

## Case 23

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### Preliminaries

The presence of a minimal zero with support of size 4 leads us to study positive semi-definite  $4 \times 4$  matrices of rank 3 with positive kernel vector. Let

$$A = \begin{pmatrix} 1 & -\cos \phi_5 & -\cos \phi_7 & \star \\ -\cos \phi_5 & 1 & -\cos \phi_8 & -\cos \phi_1 \\ -\cos \phi_7 & -\cos \phi_8 & 1 & -\cos \phi_9 \\ \star & -\cos \phi_1 & -\cos \phi_9 & 1 \end{pmatrix}$$

be a partially positive definite matrix, i.e.,  $A_{123} \succ 0$ ,  $A_{234} \succ 0$ , where  $\phi_1, \phi_5, \phi_7, \phi_8, \phi_9 \in (0, \pi)$ . The positive definiteness of the principal submatrices yields the conditions

$$\max(|\pi - \phi_5 - \phi_7|, |\pi - \phi_1 - \phi_9|) < \phi_8 < \min(\pi - |\phi_5 - \phi_7|, \pi - |\phi_1 - \phi_9|). \quad (1)$$

A consequence of these relations is

$$\phi_7 < \phi_1 + \phi_5 + \phi_9, \quad \phi_9 < \phi_1 + \phi_5 + \phi_7. \quad (2)$$

The matrix is positive semi-definite completable, and there exists a closed interval  $[a_{\min}, a_{\max}]$  for possible values of the missing corner element  $a$  which makes  $A$  positive semi-definite. The extremal values of the interval yield a rank 3 matrix. If  $a$  equals an extremal value, then there exists a non-zero kernel vector  $u$  of  $A$ . Since  $A_{123} \succ 0$ , the element  $u_4$  cannot vanish. Likewise,  $u_1$  does not vanish, because  $A_{234} \succ 0$ .

The matrix  $uu^T$  generates the face which is orthogonal to the face of  $A$  in the cone  $\mathcal{S}_+^4$ . If  $a = a_{\max}$ , then adding a positive multiple of  $E_{14}$  to  $A$  leads out of the cone  $\mathcal{S}_+^4$ , while adding a small negative multiple leads into the interior of  $\mathcal{S}_+^4$ . Hence  $\langle E_{14}, uu^T \rangle = 2u_1u_4 < 0$ . Likewise, for  $a = a_{\min}$  we get  $\langle E_{14}, uu^T \rangle = 2u_1u_4 > 0$ . Thus  $a = a_{\min}$  is a necessary condition for having a positive kernel vector. We shall henceforth assume that  $a = a_{\min}$ . We have the explicit value

$$a = \frac{\cos \phi_1 \cos \phi_5 + \cos \phi_1 \cos \phi_7 \cos \phi_8 + \cos \phi_5 \cos \phi_8 \cos \phi_9 + \cos \phi_7 \cos \phi_9}{\sin^2 \phi_8} - \frac{\sqrt{(\sin^2 \phi_1 \sin^2 \phi_8 - (\cos \phi_9 + \cos \phi_1 \cos \phi_8)^2)(\sin^2 \phi_5 \sin^2 \phi_8 - (\cos \phi_7 + \cos \phi_5 \cos \phi_8)^2)}}{\sin^2 \phi_8}.$$

We also assume that the elements  $u_1, u_4$  of the kernel vector are positive.

The submatrix  $A_{124}$  is also positive semi-definite, and hence  $a \geq \cos(\phi_1 + \phi_5)$ . Likewise,  $A_{134} \succeq 0$  yields  $a \geq \cos(\phi_7 + \phi_9)$ . Note that  $a = \cos(\phi_1 + \phi_5)$  and  $a = \cos(\phi_7 + \phi_9)$  implies

$$u = (\sin \phi_1, \sin(\phi_1 + \phi_5), 0, \sin \phi_5)^T, \quad u = (\sin \phi_9, 0, \sin(\phi_7 + \phi_9), \sin \phi_7)^T, \quad (3)$$

respectively.

Define  $v = (\sin \phi_1, \sin(\phi_1 + \phi_5), 0, \sin \phi_5)^T$  and  $w = (\sin \phi_9, 0, \sin(\phi_7 + \phi_9), \sin \phi_7)^T$ . We obtain

$$Av = ((a - \cos(\phi_1 + \phi_5)) \sin \phi_5, 0, \star, (a - \cos(\phi_1 + \phi_5)) \sin \phi_1)^T \quad Aw = ((a - \cos(\phi_7 + \phi_9)) \sin \phi_7, \star, 0, (a - \cos(\phi_7 + \phi_9)) \sin \phi_9)^T.$$

We have  $u^T Av = u^T Aw = 0$ , because  $u$  is the kernel vector of  $A$ . This yields

$$(Av)_3 u_3 = -(a - \cos(\phi_1 + \phi_5))(\sin \phi_5 u_1 + \sin \phi_1 u_4), \quad (Aw)_2 u_2 = -(a - \cos(\phi_7 + \phi_9))(\sin \phi_7 u_1 + \sin \phi_9 u_4). \quad (4)$$

Hence  $u_3 = 0$  implies  $a = \cos(\phi_1 + \phi_5)$  and  $u_2 = 0$  implies  $a = \cos(\phi_7 + \phi_9)$ . This in turn gives the values (3) for  $u$ , respectively, which by  $Au = 0$  implies  $(Av)_3 = 0$  and  $(Aw)_2 = 0$ , respectively. Hence  $u_3 = 0$  is equivalent to  $(Av)_3 = 0$  and  $u_2 = 0$  to  $(Aw)_2 = 0$ .

If  $u_3 \neq 0$  and  $u_2 \neq 0$ , then the right-hand sides of equations (4) are negative, and we obtain

$$u_3 > 0 \Leftrightarrow (Av)_3 < 0, \quad u_2 > 0 \Leftrightarrow (Aw)_2 < 0,$$

respectively.

Thus  $u > 0$  if and only if

$$\cos \phi_7 \sin \phi_1 + \cos \phi_8 \sin(\phi_1 + \phi_5) + \cos \phi_9 \sin \phi_5 > 0, \quad \cos \phi_5 \sin \phi_9 + \cos \phi_8 \sin(\phi_7 + \phi_9) + \cos \phi_1 \sin \phi_7 > 0, \quad (5)$$

implying also

$$a > \cos(\phi_1 + \phi_5), \quad a > \cos(\phi_7 + \phi_9). \quad (6)$$

Let us now derive a condition on the kernel vector. Divide  $A$  into  $2 \times 2$  blocks  $I, II$  of equal size. Then the kernel vector satisfies

$$A_{I,I}u_I + A_{I,II}u_{II} = A_{I,I}^T u_I + A_{II,II}u_{II} = 0.$$

It follows that

$$u_I^T A_{I,I}u_I = -u_I^T A_{I,II}u_{II} = u_{II}^T A_{II,II}u_{II}. \quad (7)$$

## Basic structure

The minimal zero support set is equivalent to  $\{\{3, 4, 5\}, \{4, 5, 1\}, \{5, 1, 2\}, \{1, 2, 3\}, \{1, 5, 6\}, \{2, 3, 4, 6\}\}$ . Let the corresponding zeros be  $u^1, \dots, u^6$ . It follows that  $A$  has the form

$$A = \begin{pmatrix} 1 & -\cos \phi_4 & \cos(\phi_4 + \phi_5) & \cos(\phi_2 + \phi_3) & -\cos \phi_3 & \cos(\phi_3 + \phi_6) \\ -\cos \phi_4 & 1 & -\cos \phi_5 & a_{24} & \cos(\phi_3 + \phi_4) & a_{26} \\ \cos(\phi_4 + \phi_5) & -\cos \phi_5 & 1 & -\cos \phi_1 & \cos(\phi_1 + \phi_2) & a_{36} \\ \cos(\phi_2 + \phi_3) & a_{24} & -\cos \phi_1 & 1 & -\cos \phi_2 & a_{46} \\ -\cos \phi_3 & \cos(\phi_3 + \phi_4) & \cos(\phi_1 + \phi_2) & -\cos \phi_2 & 1 & -\cos \phi_6 \\ \cos(\phi_3 + \phi_6) & a_{26} & a_{36} & a_{46} & -\cos \phi_6 & 1 \end{pmatrix}.$$

We also set  $a_{26} = -\cos \phi_7$ ,  $a_{36} = -\cos \phi_8$ ,  $a_{46} = -\cos \phi_9$ . Here  $\phi_1, \dots, \phi_9 \in (0, \pi)$ , and  $\phi_1 + \phi_2, \phi_2 + \phi_3, \phi_3 + \phi_4, \phi_4 + \phi_5, \phi_3 + \phi_6 < \pi$ .

The minimal zeros  $u_1, \dots, u_6$  are given by the columns of the matrix

$$\begin{pmatrix} 0 & \sin \phi_2 & \sin(\phi_3 + \phi_4) & \sin \phi_5 & \sin \phi_6 & 0 \\ 0 & 0 & \sin \phi_3 & \sin(\phi_4 + \phi_5) & 0 & u_{62} \\ \sin \phi_2 & 0 & 0 & \sin \phi_4 & 0 & u_{63} \\ \sin(\phi_1 + \phi_2) & \sin \phi_3 & 0 & 0 & 0 & u_{64} \\ \sin \phi_1 & \sin(\phi_2 + \phi_3) & \sin \phi_4 & 0 & \sin(\phi_3 + \phi_6) & 0 \\ 0 & 0 & 0 & 0 & \sin \phi_3 & 1 \end{pmatrix}.$$

We have the symmetry  $(123456) \mapsto (543216)$ .

## First order conditions

The minimal zero supports cover all elements, and irreducibility with respect to  $\mathcal{N}^6$  follows.

**Conditions on  $(Au_1)_1, (Au_2)_3, (Au_3)_3, (Au_4)_5$ :** We have the inequality

$$(Au_1)_1 = \cos(\phi_4 + \phi_5) \sin \phi_2 + \cos(\phi_2 + \phi_3) \sin(\phi_1 + \phi_2) - \cos \phi_3 \sin \phi_1 = (\cos(\phi_4 + \phi_5) + \cos(\phi_1 + \phi_2 + \phi_3)) \sin \phi_2 \geq 0,$$

which yields either  $\phi_1 + \phi_2 + \phi_3 + \phi_4 + \phi_5 \leq \pi$  or  $\phi_1 + \phi_2 + \phi_3 \geq \pi + \phi_4 + \phi_5$ . Further

$$(Au_2)_3 = \cos(\phi_4 + \phi_5) \sin \phi_2 - \cos \phi_1 \sin \phi_3 + \cos(\phi_1 + \phi_2) \sin(\phi_2 + \phi_3) = (Au_1)_1,$$

$(Au_3)_3 = \cos(\phi_4 + \phi_5) \sin(\phi_3 + \phi_4) - \cos \phi_5 \sin \phi_3 + \cos(\phi_1 + \phi_2) \sin \phi_4 = (\cos(\phi_3 + \phi_4 + \phi_5) + \cos(\phi_1 + \phi_2)) \sin \phi_4 \geq 0$ , which yields either  $\phi_1 + \phi_2 + \phi_3 + \phi_4 + \phi_5 \leq \pi$  or  $\phi_3 + \phi_4 + \phi_5 \geq \pi + \phi_1 + \phi_2$ . Hence if the first case does not hold, then combination with the above inequality yields  $\phi_3 \geq \pi$ , a contradiction. Thus

$$\phi_1 + \phi_2 + \phi_3 + \phi_4 + \phi_5 \leq \pi. \quad (8)$$

Similar to the relation  $(Au_2)_3 = (Au_1)_1$  we prove

$$(Au_4)_5 = -\cos \phi_3 \sin \phi_5 + \cos(\phi_3 + \phi_4) \sin(\phi_4 + \phi_5) + \cos(\phi_1 + \phi_2) \sin \phi_4 = (Au_3)_3.$$

The four quantities are hence zero if and only if in (8) we have a equality.

**Conditions on  $(Au_1)_2, (Au_2)_2, (Au_3)_4, (Au_4)_4$ :** The submatrix  $A_{2346}$  is positive semi-definite of rank 3 with positive kernel vector. This yields conditions (1),(5), and by virtue of (6)  $a_{24} > \cos(\phi_1 + \phi_5)$ ,  $a_{24} > \cos(\phi_7 + \phi_9)$ .

The strict lower bound  $\cos(\phi_1 + \phi_5)$  on  $a_{24}$  implies that the submatrix  $A_{12345}$  is a sum of a  $T$ -matrix and a positive multiple of  $E_{24}$ , and in particular copositive. It implies also that  $(Au_1)_2, (Au_2)_2, (Au_3)_4, (Au_4)_4 > 0$ , because these quantities are already nonnegative if  $a_{24} = \cos(\phi_1 + \phi_5)$ .

**Conditions on  $(Au_3)_6, (Au_5)_2, (Au_2)_6, (Au_5)_4$ :** The first two quantities give rise to the condition

$$a_{26} \geq -\cos(\phi_3 + \phi_4 + \phi_6), \quad (9)$$

while the last two yield

$$a_{46} \geq \cos(\phi_2 - \phi_6). \quad (10)$$

**Conditions on  $(Au_1)_6, (Au_4)_6$ :** The inequalities amount to

$$\begin{pmatrix} & \sin \phi_2 & \sin(\phi_1 + \phi_2) \\ \sin(\phi_4 + \phi_5) & \sin \phi_4 & \end{pmatrix} \begin{pmatrix} a_{26} \\ a_{36} \\ a_{46} \end{pmatrix} \geq \begin{pmatrix} \cos \phi_6 \sin \phi_1 \\ -\cos(\phi_3 + \phi_6) \sin \phi_5 \end{pmatrix}. \quad (11)$$

**Conditions on  $(Au_6)_1, (Au_6)_5$ :** Set  $u = (u_{62}, u_{63}, u_{64})^T$ . Then the inequalities can be written as

$$\begin{pmatrix} -\cos \phi_4 & \cos(\phi_4 + \phi_5) & \cos(\phi_2 + \phi_3) \\ \cos(\phi_3 + \phi_4) & \cos(\phi_1 + \phi_2) & -\cos \phi_2 \end{pmatrix} u \geq \begin{pmatrix} -\cos(\phi_3 + \phi_6) \\ \cos \phi_6 \end{pmatrix}.$$

Set further  $P = A_{234} \succ 0$  and  $a = (a_{26}, a_{36}, a_{46})^T$ . Then  $a = -Pu$  and conditions (11) can be rewritten as

$$\begin{pmatrix} \cos \phi_5 \sin \phi_2 - a_{24} \sin(\phi_1 + \phi_2) & \cos(\phi_1 + \phi_2) \sin \phi_1 & -\sin \phi_1 \cos \phi_2 \\ -\cos \phi_4 \sin \phi_5 & \cos(\phi_4 + \phi_5) \sin \phi_5 & -a_{24} \sin(\phi_4 + \phi_5) + \cos \phi_1 \sin \phi_4 \end{pmatrix} u \geq \begin{pmatrix} \cos \phi_6 \sin \phi_1 \\ -\cos(\phi_3 + \phi_6) \sin \phi_5 \end{pmatrix}.$$

Now

$$-a_{24} \sin(\phi_4 + \phi_5) + \cos \phi_1 \sin \phi_4 < -\cos(\phi_1 + \phi_5) \sin(\phi_4 + \phi_5) + \cos \phi_1 \sin \phi_4 = -\cos(\phi_1 + \phi_4 + \phi_5) \sin \phi_5 \leq \cos(\phi_2 + \phi_3) \sin \phi_5,$$

and hence  $(Au_4)_6 \geq 0$  implies  $(Au_6)_1 > 0$ . Likewise,

$$\cos \phi_5 \sin \phi_2 - a_{24} \sin(\phi_1 + \phi_2) < \cos(\phi_3 + \phi_4) \sin \phi_5,$$

and  $(Au_1)_6 \geq 0$  implies  $(Au_6)_5 > 0$ .

**Condition on  $(Au_5)_3$ :** The corresponding inequality yields

$$a_{36} \geq \frac{-\cos(\phi_4 + \phi_5) \sin \phi_6 - \cos(\phi_1 + \phi_2) \sin(\phi_3 + \phi_6)}{\sin \phi_3}.$$

From  $A_{346} \succ 0$  we obtain  $\phi_9 < \pi - |\phi_1 - \phi_8|$  and hence  $\cos \phi_9 > -\cos(\phi_1 - \phi_8)$ . Combined with the first condition in (11) this yields

$$\cos(\phi_1 + \phi_2 - \phi_8) \sin \phi_1 = -\sin \phi_2 \cos \phi_8 + \sin(\phi_1 + \phi_2) \cos(\phi_1 - \phi_8) > -\sin \phi_2 \cos \phi_8 - \sin(\phi_1 + \phi_2) \cos \phi_9 \geq \cos \phi_6 \sin \phi_1.$$

Thus  $|\phi_1 + \phi_2 - \phi_8| < \phi_6$ , which yields  $\phi_8 > \phi_1 + \phi_2 - \phi_6$ .

Now suppose that  $\phi_1 + \phi_2 - \phi_6 \geq 0$ . Then we obtain  $a_{36} = -\cos \phi_8 > -\cos(\phi_1 + \phi_2 - \phi_6)$ . Then, however,

$$\begin{aligned} \frac{-\cos(\phi_4 + \phi_5) \sin \phi_6 - \cos(\phi_1 + \phi_2) \sin(\phi_3 + \phi_6)}{\sin \phi_3} &\leq \frac{\cos(\phi_1 + \phi_2 + \phi_3) \sin \phi_6 - \cos(\phi_1 + \phi_2) \sin(\phi_3 + \phi_6)}{\sin \phi_3} \\ &= -\cos(\phi_1 + \phi_2 - \phi_6) < a_{36}. \end{aligned}$$

Likewise, from  $A_{236} > 0$  we obtain  $\phi_7 < \pi - |\phi_5 - \phi_8|$  and hence  $\cos \phi_7 > -\cos(\phi_5 - \phi_8)$ . Combined with the second condition in (11) this yields

$$\cos(\phi_4 + \phi_5 - \phi_8) \sin \phi_5 = \sin(\phi_4 + \phi_5) \cos(\phi_5 - \phi_8) - \sin \phi_4 \cos \phi_8 > -\sin(\phi_4 + \phi_5) \cos \phi_7 - \sin \phi_4 \cos \phi_8 \geq -\cos(\phi_3 + \phi_6) \sin \phi_5.$$

Thus  $|\phi_4 + \phi_5 - \phi_8| < \pi - \phi_3 - \phi_6$ , which yields  $\phi_3 + \phi_4 + \phi_5 + \phi_6 < \pi + \phi_8$ .

Now suppose that  $\phi_3 + \phi_4 + \phi_5 + \phi_6 \geq \pi$ , then we get  $\cos(\phi_3 + \phi_4 + \phi_5 + \phi_6) < -\cos \phi_8 = a_{36}$ . It follows that

$$\begin{aligned} \frac{-\cos(\phi_4 + \phi_5) \sin \phi_6 - \cos(\phi_1 + \phi_2) \sin(\phi_3 + \phi_6)}{\sin \phi_3} &\leq \frac{-\cos(\phi_4 + \phi_5) \sin \phi_6 + \cos(\phi_3 + \phi_4 + \phi_5) \sin(\phi_3 + \phi_6)}{\sin \phi_3} \\ &= \cos(\phi_3 + \phi_4 + \phi_5 + \phi_6) < a_{36}. \end{aligned}$$

Finally, assume that  $\phi_1 + \phi_2 - \phi_6 < 0$  and  $\phi_3 + \phi_4 + \phi_5 + \phi_6 < \pi$ . Then we get

$$\frac{-\cos(\phi_4 + \phi_5) \sin \phi_6 - \cos(\phi_1 + \phi_2) \sin(\phi_3 + \phi_6)}{\sin \phi_3} < \frac{-\cos(\pi - \phi_3 - \phi_6) \sin \phi_6 - \cos \phi_6 \sin(\phi_3 + \phi_6)}{\sin \phi_3} = -1 < a_{36}.$$

Thus in any case

$$a_{36} > \frac{-\cos(\phi_4 + \phi_5) \sin \phi_6 - \cos(\phi_1 + \phi_2) \sin(\phi_3 + \phi_6)}{\sin \phi_3}$$

and  $(Au_5)_3 > 0$ .

**Further relations on  $\phi_k$ :** From the first condition in (11) and the constraint  $\phi_8 < \pi - |\phi_1 - \phi_9|$  we get

$$\sin \phi_2 \cos(\phi_1 - \phi_9) - \sin(\phi_1 + \phi_2) \cos \phi_9 = -\cos(\phi_2 + \phi_9) \sin \phi_1 > \cos \phi_6 \sin \phi_1.$$

Hence  $|\pi - \phi_9 - \phi_2| < \phi_6$  and  $-\phi_6 < \pi - \phi_9 - \phi_2$ . On the other hand, (10) yields  $\pi - \phi_9 \leq |\phi_6 - \phi_2|$ , and hence  $\phi_2 - \phi_6 < |\phi_6 - \phi_2|$ , implying  $\phi_6 > \phi_2$ .

Likewise, from the second condition in (11) and  $\phi_8 < \pi - |\phi_5 - \phi_7|$  we get

$$-\sin(\phi_4 + \phi_5) \cos \phi_7 + \sin \phi_4 \cos(\phi_5 - \phi_7) = -\cos(\phi_4 + \phi_7) \sin \phi_5 > -\cos(\phi_3 + \phi_6) \sin \phi_5.$$

Hence  $|\pi - \phi_7 - \phi_4| < \pi - \phi_3 - \phi_6$  and  $\phi_3 + \phi_6 - \pi < \pi - \phi_7 - \phi_4$ . On the other hand, by (9) we have  $\pi - \phi_7 \leq |\pi - \phi_3 - \phi_6 - \phi_4|$ , and hence  $-\pi + \phi_3 + \phi_6 + \phi_4 < |\pi - \phi_3 - \phi_6 - \phi_4|$ , implying  $\pi > \phi_3 + \phi_4 + \phi_6$ .

Thus conditions (9),(10) can be rewritten as

$$\phi_7 \geq \phi_3 + \phi_4 + \phi_6, \quad \phi_9 \geq \pi + \phi_2 - \phi_6, \quad (12)$$

and we obtain as a consequence

$$\phi_2 < \phi_6 < \pi - \phi_3 - \phi_4, \quad \phi_7 + \phi_9 > \pi.$$

Note that  $\phi_3 + \phi_6 < \pi$  also follows.

**Again conditions on  $(Au_1)_6, (Au_4)_6$ :** We obtain  $0 < \pi - \phi_6 \leq \phi_9 - \phi_2 < \pi$  and hence  $\cos \phi_6 \leq -\cos(\phi_9 - \phi_2)$ . Multiplying with  $\sin \phi_1$  this further gives

$$-\cos \phi_9 \cos \phi_2 \sin \phi_1 - \sin \phi_9 \sin \phi_2 \sin \phi_1 = -\cos \phi_9 \sin(\phi_1 + \phi_2) + \sin \phi_2 \cos(\phi_1 + \phi_9) \geq \cos \phi_6 \sin \phi_1.$$

Now  $\cos(\phi_1 + \phi_9) = -\cos(|\pi - \phi_1 - \phi_9|) < -\cos \phi_8$ , and hence

$$-\cos \phi_9 \sin(\phi_1 + \phi_2) - \sin \phi_2 \cos \phi_8 > \cos \phi_6 \sin \phi_1.$$

Thus  $(Au_1)_6 > 0$ .

Likewise,  $0 < \phi_3 + \phi_6 \leq \phi_7 - \phi_4 < \pi$  and hence  $-\cos(\phi_3 + \phi_6) \leq -\cos(\phi_4 - \phi_7)$ . Multiplying with  $\sin \phi_5$  this further gives

$$-\cos \phi_4 \cos \phi_7 \sin \phi_5 - \sin \phi_4 \sin \phi_7 \sin \phi_5 = -\cos \phi_7 \sin(\phi_4 + \phi_5) + \sin \phi_4 \cos(\phi_5 + \phi_7) \geq -\cos(\phi_3 + \phi_6) \sin \phi_5.$$

Now  $\cos(\phi_5 + \phi_7) = -\cos(|\pi - \phi_5 - \phi_7|) < -\cos \phi_8$ , and hence

$$-\cos \phi_7 \sin(\phi_4 + \phi_5) - \sin \phi_4 \cos \phi_8 > -\cos(\phi_3 + \phi_6) \sin \phi_5.$$

Thus  $(Au_4)_6 > 0$ .

**Again conditions on  $(Au_1)_1, (Au_2)_3, (Au_3)_3, (Au_4)_5$ :** Inserting  $\cos(\phi_5 + \phi_7) < -\cos \phi_8$  into the first condition of (5) we obtain

$$\begin{aligned} 0 < \cos \phi_7 \sin \phi_1 + \cos \phi_8 \sin(\phi_1 + \phi_5) + \cos \phi_9 \sin \phi_5 &< \cos \phi_7 \sin \phi_1 - \cos(\phi_5 + \phi_7) \sin(\phi_1 + \phi_5) + \cos \phi_9 \sin \phi_5 \\ &= (\cos \phi_9 - \cos(\phi_1 + \phi_5 + \phi_7)) \sin \phi_5. \end{aligned}$$

This yields  $|\pi - \phi_1 - \phi_5 - \phi_7| < \pi - \phi_9$  and in particular

$$\phi_1 + \phi_5 + \phi_7 + \phi_9 < 2\pi. \quad (13)$$

Combining with (12) we obtain

$$\phi_1 + \phi_2 + \phi_3 + \phi_4 + \phi_5 < \pi,$$

and  $(Au_1)_1, (Au_2)_3, (Au_3)_3, (Au_4)_5 > 0$ .

**Conditions  $u_{62}, u_{63}, u_{64}, u_{66} > 0$**

We now consider constraints (5). Note that  $\phi_7 + \phi_9 > \pi$ ,  $\phi_1 + \phi_5 < \pi$ . Hence (5) can be written as

$$-\frac{\cos \phi_7 \sin \phi_1 + \cos \phi_9 \sin \phi_5}{\sin(\phi_1 + \phi_5)} < \cos \phi_8 < -\frac{\cos \phi_5 \sin \phi_9 + \cos \phi_1 \sin \phi_7}{\sin(\phi_7 + \phi_9)}.$$

From (13) and taking into account  $\phi_7 + \phi_9 > \pi$  we obtain  $\cos \phi_5 > \cos(\phi_1 + \phi_7 + \phi_9)$ . After multiplying by  $\sin \phi_9$  and transforming we get

$$\cos \phi_5 \sin \phi_9 + \cos \phi_1 \sin \phi_7 > \cos(\phi_1 + \phi_9) \sin(\phi_7 + \phi_9).$$

This further yields

$$-\frac{\cos \phi_5 \sin \phi_9 + \cos \phi_1 \sin \phi_7}{\sin(\phi_7 + \phi_9)} > \cos(\pi - \phi_1 - \phi_9) > \cos \phi_8.$$

Thus  $u_{62} > 0$  is satisfied automatically.

By the first relation in (2) and  $\phi_1 + \phi_5 < \pi < \phi_7 + \phi_9$  we have  $-\phi_9 < \phi_1 + \phi_5 - \phi_7 < \phi_9$  and hence  $\cos(\phi_1 + \phi_5 - \phi_7) > \cos \phi_9$ . Multiplying by  $\sin \phi_5$  we get

$$\cos(\phi_5 - \phi_7) \sin(\phi_1 + \phi_5) - \cos \phi_7 \sin \phi_1 = \cos(\phi_1 + \phi_5 - \phi_7) \sin \phi_5 > \cos \phi_9 \sin \phi_5.$$

It follows that

$$\cos(\pi - |\phi_5 - \phi_7|) = \cos(\pi - \phi_5 + \phi_7) < -\frac{\cos \phi_9 \sin \phi_5 + \cos \phi_7 \sin \phi_1}{\sin(\phi_1 + \phi_5)}$$

Likewise, by the second relation in (2) we get  $-\phi_7 < \phi_1 + \phi_5 - \phi_9 < \phi_7$  and hence  $\cos(\phi_1 + \phi_5 - \phi_9) > \cos \phi_7$ . Multiplying by  $\sin \phi_1$  we get

$$\cos(\phi_1 - \phi_9) \sin(\phi_1 + \phi_5) - \cos \phi_9 \sin \phi_5 = \cos(\phi_1 + \phi_5 - \phi_9) \sin \phi_1 > \cos \phi_7 \sin \phi_1.$$

It follows that

$$\cos(\pi - |\phi_1 - \phi_9|) = \cos(\pi - \phi_1 + \phi_9) < -\frac{\cos \phi_9 \sin \phi_5 + \cos \phi_7 \sin \phi_1}{\sin(\phi_1 + \phi_5)}.$$

Thus  $u_{64} > 0$  implies  $\max(|\pi - \phi_5 - \phi_7|, |\pi - \phi_1 - \phi_9|) < \phi_8$ .

## Parametrization

We parameterize  $A$  by the angles  $\phi_1, \dots, \phi_9$ . We are left with the constraints  $\phi_k \in (0, \pi)$ ,  $\phi_7 \geq \phi_3 + \phi_4 + \phi_6$ ,  $\phi_9 \geq \pi - \phi_6 + \phi_2$ ,

$$-\frac{\cos \phi_7 \sin \phi_1 + \cos \phi_9 \sin \phi_5}{\sin(\phi_1 + \phi_5)} < \cos \phi_8 < -\max(\cos(\phi_5 + \phi_7), \cos(\phi_1 + \phi_9)). \quad (14)$$

Note that (2) and (13) follow from this relation, and these are the conditions obtained by projecting out  $\phi_8$ . Projecting out  $\phi_9, \phi_7, \phi_6$  consecutively we obtain

$$\begin{aligned} \phi_7 - \phi_1 - \phi_5 &< \phi_9 < \min(2\pi - \phi_1 - \phi_5 - \phi_7, \phi_1 + \phi_5 + \phi_7), & \pi - \phi_6 + \phi_2 &\leq \phi_9, \\ \pi - \phi_1 + \phi_2 - \phi_5 - \phi_6 &< \phi_7 < \min(\pi, \pi - \phi_1 - \phi_2 - \phi_5 + \phi_6), & \phi_3 + \phi_4 + \phi_6 &\leq \phi_7, \\ \phi_2 &< \phi_6 < \pi - \phi_3 - \phi_4, \\ \phi_1 + \phi_2 + \phi_3 + \phi_4 + \phi_5 &< \pi. \end{aligned}$$

The element  $a_{24}$  is given by

$$\begin{aligned} a_{24} &= \frac{\cos \phi_1 \cos \phi_5 + \cos \phi_1 \cos \phi_7 \cos \phi_8 + \cos \phi_5 \cos \phi_8 \cos \phi_9 + \cos \phi_7 \cos \phi_9}{\sin^2 \phi_8} - \\ &= \frac{\sqrt{(\sin^2 \phi_1 \sin^2 \phi_8 - (\cos \phi_9 + \cos \phi_1 \cos \phi_8)^2)(\sin^2 \phi_5 \sin^2 \phi_8 - (\cos \phi_7 + \cos \phi_5 \cos \phi_8)^2)}}{\sin^2 \phi_8}. \end{aligned} \quad (15)$$

## Copositivity

Copositivity of  $A$  will be checked by the criterion in Theorem 4.6 of [1]. For each non-empty index set  $I \subset \{1, \dots, 6\}$  we have to find a vector  $v \in \mathbb{R}^6$  such that  $I$  contains the support of  $v$  and is contained in the nonnegative support of  $Av$ , or prove directly that  $A_I$  is copositive.

For  $I$  of size 1 or 2 we may take  $v = \sum_{i \in I} e_i$ . For  $I$  containing the support of a minimal zero  $u$  we may take  $v = u$ . Index sets which are contained in  $\{1, 2, 3, 4, 5\}$  not be considered because the corresponding submatrix is already copositive. The same holds for subsets of  $\{2, 3, 4, 6\}$ . The other index sets  $I$  are

$$\{1, 2, 6\}, \{1, 3, 6\}, \{1, 4, 6\}, \{1, 2, 4, 6\}, \{1, 3, 4, 6\}, \{2, 5, 6\}, \{3, 5, 6\}, \{2, 3, 5, 6\}, \{4, 5, 6\}, \{2, 4, 5, 6\}. \quad (16)$$

The submatrices of size 3 are copositive because

$$\begin{aligned} \phi_4 + (\pi - \phi_3 - \phi_6) + \phi_7 &\geq 2\phi_4 + \pi > \pi, & (\pi - \phi_4 - \phi_5) + (\pi - \phi_3 - \phi_6) + \phi_8 &> -\phi_4 + \pi - \phi_3 - \phi_6 + \phi_7 \geq \pi, \\ (\pi - \phi_2 - \phi_3) + (\pi - \phi_3 - \phi_6) + \phi_9 &\geq 3\pi - 2\phi_3 - 2\phi_6 > \pi, & (\pi - \phi_3 - \phi_4) + \phi_7 + \phi_6 &\geq \pi + 2\phi_6 > \pi, \\ (\pi - \phi_1 - \phi_2) + \phi_8 + \phi_6 &> -\phi_2 + \phi_9 + \phi_6 \geq \pi, & \phi_2 + \phi_9 + \phi_6 &\geq \pi + 2\phi_2 > \pi. \end{aligned}$$

For the index sets  $\{1, 2, 4, 6\}, \{2, 4, 5, 6\}$  we may choose the vectors  $e_1 + e_2, e_4 + e_5$ , respectively, because  $\cos(\phi_2 + \phi_3) + a_{24} > \cos(\phi_2 + \phi_3) + \cos(\phi_1 + \phi_5) > 0$ ,  $\cos(\phi_3 + \phi_6) > \cos \phi_7$  and  $a_{24} + \cos(\phi_3 + \phi_4) > \cos(\phi_1 + \phi_5) + \cos(\phi_3 + \phi_4) > 0$ ,  $\cos(\pi - \phi_6) > \cos \phi_9$ .

*Index set  $\{1, 3, 4, 6\}$ :* Set  $\xi_1 = \pi - \phi_4 - \phi_5$ ,  $\xi_2 = \pi - \phi_2 - \phi_3$ ,  $\xi_3 = \pi - \phi_3 - \phi_6$ . The other angles involved in the description of the off-diagonal entries of  $A_{1346}$  are  $\phi_1, \phi_8, \phi_9$ . All six angles are in  $(0, \pi)$ . Further we have the inequalities

$$\begin{aligned} \phi_1 + \phi_8 + \phi_9 &> \pi, & \xi_1 + \xi_3 + \phi_8 &> \pi - \phi_3 - \phi_4 - \phi_6 + \phi_7 \geq \pi, & \xi_1 + \xi_2 &= 2\pi - \phi_2 - \phi_3 - \phi_4 - \pi_5 > \pi, \\ \xi_1 + \phi_9 + \phi_8 &> 2\pi - \phi_4 - \phi_5 - \phi_1 > \pi, & \xi_2 + \phi_9 &\geq 2\pi - \phi_6 - \phi_3 > \pi, & \xi_1 + \xi_2 + \phi_9 + \phi_8 &> 3\pi - \phi_2 - \phi_3 - \phi_4 - \phi_5 - \phi_1 > 2\pi. \end{aligned}$$

These strict linear inequalities define the interior of a polytope with 32 extreme points, of which 28 can be obtained by increasing the elements of one of the four remaining extreme points. These four are given by

$$\begin{pmatrix} \xi_1 \\ \xi_2 \\ \xi_3 \\ \phi_1 \\ \phi_9 \\ \phi_8 \end{pmatrix} = \begin{pmatrix} \pi \\ 0 \\ 0 \\ 0 \\ \pi \\ 0 \end{pmatrix}, \begin{pmatrix} \pi \\ \pi \\ 0 \\ \pi \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ \pi \\ 0 \\ 0 \\ 0 \\ \pi \end{pmatrix}, \begin{pmatrix} 0 \\ \pi \\ 0 \\ 0 \\ \pi \\ 0 \end{pmatrix}.$$

Therefore

$$A_{1346} = \begin{pmatrix} 1 & -\cos(\psi_1 + \psi_2) & \cos \psi_1 & \cos(\psi_1 + \psi_2 + \psi_3) \\ -\cos(\psi_1 + \psi_2) & 1 & -\cos \psi_2 & -\cos \psi_3 \\ \cos \psi_1 & -\cos \psi_2 & 1 & \cos(\psi_2 + \psi_3) \\ \cos(\psi_1 + \psi_2 + \psi_3) & -\cos \psi_3 & \cos(\psi_2 + \psi_3) & 1 \end{pmatrix} + N \quad (17)$$

for some  $\psi_1, \psi_2, \psi_3 > 0$  with  $\psi_1 + \psi_2 + \psi_3 < \pi$ , where  $N$  is a non-zero nonnegative matrix. The left matrix summand is PSD of rank 2 with kernel vectors  $(0, \sin(\psi_2 + \psi_3), \sin \psi_3, \sin \psi_2)^T$  and  $(-\sin \psi_2, \sin \psi_1, \sin(\psi_1 + \psi_2), 0)^T$ . Hence  $A_{1346}$  is copositive.

In a similar way copositivity of  $A_{2356}$  is proven.

This proves copositivity of  $A$ .

## Absence of other minimal zeros

By construction there are no further minimal zeros with supports of size 1 or 2. Index sets which contain a minimal zero support are excluded by definition. The submatrix  $A_{12345}$  contains only the zeros of the  $T$ -matrix component which do not contain  $\{2, 4\}$  in their support, and these are exactly the first 4 zeros  $u_i$ . The submatrix  $A_{2346}$  does not have other zeros than  $u_6$  by construction. Hence the index sets which remain to be checked are those in (16).

The inequalities on the angles proving copositivity of the submatrices corresponding to sets with cardinality 3 are strict, and hence there does not exist a zero with these supports.

The submatrix  $A_{1346}$  cannot have a positive kernel vector because the summand  $N$  in (17) is non-zero. In a similar way there does not exist a zero with support  $\{2, 3, 5, 6\}$ .

Thus there do not exist 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:

$$(Au_1)_{3,4,5}, (Au_2)_{1,4,5}, (Au_3)_{1,2,5}, (Au_4)_{1,2,3}, (Au_5)_{1,5,6}, (Au_6)_{2,3,4,6}. \quad (18)$$

The following elements may become zero: If  $\phi_7 = \phi_3 + \phi_4 + \phi_6$ , then

$$(Au_3)_6 = (Au_5)_2 = 0.$$

If  $\phi_9 = \pi + \phi_2 - \phi_6$ , then

$$(Au_2)_6 = (Au_5)_4 = 0.$$

The following elements are always positive:

$$(Au_1)_{1,2,6}, (Au_2)_{2,3}, (Au_3)_{3,4}, (Au_4)_{4,5,6}, (Au_5)_3, (Au_6)_{1,5}.$$

We now consider these cases separately.

Case  $\phi_7 > \phi_3 + \phi_4 + \phi_6$ ,  $\phi_9 > \pi + \phi_2 - \phi_6$ : In this case there are only 19 linear relations on the 21 elements of  $B$ , and the solution space is at least 2-dimensional. Hence in this case  $A$  is not extremal.

Case  $\phi_7 = \phi_3 + \phi_4 + \phi_6$ ,  $\phi_9 > \pi + \phi_2 - \phi_6$ : Let us construct the face of  $A$  in the copositive cone. Let  $F$  be a full rank  $6 \times 3$  matrix such that  $u_1^T F = u_4^T F = u_6^T F = 0$  and let  $G$  be a full rank  $6 \times 2$  matrix such that  $u_2^T G = u_3^T G = u_5^T G = 0$ . Then for every  $B$  in the face of  $A$  there exist positive definite matrices  $P \in \mathcal{S}_+^3$ ,  $Q \in \mathcal{S}_+^2$  such that

$$FPF^T = \begin{pmatrix} b_{11} & b_{12} & b_{13} & \star & \star & \star \\ b_{12} & b_{22} & b_{23} & b_{24} & \star & b_{26} \\ b_{13} & b_{23} & b_{33} & b_{34} & b_{35} & b_{36} \\ \star & b_{24} & b_{34} & b_{44} & b_{45} & b_{46} \\ \star & \star & b_{35} & b_{45} & b_{55} & \star \\ \star & b_{26} & b_{36} & b_{46} & \star & b_{66} \end{pmatrix}, \quad GQG^T = \begin{pmatrix} b_{11} & b_{12} & \star & b_{14} & b_{15} & b_{16} \\ b_{12} & b_{22} & \star & \star & b_{25} & b_{26} \\ \star & \star & \star & \star & \star & \star \\ b_{14} & \star & \star & b_{44} & b_{45} & \star \\ b_{15} & b_{25} & \star & b_{45} & b_{55} & b_{56} \\ b_{16} & b_{26} & \star & \star & b_{56} & b_{66} \end{pmatrix}. \quad (19)$$

The products have the elements 11, 12, 22, 26, 44, 45, 55, 66 in common, which yields 8 relations on the 9 elements of  $P, Q$ . The matrix of the system in the elements  $p_{11}, p_{12}, \dots, q_{22}$  is given by

$$\begin{pmatrix} f_{11}^2 & 2f_{11}f_{12} & 2f_{11}f_{13} & f_{12}^2 & 2f_{12}f_{13} & f_{13}^2 & -g_{11}^2 & -2g_{11}g_{12} & -g_{12}^2 \\ f_{11}f_{21} & f_{11}f_{22} + f_{21}f_{12} & f_{11}f_{23} + f_{21}f_{13} & f_{12}f_{22} & f_{12}f_{23} + f_{22}f_{13} & f_{13}f_{23} & -g_{11}g_{21} & -g_{11}g_{22} - g_{21}g_{12} & -g_{12}g_{22} \\ f_{21}^2 & 2f_{21}f_{22} & 2f_{21}f_{23} & f_{22}^2 & 2f_{22}f_{23} & f_{23}^2 & -g_{21}^2 & -2g_{21}g_{22} & -g_{22}^2 \\ f_{21}f_{61} & f_{21}f_{62} + f_{61}f_{22} & f_{21}f_{63} + f_{61}f_{23} & f_{22}f_{62} & f_{22}f_{63} + f_{62}f_{23} & f_{23}f_{63} & -g_{21}g_{61} & -g_{21}g_{62} - g_{61}g_{22} & -g_{22}g_{62} \\ f_{41}^2 & 2f_{41}f_{42} & 2f_{41}f_{43} & f_{42}^2 & 2f_{42}f_{43} & f_{43}^2 & -g_{41}^2 & -2g_{41}g_{42} & -g_{42}^2 \\ f_{41}f_{51} & f_{41}f_{52} + f_{51}f_{42} & f_{41}f_{53} + f_{51}f_{43} & f_{42}f_{52} & f_{42}f_{53} + f_{52}f_{43} & f_{43}f_{53} & -g_{41}g_{51} & -g_{41}g_{52} - g_{51}g_{42} & -g_{42}g_{52} \\ f_{51}^2 & 2f_{51}f_{52} & 2f_{51}f_{53} & f_{52}^2 & 2f_{52}f_{53} & f_{53}^2 & -g_{51}^2 & -2g_{51}g_{52} & -g_{52}^2 \\ f_{61}^2 & 2f_{61}f_{62} & 2f_{61}f_{63} & f_{62}^2 & 2f_{62}f_{63} & f_{63}^2 & -g_{61}^2 & -2g_{61}g_{62} & -g_{62}^2 \end{pmatrix}.$$

A possible choice of  $F, G$  is

$$F = \begin{pmatrix} -\frac{u_{42}}{u_{41}} & -\frac{u_{43}}{u_{41}} & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & -\frac{u_{13}}{u_{15}} & -\frac{u_{14}}{u_{15}} \\ -\frac{u_{62}}{u_{66}} & -\frac{u_{63}}{u_{66}} & -\frac{u_{64}}{u_{66}} \end{pmatrix} = \begin{pmatrix} -\frac{\sin(\phi_4 + \phi_5)}{\sin \phi_5} & -\frac{\sin \phi_4}{\sin \phi_5} & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & -\frac{\sin \phi_2}{\sin \phi_1} & -\frac{\sin(\phi_1 + \phi_2)}{\sin \phi_1} \\ -\frac{u_{62}}{u_{66}} & -\frac{u_{63}}{u_{66}} & -\frac{u_{64}}{u_{66}} \end{pmatrix},$$

$$G = \begin{pmatrix} 1 & 0 \\ -\frac{u_{31}}{u_{32}} & -\frac{u_{35}}{u_{32}} \\ 0 & 0 \\ -\frac{u_{21}}{u_{24}} & -\frac{u_{25}}{u_{24}} \\ 0 & 1 \\ -\frac{u_{51}}{u_{56}} & -\frac{u_{55}}{u_{56}} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ -\frac{\sin(\phi_3 + \phi_4)}{\sin \phi_3} & -\frac{\sin \phi_4}{\sin \phi_3} \\ 0 & 0 \\ -\frac{\sin \phi_2}{\sin \phi_3} & -\frac{\sin(\phi_2 + \phi_3)}{\sin \phi_3} \\ 0 & 1 \\ -\frac{\sin \phi_6}{\sin \phi_3} & -\frac{\sin(\phi_3 + \phi_6)}{\sin \phi_3} \end{pmatrix}.$$

The coefficient matrix becomes

$$\begin{pmatrix} f_{11}^2 & 2f_{11}f_{12} & 0 & f_{12}^2 & 0 & 0 & -1 & 0 & 0 \\ f_{11} & f_{12} & 0 & 0 & 0 & 0 & -g_{21} & -g_{22} & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & -g_{21}^2 & -2g_{21}g_{22} & -g_{22}^2 \\ f_{61} & f_{62} & f_{63} & 0 & 0 & 0 & -g_{21}g_{61} & -g_{21}g_{62} - g_{61}g_{22} & -g_{22}g_{62} \\ 0 & 0 & 0 & 0 & 0 & 1 & -g_{41}^2 & -2g_{41}g_{42} & -g_{42}^2 \\ 0 & 0 & 0 & 0 & f_{52} & f_{53} & 0 & -g_{41} & -g_{42} \\ 0 & 0 & 0 & f_{52}^2 & 2f_{52}f_{53} & f_{53}^2 & 0 & 0 & -1 \\ f_{61}^2 & 2f_{61}f_{62} & 2f_{61}f_{63} & f_{62}^2 & 2f_{62}f_{63} & f_{63}^2 & -g_{61}^2 & -2g_{61}g_{62} & -g_{62}^2 \end{pmatrix}. \quad (20)$$

The solution pair  $(P, Q)$  producing the initial matrix  $A$  is positive definite. In particular, the diagonal elements of  $P, Q$  are non-zero. We look for a second linearly independent solution. We may hence



assume that for this solution  $q_{22} = 0$ . We need to check whether the left  $8 \times 8$  submatrix of the coefficient matrix has zero determinant. We shall look for a left kernel vector  $x$ .

From the first six columns we obtain  $x_4 = -2f_{61}x_8$ ,  $x_2 = -2f_{11}x_1$ ,  $x_3 = f_{11}^2x_1 + f_{61}^2x_8$ ,  $x_7 = -\frac{f_{12}^2x_1 + f_{62}^2x_8}{f_{52}^2}$ ,  $x_6 = -\frac{2f_{52}f_{53}x_7 + 2f_{62}f_{63}x_8}{f_{52}} = \frac{2f_{53}f_{12}^2x_1 + 2f_{53}f_{62}^2x_8 - 2f_{52}f_{62}f_{63}x_8}{f_{52}^2}$ ,  $x_5 = -f_{53}x_6 - f_{53}^2x_7 - f_{63}^2x_8 = \frac{-f_{53}f_{12}^2x_1 - f_{53}^2f_{62}^2x_8 + 2f_{52}f_{53}f_{62}f_{63}x_8 - f_{52}^2f_{63}^2x_8}{f_{52}^2}$ . The remaining two columns give

$$x_1 + g_{21}x_2 + g_{21}^2x_3 + g_{21}g_{61}x_4 + g_{41}^2x_5 + g_{61}^2x_8 = 0,$$

$$\frac{1}{2}(g_{22}x_2 + 2g_{21}g_{22}x_3 + g_{21}g_{62}x_4 + g_{61}g_{22}x_4 + 2g_{41}g_{42}x_5 + g_{41}x_6 + 2g_{61}g_{62}x_8) = 0.$$

Collecting the coefficients at  $x_1$  and  $x_8$  in these expressions and multiplying by  $f_{52}^2$  we obtain the matrix

$$\begin{pmatrix} f_{52}^2(1-g_{21}f_{11})^2 - g_{41}^2f_{53}^2f_{12}^2 & f_{52}^2(g_{21}f_{61} - g_{61})^2 - g_{41}^2(f_{53}f_{62} - f_{52}f_{63})^2 \\ f_{12}^2f_{53}g_{41}(1-g_{42}f_{53}) - g_{22}f_{11}f_{52}^2(1-g_{21}f_{11}) & f_{52}^2(g_{21}f_{61} - g_{61})(g_{22}f_{61} - g_{62}) + g_{41}(f_{53}f_{62} - f_{52}f_{63})(f_{62} - g_{42}f_{53}f_{62} + g_{42}f_{52}f_{63}) \end{pmatrix}.$$

We get

$$f_{52}^2(1 - g_{21}f_{11})^2 - g_{41}^2f_{53}^2f_{12}^2 = \frac{\sin^2 \phi_2 \sin^2 \phi_4 (\sin^2(\phi_3 + \phi_4 + \phi_5) - \sin^2(\phi_1 + \phi_2))}{\sin^2 \phi_1 \sin^2 \phi_3 \sin^2 \phi_5}$$

$$f_{12}^2f_{53}g_{41}(1-g_{42}f_{53}) - g_{22}f_{11}f_{52}^2(1-g_{21}f_{11}) = \frac{\sin^2 \phi_2 \sin^2 \phi_4 (\sin(\phi_3 + \phi_4 + \phi_5) \sin(\phi_4 + \phi_5) - \sin(\phi_1 + \phi_2 + \phi_3) \sin(\phi_1 + \phi_2))}{\sin^2 \phi_1 \sin^2 \phi_3 \sin^2 \phi_5}$$

$$f_{52}^2(g_{21}f_{61} - g_{61})^2 - g_{41}^2(f_{53}f_{62} - f_{52}f_{63})^2 = \frac{\sin^2 \phi_2}{\sin^2 \phi_1 \sin^2 \phi_3} ((\sin(\phi_3 + \phi_4)f_{61} - \sin \phi_6)^2 - (\sin(\phi_1 + \phi_2)f_{62} - \sin \phi_2 f_{63})^2)$$

$$\begin{aligned} & f_{52}^2(g_{21}f_{61} - g_{61})(g_{22}f_{61} - g_{62}) + g_{41}(f_{53}f_{62} - f_{52}f_{63})(f_{62} - g_{42}f_{53}f_{62} + g_{42}f_{52}f_{63}) = \\ & = \frac{\sin^2 \phi_2 ((\sin(\phi_3 + \phi_4)f_{61} - \sin \phi_6)(\sin \phi_4 f_{61} - \sin(\phi_3 + \phi_6)) - (\sin(\phi_1 + \phi_2)f_{62} - \sin \phi_2 f_{63})(\sin(\phi_1 + \phi_2 + \phi_3)f_{62} - \sin(\phi_2 + \phi_3)f_{63}))}{\sin^2 \phi_1 \sin^2 \phi_3} \end{aligned}$$

Thus the coefficient matrix is degenerate if and only if

$$\begin{aligned} & ((\sin^2(\phi_3 + \phi_4 + \phi_5) - \sin^2(\phi_1 + \phi_2))(\sin \phi_4 f_{61} - \sin(\phi_3 + \phi_6)) - (\sin(\phi_3 + \phi_4 + \phi_5) \sin(\phi_4 + \phi_5) - \sin(\phi_1 + \phi_2 + \phi_3) \sin(\phi_1 + \phi_2))(\sin(\phi_3 + \phi_4)f_{61} - \sin \phi_6))(\sin(\phi_3 + \phi_4)f_{61} - \sin \phi_6) \\ & = ((\sin^2(\phi_3 + \phi_4 + \phi_5) - \sin^2(\phi_1 + \phi_2))(\sin(\phi_1 + \phi_2 + \phi_3)f_{62} - \sin(\phi_2 + \phi_3)f_{63}) - (\sin(\phi_3 + \phi_4 + \phi_5) \sin(\phi_4 + \phi_5) - \sin(\phi_1 + \phi_2 + \phi_3) \sin(\phi_1 + \phi_2))(\sin(\phi_1 + \phi_2)f_{62} - \sin \phi_2 f_{63})). \end{aligned}$$

This simplifies to

$$\begin{aligned} & ((\sin(\phi_1 + \phi_2 + \phi_3 + \phi_4) \sin(\phi_1 + \phi_2) - \sin \phi_5 \sin(\phi_3 + \phi_4 + \phi_5))f_{61} + (\sin(\phi_1 + \phi_2 - \phi_6) \sin(\phi_1 + \phi_2) - \sin(\phi_3 + \phi_4 + \phi_5 + \phi_6) \sin(\phi_3 + \phi_4 + \phi_5))(\sin(\phi_3 + \phi_4)f_{61} - \sin \phi_6)) = \\ & = (\sin(\phi_1 + \phi_2 + \phi_3 + \phi_4 + \phi_5) \sin(\phi_3 + \phi_4 + \phi_5)f_{62} + (\sin \phi_1 \sin(\phi_1 + \phi_2) - \sin(\phi_2 + \phi_3 + \phi_4 + \phi_5) \sin(\phi_3 + \phi_4 + \phi_5))f_{63})(\sin(\phi_1 + \phi_2)f_{62} - \sin \phi_2 f_{63}). \end{aligned}$$

Hence the matrix  $A$  is not extremal if and only if

$$(\sin(\phi_1 + \phi_2 + \phi_3 + \phi_4) \sin(\phi_1 + \phi_2) - \sin \phi_5 \sin(\phi_3 + \phi_4 + \phi_5)) \sin(\phi_3 + \phi_4)u_{62}^2 + (-\sin(\phi_3 + \phi_4) \sin(\phi_1 + \phi_2 - \phi_6) \sin(\phi_1 + \phi_2) + \sin \phi_6 \sin(\phi_1 + \phi_2))u_{64}^2 = 0.$$

On the other hand, by (7) we have

$$u_{62}^2 - 2 \cos(\phi_3 + \phi_4 + \phi_6)u_{62}u_{66} + u_{66}^2 = u_{63}^2 - 2 \cos \phi_1 u_{63}u_{64} + u_{64}^2.$$

Set  $\lambda = \frac{\sin(\phi_1 + \phi_2) \cos(\phi_1 + \phi_2) + \sin(\phi_3 + \phi_4 + \phi_5) \cos(\phi_3 + \phi_4 + \phi_5)}{2}$  and subtract  $\lambda$  times this equation from the condition above. Multiplying by 2 we obtain the equivalent condition

$$\begin{aligned} & \begin{pmatrix} u_{62} \\ u_{66} \end{pmatrix}^T \begin{pmatrix} -\frac{1}{2} \sin 2(\phi_1 + \phi_2 + \phi_3 + \phi_4) - \frac{1}{2} \sin 2\phi_5 & \cos(\phi_5 + \phi_6 - \phi_1 - \phi_2) \sin(\phi_1 + \phi_2 + \phi_3 + \phi_4 + \phi_5) \\ \cos(\phi_5 + \phi_6 - \phi_1 - \phi_2) \sin(\phi_1 + \phi_2 + \phi_3 + \phi_4 + \phi_5) & -\frac{1}{2} \sin 2(\phi_3 + \phi_4 + \phi_5 + \phi_6) - \frac{1}{2} \sin 2(\phi_1 + \phi_2 - \phi_6) \end{pmatrix} \begin{pmatrix} u_{62} \\ u_{66} \end{pmatrix} = \\ & = \begin{pmatrix} u_{63} \\ u_{64} \end{pmatrix}^T \begin{pmatrix} -\frac{1}{2} \sin 2(\phi_1 + \phi_2 + \phi_3 + \phi_4 + \phi_5) & \cos(\phi_2 + \phi_3 + \phi_4 + \phi_5) \sin(\phi_1 + \phi_2 + \phi_3 + \phi_4 + \phi_5) \\ \cos(\phi_2 + \phi_3 + \phi_4 + \phi_5) \sin(\phi_1 + \phi_2 + \phi_3 + \phi_4 + \phi_5) & -\frac{1}{2} \sin 2(\phi_2 + \phi_3 + \phi_4 + \phi_5) - \frac{1}{2} \sin 2\phi_1 \end{pmatrix} \begin{pmatrix} u_{63} \\ u_{64} \end{pmatrix}. \end{aligned} \quad (21)$$

The difference of the left and right-hand side turns out to be of different sign at different points of the manifold of matrices  $A$  in the above parametrization. Hence there is an open dense subset of matrices which are extremal, and a submanifold, given by the equation (21) above, of matrices which are not extremal. We may express the condition entirely by the angles  $\phi_1, \dots, \phi_9$  by noting that the zero  $u_6$  has elements

$$\begin{aligned} u_{62} &= w_1 \sin^2 \phi_8, \\ u_{63} &= w_1(\cos \phi_5 + \cos \phi_7 \cos \phi_8) + w_5(\cos \phi_1 + \cos \phi_8 \cos \phi_9), \\ u_{64} &= w_5 \sin^2 \phi_8, \\ u_{66} &= w_1(\cos \phi_7 + \cos \phi_5 \cos \phi_8) + w_5(\cos \phi_9 + \cos \phi_1 \cos \phi_8), \end{aligned}$$

where

$$\begin{aligned} w_1 &= \sqrt{\sin^2 \phi_1 \sin^2 \phi_8 - (\cos \phi_9 + \cos \phi_1 \cos \phi_8)^2}, \\ w_5 &= \sqrt{\sin^2 \phi_5 \sin^2 \phi_8 - (\cos \phi_7 + \cos \phi_5 \cos \phi_8)^2}. \end{aligned}$$

*Case  $\phi_7 > \phi_3 + \phi_4 + \phi_6$ ,  $\phi_9 = \pi + \phi_2 - \phi_6$ :* This case is obtained from the previous one by applying the symmetry. There is again an open dense subset of extremal matrices and a submanifold of non-extremal matrices, which is given by the relation

$$\begin{aligned} \begin{pmatrix} u_{64} \\ u_{66} \end{pmatrix}^T & \begin{pmatrix} -\frac{1}{2} \sin 2(\phi_2 + \phi_3 + \phi_4 + \phi_5) - \frac{1}{2} \sin 2\phi_1 & -\cos(-\phi_1 + \phi_3 + \phi_4 + \phi_5 + \phi_6) \sin(\phi_1 + \phi_2 + \phi_3 + \phi_4 + \phi_5) \\ -\cos(-\phi_1 + \phi_3 + \phi_4 + \phi_5 + \phi_6) \sin(\phi_1 + \phi_2 + \phi_3 + \phi_4 + \phi_5) & \frac{1}{2} \sin 2(\phi_1 + \phi_2 - \phi_6) + \frac{1}{2} \sin 2(\phi_3 + \phi_4 + \phi_5 + \phi_6) \end{pmatrix} \begin{pmatrix} u_{64} \\ u_{66} \end{pmatrix} = \\ &= \begin{pmatrix} u_{63} \\ u_{62} \end{pmatrix}^T \begin{pmatrix} -\frac{1}{2} \sin 2(\phi_1 + \phi_2 + \phi_3 + \phi_4 + \phi_5) & \cos(\phi_1 + \phi_2 + \phi_3 + \phi_4) \sin(\phi_1 + \phi_2 + \phi_3 + \phi_4 + \phi_5) \\ \cos(\phi_1 + \phi_2 + \phi_3 + \phi_4) \sin(\phi_1 + \phi_2 + \phi_3 + \phi_4 + \phi_5) & -\frac{1}{2} \sin 2(\phi_1 + \phi_2 + \phi_3 + \phi_4) - \frac{1}{2} \sin 2\phi_5 \end{pmatrix} \begin{pmatrix} u_{63} \\ u_{62} \end{pmatrix}. \end{aligned} \quad (22)$$

*Case  $\phi_7 = \phi_3 + \phi_4 + \phi_6$ ,  $\phi_9 = \pi + \phi_2 - \phi_6$ :* In this case the additional linear constraints  $(Bu_2)_6 = (Bu_5)_4 = 0$  on  $B$  can be expressed as the element (4, 6) in the matrix  $GQG^T$  in (19) being equal to  $b_{46}$ . The coefficient matrix (20) then has an additional row corresponding to this element, namely

$$\begin{aligned} (f_{41}f_{61}, f_{41}f_{62} + f_{61}f_{42}, f_{41}f_{63} + f_{61}f_{43}, f_{42}f_{62}, f_{42}f_{63} + f_{62}f_{43}, f_{43}f_{63}, -g_{41}g_{61}, -g_{41}g_{62} - g_{61}g_{42}, -g_{42}g_{62}) = \\ = (0, 0, f_{61}, 0, f_{62}, f_{63}, -g_{41}g_{61}, -g_{41}g_{62} - g_{61}g_{42}, -g_{42}g_{62}) \end{aligned}$$

Consider this coefficient matrix without the rows corresponding to the elements  $b_{26}, b_{46}$ . It is given by

$$\begin{pmatrix} f_{11}^2 & 2f_{11}f_{12} & 0 & f_{12}^2 & 0 & 0 & -1 & 0 & 0 \\ f_{11} & f_{12} & 0 & 0 & 0 & 0 & -g_{21} & -g_{22} & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & -g_{21}^2 & -2g_{21}g_{22} & -g_{22}^2 \\ 0 & 0 & 0 & 0 & 0 & 1 & -g_{41}^2 & -2g_{41}g_{42} & -g_{42}^2 \\ 0 & 0 & 0 & 0 & f_{52} & f_{53} & 0 & -g_{41} & -g_{42} \\ 0 & 0 & 0 & f_{52}^2 & 2f_{52}f_{53} & f_{53}^2 & 0 & 0 & -1 \\ f_{61}^2 & 2f_{61}f_{62} & 2f_{61}f_{63} & f_{62}^2 & 2f_{62}f_{63} & f_{63}^2 & -g_{61}^2 & -2g_{61}g_{62} & -g_{62}^2 \end{pmatrix}. \quad (23)$$

Its rows are linearly independent. Indeed, let  $x$  be a left kernel vector of this matrix. Then the third column implies that  $x_7 = 0$ . Columns 1, 2, 4, 5, 6 allow to express all elements of  $x$  as a linear function of  $x_1$ . The last three columns then after simplification yield the conditions

$$\begin{aligned} (\sin(\phi_3 + \phi_4 + \phi_5) - \sin(\phi_1 + \phi_2))x_1 &= 0, \\ (\sin(\phi_3 + \phi_4 + \phi_5) \sin(\phi_4 + \phi_5) - \sin(\phi_1 + \phi_2 + \phi_3) \sin(\phi_1 + \phi_2))x_1 &= 0, \\ (\sin(\phi_4 + \phi_5) - \sin(\phi_1 + \phi_2 + \phi_3))x_1 &= 0. \end{aligned}$$

By  $\phi_1 + \phi_2 + \phi_3 + \phi_4 + \phi_5 < \pi$  this has only the solution  $x_1 = 0$  and hence  $x = 0$ .

It follows that  $A$  is not extremal if and only if both rows corresponding to the elements  $b_{26}, b_{46}$  can be expressed as a linear combination of the rows in (23). Equivalently, both relations (21), (22) hold.

## Result

In Case 23 the extremal matrices with unit diagonal are given by

$$A = \begin{pmatrix} 1 & -\cos \phi_4 & \cos(\phi_4 + \phi_5) & \cos(\phi_2 + \phi_3) & -\cos \phi_3 & \cos(\phi_3 + \phi_6) \\ -\cos \phi_4 & 1 & -\cos \phi_5 & a_{24} & \cos(\phi_3 + \phi_4) & -\cos \phi_7 \\ \cos(\phi_4 + \phi_5) & -\cos \phi_5 & 1 & -\cos \phi_1 & \cos(\phi_1 + \phi_2) & -\cos \phi_8 \\ \cos(\phi_2 + \phi_3) & a_{24} & -\cos \phi_1 & 1 & -\cos \phi_2 & -\cos \phi_9 \\ -\cos \phi_3 & \cos(\phi_3 + \phi_4) & \cos(\phi_1 + \phi_2) & -\cos \phi_2 & 1 & -\cos \phi_6 \\ \cos(\phi_3 + \phi_6) & -\cos \phi_7 & -\cos \phi_8 & -\cos \phi_9 & -\cos \phi_6 & 1 \end{pmatrix},$$

where  $a_{24}$  is given by (15) and the angles  $\phi_1, \dots, \phi_9 \in (0, \pi)$  satisfy

$$\min(\phi_7 - \phi_3 - \phi_4 - \phi_6, \phi_9 - \pi + \phi_6 - \phi_2) = 0$$

and (14). If  $\phi_7 = \phi_3 + \phi_4 + \phi_6$ , then (21) does not hold, if  $\phi_9 = \pi - \phi_6 + \phi_2$ , then relation (22) does not hold. The submanifolds defined by these relations consist of non-extremal copositive matrices. The set of extremal matrices corresponding to this case is hence parameterized by 8 angles.

## 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):1184–1195, 2016.