus case a has zeros (11100), (10011) and case b has zeros (11100), (11010).

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 $u_2 u_5 \neq 0$ 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 4.2 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 $u_3 u_4 \neq 0$ 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 4.2 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 by Corollary 3.10. 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 his point all of a. 1. a. 1 has been either eliminated or subsumed, 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; re-labeling the variables gives

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

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 $q_{ii} = 1$ ($i = 1, \ldots, 5$) and hence that $-1 \leq q_{ii} \leq 1$ (Corollary 3. 9). 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 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 $Q_4 = Q' + bx_3x_4$ where Q' has $A^*(4)$ for $b \geq 0$ large enough. Thus Q' is positive semi-definite and (Thm. 4, Diananda) has a zero in $S(4)$ with all components positive. So Corollary 3. 10 implies that Q is positive semi-definite if $b = 0$. Thus we may assume $b > 0$; hence applying Corollary 3. 9 to Q' 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

	q_{12}	q_{23}	q_{14}	q_{24}	q_{15}	q_{25}
B1	1	−1	−1	−1	−1	−1
B2	−1	1	1	−1	1	−1
B3	−1	1	1	−1	−1	1
B4	−1	1	−1	1	1	−1
B5	−1	1	−1	1	−1	1

For B1 we have $Q(x_1, 0, x_3, x_4, 0)$ copositive, thus $q_{34} = 1$; 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 $q_{ii} = 1$ $(i = 1, \ldots, 5)$ 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, $Q(x_1, 0, x_3, x_4, 0)$ copositive yields $q_{34} = 1$ and proceeding similarly we establish that $q_{35} = q_{45} = 1$ which contradicts $Q(z) = 0$. Only case A remains, here $q_{12} = -1$ whence one of $q_{13}, q_{23} = -1$ and thus we have a sub-case of B. So we conclude that a. 3. c cannot have any further zero patterns, which implies $q_{ij} > -1$ $(i, j = 1, \ldots, 5)$. Further if $q_{ij} = 1$ for some $i \neq j$

$(i, j = 1, \ldots, 5)$ 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 $-1 < q_{ij} < 1$ $i \neq j$ $(i, j = 1, \ldots, 5)$. 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 zeros of Q in $S(5)$ are u, v, w, z and these are unique.

Since u is a unique zero of Q we know that

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

$$k, u_2, u_3 > 0$$

and hence that

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

where $b > 0, c \geq 0$ follow from Corollary 3.2 and a relabeling of the variables if necessary. (We note that this is the first time that the extremity of Q is crucial. Note further that if the variables need to be relabeled no change in the zero patterns is produced.) $A, C \leq 0$

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 $b > 0, c \geq 0$. Now let $r = v + w$, then $Q(r) = L_1^2(r) + kL_2^2(r) + Br_4 r_5 < 0$ 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 $u = (u_1, u_2, u_3, 0, 0)$, $v = (0, v_2, v_3, v_4, 0)$, $w = (0, 0, w_3, w_4, w_5)$, $y = (y_1, 0, 0, y_4, y_5)$, 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 $b \geq 0$ large enough. Thus Q' is positive semi-definite and (Thm. 4, Diananda) has a zero in $S(4)$ with all components positive. So Corollary 3. 10 implies that Q is positive semi-definite if $b = 0$. Thus we may assume $b > 0$; hence applying Corollary 3. 9 to Q' yields $q_{14} > -1$. 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 $Q(0, 0, x_3, x_4, x_5) = (x_3 - x_4 + x_5)^2$, $Q(x_1, 0, 0, x_4, x_5) = (x_4 - x_5 + x_1)^2$ 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 zeros in S(5) 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 zeros of Q in S(5) are u, v, w, y, z, and these are unique.

For computational convenience we normalize the zeros so that $u_3 = v_4 = w_5 = y_1 = z_2 = 1$; this takes the zeros out of S(5) but does no other damage. Consider $Q_5 = Q(x_1, x_2, x_3, x_4, 0)$, it is a co-positive 4-variable form and hence (Thm. 2, Diananda) belongs to P + S. Further $Q_5(u) = Q_5(v) = 0$ and so the part from P is necessarily $t_5 x_1 x_4$ with $t_5 \geq 0$. But if $t_5 = 0$ then Q_5 would be positive semi-definite and hence would have the 4-variable zero u + v [since $Q_5(u) = Q_5(v) = 0$]. But Corollary 3. 10 then implies that Q itself is positive semi-definite. So we may assume that $t_5 > 0$. Thus

$$
\begin{aligned}
Q_5 = \; & t_5 x_1 x_4 + [x_1 + q_{12} x_2 + q_{13} x_3 + (q_{14} - \tfrac{1}{2} t_5) x_4]^2 \\
& + g_5 (x_2 + b_{23} x_3 + b_{24} x_4)^2 \\
& + h (x_3 + c_{34} x_4)^2 \\
& + j \, x_4^2
\end{aligned}
$$

with $t_5, g_5, h, j \geq 0$. But $Q_5(u) = Q_5(v) = 0$ hence $h = j = 0$ and the uniqueness of the zero u implies $g_5 > 0$, thus

$$Q_5 = t_5x_1x_4 + [x_1 + q_{12}x_2 + q_{13}x_3 + (q_{14} - \tfrac{1}{2}t_5)x_4]^2$$

$$+ g_5(x_2 + b_{23}x_3 + b_{24}x_4)^2 \qquad t_5, g_5 > 0$$

Now $Q_5(u) = 0$ implies $u_2 + b_{23} = 0$, i.e. $b_{23} = -u_2 < 0$. Also $Q_5(v) = 0$ implies $v_2 + b_{23}v_3 + b_{24} = 0$, i.e. $b_{24} = -v_2 + u_2v_3$. $Q_5(u) = 0$, $Q_5(v) = 0$ imply

$$u_1 + q_{12}u_2 + q_{13} = 0 \tag{4.1}$$

$$q_{12}v_2 + q_{13}v_3 + (q_{14} - \tfrac{1}{2}t_5) = 0 \tag{4.2}$$

and the coefficients of x_2^2, x_2x_3, x_3^2 yield

$$q_{12}^2 + g_5 = 1 \tag{4.3}$$

$$q_{12}q_{13} - g_5u_2 = q_{23} \tag{4.4}$$

$$q_{13}^2 + g_5u_2^2 = 1 \tag{4.5}$$

Solving (4.3) for g_5 and using this in equation 4.4 together with equation 4.1 yields

$$u_1q_{12} + u_2 + q_{23} = 0 \tag{4.6}$$

Similarly, solving for g_5 in equation 4.5 and using it in equation 4.4 one gets

$$u_1q_{13} + u_2q_{23} + 1 = 0 \tag{4.7}$$

Hence using equations 4.1, 4.6 and 4.7 we get the system

$$\begin{bmatrix} u_2 & 1 & 0 \\ u_1 & 0 & 1 \\ 0 & u_1 & u_2 \end{bmatrix} \begin{bmatrix} q_{12} \\ q_{13} \\ q_{23} \end{bmatrix} = \begin{bmatrix} -u_1 \\ -u_2 \\ -1 \end{bmatrix} \qquad (4.8)$$

which has determinant $-2u_1u_2 < 0$, and thus may be solved for q_{12}, q_{13}, q_{23}. We obtain similar equations for each of the 4-variable sub-forms of Q and as we shall have to refer to them later, we list them here.

$$\begin{aligned} u_1 + u_2q_{12} + q_{13} &= 0 \\ u_1q_{12} + u_2 + q_{23} &= 0 \\ u_1q_{13} + u_2q_{23} + 1 &= 0 \end{aligned} \qquad (4.9)$$

$$\begin{aligned} v_2 + v_3q_{23} + q_{24} &= 0 \\ v_2q_{23} + v_3 + q_{34} &- 0 \\ v_2q_{24} + v_3q_{34} + 1 &= 0 \end{aligned} \qquad (4.10)$$

$$\begin{aligned} w_3 + w_4q_{34} + q_{35} &= 0 \\ w_3q_{34} + w_4 + q_{45} &= 0 \\ w_3q_{35} + w_4q_{45} + 1 &= 0 \end{aligned} \qquad (4.11)$$

$$\begin{aligned} y_4 + y_5 q_{45} + q_{14} &= 0 \\ y_4 q_{45} + y_5 + q_{15} &= 0 \\ y_4 q_{14} + y_5 q_{15} + 1 &= 0 \end{aligned} \tag{4.12}$$

$$\begin{aligned} z_5 + z_1 q_{15} + q_{25} &= 0 \\ z_5 q_{15} + z_1 + q_{12} &= 0 \\ z_5 q_{25} + z_1 q_{12} + 1 &= 0 \end{aligned} \tag{4.13}$$

Solving equations 4.9, . . . , 4.13 for the q_{ij} yields

$$q_{12} = \frac{-1 + u_1^2 + u_2^2}{-2u_1 u_2} = \frac{1 - z_5^2 + z_1^2}{-2z_1} \tag{4.14}$$

$$q_{13} = \frac{1 + u_1^2 - u_2^2}{-2u_1} \tag{4.15}$$

$$q_{14} = \frac{1 + y_4^2 - y_5^2}{-2y_4} \tag{4.16}$$

$$q_{15} = \frac{-1 + z_5^2 + z_1^2}{-2z_1 z_5} = \frac{1 - y_4^2 + y_5^2}{-2y_5} \tag{4.17}$$

$$q_{23} = \frac{-1 + v_2^2 + v_3^2}{-2v_2 v_3} = \frac{1 - u_1^2 + u_2^2}{-2u_2} \tag{4.18}$$

$$q_{24} = \frac{1 + v_2^2 - v_3^2}{-2v_2} \tag{4.19}$$

$$q_{25} = \frac{1 + z_5^2 - z_1^2}{-2z_5} \tag{4.20}$$

$$q_{34} = \frac{-1 + w_3^2 + w_4^2}{-2w_3w_4} = \frac{1 - v_2^2 + v_3^2}{-2v_3} \tag{4.21}$$

$$q_{35} = \frac{1 + w_3^2 - w_4^2}{-2w_3} \tag{4.22}$$

$$q_{45} = \frac{-1 + y_4^2 + y_5^2}{-2y_4y_5} = \frac{1 - w_3^2 + w_4^2}{-2w_4} \tag{4.23}$$

which are subject to the constraint (4.2), and similar constraints arising from the other 4-variable sub-forms, these are

$$\begin{aligned}
q_{12}v_2 + q_{13}v_3 + q_{14} &= \tfrac{1}{2}t_5 > 0 \\
q_{23}w_3 + q_{24}w_4 + q_{25} &= \tfrac{1}{2}t_1 > 0 \\
q_{34}y_4 + q_{35}y_5 + q_{13} &= \tfrac{1}{2}t_2 > 0 \\
q_{45}z_5 + q_{14}z_1 + q_{24} &= \tfrac{1}{2}t_3 > 0 \\
q_{15}u_1 + q_{25}u_2 + q_{35} &= \tfrac{1}{2}t_4 > 0
\end{aligned} \tag{4.24}$$

Further constraints are those imposed initially, i.e.

$$\begin{gathered}
u_1, u_2, v_2, v_3, w_3, w_4, y_4, y_5, z_5, z_1 > 0 \\
-1 < q_{ij} < 1 \qquad (i \neq j) \\
q_{ii} = 1 \ (i = 1, \ldots, 5) \\
u_3 = v_4 = w_5 = y_1 = z_2 = 1
\end{gathered} \tag{4.25}$$

Equations 4.9, . . . , 4.25 have a wide range of solutions, but the constraints (4.24) only insure that all 4-variable sub-forms of a solution are copositive (see preceding where t_5 was introduced). Hence a solution of these equations must be checked for copositivity in 5 variables. (Fortunately, such a test exists, see Motzkin Ref. 3.) Even so equations 4.9, . . . , 4.25 appear to yield a large family of copositive quadratic forms which has not as yet been parameterized. We give the following example of a solution, listing first the zeros and then the coefficients

$$u = \{\tfrac{1}{8}, \tfrac{1}{8^2}(7 + \sqrt{8^4 - 15}), 1, 0, 0\} = \{0.125, 1.1075+, 1, 0, 0\}$$

$$v = \{0, \tfrac{1}{8}, \tfrac{1}{8^3}(\sqrt{8^4 - 15} + \sqrt{8^6 - 15}), 1, 0\} = \{0, 0.125, 1.1247+, 1, 0\}$$

$$w = \{0, 0, \tfrac{1}{8}, \tfrac{1}{8^4}(\sqrt{8^6 - 15} + \sqrt{8^8 - 15}), 1\} = \{0, 0, 0.125, 1.1249+, 1\}$$

$$y = \{1, 0, 0, \tfrac{1}{8}, \tfrac{1}{8^5}(\sqrt{8^8 - 15} + \sqrt{8^{10} - 15})\} = \{1, 0, 0, 0.125, 1.1249+\}$$

$$z = \{\tfrac{1}{8}(7 + \sqrt{8^{10} - 15}), 1, 0, 0, 8^4\} = \{4096.874+, 1, 0, 0, 4096\}$$

$$q_{11} = q_{22} = q_{33} = q_{44} = q_{55} = 1$$

$$q_{12} = \frac{-7}{8} = -0.875$$

$$q_{13} = \frac{1}{8^3}(7\sqrt{8^4 - 15} - 15) = 0.844099482+$$

$$q_{14} = \frac{1}{8^9}\{\sqrt{(8^8 - 15)(8^{10} - 15)} - 15\} = 0.999999434+$$

$$q_{15} = \frac{-1}{8^5}\sqrt{8^{10} - 15} = -(0.999999993+)$$

$$q_{23} = \frac{-1}{8^2}\sqrt{8^4-15} \qquad = -(0.998167265+)$$

$$q_{24} = \frac{1}{8^5}\{\sqrt{(8^4-15)(8^6-15)} - 15\} \qquad = 0.997680943+$$

$$q_{25} = \frac{1}{8^6}(7\sqrt{8^{10}-15}-15) = \frac{1}{8^6}\sqrt{8^{12}-15(7+\sqrt{8^{10}-15})^2}$$
$$= 0.874942773+$$

$$q_{34} = \frac{-1}{8^3}\sqrt{8^6-15} \qquad = -(0.999971389+)$$

$$q_{35} = \frac{1}{8^7}\{\sqrt{(8^6-15)(8^8-15)} - 15\} \qquad = 0.999963789+$$

$$q_{45} = \frac{-1}{8^4}\sqrt{8^8-15} \qquad = -(0.999999552+)$$

Here the t_i are:

$$t_1 = 3.745+,\ t_2 = 3.688+,\ t_3 = 3.744+,\ t_4 = 3.687+,\ t_5 = 3.680+$$

One notes, among other things, that in this solution $u_1v_2w_3y_4z_5 = 1$. In fact this is generally the case as will be shown later (Thm. 4.3).

As mentioned above $t_i > 0$ $(i = 1, \ldots, 5)$ implies that our form Q is copositive in any four variables. Thus in order to establish the copositivity of Q we need only determine whether $Q(x) \geq 0$ for $x_i > 0$ $(i = 1, \ldots, 5)$. Using homogeneity, we can ascertain this from the values of $Q(x)$ restricted to $x_5 = 1$. To do this we first note that $Q(x) \geq 0$ for all x on the boundary of $J = \{x : x_5 = 1,\ x_i \geq 0$ $(i = 1, \ldots, 4)\}$. For those portions of the boundary which have $x_i = 0$ for some i $(i = 1, \ldots, 4)$ this follows from $t_1, \ldots, t_4 > 0$, i.e. from the 4-variable sub-forms. A typical point on the other part of the boundary might be $y = \lim_{m \to \infty} (951, M, 3, M, 1)$. Now let y_j be any sequence of points of J which converges to y. For each $y_j = (y_{j1}, \ldots, y_{j4}, 1)$ let $N_j = y_{j1} + \ldots + y_{j4} + 1$, then by homogeneity we have

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

and thus in particular $Q(y_j)$ and $Q(y_j/N_j)$ have the same sign for all j. Hence $Q(y)$ has the same sign as $Q(0, \frac{1}{2}, 0, \frac{1}{2}, 0)$ which is ≥ 0 since $x_5 = 0$ and $t_5 > 0$. As the same proof works for all such boundary points we see that $Q(x) \geq 0$ on the boundary of J. Further we note that $\lim_{j \to \infty} Q(y_j) \geq 0$ no matter what sequence y_j approaching y we choose.

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.) Then consider the set $T = \{x \text{ in } J: Q(x) \leq \frac{1}{2}d\}$, clearly s belongs to T and T is closed. Suppose T was not bounded, then there would exist a sequence of points of T which would approach a boundary point of J. But T is closed, thus this boundary point must have a function value $\leq \frac{1}{2}d$, 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 $Q > \frac{1}{2}d$, thus Q has a minimum $\leq d$ in this region. Since Q is continuous this minimum cannot appear on the boundary, hence Q has a stationary point in the interior of this region — hence in the interior of J.

Thus if we wish to prove that $Q(x) \geq 0$ in J, we need only examine the stationary points of Q which lie in J. For this purpose we write $Q(x) = x^t Ax$ and apply Lagrange's method to $Q(x) + \lambda x_5$. So we are led to solve

$$2Ax = (0, 0, 0, 0, -\lambda)^t$$

for the vector x. As $|A| \sim 11.925$ this is possible and we determine λ by Cramer's rule from $x_5 = 1 = -\lambda D_{n-1}/2|A|$ where $D_{n-1} \sim -0.0124$ is the determinant of the first four rows and columns of A. This yields $x \sim (-0.1272, -513.6, -521.6, -8.017, 1)$ with the associated value $Q(x) = x^t Ax = x^t(0, 0, 0, 0, -\frac{1}{2}\lambda)^t = -\frac{1}{2}\lambda \sim -961.8$. Thus Q has no stationary point in J and hence $Q(x) \geq 0$ in J by the previous paragraph. That is, Q is copositive.

So at this point we have a copositive quadratic form Q which has $A^*(5)$ — as follows from its zero patterns — but we do not know whether it is extreme. Letting H be the class of forms of the Horn type, i.e. $H = \{Q : Q = \sum_i R_i(t_{i1}x_1, \ldots, t_{i5}x_5)$ where $R_i(x_1, \ldots, x_5)$ is equivalent to the Horn form by a relabeling of the variables and $t_{i1}, \ldots, t_{i5} > 0$ for all $i\}$, and letting N be the class of all other copositive quadratic forms which might exist outside $H + P + S$, we must have $Q \in P + S + H + N$. Thus

$$Q(x) \equiv P(x) + S(x) + H(x) + N(x)$$

Now $P(x) \equiv 0$ since $Q(x)$ has zeros with $x_i x_j \neq 0$ $(i, j = 1, \ldots, 5)$. Further $S(x) \equiv 0$ since the determinant of the zeros of $Q(x)$ — hence also zeros of $S(x)$ — has value $\sim 3.678 \neq 0$. So $Q \in H + N$; suppose $Q(x) \equiv H_1(x) + Q_1(x)$ where Q_1 is copositive and H_1 is a particular scaled Horn form, i.e. $H_1(x_1, \dots, x_5) = R(p_1'x_1', \dots, p_5'x_5')$ with R the Horn form, $p_i' > 0$ $(i = 1, \dots, 5)$ and each $x_i' = x_j$ for a different value of j $(i, j = 1, \dots, 5)$. Now the zero patterns of Q, hence also of H_1, imply that $j = i + k$ for some fixed k (where we define $x_{5+m} = x_m$, $m \geq 0$). Thus (since R is fixed under cyclic relabeling of the variables) we may assume that $Q(x) \equiv H_1(x) + Q_1(x) \equiv R(p_1x_1, \dots, p_5x_5) + Q_1(x)$ where R is the Horn form. Making the transformation $x_i \to x_i/p_i$ we see that the transformed Q has zeros $(p_1u_1, p_2u_2, p_3, 0, 0)$ $, \dots, (p_1z_1, p_2, 0, 0, p_5z_5)$. But these are also the zeros of R, thus from our listing of the zeros of R (see section 2) we know that $p_1u_1 - p_2u_2 + p_3 = 0, \dots, p_5z_5 - p_1z_1 + p_2 = 0$; that is

$$\begin{bmatrix} u_1 & -u_2 & 1 & 0 & 0 \\ 0 & v_2 & -v_3 & 1 & 0 \\ 0 & 0 & w_3 & -w_4 & 1 \\ 1 & 1 & 0 & y_4 & -y_5 \\ -z_1 & 1 & 0 & 0 & z_5 \end{bmatrix} \begin{bmatrix} p_1 \\ p_2 \\ p_3 \\ p_4 \\ p_5 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

But the determinant in question has value $\sim 0.32112 > 0$, so $p_1 = \dots = p_5 = 0$ thus $H_1(x) \equiv 0$. Thus $H(x) \equiv 0$, and so Q lies outside the convex hull $P + S + H$. That is, Q is a sum of new extremes. We note that any new extreme must satisfy all the conditions that Q has satisfied, hence we state:

Theorem 4.3. If $Q(x_1, \ldots, x_5)$ is an extreme copositive quadratic form having $q_{ii} = 1$ $(i = 1, \ldots, 5)$ then (i) Q is a positive semi-definite extreme or (ii) Q is a replica of the Horn form in which the variables have been relabeled or (iii) after a relabeling of the variables Q is a solution of equations 4.9, ..., 4.25. In this later case, Q has exactly 5 zeros in S(5) which are thus isolated in S(5) and can be assumed to be multiples of $u = (u_1, u_2, 1, 0, 0)$, $v = (0, v_2, v_3, 1, 0)$, $w = (0, 0, w_3, w_4, 1)$, $y = (1, 0, 0, y_4, y_5)$, $z = (z_1, 1, 0, 0, z_5)$, where $u_1 v_2 w_3 y_4 z_5 = 1$.

Proof. The only assertion which we have not yet established is that $u_1 v_2 w_3 y_4 z_5 = 1$. To this end we first show that not both q_{12}, $q_{15} = 0$. Suppose so, then

$$Q(x_1, x_2, 0, 0, x_5) = x_1^2 + x_2^2 + x_5^2 + 2q_{25}x_2x_5$$

$$= (x_2 + q_{25}x_5)^2 + sx_5^2 + x_1^2$$

where $-1 < q_{25} < 1$ and hence $s > 0$. Now $Q(z) = 0$, but this is impossible by the above representation. Hence at least one of q_{12}, $q_{15} \neq 0$.

We now establish $u_1 v_2 w_3 y_4 z_5 = 1$ using $q_{15} \neq 0$ (an analogous proof holds for $q_{12} \neq 0$). Since the $u_i, \ldots, z_i \geq 0$ we need only prove that $(u_1 v_2 w_3 y_4 z_5)^2 = 1$. By equation 4.13 we have

$$(u_1 v_2 w_3 y_4 z_5)^2 = (u_1 v_2 w_3 y_4)^2 \left(\frac{z_1 + q_{12}}{q_{15}}\right)^2 \qquad (q_{15} \neq 0)$$

and solving (4. 14) and (4. 17) simultaneously for z_1 yields

$$z_1 = -q_{12} \pm \frac{q_{15}}{q_{15}^2-1} \sqrt{(q_{15}^2-1)(q_{12}^2-1)} \qquad (\text{as } -1 < q_{15} < 1)$$

thus

$$(u_1 v_2 w_3 y_4 z_5)^2 = (u_1 v_2 w_3 y_4)^2 \; \frac{(q_{12}^2-1)}{(q_{15}^2-1)}$$

But

$$q_{15}^2 = (q_{45}^2 - 1) y_4^2 + 1 \qquad (4.12, 4.23)$$

$$q_{45}^2 = (q_{34}^2 - 1) w_3^2 + 1 \qquad (4.11, 4.21)$$

$$q_{34}^2 = (q_{23}^2 - 1) v_2^2 + 1 \qquad (4.10, 4.18)$$

$$q_{23}^2 = (q_{12}^2 - 1) u_1^2 + 1 \qquad (4.9, 4.14)$$

and using these in turn gives the desired result, since $-1 < q_{ij} < 1$, for $i \neq j$.

Corollary 4. 4. There exists an extreme copositive quadratic form in 5 variables with $q_{ii} = 1$ $(i = 1, \ldots, 5)$ which does not have $q_{ij} = \pm 1$ $(i, j = 1, \ldots, 5)$.

Proof. Follows immediately from the theorem if we use Lemma 4. 1.

At this point only Conjecture 2. 7 remains; we prove it for $n \leq 5$ variables.

Corollary 4. 5. Let u be a maximal zero in $S(n)$ of an extreme copositive quadratic form in $n \leq 5$ variables, then $u_i = 0$

implies $\partial Q(u)/\partial x_i > 0$ for any $i = 1, \ldots, n$.

Proof. The copositive extremes for $n \leq 4$ variables all belong to $P + S$ (Thm. 2, Diananda). These have been determined (Thm. 3.2, Hall and Newman), see the first part of section 2 for a listing of them. The corollary is obviously true for all these and also for the Horn form as the exhaustive listing of its zeros in section 2 indicates. Thus (Thm. 4.3) we need only concern ourselves with our new category of extremes. Any of these may be written

$$
\begin{aligned}
Q = {} & (x_1 + q_{12}x_2 + q_{13}x_3 + q_{14}x_4 + q_{15}x_5)^2 && && (= M_1^2) \\
& + k\left(\frac{x_2}{u_2} - \frac{x_3}{u_3} + ex_4 + fx_5\right)^2 && k > 0 && (= kM_2^2) \\
& + bx_3x_4 + cx_3x_5 && b, c \geq 0 && \\
& + Ax_4^2 + Bx_4x_5 + Cx_5^2 && &&
\end{aligned}
$$

where $k > 0$ is implied by the isolation of the zero $u = (u_1, u_2, 1, 0, 0)$ in $S(5)$. Further $b, c \geq 0$ since $\partial Q(u)/\partial x_4 = bu_3 = b \geq 0$ (by copositivity), similarly $\partial Q(u)/\partial x_5 = c \geq 0$. Now $Q(z) = 0$ where $z = (z_1, 1, 0, 0, z_5)$ hence $C \leq 0$, but $Q(x_1, x_2, 0, 0, x_5)$ is positive semi-definite (Lemma 1, Diananda) and so $C = 0$. Thus from $M_1(u) = M_2(u) = M_1(z) = M_2(z) = 0$ we get $Q(u + z) = cu_3z_5 = cz_5 \geq 0$. If $c = 0$ then $u + z$ is a 4-variable zero of Q, which contradicts Corollary 3.11. Hence $c > 0$ (i.e. $\partial Q(u)/\partial x_5 > 0$). Now if $\partial Q(u)/\partial x_4 = b = 0$ then $Q(x_1, x_2, x_3, x_4, 0) = L_1^2 + \ldots + L_s^2 + Q_1(x_4)$ with Q_1 copositive, by Lemma 3.1 (using the zero u). Hence $Q_1(x_4) = ax_4^2$ with $a \geq 0$. But

$v = (0, v_2, v_3, 1, 0)$ is also a zero of Q and hence of $Q(x_1, x_2, x_3, x_4, 0)$, thus $Q(v) = L_1^2(v) + \ldots + L_s^2(v) + a = 0$ and hence $L_1(v) = \ldots = L_s(v) = a = 0$. But this implies $Q(u + v) = 0$, that is Q must have the 4-variable zero $u + v$, contradiction. Hence we are forced to conclude that $b > 0$ also. So for the zero u of Q we have shown that $u_i = 0$ implies $\partial Q(u)/\partial x_i > 0$. This is true for the other zeros v, w, y, z of Q, since a cyclic relabelling of the variables takes u into any one of these.

Finally we show that our solution for equations (4.9), ..., (4.25) is actually an extreme form. Suppose not, then $Q = Q_1 + Q_2$ where Q_1, Q_2 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 $Q_1 = aQ$, $Q_2 = (1 - a)Q$ $(0 \leq a \leq 1)$.

Let us assume that $R(x_1, \ldots, x_5)$ is a copositive quadratic form having the zeros u, v, w, y, z, then R has A*(5) and thus R has $r_{ii} > 0$ $(i = 1, \ldots, 5)$. So by multiplying R by a suitable scalar we may assume that $r_{11} = 1$. Since R is copositive and has the zero u, $R(x_1, x_2, x_3, 0, 0)$ 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 analoguous 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

$$r_{11} = 1, \quad r_{12} = b, \quad r_{13} = -u_1 - bu_2, \quad r_{14} = (by_5 + z_1y_5 - z_5)/y_4z_5,$$

$$r_{15} = (-b-z_1)/z_5, \quad r_{22} = e, \quad r_{23} = -bu_1 - eu_2,$$

$$r_{24} = -v_2e + (bu_1+eu_2)v_3, \quad r_{25} = (-e-bz_1)/z_5,$$

$$r_{33} = u_1^2 + 2bu_1u_2 + eu_2^2,$$

$$r_{34} = v_2(bu_1+eu_2) - v_3(u_1^2+2bu_1u_2+eu_2^2),$$

$$r_{35} = (v_3w_4-w_3)(u_1^2+2bu_1u_2+eu_2^2) - v_2w_4(bu_1+eu_2),$$

$$r_{44} = v_2^2e - 2v_2v_3(bu_1+eu_2) + v_3^2(u_1^2+2bu_1u_2+eu_2^2),$$

$$r_{45} = (bz_5+z_1z_5-z_1^2y_5-2bz_1y_5-ey_5)/y_4z_5^2,$$

$$r_{55} = (z_1^2+2bz_1+e)/z_5^2.$$

An examination of these equations would show that they were obtained without the use of relations $r_{35}w_3 + r_{45}w_4 + r_{55} = 0$ and $r_{34}w_3 + r_{44}w_4 + r_{45} = 0$. Using these and $u_1v_2w_3y_4z_5 = 1$ yields

$$\begin{aligned}
&(u_1^2v_3w_3w_4y_4z_5^2 - u_1^2w_3^2y_4z_5^2 + w_4z_5z_1 - w_4y_5z_1^2 + y_4z_1^2) \\
+\;&(2u_1u_2v_3w_3w_4y_4z_5^2 - 2u_1u_2w_3^2y_4z_5^2 - 2w_4y_5z_1 + 2y_4z_1)b \\
+\;&(u_2^2v_3w_3w_4y_4z_5^2 - u_2^2w_3^2y_4z_5^2 - u_2v_2w_3w_4y_4z_5^2 - w_4y_5 + y_4)\,e = 0
\end{aligned}$$

$$\begin{aligned}
&(-u_1^2v_3w_3y_4z_5^2 + u_1^2v_3^2w_4y_4z_5^2 + z_1z_5 - y_5z_1^2) \\
+\;&(-2u_1u_2v_3w_3y_4z_5^2 - 2u_1v_2v_3w_4y_4z_5^2 + 2u_1u_2v_3^2w_4y_4z_5^2 + 2z_5)b \\
+\;&(u_2v_2w_3y_4z_5^2 - u_2^2v_3w_3y_4z_5^2 + v_2^2w_4y_4z_5^2 - 2u_2v_2v_3w_4y_4z_5^2)e \\
+\;&(-2z_1y_5)b + (u_2^2v_3^2w_4y_4z_5^2 - y_5)e = 0
\end{aligned}$$

For our particular values of $u_i, \ldots, z_i$ these two equations have the unique solution $b = -7/8$, $e = 1$. Hence R is unique and thus Q is extreme.

REFERENCES

1. P. H. Diananda, ''On Non-negative Forms in Real Variables Some or All of Which are Non-negative,'' Proc. Cambridge Philos. Soc. 58 (1962), 17-25.

2. M. Hall, Jr. and M. Newman, ''Copositive and Completely Positive Quadratic Forms,'' Proc. Cambridge Philos. Soc. 59 (1963), 329-339.

3. T. Motzkin, ''Copositive Quadratic Forms,'' National Bureau of Standards Report 1818 (1952), 11-12.