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EXTREME COPOSITIVE QUADRATIC FORMS

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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 covex 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 $Q_1 = aQ, Q_2 = (1-a)Q, 0 \leqq a \leqq 1$. We show that if $Q(x_1, \cdots, x_n), n \geqq 2$, is an extreme copositive quadratic form then for any index i $(1 \leqq i \leqq n), Q$ has a zero u with $u_1 \cdots, u_n \geqq 0$ where $u_i > 0$. Further, using this fact, we establish an extension process whereby extreme forms in n variables can be used to construct extreme form in n' variables, for all $n' > n$.

Copositive quadratic forms arise in the theory of inequalities (see the references in Diananda, [2]) and also in the study of block designs (Hall and Newman, [3]). The interested reader should also see Motzkin [4, 5].

In § 2 we indicate some of the basic results on copositive quadratic forms and describe some normalizations which will be of use later.

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 is clearly copositive. Thus, denoting the class of positive semi-definite quadratic forms by S and the nonnegative coefficient forms by P, we see that any quadratic form which is expressible as a sum of elements of P and S is necessarily copositive (i.e., $Q \in P + S$ implies Q is copositive). In fact, Diananda [2] has shown that there are no other copositive quadratic forms in $n \leqq 4$ variables. 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]. Thus whenever it is convenient to do so we shall restrict attention to extreme copositive forms *not* belonging to $P + S$.

Suppose $Q = Q(x_1, \cdots, x_n)$ is copositive; then so is $Q' = Q(p_1x_1, \cdots, p_nx_n)$ for any choice of $p_i > 0$ $(i = 1, \cdots, n)$. Similarly Q is an extreme form if and only if Q' is also. Hence in questions of copositivity or extremity we may restrict ourselves to the case $q_{ii} = 1$ $(i = 1, \cdots, n)$, provided $q_{ii} > 0$ $(i = 1, \cdots, n)$. As copositivity implies $q_{ii} \geqq 0$ $(i = 1, \cdots, n)$ the only alternative is that $q_{ii} = 0$ (some i). Here the form, if copositive, is of an extremely simple type (Lemma 2, Diananda) which often allows us to consider only those variables for which $q_{ii} > 0$. That is, we can often restrict attention to a sub-form for which we can insist that $q_{ii} = 1$ $(i = 1, \cdots, n' < n)$. Relabeling of the variables is another transformation which does not effect copositivity or extremity and we shall resort to it in order to simplify the statements of results.

In many instances the concept of extremity is hard to handle—and it often suffices to replace it with the weaker property which (following Diananda) we call $A^*(n)$.

DEFINITION 2.1. 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 $(i, j = 1, \cdots, n)$ $Q - \varepsilon x_i x_j$ is not copositive for any $\varepsilon > 0$. (That is, Q is a copositive quadratic form which is "reduced" with respect to the extremes of P).

We shall be concerned with the values taken by a quadratic form for $x_i \geqq 0$ $(i = 1, \cdots, n)$; to which end homogeneity usually permits us to restrict attention to those x for which $x_1 + \cdots + x_n = 1$. Again following Diananda we call this $S(n)$, that is:

DEFINITION 2.2. $S(n) = \{x \text{ in } E_n\colon x_1 + \cdots + x_n = 1, x_i \geqq 0 \ (i = 1, \cdots, n)\}$.

3. General results. We prove first a lemma which will be required later. It has an immediately corollary which serves to characterize the extreme copositive quadratic forms *not* belonging to $P + S$.

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

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

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

Proof. By Lemma 1 of Diananda $Q(x_1, \cdots, x_m, 0, \cdots, 0)$ is positive semi-definite and we collect squares with respect to $x_1, \cdots, x_m$ yielding

$$Q(x_1, \cdots, x_m, 0, \cdots, 0) = K_1^2 + \cdots + K_s^2$$

where by renumbering the x_i $(i = 1, \cdots, m)$ we may assume that K_i is a linear form in $x_i, \cdots, x_m (i = 1, \cdots, s)$. Note that $Q(u) = 0$ implies $s < m$. Thus we may express $Q(x_1, \cdots, x_n)$ as follows

$$(3.1) \qquad Q = L_1^2 + \cdots + L_s^2 + 2 \sum_{i=s+1}^{m} \sum_{j=m+1}^{n} a_{ij} x_i x_j + Q_1(x_{m+1}, \cdots, x_n)$$

where we may assume that L_i is a linear form in $x_i, \cdots, x_n (i = 1, \cdots, s)$. Now for any set of $x_i \geqq 0$ $(i = s + 1, \cdots, n)$ there exist values (possibly negative) for $x_i (i = 1, \cdots, s)$ for which $L_1 = \cdots = L_s = 0$. Let z be such a vector. Since $\partial Q(u)/\partial x_i = 0$ $(i = 1, \cdots, n)$

$$(3.2) \qquad Q(z) = Q(z + ku)$$

for all real k. But for $k > 0$ sufficiently large $z + ku$ has all non-negative components. Hence the copositivity of Q together with equation 3.2 implies $Q(z) \geqq 0$. As $L_1(z) = \cdots = L_s(z) = 0$, we see from (3.1) that

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

is copositive in the variables $x_{s+1}, \cdots, x_n$ and hence (Lemma 2, Diananda) $a_{ij} \geqq 0$ $(i = s + 1, \cdots, m; j = m + 1, \cdots, n)$.

Let $m + 1 \leqq j \leqq n$, then by (3.1)

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

where g_k is the coefficient of x_j in $L_k (k = 1, \cdots, s)$. Now $Q(u) = 0$ and Q_2 copositive imply by (3.1) that $L_k(u) = 0$ $(k = 1, \cdots, s)$; further $\partial Q_1(u)/\partial x_j = 0$ as $u_{m+1} = \cdots = u_n = 0$. Thus as $u_i > 0$ $(i = s + 1, \cdots, m)$ we have $a_{ij} = 0$ $(i = s + 1, \cdots, m; j = m + 1, \cdots, n)$. Hence

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

where Q_1 is copositive and the L_i's are constituted as desired, which completes the proof.

Note that if $u_1, \cdots, u_{n-1} > 0 = u_n$ then $Q_1 = a x_n^2$ and is copositive, hence $a \geqq 0$. Thus we have:

COROLLARY 3.2. *If $Q(x_1, \cdots, x_n)$ is a copositive quadratic form having a zero u on $S(n)$, at which $u_1, \cdots, u_{n-1} > 0 = u_n$ and $\partial Q(u)/\partial x_i = 0$ $(i = 1, \cdots, n)$, then Q is positive semi-definite.*

COROLLARY 3.3. *If $Q(x_1, \cdots, x_n)$ 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 $(i = 1, \cdots, n)$ *then* Q *is positive semi-definite.*

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

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

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

Now every extreme copositive quadratic form in $n \geqq 2$ variables has zeros in $S(n)$, Lemma 4 of Diananda. Further if u in $S(n)$ is a zero of a copositive quadratic form Q then $\partial Q(u)/\partial x_i \geqq 0$ $(i = 1, \cdots, n)$, as one easily sees from copositivity. In fact $u_i > 0$ implies $\partial Q(u)/\partial x_i = 0$ and thus $\partial Q(u)/\partial x_i > 0$ only if $u_i = 0$. Thus the Corollary above allows us to conclude that every extreme copositive quadratic form *not* belonging to $P + S$ has at each of its zeros u in $S(n)$ a component $u_j = 0$, where $\partial Q(u)/\partial x_j > 0$.

Our next theorem is the most important result of this paper; almost everything that is new here depends upon it in one way or another. In many respects it is related to Theorem 4.1 of Hall and Newman, [3].

THEOREM 3.4. *A copositive quadratic form* $Q(x_1, \cdots, x_n)$ *has a zero* u *on* $S(n)$ *with* $u_i > 0$ *if and only if* $Q - \varepsilon x_i^2$ *is not copositive for any* $\varepsilon > 0$, $(1 \leqq i \leqq n)$.

Proof. If Q has such a zero u then $Q(u) - \varepsilon u_i^2 = - \varepsilon u_i^2 < 0$ for any $\varepsilon > 0$. On the other hand, proceeding by induction on n, let $n = 1$, then $Q = qx_1^2$ $(q \geqq 0)$, but $Q - \varepsilon x_1^2$ not copositive for all $\varepsilon > 0$ 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) $qx_1x_2 (q \geqq 0)$, (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 $x_1 = 0, x_2 = 1$.

Case 2. $Q - \varepsilon x_i^2$ not copositive for all $\varepsilon > 0$ implies that $i = 2$, 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

$k \geqq 0$ since Q is copositive. Now $Q - \varepsilon x_i^2$ not copositive for all $\varepsilon > 0$ implies (Lemma 4, Diananda [2] that $Q = (x_1 - x_2)^2 + kx_1x_2$, $k \geqq 0$ has a zero on $S(2)$ which can only be $x_1 = x_2 = 1/2$, thus $k = 0$. So $x_1 = x_2 = 1/2$ is the desired zero on $S(2)$.

More generally, since $Q - \varepsilon x_i^2$ is not copositive for $\varepsilon > 0$, there exists a nonnegative n-tuple z [which may be assumed to be on $S(n)$] for which $Q(z) < \varepsilon z_i^2$. By taking successively smaller positive ε's we construct a sequence of nonnegative 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 $Q(u) = 0$. If $u_i > 0$ we are done, so we assume $u_i = 0$. Now relabel the variables so that $i = 1$, and $u_2, \cdots, u_m > 0$ and further $\partial Q(u)/\partial x_j = 0$ for $j = m + 1, \cdots, k$ and $\partial Q(u)/\partial x_j > 0$ $(k + 1 \leqq j \leqq n)$.

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

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

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

$$0 \leqq Q(v_1, \cdots, v_{n-1}, 0) < Q(v) < \varepsilon v_1^2 \tag{3.3}$$

Thus there exists a subsequence of the v's in which we may replace $v = (v_1, \cdots, v_n)$ by $v' = (v_1, \cdots, v_{n-1}, 0)$ to yield a sequence which approaches u and has the property $Q(v') < \varepsilon v_1^2$. Repeating this process we replace all the nonzero $v_{k+1}, \cdots, v_n$ in some suitable subsequence of the v's by zero. This yields a form $Q_1(x_1, \cdots, x_k) = Q(x_1, \cdots, x_k, 0, \cdots, 0)$ and a sequence of k-tuples (in which we again designate the generic member by v) $v = (v_1, \cdots, v_k)$ approaching $u = (u_1, \cdots, u_k)$ for which $Q_1(v_1, \cdots, v_k) < \varepsilon v_1^2$ and for which $\partial Q_1(u)/\partial x_i = 0$ for $i = 2, \cdots, k$ (copositivity implies $\partial Q_1(u)/\partial x_i = 0$ if $u_i > 0$). Since $u_1 = 0$ we have

$$\begin{aligned} Q_1(v_1, \cdots, v_k) &= w_1\left(q_{11}w_1 + \frac{\partial Q_1(u)}{\partial x_1} + 2q_{12}w_2 + \cdots + 2q_{1k}w_k\right) \\ &\quad + Q_1(0, v_2, \cdots, v_k) \end{aligned}$$

with $w_1 = v_1 > 0$ (follows from 3.3). Since $Q_1(0, v_2, \cdots, v_k) \geqq 0$ the inequality $Q_1(v_1, \cdots, v_k) < \varepsilon v_1^2$ can only hold for sufficiently small w's if $\partial Q_1(u)/\partial x_1 = 0$. Hence for $Q_1(x_1, \cdots, x_k)$ we have $Q_1(u) = 0$ and

$\partial Q_1(u)/\partial x_i = 0$ $(i = 1, \cdots, k)$.

Applying Lemma 3.1 we get

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

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

If $(v_1, \cdots, v_k) = v$ is one of our k-tuples for which $Q_1(v) < \varepsilon v_1^2$ then (3.4) shows that $Q_2(v_1, v_{m+1}, \cdots, v_k) < \varepsilon v_1^2$. If Q_2 does not contain x_1^2 then $Q_2(1, 0, \cdots, 0) = 0$; whereas if x_1^2 appears in Q_2 the induction hypothesis applies as $0 < k - m + 1 < n$. So in either case Q_2 has a zero $z = (z_1, z_{m+1}, \cdots, z_k)$ on $S(k - m + 1)$ with $z_1 \neq 0$. Now $Q_1(u) = 0$, hence (by 3.4) $L_2(u) = \cdots = L_s(u) = 0$ where $u_1 = 0 = u_{m+1} = \cdots = u_k$ and $u_i > 0$ $(i = 2, \cdots, m)$. Due to the structure of the L_i's, the equations

$$L_2 = \cdots = L_s = x_{s+1} = \cdots = x_m = 0\ ,$$
$$x_1 = z_1,\ x_{m+1} = z_{m+1}, \cdots, x_k = z_k$$

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

If we apply this result to forms having $A^*(n)$ we get

COROLLARY 3.5. *If $Q(x_1, \cdots, x_n)$ is a quadratic form having $A^*(n)$ then for every index i $(1 \leqq i \leqq n)$, Q has a zero u on $S(n)$ with $u_i > 0$.*

In stating the associated result for extreme forms we must be careful to exclude extremes of the type $ax_i^2, a > 0$, hence we limit ourselves to the case where $n \geqq 2$.

COROLLARY 3.6. *If $Q(x_1, \cdots, x_n)$, $n \geqq 2$, is an extreme copositive quadratic form then for every index i $(1 \leqq i \leqq n)$, Q has a zero u on $S(n)$ with $u_i > 0$.*

Another immediate consequence of Theorem 3.4 is:

COROLLARY 3.7. *If $Q(x_1, \cdots, x_n)$ is a quadratic form having $A^*(n)$, and if, among its zeros on $S(n)$, Q has a zero u with*

$$u_1, \cdots, u_{k-1}, u_{k+1}, \cdots, u_n > 0 = u_k$$

then Q is positive semi-definite.

Proof. By Lemma 11, Diananda [2] we are done if we can show that Q has a zero with $u_k > 0$, but this follows from Corollary 3.5.

As extreme forms in $n \geqq 3$ variables have $A^*(n)$ Corollary 3.7 is immediately applicable to them. Our final result of this section allows us to construct extreme copositive forms in n variables from those in n' variables, for $2 < n' < n$.

THEOREM 3.8. *If Q_n is an extreme copositive quadratic form in $n \geqq 3$ variables $x_1, \cdots, x_n$ then replacing any 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 $n \geqq 3$ and Q_n is extreme, see Lemma 2, Diananda). 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

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

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

$$Q' = a\Big(Q_n + x_{n+1}^2 + 2\sum_{i=1}^{n-1} q_{in}x_i x_{n+1}\Big) + kx_n x_{n+1}$$
$$Q'' = (1 - a)\Big(Q_n + x_{n+1}^2 + 2\sum_{i=1}^{n-1} q_{in}x_i x_{n+1}\Big) + tx_n x_{n+1}$$

with $k + t = 2$. Thus

$$Q' = aQ_{n+1} + (k - 2a)x_n x_{n+1} ,$$
$$Q'' = (1 - a)Q_{n+1} + (t + 2a - 2)x_n x_{n+1}$$

Since Q_n is extreme it has a zero u in $S(n)$ with $u_n > 0$ (Corollary 3.6), thus $(u_1, \cdots, u_{n-1}, u_n/2, u_n/2)$ is a zero of Q_{n+1} in $S(n + 1)$ with $x_n x_{n+1} > 0$. At this zero $4Q' = (k - 2a)u_n^2$ and $4Q'' = (t + 2a - 2)u_n^2$, thus the copositivity of Q', Q'' insures that $(k - 2a) \geqq 0$ and $(t + 2a - 2) \geqq 0$ 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.

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References

1. L. D. Baumert, *Extreme copositive quadratic forms*, Dissertation, California Institute of Technology, 1965.
2. 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.
3. M. Hall, Jr. and M. Newman, *Copositive and completely positive quadratic forms*, Proc. Cambridge Philos. Soc. **59** (1963), 329-339.
4. T. S. Motzkin, *Copositive quadratic forms*, National Bureau of Standards Report **1818** (1952), 11-12.
5. ———, *Quadratic forms positive for non-negative variables not all zero*, Notices of Amer. Math. Soc. **12** (1965), 224.

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