Case 34

Roland Hildebrand

April 7, 2016

Parametrization. We first find a parametrization of the reduced exceptional copositive matrices A with the minimal zero pattern in question. After a permutation of the indices the supports of the minimal zeros of A are given by

$$\{1,2,3\},\{2,3,4\},\{3,4,5\},\{4,5,6\},\{5,6,1\},\{6,1,2\}. \tag{1}$$

Hence A has the form

$$\begin{pmatrix} 1 & -\cos\varphi_1 & \cos(\varphi_1+\varphi_2) & a & \cos(\varphi_5+\varphi_6) & -\cos\varphi_6 \\ -\cos\varphi_1 & 1 & -\cos\varphi_2 & \cos(\varphi_2+\varphi_3) & b & \cos(\varphi_1+\varphi_6) \\ \cos(\varphi_1+\varphi_2) & -\cos\varphi_2 & 1 & -\cos\varphi_3 & \cos(\varphi_3+\varphi_4) & c \\ a & \cos(\varphi_2+\varphi_3) & -\cos\varphi_3 & 1 & -\cos\varphi_4 & \cos(\varphi_4+\varphi_5) \\ \cos(\varphi_5+\varphi_6) & b & \cos(\varphi_3+\varphi_4) & -\cos\varphi_4 & 1 & -\cos\varphi_5 \\ -\cos\varphi_6 & \cos(\varphi_1+\varphi_6) & c & \cos(\varphi_4+\varphi_5) & -\cos\varphi_5 & 1 \end{pmatrix}, \tag{2}$$

and the minimal zeros are the columns of the matrix

$$\begin{pmatrix} \sin\varphi_2 & 0 & 0 & 0 & \sin\varphi_5 & \sin(\varphi_1+\varphi_6) \\ \sin(\varphi_1+\varphi_2) & \sin\varphi_3 & 0 & 0 & 0 & \sin\varphi_6 \\ \sin\varphi_1 & \sin(\varphi_2+\varphi_3) & \sin\varphi_4 & 0 & 0 & 0 \\ 0 & \sin\varphi_2 & \sin(\varphi_3+\varphi_4) & \sin\varphi_5 & 0 & 0 \\ 0 & 0 & \sin\varphi_3 & \sin(\varphi_4+\varphi_5) & \sin\varphi_6 & 0 \\ 0 & 0 & 0 & \sin\varphi_4 & \sin(\varphi_5+\varphi_6) & \sin\varphi_1 \end{pmatrix}. \tag{3}$$

Denote these columns by $u^1,\dots,u^6$. Here $\varphi_1,\dots,\varphi_6 > 0$, $\varphi_j+\varphi_{j+1} < \pi$, $j = 1,\dots,5$, and $\varphi_1+\varphi_6 < \pi$. Copositivity of the submatrix A_{246} and the absence of a minimal zero with support in $\{2,4,6\}$ lead to the condition $(\pi-\varphi_1-\varphi_2)+(\pi-\varphi_3-\varphi_4)+(\pi-\varphi_5-\varphi_6) > \pi$. It follows that $\sum_{j=1}^6 \varphi_j \in (0,2\pi)$.

The determinant of the matrix $(u^1,\dots,u^6)$ equals $2(1-\cos(\varphi_1+\dots+\varphi_6))\prod_{i=1}^6 \sin\varphi_i > 0$, hence A is reduced with respect to $\mathcal{S}_+^6$.

Consider the entry $A_{14} = a$ of A. There is no minimal zero u of A such that u_1, u_4 are both nonzero. Since A is reduced with respect to E_{14}, we have $(Au^j)_4 = 0$ for some $j \in \{1,5,6\}$, or $(Au^j)_1 = 0$ for some $j \in \{2,3,4\}$. In general, these numbers have to be nonnegative. We have

$$\begin{aligned}
(Au^3)_1 &= a\sin(\varphi_3+\varphi_4) + \cos(\varphi_1+\varphi_2)\sin\varphi_4 + \cos(\varphi_5+\varphi_6)\sin\varphi_3, \\
(Au^2)_1 &= a\sin\varphi_2 - \cos\varphi_1\sin\varphi_3 + \cos(\varphi_1+\varphi_2)\sin(\varphi_2+\varphi_3) = \sin\varphi_2(a+\cos(\varphi_1+\varphi_2+\varphi_3)), \\
(Au^4)_1 &= a\sin\varphi_5 + \cos(\varphi_5+\varphi_6)\sin(\varphi_4+\varphi_5) - \cos\varphi_6\sin\varphi_4 = \sin\varphi_5(a+\cos(\varphi_4+\varphi_5+\varphi_6)).
\end{aligned}$$

Note that $\sin\varphi_2, \varphi_5, \sin(\varphi_3+\varphi_4)$ are all positive.

Suppose for the sake of contradiction that $(Au^3)_1 = 0$. Then we get $a = -\frac{\cos(\varphi_1+\varphi_2)\sin\varphi_4+\cos(\varphi_5+\varphi_6)\sin\varphi_3}{\sin(\varphi_3+\varphi_4)}$, and upon insertion into the other two expressions and division by the positive factor

$$\begin{aligned}
\cos(\varphi_1+\varphi_2+\varphi_3) - \frac{\cos(\varphi_1+\varphi_2)\sin\varphi_4+\cos(\varphi_5+\varphi_6)\sin\varphi_3}{\sin(\varphi_3+\varphi_4)} &= \frac{\sin\varphi_3(\cos(\varphi_1+\varphi_2+\varphi_3+\varphi_4)-\cos(\varphi_5+\varphi_6))}{\sin(\varphi_3+\varphi_4)} \geq 0, \\
\cos(\varphi_4+\varphi_5+\varphi_6) - \frac{\cos(\varphi_1+\varphi_2)\sin\varphi_4+\cos(\varphi_5+\varphi_6)\sin\varphi_3}{\sin(\varphi_3+\varphi_4)} &= \frac{\sin\varphi_4(\cos(\varphi_3+\varphi_4+\varphi_5+\varphi_6)-\cos(\varphi_1+\varphi_2))}{\sin(\varphi_3+\varphi_4)} \geq 0.
\end{aligned}$$

We then get $\cos(\varphi_1+\varphi_2+\varphi_3+\varphi_4) \geq \cos(\varphi_5+\varphi_6)$, $\cos(\varphi_3+\varphi_4+\varphi_5+\varphi_6) \geq \cos(\varphi_1+\varphi_2)$, which by virtue of $\sum_{j=1}^6 \varphi_j < 2\pi$ yields $\varphi_1+\varphi_2+\varphi_3+\varphi_4 \leq \varphi_5+\varphi_6$, $\varphi_3+\varphi_4+\varphi_5+\varphi_6 \leq \varphi_1+\varphi_2$. Adding these two inequalities leads to $\varphi_3+\varphi_4 \leq 0$, a contradiction.

Therefore $(Au^3)_1 > 0$, and in a similar manner $(Au^6)_4 > 0$. Hence $\min\{(Au^1)_4,(Au^5)_4,(Au^2)_1,(Au^4)_1\} = 0$, which is equivalent to $a = -\min\{\cos(\varphi_1+\varphi_2+\varphi_3),\cos(\varphi_4+\varphi_5+\varphi_6)\}$. In a similar manner,

$b = -\min\{\cos(\varphi_2+\varphi_3+\varphi_4), \cos(\varphi_1+\varphi_5+\varphi_6)\}$, $c = -\min\{\cos(\varphi_3+\varphi_4+\varphi_5), \cos(\varphi_1+\varphi_2+\varphi_6)\}$. Note that if in any of these minima the two numbers are equal, then also the arguments of the cosinus function are equal, otherwise the condition $\sum_{j=1}^6 \varphi_j < 2\pi$ is violated.

Copositivity. We consider matrices A given by (2), with angles φ_j and elements a, b, c satisfying the conditions

$$\varphi_j > 0,\ j = 1,\dots,6; \quad \varphi_j + \varphi_{j+1} < \pi,\ j = 1,\dots,5; \quad \varphi_1 + \varphi_6 < \pi; \quad \sum_{j=1}^{6} \varphi_j < 2\pi, \tag{4}$$

$$\begin{aligned} a &= -\min\{\cos(\varphi_1+\varphi_2+\varphi_3), \cos(\varphi_4+\varphi_5+\varphi_6)\}, \\ b &= -\min\{\cos(\varphi_2+\varphi_3+\varphi_4), \cos(\varphi_1+\varphi_5+\varphi_6)\}, \\ c &= -\min\{\cos(\varphi_3+\varphi_4+\varphi_5), \cos(\varphi_1+\varphi_2+\varphi_6)\}. \end{aligned} \tag{5}$$

Let us prove copositivity of A. Consider the principal submatrix $A_{\{1,2,3,4,5\}}$. If $\cos(\varphi_5+\varphi_6) \geq \cos(\varphi_1+\varphi_2+\varphi_3+\varphi_4)$, then this submatrix is in $\mathcal{S}_+^5 + \mathcal{N}^5$.

Assume the contrary, yielding $\varphi_1+\varphi_2+\varphi_3+\varphi_4 < \varphi_5+\varphi_6$. Then $\varphi_1+\varphi_2+\varphi_3 < \varphi_4+\varphi_5+\varphi_6$, and hence $\cos(\varphi_1+\varphi_2+\varphi_3) > \cos(\varphi_4+\varphi_5+\varphi_6)$. It follows that $a = -\cos(\varphi_4+\varphi_5+\varphi_6)$. In a similar way, $b = -\cos(\varphi_1+\varphi_5+\varphi_6)$. Set $\varphi' = \pi-\varphi_5-\varphi_6 \in (0,\pi)$. We have $\varphi_1+\varphi_2+\varphi_3+\varphi_4+\varphi' < \varphi_5+\varphi_6+\varphi' = \pi$. Therefore the T-matrix with arguments $\varphi = (\varphi_1,\varphi_2,\varphi_3,\varphi_4,\varphi')$ is exceptional extremal. We have that

$$A_{\{1,2,3,4,5\}} - T(\varphi) = \begin{pmatrix} 0 & 0 & 0 & -\cos(\varphi_4+\varphi_5+\varphi_6)-\cos(\varphi_4+\varphi') & \cos(\varphi_5+\varphi_6)+\cos\varphi' \\ 0 & 0 & 0 & 0 & -\cos(\varphi_1+\varphi_5+\varphi_6)-\cos(\varphi_1+\varphi') \\ 0 & 0 & 0 & 0 & 0 \\ * & 0 & 0 & 0 & 0 \\ * & * & 0 & 0 & 0 \end{pmatrix}$$
$$= 2\begin{pmatrix} 0 & 0 & 0 & \sin\varphi_4\sin\varphi' & 0 \\ 0 & 0 & 0 & 0 & \sin\varphi_1\sin\varphi' \\ 0 & 0 & 0 & 0 & 0 \\ \sin\varphi_4\sin\varphi' & 0 & 0 & 0 & 0 \\ 0 & \sin\varphi_1\sin\varphi' & 0 & 0 & 0 \end{pmatrix}$$

is nonnegative, and hence $A_{\{1,2,3,4,5\}} \in \mathcal{C}^5$.

In a similar way the other 5×5 principal submatrices of A are copositive. Hence the quadratic form A is nonnegative on the boundary of the positive orthant. Let $\Delta = \{x \in \mathbb{R}_+^6 \mid \mathbf{1}^T x = 0\}$ be the standard simplex. If A is not copositive, then it must have a strict minimum in the interior of Δ and hence be strictly convex on Δ. Let l be the line segment between the multiples of the zeros u^1 and u^2 lying in Δ. Then l lies on the boundary of Δ, and A is zero at the endpoints of l and strictly convex on l. Therefore A attains negative values on the boundary of Δ, a contradiction. This proves that $A \in \mathcal{C}^6$.

Extremality. We now investigate the extremality of A. Let $X \in \mathcal{S}^6$ be a matrix such that $(Xu^j)_{\operatorname{supp} u^j} = 0$ for all $j = 1,\dots,6$. Then there exists a matrix $B \in \mathcal{S}^2$ such that

$$X_{\{1,2,3\}} = \begin{pmatrix} 1 & 0 \\ -\cos\varphi_1 & \sin\varphi_1 \\ \cos(\varphi_1+\varphi_2) & -\sin(\varphi_1+\varphi_2) \end{pmatrix} B \begin{pmatrix} 1 & 0 \\ -\cos\varphi_1 & \sin\varphi_1 \\ \cos(\varphi_1+\varphi_2) & -\sin(\varphi_1+\varphi_2) \end{pmatrix}^T,$$

because $(Xu^1)_{\operatorname{supp} u^1} = 0$. The relation $(Xu^2)_{\operatorname{supp} u^2} = 0$ then implies that

$$X_{\{2,3,4\}} = \begin{pmatrix} -\cos\varphi_1 & \sin\varphi_1 \\ \cos(\varphi_1+\varphi_2) & -\sin(\varphi_1+\varphi_2) \\ -\cos(\varphi_1+\varphi_2+\varphi_3) & \sin(\varphi_1+\varphi_2+\varphi_3) \end{pmatrix} B \begin{pmatrix} -\cos\varphi_1 & \sin\varphi_1 \\ \cos(\varphi_1+\varphi_2) & -\sin(\varphi_1+\varphi_2) \\ -\cos(\varphi_1+\varphi_2+\varphi_3) & \sin(\varphi_1+\varphi_2+\varphi_3) \end{pmatrix}^T.$$

Continuing in this manner, we express all elements of X except X_{14}, X_{25}, X_{36} in dependence of B. However, after six steps we obtain again

$$X_{\{1,2,3\}} = \begin{pmatrix} 1 & 0 \\ -\cos\varphi_1 & \sin\varphi_1 \\ \cos(\varphi_1+\varphi_2) & -\sin(\varphi_1+\varphi_2) \end{pmatrix} UBU^T \begin{pmatrix} 1 & 0 \\ -\cos\varphi_1 & \sin\varphi_1 \\ \cos(\varphi_1+\varphi_2) & -\sin(\varphi_1+\varphi_2) \end{pmatrix}^T,$$

where U is a rotation by $-\sum_{j=1}^6 \varphi_j$. Therefore $B = UBU^T$, which yields $B = const \cdot I_2$ if $\sum_{j=1}^6 \varphi_j \neq \pi$. If $\sum_{j=1}^6 \varphi_j = \pi$, then B is unrestricted.

The linear system determining the extremality of A consists also of relations other than $(Xu^j)_{\operatorname{supp} u^j} = 0$. If a minimum in (5) is attained only by one of the two corresponding terms, then the corresponding relation determines the corresponding element X_{14}, X_{25}, or X_{36}, but does not give a relation on B. If a minimum is attained at both terms, then a relation on B arises. In any case, the elements X_{14}, X_{25}, X_{36} are determined as linear functions of B.

Thus the linear system determining the extremality has a 1-dimensional solution space if $\sum_{j=1}^6 \varphi_j \neq \pi$. Let us hence assume that $\sum_{j=1}^6 \varphi_j = \pi$.

Let, e.g., $\varphi_1 + \varphi_2 + \varphi_3 = \varphi_4 + \varphi_5 + \varphi_6$. Then the linear system determining the extremality of A contains the relations $(Xu^1)_4 = (Xu^4)_1 = 0$. Eliminating the variable X_{14}, we obtain

$$\sin(\varphi_1+\varphi_2)\sin\varphi_5 X_{24} + \sin\varphi_1 \sin\varphi_5 X_{34} = \sin\varphi_2 \sin(\varphi_4+\varphi_5) X_{15} + \sin\varphi_2 \sin\varphi_4 X_{16}.$$

Expressing the occurring elements of X in dependence of B, we get $-2\sin\varphi_2 \sin\varphi_5 B_{12} = 0$.

The condition $\varphi_2 + \varphi_3 + \varphi_4 = \varphi_5 + \varphi_6 + \varphi_1$ leads in a similar way to $\sin\varphi_3 \sin\varphi_6(\sin(2\varphi_1)(B_{22} - B_{11}) - 2\cos(2\varphi_1)B_{12}) = 0$, and the condition $\varphi_3 + \varphi_4 + \varphi_5 = \varphi_6 + \varphi_1 + \varphi_2$ to $\sin\varphi_1 \sin\varphi_4(\sin(2\varphi_1 + 2\varphi_2)(B_{22} - B_{11}) - 2\cos(2\varphi_1 + 2\varphi_2)B_{12}) = 0$.

The three supplementary conditions are pairwise linearly independent, but linearly dependent as an ensemble. Thus if $\sum_{j=1}^6 \varphi_j = \pi$, then the system has a 3-dimensional solution space if the minimum in (5) is attained only at one term everywhere, a 2-dimensional solution space if the minimum is attained by both terms in one instance, and 1-dimensional if the minimum is attained at least in two equations by both terms.

Thus if none or only one of the minima in (5) is attained by both terms, then the matrix A is not extremal. If, however, two or three minima are attained by both terms, then A is extremal.

Absence of other minimal zeros. Let A be given by (2) under the conditions (4),(5). Then the columns of (3) are minimal zeros of A. If there were other minimal zeros and A were an exceptional extremal matrix, then the minimal zero pattern of A would be a strict superset of the set in (1) and isomorphic to one of the 44 sets in the table. There is only one set in the table having this property, namely that in Case 44. Then there must be two additional minimal zeros of A, with supports $\{1,3,5\}$ and $\{2,4,6\}$, respectively. But this is only possible when $\sum_{j=1}^6 \varphi_j = 2\pi$, as shown above. Hence A has no additional minimal zeros.

Result

A matrix $A \in \mathcal{C}^6$ with all ones on the diagonal is exceptional extremal with minimal zero pattern (1) if and only if A is given by (2), where the angles φ_j and the elements a, b, c obey (4),(5), and where either $\sum_{j=1}^6 \varphi_j \neq \pi$, or at least four of the sums $\sum_{j \in I_k} \varphi_j$ equal $\frac{\pi}{2}$, where $I_k \subset \{1, 2, \ldots, 6\}$ is the support of column k of (3). The minimal zeros of A are then given by the columns of (3).