Case 8

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Basic structure

The minimal zero supports are given by $\{1,2\},\{1,3\},\{2,4,5\},\{2,4,6\},\{3,4,5\},\{3,5,6\}$. There is a symmetry $(123456)\mapsto(132546)$. We may write a copositive matrix with this minimal zero support set as

$$A=\begin{pmatrix} 1 & -1 & -1 & b_1 & b_2 & b_3 \\ -1 & 1 & 1 & -\cos\phi_2 & \cos(\phi_2+\phi_3) & \cos(\phi_2+\phi_4) \\ -1 & 1 & 1 & \cos(\phi_1+\phi_3) & -\cos\phi_1 & -\cos\phi_5 \\ b_1 & -\cos\phi_2 & \cos(\phi_1+\phi_3) & 1 & -\cos\phi_3 & -\cos\phi_4 \\ b_2 & \cos(\phi_2+\phi_3) & -\cos\phi_1 & -\cos\phi_3 & 1 & \cos(\phi_1+\phi_5) \\ b_3 & \cos(\phi_2+\phi_4) & -\cos\phi_5 & -\cos\phi_4 & \cos(\phi_1+\phi_5) & 1 \end{pmatrix},$$

where $\phi_j\in(0,\pi)$, $j=1,\dots,5$; $\phi_i+\phi_j<\pi$, for the terms $\cos(\phi_i+\phi_j)$ appearing in the matrix. The symmetry leads to the transformation $(\phi_1,\phi_2,\phi_3,\phi_4,\phi_5)\mapsto(\phi_2,\phi_1,\phi_3,\pi-\phi_1-\phi_5,\pi-\phi_2-\phi_4)$. Hence $\phi_2+\phi_4+\phi_5\mapsto 2\pi-\phi_5-\phi_2-\phi_4$, and the cases $\phi_2+\phi_4+\phi_5\le\pi$, $\phi_2+\phi_4+\phi_5\ge\pi$ are exchanged. We then need to consider only $\phi_2+\phi_4+\phi_5\le\pi$.

The minimal zeros of A are given by

$$(u_1,u_2,u_3,u_4,u_5,u_6)=\begin{pmatrix}1\\1\\0\\0\\0\\0\end{pmatrix}\begin{pmatrix}1\\0\\1\\0\\0\\0\end{pmatrix}\begin{pmatrix}0\\ \sin\phi_3\\0\\ \sin(\phi_2+\phi_3)\\ \sin\phi_2\\0\end{pmatrix}\begin{pmatrix}0\\0\\ \sin\phi_3\\ \sin\phi_1\\ \sin(\phi_1+\phi_3)\\0\end{pmatrix}\begin{pmatrix}0\\ \sin\phi_4\\0\\ \sin(\phi_2+\phi_4)\\0\\ \sin\phi_2\end{pmatrix}\begin{pmatrix}0\\0\\ \sin(\phi_1+\phi_5)\\0\\ \sin\phi_5\\ \sin\phi_1\end{pmatrix}$$

First order conditions

The conditions $(Au_i)_j\ge 0$ amount to

1. $$Au_1=\begin{pmatrix}0\\0\\0\\ b_1-\cos\phi_2\\ b_2+\cos(\phi_2+\phi_3)\\ b_3+\cos(\phi_2+\phi_4)\end{pmatrix}\Rightarrow\begin{cases} b_1\ge\cos\phi_2\\ b_2\ge-\cos(\phi_2+\phi_3)\\ b_3\ge-\cos(\phi_2+\phi_4)\end{cases}$$

2. $$Au_2=\begin{pmatrix}0\\0\\0\\ b_1+\cos(\phi_1+\phi_3)\\ b_2-\cos\phi_1\\ b_3-\cos\phi_5\end{pmatrix}\Rightarrow\begin{cases} b_1\ge-\cos(\phi_1+\phi_3)\\ b_2\ge\cos\phi_1\\ b_3\ge\cos\phi_5\end{cases}$$

3. $$Au_3=\begin{pmatrix} b_2\sin\phi_2-\sin\phi_3+b_1\sin(\phi_2+\phi_3)\\ 0\\ \sin\phi_3+\sin\phi_3\cos(\phi_1+\phi_2+\phi_3)\\ 0\\ 0\\ \sin\phi_2(\cos(\phi_1+\phi_5)-\cos(\phi_3-\phi_4))\end{pmatrix}\Rightarrow\begin{cases} b_2\sin\phi_2-\sin\phi_3+b_1\sin(\phi_2+\phi_3)\ge 0\\ 1\ge-\cos(\phi_1+\phi_2+\phi_3)\\ \cos(\phi_1+\phi_5)-\cos(\phi_3-\phi_4)\ge 0\end{cases}$$

4. $Au_4 = \begin{pmatrix} b_1 \sin\phi_1 - \sin\phi_3 + b_2 \sin(\phi_1+\phi_3) \\ \sin\phi_3 + \sin\phi_3 \cos(\phi_1+\phi_2+\phi_3) \\ 0 \\ 0 \\ 0 \\ \sin\phi_1(\cos(\phi_1+\phi_3+\phi_5) - \cos\phi_4) \end{pmatrix} \Rightarrow \begin{cases} b_1 \sin\phi_1 - \sin\phi_3 + b_2 \sin(\phi_1+\phi_3) \geq 0 \\ 1 \geq -\cos(\phi_1+\phi_2+\phi_3) \\ \cos(\phi_1+\phi_3+\phi_5) - \cos\phi_4 \geq 0 \end{cases}$

5. $Au_5 = \begin{pmatrix} b_3 \sin\phi_2 - \sin\phi_4 + b_1 \sin(\phi_2+\phi_4) \\ 0 \\ \sin\phi_4 + \sin(\phi_2+\phi_4)\cos(\phi_1+\phi_3) - \sin\phi_2 \cos\phi_5 \\ 0 \\ \sin\phi_2(\cos(\phi_1+\phi_5) - \cos(\phi_3-\phi_4)) \\ 0 \end{pmatrix} \Rightarrow \begin{cases} b_3 \sin\phi_2 - \sin\phi_4 + b_1 \sin(\phi_2+\phi_4) \geq 0 \\ \sin\phi_4(1+\cos(\phi_2+\phi_4)) + \sin(\phi_2+\phi_4)(\cos(\phi_1+\phi_3) - \mathrm{c} \\ \cos(\phi_1+\phi_5) - \cos(\phi_3-\phi_4) \geq 0 \end{cases}$

6. $Au_6 = \begin{pmatrix} b_3 \sin\phi_1 + b_2 \sin\phi_5 - \sin(\phi_1+\phi_5) \\ \sin(\phi_1+\phi_5) + \sin\phi_1 \cos(\phi_2+\phi_4) + \sin\phi_5 \cos(\phi_2+\phi_3) \\ 0 \\ \sin\phi_1(\cos(\phi_1+\phi_3+\phi_5) - \cos\phi_4) \\ 0 \\ 0 \end{pmatrix} \Rightarrow \begin{cases} b_3 \sin\phi_1 + b_2 \sin\phi_5 - \sin(\phi_1+\phi_5) \geq 0 \\ \sin\phi_1(\cos\phi_5 + \cos(\phi_2+\phi_4)) + \sin\phi_5(\cos\phi_1 + \mathrm{co} \\ \cos(\phi_1+\phi_3+\phi_5) - \cos\phi_4 \geq 0 \end{cases}$

The conditions $(Au_3)_6 \geq 0$ and $(Au_4)_6 \geq 0$ combined lead to the inequality $\phi_1+\phi_3+\phi_5 \leq \phi_4$. It follows that $\phi_1+\phi_2+\phi_3+\phi_5 \leq \phi_2+\phi_4 < \pi$. In particular, $\phi_1+\phi_2+\phi_3 < \pi$ and $\cos\phi_2 > -\cos(\phi_1+\phi_3)$, $\cos\phi_1 > -\cos(\phi_2+\phi_3)$. Our assumption $\phi_2+\phi_4+\phi_5 \leq \pi$ leads also to $\cos\phi_5 \geq -\cos(\phi_2+\phi_4)$.

If we insert the values $b_1 = \cos\phi_2$, $b_2 = \cos\phi_1$, $b_3 = \cos\phi_5$ into the inequalities involving the variables b_i, then they are all fulfilled automatically. Hence b_i are equal to these values by the irreducibility condition with respect to $\mathcal{N}^6$.

Parametrization

We arrive at the parametrization

$$A = \begin{pmatrix} 1 & -1 & -1 & \cos(\phi_2) & \cos(\phi_1) & \cos\phi_5 \\ -1 & 1 & 1 & -\cos(\phi_2) & \cos(\phi_2+\phi_3) & \cos(\phi_2+\phi_4) \\ -1 & 1 & 1 & \cos(\phi_1+\phi_3) & -\cos(\phi_1) & -\cos(\phi_5) \\ \cos(\phi_2) & -\cos(\phi_2) & \cos(\phi_1+\phi_3) & 1 & -\cos(\phi_3) & -\cos(\phi_4) \\ \cos(\phi_1) & \cos(\phi_2+\phi_3) & -\cos(\phi_1) & -\cos(\phi_3) & 1 & \cos(\phi_1+\phi_5) \\ \cos\phi_5 & \cos(\phi_2+\phi_4) & -\cos(\phi_5) & -\cos(\phi_4) & \cos(\phi_1+\phi_5) & 1 \end{pmatrix} \quad (1)$$

with $\phi_i \in (0,\pi)$, $\phi_2+\phi_4+\phi_5 \leq \pi$, $\phi_1+\phi_3+\phi_5 \leq \phi_4$.

Copositivity / Absence of other minimal zeros

Copositivity of A will be checked by the criterion in Theorem 4.6 of [1]. For each index set $I \subset \{1,\dots,6\}$, of cardinality not smaller than 3 and not containing a known minimal zero support, we have to find a vector $u \in \mathbb{R}^6$ with at least one positive element such that $\mathrm{supp}(u) \subset I \subset \mathrm{supp}_{\geq 0}(Au)$ or show that the submatrix A_I is copositive. For index sets of cardinality three this reduces to checking an inequality on the corresponding angles. We have to consider the index sets $(2,3,4), (2,3,5), (1,4,5), (2,3,6), (1,4,6), (3,4,6), (1,5,6), (2,5,6), (4,5,6), (1,4,5,6)$. All inequalities for triple sets fulfilled strictly:

1. $I = (2,3,4) : \phi_2 + \pi - \phi_1 - \phi_3 \geq 0, \pi - \phi_1 - \phi_3 \geq 0 \Rightarrow \phi_2 + \pi - \phi_1 - \phi_3 > 0$
2. $I = (2,3,5) : \pi - \phi_2 - \phi_3 + \phi_1 \geq 0, \pi - \phi_2 - \phi_3 \geq 0 \Rightarrow \pi - \phi_2 - \phi_3 + \phi_1 > 0$
3. $I = (1,4,5) : \pi - \phi_1 - \phi_2 + \phi_4 \geq 0, \phi_4 > \phi_1 \Rightarrow \pi - \phi_1 - \phi_2 + \phi_4 > 0$

4. $I=(2,3,6): \pi-\phi_2-\phi_4+\phi_5\geq 0, \pi-\phi_2-\phi_4\geq 0 => \pi-\phi_2-\phi_4+\phi_5>0$
5. $I=(1,4,6),(1,5,6)\subset(1,4,5,6)$ Inequalities fulfilled strictly
6. $I=(3,4,6): -\phi_1-\phi_3+\phi_5+\phi_4\geq 0, \phi_4>-\phi_1-\phi_3 => -\phi_1-\phi_3+\phi_5+\phi_4>0$
7. $I=(2,5,6): \pi-\phi_2-\phi_3+\pi-\phi_2-\phi_4-\phi_1-\phi_5\geq 0, \pi-\phi_2-\phi_4+\pi-\phi_2-\phi_4>0 => \pi-\phi_2-\phi_3+\pi-\phi_2-\phi_4-\phi_1-\phi_5>0$
8. $I=(4,5,6): \phi_3+\phi_4-\phi_1-\phi_5\geq 0, \phi_4>-\phi_1-\phi_5 => \phi_3+\phi_4-\phi_1-\phi_5>0$

$I=(1,4,5,6): u=e_4+e_5$
$\cos(\phi_2)+\cos(\phi_1)\geq 0 => \phi_2+\phi_1\leq\pi, \phi_1\leq\phi_4, \phi_2+\phi_4<\pi$
$\cos(\phi_1+\phi_5)-\cos(\phi_4)\geq 0 => \phi_1+\phi_5\leq\phi_4$ This proves copositivity.

All angle inequalities are satisfied strictly and the vector u in the last case is not positive. Hence there are no additional minimal zeros.

Extremality

We use the extremality criterion Theorem 17 point 5 in [2]. The matrix A is extremal whenever every matrix B satisfying $(Bu_i)_j=0$ whenever $(Au_i)_j=0$ is proportional to A. Let us consider the elements $(Au_i)_j$.

The following elements are always zero:

$$(Au_1)_{1,2,3,4},\ (Au_2)_{1,2,3,5,6},\ (Au_3)_{2,4,5},\ (Au_4)_{3,4,5},\ (Au_5)_{2,4,6},\ (Au_6)_{1,3,5,6}. \tag{2}$$

The following elements may become zero: If $\phi_2+\phi_4+\phi_5=\pi$, then

$$(Au_1)_6=(Au_5)_1=0.$$

If $\phi_1+\phi_3+\phi_5=\phi_4$, then

$$(Au_3)_6=(Au_4)_6=(Au_5)_5=(Au_6)_4=0.$$

The following elements are always positive:

$$(Au_1)_5,(Au_2)_4,(Au_3)_{1,3},(Au_4)_{1,2},(Au_5)_3,(Au_6)_2.$$

We now use relations (2), which translate to corresponding relations on B. Consider the face of A. For every B in this face there exist matrices $P,Q\in\mathcal{S}_+^2$ such that $X=FPF^T$, $Y=GQG^T$ with

$$X=\begin{pmatrix} b_{22} & * & b_{24} & b_{25} & b_{26}\\ * & b_{33} & b_{34} & b_{35} & *\\ b_{42} & b_{43} & b_{44} & b_{45} & b_{46}\\ b_{52} & b_{53} & b_{54} & b_{55} & *\\ b_{62} & * & b_{64} & * & b_{66}\end{pmatrix}, F=\begin{pmatrix} f_2\\ f_3\\ f_4\\ f_5\\ f_6\end{pmatrix}, \begin{cases} u_{32}f_2+u_{34}f_4+u_{35}f_5=0\\ u_{52}f_2+u_{54}f_4+u_{56}f_6=0\\ u_{43}f_3+u_{44}f_4+u_{45}f_5=0\end{cases}, F=\begin{pmatrix} \sin(\phi_2+\phi_3) & 0\\ \sin\phi_1 & -\sin(\phi_1+\phi_2+\phi_3)\\ -\sin\phi_3 & -\sin\phi_2\\ 0 & \sin(\phi_2+\phi_3)\\ \sin(\phi_3-\phi_4) & \sin(\phi_2+\phi_4)\end{pmatrix}$$

$$Y=\begin{pmatrix} b_{11} & b_{12} & b_{13} & b_{15} & b_{16}\\ b_{21} & b_{22} & b_{23} & * & *\\ b_{31} & b_{23} & b_{33} & b_{35} & b_{36}\\ b_{15} & * & b_{53} & b_{55} & b_{56}\\ b_{16} & * & b_{63} & b_{65} & b_{66}\end{pmatrix}, G=\begin{pmatrix} g_1\\ g_2\\ g_3\\ g_5\\ g_6\end{pmatrix}, \begin{cases} u_{63}g_3+u_{65}g_5+u_{66}g_6=0\\ g_1=-g_3\\ g_2=-g_1\end{cases}, G=\begin{pmatrix} -\sin\phi_1 & 0\\ \sin\phi_1 & 0\\ \sin\phi_1 & 0\\ 0 & \sin\phi_1\\ -\sin(\phi_1+\phi_5) & -\sin\phi_5\end{pmatrix}.$$

Here we used all of (2) except $(Bu_1)_4=0$, which determines $b_{14}=-b_{24}$ by an element of X.

Hence equations (2) describe all elements of B by elements of X,Y, or equivalently, P,Q. Elements of B which appear in both X,Y yield linear relations on the elements of P,Q. $\begin{cases} x_{22}=y_{22}\\ x_{33}=y_{33}\\ x_{53}=y_{53}\\ x_{55}=y_{55}\\ x_{66}=y_{66}\end{cases}$ yields the system

$$\begin{pmatrix} \sin^2(\phi_2+\phi_3) & 0 & 0 & \sin^2\phi_1 & 0 & 0 \\ \sin^2\phi_1 & -2\sin\phi_1\sin(\phi_1+\phi_2+\phi_3) & \sin^2(\phi_1+\phi_2+\phi_3) & \sin^2\phi_1 & 0 & 0 \\ 0 & \sin\phi_1\sin(\phi_2+\phi_3) & -\sin(\phi_1+\phi_2+\phi_3)\sin(\phi_2+\phi_3) & 0 & \sin^2\phi_1 & 0 \\ 0 & 0 & \sin^2(\phi_2+\phi_3) & 0 & 0 & \sin^2\phi_1 \\ \sin^2(\phi_3-\phi_4) & 2\sin(\phi_3-\phi_4)\sin(\phi_2+\phi_4) & \sin^2(\phi_2+\phi_4) & \sin^2(\phi_1+\phi_5) & 2\sin(\phi_1+\phi_5)\sin\phi_5 & \sin^2\phi_5 \end{pmatrix}$$

Let us assume that the solution B is such that $B_{55}=0$, which can always be achieved by adding a multiple of the solution A. Then $p_{22}=q_{22}=0$. Eliminating the corresponding columns and the zero row from the coefficient matrix, we arrive at a 4×4 matrix whose determinant is proportional to

$$(\sin^2\phi_1-\sin^2(\phi_2+\phi_3))(\sin(\phi_3-\phi_4)\sin(\phi_2+\phi_4)\sin\phi_1-\sin(\phi_1+\phi_5)\sin\phi_5\sin(\phi_2+\phi_3))+\sin(\phi_1+\phi_2+\phi_3)(\sin^2\phi_1\sin^2(\phi_3-\phi_4)-\sin^2$$

This is further proportional to

$$(\sin(\phi_2+\phi_3)\cos(\phi_2+\phi_3)+\sin\phi_1\cos\phi_1)(\cos^2(\phi_1+\phi_5)-\sin^2(\phi_1+\phi_5)+\sin^2(\phi_3-\phi_4)-\cos^2(\phi_3-\phi_4))+2(\sin^2\phi_1-\sin^2(\phi_2+\phi_3))(\sin(\phi$$

and $(\sin 2(\phi_2+\phi_3)+\sin 2\phi_1)(\cos 2(\phi_1+\phi_5)-\cos 2(\phi_3-\phi_4))+(\cos 2(\phi_2+\phi_3)-\cos 2\phi_1)(\sin 2(\phi_1+\phi_5)+\sin 2(\phi_3-\phi_4))=\sin\xi_1+\sin\xi_2+\sin\xi_3+\sin\xi_4$, where

$$\xi_1=2(-\phi_1-\phi_3+\phi_4),\ \xi_2=-2\phi_5,\ \xi_3=-2(\phi_2+\phi_4),\ \xi_4=2(\phi_1+\phi_2+\phi_3+\phi_5).$$

The angles ξ are linked by the relation $\sum_i \xi_i=0$ and the quadruple $(\xi_1,\dots,\xi_4)$ is located in the simplex with vertices

$$\pi(0,0,0,0),\ \pi(0,0,-2,2),\ \pi(1,-1,-1,1),\ \pi(2,0,-2,0).$$

But $\sin(\varphi+\delta)-\sin\varphi\geq\sin\psi-\sin(\psi-\delta)$ if $\varphi+\delta\leq\psi\leq 2\pi-\varphi$, $\varphi\geq 0$, $\delta\geq 0$. We have equality only if $\delta=0$ or $\psi=2\pi-\varphi$ or if $\psi=\varphi+\delta$. Hence in the interior of the simplex the system of equations is non-degenerate and the matrix A is extremal.

If $\phi_2+\phi_4+\phi_5=\pi$ or $\phi_1+\phi_3+\phi_5=\phi_4$, then the determinant is zero and the last row of the coefficient matrix is a linear combination of the first 4 rows, which are always linearly independent. Then we have other equalities on B, however.

Consider the case $\phi_2+\phi_4+\phi_5=\pi$. Then b_{26} appears at the corresponding place in Y and $b_{12}\sin\phi_4+b_{14}\sin(\phi_2+\phi_4)+b_{16}\sin\phi_2=g_1Qg_2^T\sin\phi_4-f_2Pf_4^T\sin(\phi_2+\phi_4)+g_1Qg_6^T\sin\phi_2=0$. This yields the two additional rows

$$\begin{pmatrix} \sin(\phi_2+\phi_3)\sin(\phi_3-\phi_4) & \sin(\phi_2+\phi_3)\sin(\phi_2+\phi_4) & 0 & -\sin\phi_1\sin(\phi_1+\phi_5) & -\sin \\ -\sin(\phi_2+\phi_3)\sin\phi_3\sin(\phi_2+\phi_4) & -\sin(\phi_2+\phi_3)\sin\phi_2\sin(\phi_2+\phi_4) & 0 & -\sin^2\phi_1\sin\phi_4+\sin\phi_1\sin(\phi_1+\phi_5)\sin\phi_2 & \sin\phi_1 \end{pmatrix}$$

Nevertheless, these rows are linearly dependent on the previous 4 rows. Hence the corresponding matrices A are not extremal.

Consider the case $\phi_1+\phi_3+\phi_5=\phi_4$. Then the elements b_{63},b_{65} appear in X, and we have $b_{43}\sin(\phi_1+\phi_5)+b_{45}\sin\phi_5+b_{46}\sin\phi_1=f_3Pf_4^T\sin(\phi_1+\phi_5)+f_4Pf_5^T\sin\phi_5+f_4Pf_6^T\sin\phi_1=0$. This yields the three additional rows

$$\begin{pmatrix} \sin\phi_1\sin(\phi_3-\phi_4) & \sin\phi_1\sin(\phi_2+\phi_4)-\text{s} \\ 0 & \sin(\phi_2+ \\ -\sin\phi_1\sin\phi_3\sin(\phi_1+\phi_5)-\sin\phi_3\sin(\phi_3-\phi_4)\sin\phi_1 & \sin(\phi_1+\phi_2+\phi_3)\sin\phi_3\sin(\phi_1+\phi_5)-\sin\phi_1\sin\phi_2\sin(\phi_1+\phi_5)-\sin \end{pmatrix}$$

These rows are also linearly dependent on the previous 4 rows. Hence the corresponding matrices A are not extremal.

Result

In Case 8 the extremal matrices with unit diagonal are given by (1) with $\phi_1,\dots,\phi_5>0$, $\phi_1+\phi_3+\phi_5<\phi_4$, $\phi_2+\phi_4+\phi_5<\pi$, as well as those obtained by the index transformation $(123456)\mapsto(132546)$.

References

[1] Peter J.C. Dickinson. *A new certificate for copositivity. Optimization Online.*

[2] Peter J.C. Dickinson and Roland Hildebrand. *Considering copositivity locally.* J.Math. Anal.Appl., 437(2):11841195, 2016