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# The real positive definite completion problem for a 4-cycle

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## Abstract

The positive semidefinite (PSD) completion problem is concerned with determining the set of PSD completions of a partial matrix. Previous work has focused on determining whether or not a given partial PSD matrix has a PSD completion, by examining characteristics of the graph of the matrix. Our aim is to move beyond the existence question to that of describing the set of all PSD completions of a given partial matrix. To this end, we consider the most fundamental nontrivial instance of the problem. Let  $A(x, y)$  be a real PSD matrix of order 4 whose graph is  $C_4$ , a 4-cycle, with  $x$  and  $y$  the two unspecified entries corresponding to the two missing edges of  $C_4$ . We investigate the problem of giving a precise description of the convex region  $R$  inside the square  $|x| \leq 1, |y| \leq 1$  for which  $A(x, y)$  is PSD. The boundary curve  $\partial R$  is determined by the quartic polynomial equation  $\det A(x, y) = 0$ ; an important feature of our description is the set of singular points on  $\partial R$ . We find necessary and sufficient conditions on the specified entries of  $A(x, y)$  so that  $\det A(x, y)$  factors with 1, 2, 3 or 4 singular points on  $\partial R$  corresponding to the points of intersection of the curves of all factors of  $\det A(x, y)$ . We then find necessary and sufficient conditions on the specified entries of  $A(x, y)$  so that  $A(x, y)$  has rank 2 PSD completions. We show that this can occur in three ways: either there is a unique PSD completion ( $R$  is a single point), or  $\det A(x, y)$  factors (with the occurrence of singular points), or the PSD completion region  $R$  contains a unique rank 2 PSD completion which is a singular point, but  $R$  is not a single point. We also show that the results mentioned above can be generalized for any partial PSD matrix of order  $n > 4$  whose graph is missing two nonadjacent edges. © 2001 Elsevier Science Inc. All rights reserved.

*Keywords:* 4-Cycle; Matrix completion problem; Nonchordal graph; Partial matrix; Positive definite completion problem; Singular points; Two unspecified entries

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## 1. Introduction

A *real partial matrix* is one in which some entries are specified real numbers and the remainder are unspecified, i.e., free variables over the real numbers. An example is

$$\begin{bmatrix} 2 & 3 & ? \\ 3 & 6 & -4 \\ ? & -4 & 3 \end{bmatrix}, \quad (1)$$

in which the ?'s indicate unspecified entries. We say that a matrix  $A$  is *partial symmetric* if  $A$  is square,  $a_{ji}$  is specified whenever  $a_{ij}$  is, and  $a_{ji} = a_{ij}$ . We shall assume throughout that the diagonal entries of  $A$  are specified.

**Notation.** In this paper, we will write PD (PSD) to mean positive definite (positive semidefinite), respectively. We will also write  $A^\dagger$  to mean the Moore–Penrose generalized inverse of the matrix  $A$ .

By a *partial PD (PSD) matrix* we mean a real partial symmetric matrix each of whose specified principal submatrices is PD (PSD). The matrix given by (1) is partial PD.

A *PD completion* of a partial PD matrix is a real PD matrix resulting from a specification of the unspecified entries. For example,

$$\begin{bmatrix} 2 & 3 & -2 \\ 3 & 6 & -4 \\ -2 & -4 & 3 \end{bmatrix}$$

is a PD completion of the matrix in (1). A *PSD completion* is defined similarly.

Much is known about the existence of PD (PSD) completions and we summarize the essential results here. We first discuss the case in which there is just one (two symmetrically placed) unspecified entry in a partial PD (PSD) matrix  $A$ . Because the problem of existence is unchanged under permutation similarity, we may assume that the missing entry lies in the upper right (and lower left) corner. Then

$$A = \begin{bmatrix} a & b^T & x \\ b & B & c \\ x & c^T & d \end{bmatrix}, \quad (2)$$

where  $x$  is the unspecified entry. We have from [5, p. 175]:

**Proposition 1.** *If  $A$  given by (2) is partial PD, then  $A$  has PD completions. The set of all such completions is the interval given by the inequality*

$$|x - b^T B^{-1} c|^2 < \det \begin{bmatrix} a & b^T \\ b & B \end{bmatrix} \cdot \det \begin{bmatrix} B & c \\ c^T & d \end{bmatrix} / (\det B)^2. \quad (3)$$

*The endpoints of this interval give PSD completions of  $A$ .*

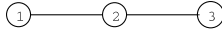


Fig. 1. A graph on three vertices.

If  $A$  is partial PSD, we have a similar result [7, p. 18]:

**Proposition 2.** *If  $A$  given by (2) is partial PSD, then  $A$  has PSD completions. The set of all such completions is the interval given by the inequality*

$$|x - b^T B^\dagger c|^2 \leq (a - b^T B^\dagger b)(d - c^T B^\dagger c). \tag{4}$$

The question of existence of a PSD completion in the case there is more than one unspecified entry in a partial PSD matrix depends on its graph.

**Definition 1.** Let  $A$  be a partial symmetric  $n$ -by- $n$  matrix. The undirected graph  $G = (N, E)$  of  $A$  has vertex set  $N = \{1, 2, \dots, n\}$  and edge set  $E$  such that  $ij \in E, i \neq j$ , if and only if  $a_{ij}, i, j = 1, \dots, n$ , is specified.

For example, the graph of the matrix in (1) is shown in Fig. 1.

**Definition 2.** A graph  $G$  is *chordal* if it has no minimal cycle of four or more edges.

Previously, considerable work has been done on the existence aspect of the PD (PSD) completion problem; i.e., given a partial PD (PSD) matrix, is there a PD (PSD) completion? The first major graph theoretic result about PD (PSD) completions states that if  $A$  is a partial PD (PSD) matrix whose graph is chordal, then  $A$  has a PD (PSD) completion [4]. It is also shown that for nonchordal graphs one must impose additional conditions on  $A$ . The simplest nonchordal graphs are the  $n$ -cycles,  $n \geq 4$ . Necessary and sufficient conditions for the existence of a PD (PSD) completion for a partial PD (PSD) matrix whose graph is an  $n$ -cycle are given in [2]. Conditions for a completion for a class of graphs significantly generalizing the chordal graphs and including the  $n$ -cycles are given in [1].

The set of all PD (PSD) completions of a given partial PD (PSD) matrix is, in general, not well understood. In fact, it has only been investigated for a very restricted class of partial PD (PSD) matrices. Our main aim in this paper is to describe the set of PSD completions of the class of real partial PSD matrices with only two unspecified entries and whose graph is missing two nonadjacent edges. As it will be shown, even in this case, there are myriad possibilities.

## 2. The problem for two unspecified entries

The simplest example of a partial PSD matrix with two unspecified entries is the 3-by-3 matrix

$$A = \begin{bmatrix} 1 & a & x \\ a & 1 & y \\ x & y & 1 \end{bmatrix}, \quad |a| \leq 1, \quad (5)$$

where  $x$  and  $y$  are the unspecified entries. We have normalized the diagonal entries to be one as we will do throughout. Because the set of PSD matrices of a given size is a convex set, we know a priori that the completion region  $R = \{(x, y) \in \mathbb{R}^2 \mid A \text{ is PSD}\}$  is a closed convex subset of the square  $S = \{(x, y) \in \mathbb{R}^2 \mid |x| \leq 1, |y| \leq 1\}$ . Since all proper principal minors of  $A$  are nonnegative if  $x, y \in S$ ,  $A$  is PSD if and only if

$$\det A = 1 + 2axy - a^2 - x^2 - y^2 \quad (6)$$

is nonnegative. We first consider the case  $a = \pm 1$ . If  $a = 1$ , then

$$\begin{bmatrix} 1 & 1 & x \\ 1 & 1 & y \\ x & y & 1 \end{bmatrix}$$

is PSD if and only if  $y = x$ ; hence, the region  $R$  is the diagonal of the square  $S$  given by  $y = x$ . If  $a = -1$ , then

$$\begin{bmatrix} 1 & -1 & x \\ -1 & 1 & y \\ x & y & 1 \end{bmatrix}$$

is PSD if and only if  $y = -x$ ; hence, the region  $R$  is the diagonal of the square  $S$  given by  $y = -x$ . We now summarize this case for future reference.

**Observation 1.** *Let  $x, y \in [-1, 1]$ . Then*

$$\begin{bmatrix} 1 & 1 & x \\ 1 & 1 & y \\ x & y & 1 \end{bmatrix}$$

*is PSD if and only if  $y = x$ , and*

$$\begin{bmatrix} 1 & -1 & x \\ -1 & 1 & y \\ x & y & 1 \end{bmatrix}$$

*is PSD if and only if  $y = -x$ .*

We now consider the case  $|a| < 1$ . Then the boundary of  $R$  is determined by  $1 + 2axy - a^2 - x^2 - y^2 = 0$ . This equation, which appears in [2, pp. 25–27], describes an ellipse whose axes lie along the lines  $y = \pm x$  and which is tangent to the sides of the square  $S$ . For example, if  $a = \frac{1}{2}$ , the graph is shown in Fig. 2. (This and subsequent graphs in Figs. 4 and 5 are generated by a MAPLE program.)

Since  $\det A > 0$  at  $(0, 0)$ ,  $\det A \geq 0$  in the interior and on the boundary of the ellipse. Thus, the set  $R$  is completely understood for  $n = 3$ .

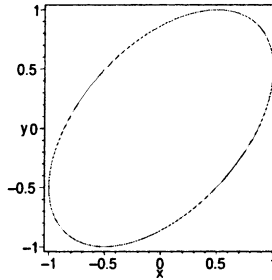


Fig. 2. PSD completion region for  $n = 3$ .

For  $n = 4$ , there are two possible configurations with two unspecified entries,

$$\begin{bmatrix} 1 & a & d & x \\ a & 1 & b & y \\ d & b & 1 & c \\ x & y & c & 1 \end{bmatrix} \tag{7}$$

and

$$A(x, y) = \begin{bmatrix} 1 & a & x & d \\ a & 1 & b & y \\ x & b & 1 & c \\ d & y & c & 1 \end{bmatrix}, \tag{8}$$

whose graphs are shown in Fig. 3(a) and (b), respectively. The edges have been labeled by the corresponding matrix entries.

We always assume  $|a| \leq 1$ ,  $|b| \leq 1$ ,  $|c| \leq 1$ ,  $|d| \leq 1$ . As the graphs in Fig. 3(a) and (b) are the only graphs on four vertices with four edges, any other 4-by-4 matrix with two unspecified entries is permutation similar to either (7) or (8). Likewise, if  $n > 4$ , there are just two graphs with two missing edges (depending on whether or not the missing edges are adjacent).

In [7, Section 2.2] it is shown that for any partial PSD matrix of order  $n \geq 4$  whose graph is missing two adjacent edges, the possible completion regions are either a single point, a line segment, or an ellipse. The matrix in (7) is a special case.

The graph in Fig. 3(b), a 4-cycle, is the simplest nonchordal graph. Our aim in this paper is to give a fairly complete description of the PSD completion region,

$$R = \left\{ (x, y) \in \mathbb{R}^2 \mid A(x, y) \text{ is PSD} \right\}.$$

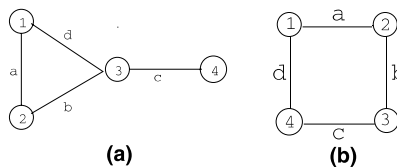


Fig. 3. Nonisomorphic graphs on four vertices with two unspecified entries.

We first show that the PSD completion problem for any partial PSD matrix whose graph is missing two nonadjacent edges can be reduced to the case of a 4-cycle.

### 3. Reduction to a 4-cycle

We need the following lemma from [6, p. 93].

**Lemma 1.** *If*

$$\begin{bmatrix} B & C \\ C^T & A \end{bmatrix}$$

*is PSD, then  $\mathfrak{R}(C) \subseteq \mathfrak{R}(B)$  and  $\mathfrak{R}(C^T) \subseteq \mathfrak{R}(A)$ .*

We note that Observation 1 is a special case of this lemma.

Let  $G$  be a graph on  $n$  vertices obtained from  $K_n$  by deleting two nonadjacent edges. Let  $\{1, 2, \dots, n\}$  be the vertex set of  $G$  and let  $\{n - 3, n - 1\}$  and  $\{n - 2, n\}$  be the two deleted edges.

Let

$$H(x, y) = \begin{bmatrix} B & C \\ C^T & A(x, y) \end{bmatrix}$$

be a partial PSD matrix with graph  $G$ , where  $A(x, y)$ , as before, is given by (8). We allow the possibility that  $B$  is singular. By Lemma 1,  $C = BE$  for some  $(n - 4)$ -by-4 matrix  $E$ . Multiplying  $H(x, y)$  on the right by

$$\begin{bmatrix} I & -B^\dagger C \\ 0 & I \end{bmatrix}$$

and on left by its transpose, we see that  $H(x, y)$  is PSD if and only if the Schur complement

$$S(x, y) = A(x, y) - C^T B^\dagger C,$$

of  $B$  in  $H(x, y)$ , is PSD. So, we analyze the PSD completion region for  $S(x, y)$ , which we express as

$$S(x, y) = \begin{bmatrix} d_1 & a_1 & x - x_0 & a_4 \\ a_1 & d_2 & a_2 & y - y_0 \\ x - x_0 & a_2 & d_3 & a_3 \\ a_4 & y - y_0 & a_3 & d_4 \end{bmatrix}.$$

If  $S(x, y)$  is not partial PSD, then the completion region is empty. If any  $d_i$  is 0, we have the completion problem for a 3-by-3 matrix with one unspecified entry, which we covered in Section 1. So assume all  $d_i$  are positive. Multiply  $S(x, y)$  on the left and right by  $\text{diag}(\frac{1}{\sqrt{d_1}}, \frac{1}{\sqrt{d_2}}, \frac{1}{\sqrt{d_3}}, \frac{1}{\sqrt{d_4}})$  to give the normalized

$$\bar{S}(x, y) = \begin{bmatrix} 1 & \frac{a_1}{\sqrt{d_1d_2}} & \frac{x-x_0}{\sqrt{d_1d_3}} & \frac{a_4}{\sqrt{d_1d_4}} \\ \frac{a_1}{\sqrt{d_1d_2}} & 1 & \frac{a_2}{\sqrt{d_2d_3}} & \frac{y-y_0}{\sqrt{d_2d_4}} \\ \frac{x-x_0}{\sqrt{d_1d_3}} & \frac{a_2}{\sqrt{d_2d_3}} & 1 & \frac{a_3}{\sqrt{d_3d_4}} \\ \frac{a_4}{\sqrt{d_1d_4}} & \frac{y-y_0}{\sqrt{d_2d_4}} & \frac{a_3}{\sqrt{d_3d_4}} & 1 \end{bmatrix}.$$

Letting

$$a = \frac{a_1}{\sqrt{d_1d_2}}, \quad b = \frac{a_2}{\sqrt{d_2d_3}}, \quad c = \frac{a_3}{\sqrt{d_3d_4}},$$

$$d = \frac{a_4}{\sqrt{d_1d_4}}, \quad x' = \frac{x - x_0}{\sqrt{d_1d_3}}, \quad y' = \frac{y - y_0}{\sqrt{d_2d_4}},$$

we find the PSD completion region inside the square  $S$  in  $x', y'$  coordinates as in the case  $n = 4$ . Then, by scaling and translation, we find the PSD completion region in terms of the given  $x, y$  coordinates inside the square  $[x_0 - \sqrt{d_1d_3}, x_0 + \sqrt{d_1d_3}] \times [y_0 - \sqrt{d_2d_4}, y_0 + \sqrt{d_2d_4}]$ . Hence, the reduction to the 4-cycle is done.

#### 4. Elementary cases of PSD completion region for the 4-cycle

Let  $A(x, y)$  be a partial PSD matrix as given in (8).

**Case I.** We determine conditions on  $(a, b, c, d)$  so that the PSD completion region  $R$  is a single point.

In order to do so, we consider the 3-by-3 principal submatrices of  $A(x, y)$  in which  $x$  appears:

$$A(x, y)[\{1, 2, 3\}] = \begin{bmatrix} 1 & a & x \\ a & 1 & b \\ x & b & 1 \end{bmatrix}, \quad A(x, y)[\{1, 3, 4\}] = \begin{bmatrix} 1 & x & d \\ x & 1 & c \\ d & c & 1 \end{bmatrix}.$$

If  $(x, y)$  is a point in  $R$ , these two matrices are PSD. By Proposition 2, we have  $|x - ab|^2 \leq (1 - a^2)(1 - b^2)$  and  $|x - cd|^2 \leq (1 - c^2)(1 - d^2)$ . Equivalently,  $x$  lies in the intersection of the intervals

$$I_1 = \left[ ab - \sqrt{(1 - a^2)(1 - b^2)}, ab + \sqrt{(1 - a^2)(1 - b^2)} \right]$$

and

$$I_2 = \left[ cd - \sqrt{(1 - c^2)(1 - d^2)}, cd + \sqrt{(1 - c^2)(1 - d^2)} \right].$$

Thus, a necessary condition that  $R \neq \emptyset$  is that  $I_1 \cap I_2 \neq \emptyset$  or equivalently,

$$|ab - cd| \leq \sqrt{(1 - a^2)(1 - b^2)} + \sqrt{(1 - c^2)(1 - d^2)}. \tag{9}$$

Conversely, if  $x_0 \in I_1 \cap I_2$ , then  $A(x_0, y)[\{1, 2, 3\}]$  and  $A(x_0, y)[\{1, 3, 4\}]$  are PSD and  $A(x_0, y)$  has a PSD completion by Proposition 2. Therefore, in order that  $A(x, y)$  have a PSD completion ( $R \neq \emptyset$ ) it is necessary and sufficient that inequality (9) holds. (This criterion is given in [2].)

Now assume that  $A(x, y)$  has a unique PSD completion. Then  $I_1 \cap I_2$  must be a single point. If  $I_1$  and  $I_2$  are nondegenerate intervals, this occurs if and only if

$$ab \pm \sqrt{(1 - a^2)(1 - b^2)} = cd \mp \sqrt{(1 - c^2)(1 - d^2)},$$

equivalently,

$$|ab - cd| = \sqrt{(1 - a^2)(1 - b^2)} + \sqrt{(1 - c^2)(1 - d^2)}.$$

Otherwise  $I_1 = \{ab\}$  and  $|a| = 1$  or  $|b| = 1$ , or  $I_2 = \{cd\}$  and  $|c| = 1$  or  $|d| = 1$ . If  $|a| = 1$ , then  $ab \in I_2$ , i.e.,  $|ab - cd| \leq \sqrt{(1 - c^2)(1 - d^2)}$ , or on simplifying  $1 + 2abcd - b^2 - c^2 - d^2 \geq 0$ . Adding and subtracting  $a^2 = 1$ , we can write this in a symmetric form as  $2 + 2abcd - a^2 - b^2 - c^2 - d^2 \geq 0$ . The cases  $|b| = 1$ ,  $|c| = 1$ , and  $|d| = 1$  give the same inequality. It remains to observe that if  $I_1 \cap I_2$  is a single point  $x_0$ , then at least one of  $A(x_0, y)[\{1, 2, 3\}]$ ,  $A(x_0, y)[\{1, 3, 4\}]$  is singular. Regarding  $y$  as the unspecified entry in  $A(x_0, y)$ , it follows from Proposition 2 that there is a unique  $y_0$  such that  $A(x_0, y_0)$  is PSD. We have proved:

**Proposition 3.** *The completion region  $R$  of the partial PSD matrix  $A(x, y)$  given in (8) is a single point if and only if either*

$$|ab - cd| = \sqrt{(1 - a^2)(1 - b^2)} + \sqrt{(1 - c^2)(1 - d^2)}, \tag{10}$$

or

$$\begin{aligned} &\text{one of } a, b, c, d \text{ has modulus 1 and} \\ &a^2 + b^2 + c^2 + d^2 \leq 2(1 + abcd). \end{aligned}$$

In Section 7 we give another formulation of this result in Proposition 6.

The argument preceding Proposition 3 also shows that the completion region  $R$  for  $A(x, y)$  cannot be a horizontal or vertical line segment. However, it can be any point  $(x_0, y_0)$  in the square  $S$ . To see this, choose any  $c$ ,  $|c| \leq 1$ , such that

$$\begin{bmatrix} 1 & x_0 & y_0 \\ x_0 & 1 & c \\ y_0 & c & 1 \end{bmatrix}$$

is PSD, which is possible by Proposition 2. Then  $1 + 2x_0y_0c \geq x_0^2 + y_0^2 + c^2$ , so by Observation 1 and Proposition 3, the completion region  $R$  of the matrix

$$\begin{bmatrix} 1 & 1 & x & y_0 \\ 1 & 1 & x_0 & y \\ x & x_0 & 1 & c \\ y_0 & y & c & 1 \end{bmatrix}$$



is  $\{(x_0, y_0)\}$ .

**Case II.** At the other extreme, suppose that  $a = b = c = d = 0$ . Then  $A(x, y)$  is permutation similar to

$$\begin{bmatrix} 1 & x \\ x & 1 \end{bmatrix} \oplus \begin{bmatrix} 1 & y \\ y & 1 \end{bmatrix},$$

so the PSD completion region is all of  $S$ . The converse is also true. In fact, if the PSD completion region contains two corners of the square  $S$ , then necessarily  $a = b = c = d = 0$ . To see this, assume that

$$A(1, 1) = \begin{bmatrix} 1 & a & 1 & d \\ a & 1 & b & 1 \\ 1 & b & 1 & c \\ d & 1 & c & 1 \end{bmatrix} \quad \text{and} \quad A(-1, 1) = \begin{bmatrix} 1 & a & -1 & d \\ a & 1 & b & 1 \\ -1 & b & 1 & c \\ d & 1 & c & 1 \end{bmatrix}$$

are PSD. Then, by Observation 1,  $A(1, 1)[1, 2, 3]$ ,  $A(1, 1)[1, 3, 4]$  and  $A(1, 1)[1, 2, 4]$  are PSD if and only if  $a = b$ ,  $c = d$  and  $a = d$ , respectively. Hence, we must have  $a = b = c = d$ . Similarly,  $A(-1, 1)[1, 2, 3]$  is PSD if and only if  $a = -b$ , so we have  $a = b = c = d = 0$ . A similar argument applies for any other pair of corners of  $S$ .

So we may assume, whenever convenient, that  $|a|, |b|, |c|, |d| < 1$  and are not all 0. If  $(x, y)$  is a boundary point of the completion region  $R$ , then  $\det A(x, y) = 0$ . We have

$$\det A(x, y) = D + 2Ex + 2Gy - 2Fxy - x^2 - y^2 + x^2y^2, \tag{11}$$

where

$$\begin{aligned} D &= 1 - a^2 - b^2 - c^2 - d^2 + a^2c^2 - 2abcd + b^2d^2, \\ E &= ab + cd, \quad F = ac + bd, \quad G = ad + bc. \end{aligned} \tag{12}$$

We wish to observe that the function  $\det A(x, y)$  has no relative minima. For if  $(x_0, y_0)$  is a relative minimum,

$$\frac{\partial^2 \det A}{\partial x^2}(x_0, y_0) = 2(y_0^2 - 1) \geq 0 \quad \text{and} \quad \frac{\partial^2 \det A}{\partial y^2}(x_0, y_0) = 2(x_0^2 - 1) \geq 0$$

so that  $|x_0| = |y_0| = 1$ . But then positive semidefiniteness of the 2-by-2 Hessian matrix of  $\det A(x, y)$  requires that

$$\frac{\partial^2 A}{\partial x \partial y}(x_0, y_0) = 4x_0y_0 - 2F = 0$$

so  $|F| = 2|x_0| |y_0| = 2$  which implies  $|a| = |b| = |c| = |d| = 1$ .

One consequence of particular interest is that  $\det A(x, y)$  cannot vanish at an interior point of  $R$ . Therefore  $A(x, y)$  is PD at all interior points of  $R$ .

**Case III.** For our final elementary case, we assume that  $A(0, 0)$  is PD and that the boundary of  $R$  is symmetric with respect to the origin. In particular, there must be

boundary points  $(x_0, 0)$ ,  $(-x_0, 0)$ ,  $0 < x_0 \leq 1$ , and  $(0, y_0)$ ,  $(0, -y_0)$ ,  $0 < y_0 \leq 1$ . Then,  $\det A(x_0, 0) = \det A(-x_0, 0) = 0$  implies that  $E = 0$ , while  $\det A(0, y_0) = \det A(0, -y_0) = 0$  implies that  $G = 0$ . Then the equation  $\det A(x, y) = 0$  becomes  $D - 2Fxy - x^2 - y^2 + x^2y^2 = 0$ , which is clearly symmetric about the origin.

We now determine the ordered quadruples  $(a, b, c, d)$  so that

$$E = ab + cd = 0, \quad G = ad + bc = 0. \tag{13}$$

**Subcase 1.**  $abcd = 0$ . Without loss of generality, assume that  $d = 0$ . Then from (13),  $ab = bc = 0$ .

(i) If  $b = 0$ , then  $A(x, y)$  becomes

$$\begin{bmatrix} 1 & a & x & 0 \\ a & 1 & 0 & y \\ x & 0 & 1 & c \\ 0 & y & c & 1 \end{bmatrix},$$

and  $\det A(x, y) = 0$  reduces to

$$(1 - a^2)(1 - c^2) - 2acxy - x^2 - y^2 + x^2y^2 = 0. \tag{14}$$

The graph of the curve in (14) inside  $S$  for  $a = .9, c = .8$  is shown in Fig. 4, and this is typical if  $ac > 0$  and  $a \neq c$ . If  $ac < 0, a \neq -c$ , the graph is a  $90^\circ$  rotation of the graph for  $a, -c$ . The completion region  $R$  is the interior and boundary of the inner “ellipse like” region.

We will not give a complete description of the entire curve (14) here; we only verify that the boundary of  $R$  is a proper subset of the curve for  $|a| \neq |c|$ . Along the line  $y = -x$ ,  $\det A(x, -x) = x^4 - 2(1 - ac)x^2 + (1 - a^2)(1 - c^2)$  vanishes at  $x = \pm\sqrt{(1 + a)(1 - c)}$ ,  $x = \pm\sqrt{(1 - a)(1 + c)}$  and, for  $a \neq c$ , is negative at the intermediate values  $x = \pm\sqrt{1 - ac}$ . Similarly, along  $y = x$ ,  $\det A(x, x)$  vanishes at  $x = \pm\sqrt{(1 + a)(1 + c)}$ ,  $x = \pm\sqrt{(1 - a)(1 - c)}$  and, for  $c \neq -a$ , is negative at the intermediate values  $x = \pm\sqrt{1 + ac}$ . (For the values of  $a, c$  in Fig. 4, there are two zeros of  $\det A(x, y)$  along  $y = x$  that lie outside  $S$ .) We will consider the case  $|a| = |c|$  after a discussion of singular points. Since  $R$  is a closed convex set, it must

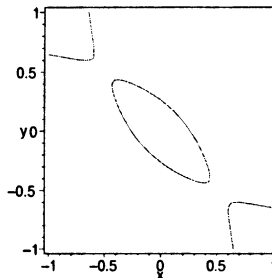


Fig. 4. A smooth PSD completion region for the 4-cycle.

be the inner “ellipse like” region as claimed. Thus we have shown that there can be points  $(x, y)$  not in  $\partial R$  for which  $\det A(x, y) = 0$ . It is easily seen that the curve  $\det A(x, y) = 0$  is symmetric about the lines  $y = \pm x$ . If  $c = 0$ , then  $\det A(x, y) = 0$  reduces to  $1 - a^2 - x^2 - y^2 + x^2y^2 = 0$ , which is also symmetric about the two axes. The boundary of  $R$  is a smooth simple closed curve as can be seen by writing the equation in polar form,  $r^2 - \frac{1}{4}r^4 \sin^2 2\theta = 1 - a^2$ .

(ii) If  $b \neq 0$ , then  $a = c = 0$  and, upon interchanging the pairs  $(a, c)$  and  $(b, d)$ , this is the same as the case discussed in (i)

**Subcase 2.**  $abcd \neq 0$ . Then from (13),  $d = -ab/c = -bc/a$ , which implies  $a^2 = c^2$ , giving two isomorphic cases:  $c = a, d = -b$  and  $c = -a, d = b$ .

We consider just the first case:  $c = a, d = -b$ . Then  $A(x, y)$  becomes

$$\begin{bmatrix} 1 & a & x & -b \\ a & 1 & b & y \\ x & b & 1 & a \\ -b & y & a & 1 \end{bmatrix},$$

and  $\det A(x, y) = 0$  reduces to

$$(1 - a^2 - b^2)^2 - 2(a^2 - b^2)xy - x^2 - y^2 + x^2y^2 = 0. \tag{15}$$

By (9),  $A(x, y)$  has a PSD completion if and only if

$$a^2 + b^2 \leq 1. \tag{16}$$

Note that (15) has much in common with (14); in fact, it can always be written in that form. To see this, first replace  $a$  by  $h$  in (14), so

$$(1 - h^2)(1 - c^2) - 2hcxy - x^2 - y^2 + x^2y^2 = 0.$$

To show that (15) can be put in this form, it suffices to show that given  $a, b$  with  $a^2 + b^2 \leq 1$ , there exist  $h, c$  with  $|h|, |c| \leq 1$  such that

$$hc = a^2 - b^2, \quad (1 - h^2)(1 - c^2) = (1 - a^2 - b^2)^2. \tag{17}$$

If  $b^2 = a^2$ , take  $c = 0$  and  $h^2 = 4a^2(1 - a^2)$ . So suppose  $b^2 \neq a^2$ ; we just give the argument in the case  $a^2 > b^2$ . If  $b = 0$ , let  $h = c = a$ ; so assume  $b \neq 0$ . Then, in the variables  $h$  and  $c$ , the curve  $hc = a^2 - b^2$  is a hyperbola intersecting the first and third quadrants of  $S$ , and  $(\sqrt{a^2 - b^2}, \sqrt{a^2 - b^2})$  lies on the curve. Moreover,  $(\sqrt{a^2 + b^2}, \sqrt{a^2 + b^2})$  and  $(\sqrt{1 - (1 - a^2 - b^2)^2}, 0)$  are points on the curve  $(1 - h^2)(1 - c^2) = (1 - a^2 - b^2)^2$ . Since these are on opposite sides of the branch of  $hc = a^2 - b^2$  in the first quadrant, by a continuity argument there is a point  $(h_0, c_0)$  in the first quadrant lying on both of the curves in (17). This concludes the argument. It follows that the set of possible completion regions in Subcase 2 coincides with the set of completion regions in (i) of Subcase 1 (excluding those for which  $|a| = |c|$ ).

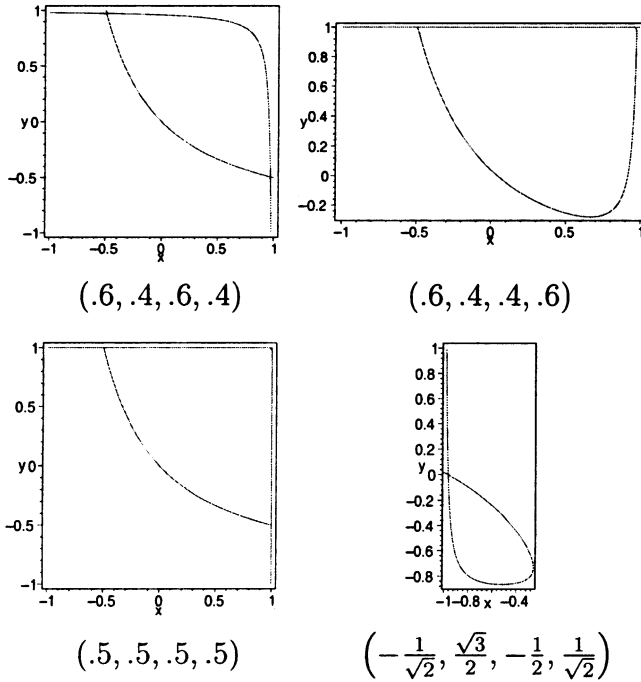


Fig. 5. PSD completion regions with singular points.

**5. Singular points on the boundary of  $R$**

The completion region  $R$  for  $A(x, y)$  is extremely sensitive to the values of the specified entries  $a, b, c, d$ . Four examples are given in Fig. 5.

Unlike the region in Fig. 4, the boundary of  $R$  in these four cases is not smooth because there are points on the boundary of  $R$  at which there is not a unique tangent line. These points on the boundary of  $R$  are singular points, defined as follows:

**Definition 3.** A singular point  $(x_0, y_0)$  of  $R$  is a point on the boundary of  $R$  simultaneously satisfying the equations:

$$\det A(x, y) = 0, \quad \frac{\partial}{\partial x} \det A(x, y) = 0, \quad \frac{\partial}{\partial y} \det A(x, y) = 0. \tag{18}$$

(We note that singular points of a curve need not always be sharp points; they may in some cases appear smooth.)

From Eq. (11), these three equations are

$$D + 2Ex + 2Gy - 2Fxy - x^2 - y^2 + x^2y^2 = 0, \tag{19}$$

$$E - Fy + x(y^2 - 1) = 0 \tag{20}$$

and

$$G - Fx + y(x^2 - 1) = 0, \tag{21}$$

respectively.

As a simple example, consider (i) of Subcase 1 of Case III in Section 4, in which  $b = d = 0$ . We also assume  $|a|, |c| < 1$  (otherwise  $R$  is the single point  $(0, 0)$ ). Then Eqs. (19), (20) and (21) become

$$\begin{aligned} (1 - a^2)(1 - c^2) - 2acxy - x^2 - y^2 + x^2y^2 &= 0, \\ -acy - x + xy^2 &= 0, \\ -acx - y + x^2y &= 0. \end{aligned}$$

We now show that there are two singular points on the boundary  $\partial R$  if and only if  $|c| = |a|$ . For the only if part, adding  $-x$  times the second equation to  $y$  times the third equation gives  $x^2 - y^2 = 0$ , so  $y = \pm x$ . First substituting  $y = x$  in the first and second equations gives

$$\begin{aligned} x^4 - 2(1 + ac)x^2 + (1 - a^2)(1 - c^2) &= 0, \\ x^3 - (1 + ac)x &= 0. \end{aligned}$$

Since  $|a|, |c| < 1$ ,  $x \neq 0$  and we find that  $x^2 = 1 + ac$  so that  $(1 + ac)^2 = (1 - a^2)(1 - c^2)$ , which reduces to  $(a + c)^2 = 0$ . Hence,  $c = -a$ . In this case, the two points  $(\pm\sqrt{1 - a^2}, \pm\sqrt{1 - a^2})$  both satisfy Eqs. (19), (20) and (21), and hence they are singular points on  $\partial R$ . Similarly, if  $y = -x$ , then  $c = a$  and the singular points are then  $(\pm\sqrt{1 - a^2}, \mp\sqrt{1 - a^2})$ . For  $|c| \neq |a|$ , the boundary is smooth as in Fig. 4, and this completes the special case.

It is also convenient to give Eqs. (20) and (21) in the form obtained by applying partial derivatives directly to  $\det A(x, y)$  in (8) (by the product rule for derivatives, the derivative of a determinant is the sum of the determinants obtained by differentiating one row at a time):

$$\frac{1}{2} \frac{\partial}{\partial x} \det A(x, y) = \det A[\{2, 3, 4\}, \{1, 2, 4\}] = \det \begin{bmatrix} a & 1 & y \\ x & b & c \\ d & y & 1 \end{bmatrix} = 0, \tag{22}$$

$$\frac{1}{2} \frac{\partial}{\partial y} \det A(x, y) = \det A[\{1, 3, 4\}, \{1, 2, 3\}] = \det \begin{bmatrix} 1 & a & x \\ x & b & 1 \\ d & y & c \end{bmatrix} = 0. \tag{23}$$

In Section 6 we investigate all the possible factorizations of  $\det A(x, y)$ . We call a factor of  $\det A(x, y)$  simple if its multiplicity is one. The following lemma shows that the number of singular points cannot exceed the number of simple irreducible factors of  $\det A(x, y)$ .

**Lemma 2.** Assume  $\det A(x, y)$  given by (11) factors into  $c$  simple nonconstant irreducible polynomials. Then the number of singular points on the boundary of the curve  $\det A(x, y) = 0$  is bounded above by  $c$ .

**Proof.** Consider (19) for  $\det A(x, y) = 0$  and homogenize with a third variable  $z$  to obtain the polynomial

$$f(x : y : z) = Dz^4 + 2Exz^3 + 2Gyz^3 - 2Fxyz^2 - x^2z^2 - y^2z^2 + x^2y^2, \quad (24)$$

which defines a curve in the complex projective plane.

Since  $f(1:0:0) = f(0:1:0) = 0$ ,  $(1:0:0)$  and  $(0:1:0)$  are points at infinity of the curve in (24). The partial derivatives of  $f$  are

$$\begin{aligned} \frac{\partial f}{\partial x} &= 2Ez^3 - 2Fyz^2 - 2xz^2 + 2xy^2, \\ \frac{\partial f}{\partial y} &= 2Gz^3 - 2Fxz^2 - 2yz^2 + 2x^2y, \\ \frac{\partial f}{\partial z} &= 4Dz^3 + 6Exz^2 + 6Gyz^2 - 4Fxyz - 2x^2z - 2y^2z. \end{aligned}$$

At  $(1:0:0)$  and  $(0:1:0)$ ,  $\nabla f = (0:0:0)$ , so  $f$  is singular at both points at infinity.

We now make use of the following result for a reduced projective plane curve (i.e., one with no irreducible components of multiplicity greater than one), which is an immediate consequence of problem 5-25 [3]. If such a curve has degree  $n$  and  $c$  irreducible components, we have

$$\# \text{ of singular points} \leq \frac{(n-1)(n-2)}{2} + c - 1. \quad (25)$$

Since by hypothesis  $\det A(x, y)$  has only simple irreducible factors, so does  $f(x : y : z)$ . Since  $\deg f(x : y : z) = 4$ , by (25), # of singular points  $\leq c + 2$ . Excluding the two singular points at infinity,  $f$  has at most  $c$  singular points in the affine plane and consequently there can be at most  $c$  singular points of the curve  $\det A(x, y) = 0$ .  $\square$

In the following two sections we examine ways that singular points arise and their connection with the rank of a completion of  $A(x, y)$ ,

## 6. Factorization of $\det A(x, y)$

In this section we assume that the PSD completion region  $R$  of  $A(x, y)$  is not empty.

If  $\det A(x, y)$  can be factored as

$$\det A(x, y) = f(x, y)g(x, y), \quad (26)$$

where  $f$  and  $g$  are nonconstant polynomials in  $x$  and  $y$ , then since

$$\frac{\partial}{\partial x} \det A(x, y) = f \frac{\partial g}{\partial x} + \frac{\partial f}{\partial x} g, \quad \frac{\partial}{\partial y} \det A(x, y) = f \frac{\partial g}{\partial y} + \frac{\partial f}{\partial y} g,$$

we have the elementary, but useful result:

**Proposition 4.** *If Eq. (26) holds and  $(x_0, y_0)$  is a point on the boundary of  $R$  that is a common zero of  $f(x, y) = 0$  and  $g(x, y) = 0$ , then  $(x_0, y_0)$  is a singular point of  $R$ .*

We now proceed to determine the ordered quadruples  $(a, b, c, d)$  for which  $\det A(x, y)$  can be factored, and the coordinates of the singular points in each case.

**Case 1.**  *$f$  and  $g$  are both quadratic polynomials in  $x$  and  $y$ .*

Let

$$f(x, y) = a_{20}x^2 + a_{11}xy + a_{02}y^2 + a_{10}x + a_{01}y + a_{00}$$

and

$$g(x, y) = b_{20}x^2 + b_{11}xy + b_{02}y^2 + b_{10}x + b_{01}y + b_{00}.$$

I. Suppose  $a_{20} \neq 0$ . Comparing the terms of the product  $f(x, y)g(x, y)$  with those of (11), we set the coefficients of  $x^4, x^3y$  and  $x^3$  equal to 0. That is,  $a_{20}b_{20} = 0$ ,  $a_{20}b_{11} + a_{11}b_{20} = 0$  and  $a_{20}b_{10} + a_{10}b_{20} = 0$ , which give us  $b_{20} = b_{11} = b_{10} = 0$ . This leaves  $a_{20}b_{02}$  as the coefficient of  $x^2y^2$ , so  $b_{02} \neq 0$ . Similarly,  $a_{02} = a_{11} = a_{01} = 0$ , hence,  $f$  and  $g$  reduce to  $a_{20}x^2 + a_{10}x + a_{00}$  and  $b_{02}y^2 + b_{01}y + b_{00}$ , respectively. Comparing terms again yields  $a_{20}b_{01} = 0$ ,  $a_{10}b_{02} = 0$ ,  $a_{20}b_{02} = 1$ ,  $a_{20}b_{00} = -1$ ,  $a_{00}b_{02} = -1$  and  $a_{00}b_{00} = D$ , which give us  $a_{10} = b_{01} = 0$ ,  $b_{02} = 1/a_{20}$ ,  $a_{00} = -a_{20}$  and  $b_{00} = -b_{02}$ . So,  $f(x, y)g(x, y)$  reduces to  $(x^2 - 1)(y^2 - 1)$  and, hence,

$$(1 - x)(1 + x)(1 - y)(1 + y), \tag{27}$$

a linear factorization of (11).

We now find necessary conditions on  $a, b, c, d$  so that (27) is obtained. Comparing the terms of (27) with (11), we must have  $E = F = G = 0$  and  $D = 1$ . From Subcases 1 and 2 of Case III in Section 4,  $E = G = 0$  implies either  $b = d = 0$  ( $c = a = 0$ ) or  $c = a$ ,  $d = -b$  ( $c = -a$ ,  $d = b$ ).

With  $d = b = 0$ , then  $F = 0$ , implies  $c = 0$  or  $a = 0$ . If  $c = 0$ , then  $D = 1$  implies  $a = 0$ . Hence,  $a = b = c = d = 0$ . If  $c = a$ ,  $d = -b$ , then  $1 = D = (1 - (a^2 + b^2))^2$ . If  $a^2 + b^2 = 2$ , then  $|a| = |b| = 1$ . For example, if  $a = b = 1$ , then

$$A(x, y) = \begin{bmatrix} 1 & 1 & x & -1 \\ 1 & 1 & 1 & y \\ x & 1 & 1 & 1 \\ -1 & y & 1 & 1 \end{bmatrix},$$

which has no PSD completion [5, p. 178]. The other three possibilities for  $(a, b, c, d)$  are  $(1, -1, 1, 1)$ ,  $(-1, 1, -1, -1)$  and  $(-1, -1, -1, 1)$ , which also yield an empty completion region  $R$ . Thus  $a^2 + b^2$  cannot be 2, so  $a^2 + b^2 = 0$ , and again  $a = b = c = d = 0$ . Thus, (27) is a factorization of (11) if and only if  $a, b, c, d$  are all zero, and in this case the singular points are  $(-1, -1), (-1, 1), (1, -1), (1, 1)$ . By (27) and Lemma 2, these are the only singular points of  $R$ .

II. Suppose  $a_{20} = a_{02} = b_{20} = b_{02} = 0$ . Then,  $f$  and  $g$  reduce to

$$a_{11}xy + a_{10}x + a_{01}y + a_{00}$$

and

$$b_{11}xy + b_{10}x + b_{01}y + b_{00},$$

respectively. Comparing the coefficient of  $x^2y^2$  in (11) with that of the product  $f(x, y)g(x, y)$  implies  $a_{11}b_{11} = 1$ . Without loss of generality, we may assume  $a_{11} = b_{11} = 1$ . Otherwise,  $b_{11} = 1/a_{11}$ , and by factoring  $a_{11}$  from  $f$ ,  $1/a_{11}$  from  $g$ , and by renaming the coefficients of  $f$  and  $g$ , the product  $f(x, y)g(x, y)$  becomes

$$(xy + c_{10}x + c_{01}y + c_{00})(xy + d_{10}x + d_{01}y + d_{00}). \tag{28}$$

Comparing the coefficients of  $x^2y$  and  $x^2$  in (11) and (28) gives, respectively,  $c_{10} + d_{10} = 0$ ,  $c_{10}d_{10} = -1$  which yield  $d_{10} = -c_{10} = -1/c_{10}$  and this implies  $d_{10} = -c_{10} = \pm 1$ . Similarly,  $d_{01} = -c_{01} = \pm 1$ . So (28) becomes

$$(xy + c_{10}x + c_{01}y + c_{00})(xy - c_{10}x - c_{01}y + d_{00}). \tag{29}$$

Again, comparing the coefficients of  $x, y, xy$  and  $1$  in (11) with those of the product (29) yields  $c_{10}(d_{00} - c_{00}) = 2E$ ,  $c_{01}(d_{00} - c_{00}) = 2G$ ,  $d_{00} - 2c_{01}c_{10} + c_{00} = -2F$  and  $c_{00}d_{00} = D$  which gives

$$d_{00} - c_{00} = 2E/c_{10} = 2G/c_{01}, \tag{30}$$

$d_{00} = -c_{00} + 2c_{01}c_{10} - 2F$  and  $c_{00}^2 + 2(F - c_{01}c_{10})c_{00} + D = 0$ . Hence, solving the last two equations for  $c_{00}$  and then  $d_{00}$  yields

$$c_{00} = c_{01}c_{10} - F \pm \sqrt{F^2 - 2c_{01}c_{10}F + c_{01}^2c_{10}^2 - D}$$

and

$$d_{00} = c_{01}c_{10} - F \mp \sqrt{F^2 - 2c_{01}c_{10}F + c_{01}^2c_{10}^2 - D}.$$

With (30),

$$d_{00} - c_{00} = 2E/c_{10} = 2G/c_{01} = \pm 2\sqrt{F^2 - 2c_{01}c_{10}F + c_{01}^2c_{10}^2 - D}. \tag{31}$$

Since  $|c_{01}| = |c_{10}| = 1$ , we have two subcases to consider:

(i)  $c_{10}c_{01} = 1$ . Then (31) gives

$$E = G = \pm\sqrt{(F - 1)^2 - D} \tag{32}$$



From  $E = G$ , either  $c = a$  or  $d = b$ . Without loss of generality, assume  $c = a$ . Then,  $E = a(b + d)$ ,  $F = a^2 + bd$ ,  $D = 1 - 2a^2 - b^2 - d^2 + a^4 - 2a^2bd + b^2d^2$ , and with a little algebra, (32) reduces to  $(1 - a^2)(b - d)^2 = 0$ , so either  $d = b$  or  $|a| = 1$ . We first show that  $|a| = 1$  implies  $d = b$ . So suppose  $a = 1$ . Then  $c = a = 1$  and

$$A(x, y) = \begin{bmatrix} 1 & 1 & x & d \\ 1 & 1 & b & y \\ x & b & 1 & 1 \\ d & y & 1 & 1 \end{bmatrix}.$$

By Observation 1,  $A(x, y)[1, 2, 3]$  and  $A(x, y)[1, 3, 4]$  are PSD if and only if  $x = b$  and  $x = d$ , respectively. So,  $d = b$ . A similar argument shows if  $a = -1$  then  $d = b$ . So, we have  $a = c$  and  $d = b$ . Then  $E = G = 2ab$ ,  $F = a^2 + b^2$ ,  $D = (1 - a^2 - b^2)^2 - 4a^2b^2$ ,  $c_{00} = 1 - a^2 - b^2 \pm 2ab$  and  $d_{00} = 1 - a^2 - b^2 \mp 2ab$ . Since,  $d_{00} - c_{00} = 2E/c_{10}$ , then  $c_{10} = 1$  implies that  $c_{00} = 1 - a^2 - b^2 - 2ab$  and  $d_{00} = 1 - a^2 - b^2 + 2ab$ , while  $c_{10} = -1$  implies that  $c_{00} = 1 - a^2 - b^2 + 2ab$  and  $d_{00} = 1 - a^2 - b^2 - 2ab$ . In either case, (29) becomes

$$(xy + x + y + 1 - a^2 - b^2 - 2ab)(xy - x - y + 1 - a^2 - b^2 + 2ab). \quad (33)$$

We now describe the completion region  $R$  for the matrix

$$M(x, y) = \begin{bmatrix} 1 & a & x & b \\ a & 1 & b & y \\ x & b & 1 & a \\ b & y & a & 1 \end{bmatrix}.$$

There are several cases to consider.

$|b| \neq |a|$ ,  $|a|, |b| < 1$ : In this case (33) does not factor any further and  $\det M(x, y) = 0$  describes two hyperbolas symmetric about  $y = x$ . Writing these as

$$(x + 1)(y + 1) = (a + b)^2, \quad (x - 1)(y - 1) = (a - b)^2,$$

we see that they have asymptotes  $x = -1, y = -1$ , and  $x = 1, y = 1$ , respectively. The first graph in Fig. 5 is an example of this case. Each hyperbola has one branch passing through the square  $S$ . Let  $B_+(B_-)$  be the branch passing through  $S$  corresponding to the hyperbola with asymptotes  $x = 1, y = 1$  ( $x = -1, y = -1$ ). We claim that the PSD completion region  $R$  is the region bounded by  $B_+$  and  $B_-$ . Solving for the common zeros of the two factors in (33) we find that  $B_+$  and  $B_-$  intersect at the two points

$$P_1: \left( ab - \sqrt{(1 - a^2)(1 - b^2)}, ab + \sqrt{(1 - a^2)(1 - b^2)} \right)$$

and

$$P_2: \left( ab + \sqrt{(1 - a^2)(1 - b^2)}, ab - \sqrt{(1 - a^2)(1 - b^2)} \right).$$

The midpoint of  $P_1$  and  $P_2$  is  $(ab, ab)$ . Substituting  $x = y = ab$  in  $M$ , we have

$$M(ab, ab) = \begin{bmatrix} 1 & a & ab & b \\ a & 1 & b & ab \\ ab & b & 1 & a \\ b & ab & a & 1 \end{bmatrix}.$$

Since  $\det M(ab, ab) = (1 - a^2)^2(1 - b^2)^2 > 0$ , and each principal submatrix of order 3 has determinant equal to  $(1 - a^2)(1 - b^2) > 0$ ,  $M(ab, ab)$  is PD. It follows that  $M(x, y)$  is PD at each point in the region bounded by  $B_+$  and  $B_-$ . Moreover, at the centers of the two hyperbolas,  $\det M(1, 1) = (a - b)^2[(a + b)^2 - 4] < 0$  and  $\det M(-1, -1) = (a + b)^2[(a - b)^2 - 4] < 0$ . Consequently,  $\det M(x, y)$  is negative at all interior points of any line segment from  $(1, 1)$  to a point on  $B_+$  between  $P_1$  and  $P_2$  and at all interior points of any line segment from  $(-1, -1)$  to a point on  $B_-$  between  $P_1$  and  $P_2$ . Because  $R$  is a convex set, it is contained in, and therefore equal to, the region bounded by  $B_+$  and  $B_-$ . By Proposition 4,  $P_1$  and  $P_2$  are singular points and by Lemma 2, there are at most two singular points.

$0 \neq a = b \neq \pm 1$ : Then (33) factors further to

$$(x - 1)(y - 1)(xy + x + y + 1 - 4a^2),$$

and  $M(x, y)$  reduces to

$$K(x, y) = \begin{bmatrix} 1 & a & x & a \\ a & 1 & a & y \\ x & a & 1 & a \\ a & y & a & 1 \end{bmatrix}.$$

The point  $(|a|, |a|)$  is inside the region  $R$  bounded by  $x = 1, y = 1$  and the branch of  $xy + x + y + 1 - 4a^2 = 0$  passing through  $S$ . Since  $K(|a|, |a|)$  is PD, and  $K(-1, -1)$  is not PD, it follows that  $R$  is the PD completion region for  $K(x, y)$ . The singular points are  $(1, 1), (1, 2a^2 - 1)$ , and  $(2a^2 - 1, 1)$ . By Lemma 2 there can be no others. The third graph in Fig. 5 illustrates this case.

$0 \neq a = -b \neq \pm 1$ : Then (33) factors as  $(x + 1)(y + 1)(xy - x - y + 1 - 4a^2)$ , and the PSD completion region is the region bounded by  $x = -1, y = -1$ , and the branch of  $xy - x - y + 1 - 4a^2$  passing through  $S$ . The singular points are  $(-1, -1), (-1, 1 - 2a^2)$  and  $(1 - 2a^2, -1)$ .

$a = b = 0$ : This was done in part I.

$|a| = 1$  or  $|b| = 1$ : By Proposition 3 the completion region is a single point. For example, if  $a = 1$ , it is  $(b, b)$ , which is a singular point.

(ii)  $c_{10}c_{01} = -1$ . By following an argument similar to (i) above,  $c = -a$  and  $d = -b$ . Then (29) factors as

$$(xy - x + y - 1 + a^2 + b^2 + 2ab)(xy + x - y - 1 + a^2 + b^2 - 2ab). \quad (34)$$

The results are like those in (i). There is one singular point if  $|a| = 1$  or  $|b| = 1$ , there are two singular points if  $1 \neq |b| \neq |a| \neq 1$ , three if  $a = b = -c = -d$  or  $a = -b = -c = d$  with  $|a| \neq 0, 1$ , and four if  $a = b = c = d = 0$ .

**Case 2.**  $f$  is cubic and  $g$  is linear in  $x$  and  $y$ .

Let

$$f(x, y) = a_{30}x^3 + a_{21}x^2y + a_{12}xy^2 + a_{03}y^3 + a_{20}x^2 + a_{11}xy + a_{02}y^2 + a_{10}x + a_{01}y + a_{00}$$

and

$$g(x, y) = b_{10}x + b_{01}y + b_{00}.$$

I. Suppose  $a_{30} \neq 0$ . As in I of Case 1 above, setting the coefficients of  $x^4$  and  $x^3y$  equal to 0 gives  $b_{10} = b_{01} = 0$  and hence, no factorization exists.

II. Suppose  $a_{30} = a_{03} = 0$ ,  $a_{21} \neq 0$ . Then  $f$  reduces to  $a_{21}x^2y + a_{12}xy^2 + a_{20}x^2 + a_{11}xy + a_{02}y^2 + a_{10}x + a_{01}y + a_{00}$ .

Following an analysis similar to Case 1 we obtain

$$f(x, y)g(x, y) = (x^2y + c_{20}x^2 + c_{10}x + c_{01}y + c_{00})(y + d_{00}). \tag{35}$$

Comparing coefficients of  $x^2y$ ,  $x^2$ ,  $y^2$ ,  $xy$ ,  $x$ , 1 and  $y$  with the terms of (11) yields  $c_{20} = -d_{00} = \pm 1$ ,  $c_{01} = -1$ ,  $c_{10} = -2F$ ,  $E = c_{20}F$ ,  $c_{00} = -D/c_{20}$  and  $2G = (c_{20}^2 - D)/c_{20}$ . Then  $f(x, y)g(x, y)$  becomes

$$(x^2y + c_{20}x^2 - 2Fx - y - D/c_{20})(y - c_{20}), \tag{36}$$

where  $c_{20} = \pm 1$ .

If  $c_{20} = 1$ , then  $E = F$  and  $2G = 1 - D$ . With  $E = F$ , then either  $c = b$  or  $d = a$ . Without loss of generality, assume  $c = b$ . Then, from  $2G = 1 - D$ , either  $d = a$  or  $|b| = 1$ . An argument similar to that of II of Case 1 shows that if  $b = \pm 1$ , then  $d = a$ . So we have  $c = b$  and  $d = a$ . Then  $F = 2ab$ ,  $D = 1 - 2a^2 - 2b^2$  and (36) reduces to

$$(x^2y + x^2 - 4abx - y - 1 + 2a^2 + 2b^2)(y - 1). \tag{37}$$

If  $|b| \neq |a|$ , then (37) does not factor any further. The completion region is the region bounded by  $x^2y + x^2 - 4abx - y - 1 + 2a^2 + 2b^2 = 0$  and  $y = 1$ . The points  $(ab - \sqrt{(1 - a^2)(1 - b^2)}, 1)$  and  $(ab + \sqrt{(1 - a^2)(1 - b^2)}, 1)$  are the two common roots of the two factors in (37), hence they are singular points. The second graph in Fig. 5 illustrates this case. If  $1 \neq |b| = |a| \neq 0$ , then (35) reduces to one of the factorizations in Case 1 above with three singular points. If  $b = 1$ , then  $(a, 1)$  is the only singular point and if  $b = -1$ , then  $(-a, 1)$  is the only singular point. The case  $a = \pm 1$  is similar.

If  $c_{20} = -1$ , then following the above argument, (36) becomes  $(x^2y - x^2 - 2Fx - y + D)(y + 1)$  with  $E = -F$  and  $2G = -1 + D$ , which gives  $c = -b$ ,  $d = -a$  and (36) reduces to

$$(x^2y - x^2 + 4abx - y + 1 - 2a^2 - 2b^2)(y + 1). \tag{38}$$

As in the case  $c_{20} = 1$ , there is one singular point if  $|a| = 1$  or  $|b| = 1$ , and there are two singular points if  $1 \neq |b| \neq |a| \neq 1$ .

Table 1

$(a, b, c, d)$	Factors
$(0, 0, 0, 0)$	$(x - 1)(x + 1)(y - 1)(y + 1)$
$a \neq 0$	
$(a, a, a, a)$	$(xy + x + y + 1 - 4a^2)(x - 1)(y - 1)$
$(a, -a, a, -a)$	$(xy - x - y + 1 - 4a^2)(x + 1)(y + 1)$
$(a, a, -a, -a)$	$(xy - x + y - 1 + 4a^2)(x - 1)(y + 1)$
$(a, -a, -a, a)$	$(xy + x - y - 1 + 4a^2)(x + 1)(y - 1)$
$ b ,  c  \neq  a $	
$(a, b, a, b)$	$(xy + x + y + 1 - a^2 - b^2 - 2ab)(xy - x - y + 1 - a^2 - b^2 + 2ab)$
$(a, b, -a, -b)$	$(xy - x + y - 1 + a^2 + b^2 + 2ab)(xy + x - y - 1 + a^2 + b^2 - 2ab)$
$(a, b, b, a)$	$(x^2y + x^2 - 4abx - y - 1 + 2a^2 + 2b^2)(y - 1)$
$(a, b, -b, -a)$	$(x^2y - x^2 + 4abx - y + 1 - 2a^2 - 2b^2)(y + 1)$
$(a, a, c, c)$	$(xy^2 + y^2 - x - 4acy - 1 + 2a^2 + 2c^2)(x - 1)$
$(a, -a, c, -c)$	$(xy^2 - y^2 - x - 4acy + 1 - 2a^2 - 2c^2)(x + 1)$

III. Now suppose  $a_{21} = 0$  and  $a_{12} \neq 0$ . This is equivalent to reversing the roles of  $x$  and  $y$  and the roles of  $c$  and  $a$  in the above argument, and results in the factorizations:

$$(xy^2 + y^2 - x - 4acy - 1 + 2a^2 + 2c^2)(x - 1)$$

and

$$(xy^2 - y^2 - x - 4acy + 1 - 2a^2 - 2c^2)(x + 1).$$

Summarizing, we have:

**Theorem 1.** *Let  $A(x, y)$  be given by (8) and assume that the PSD completion region of  $A(x, y)$  is not empty. Then the polynomial  $\det A(x, y)$  factors into nonconstant polynomials if and only if the quadruple  $(a, b, c, d)$  satisfies one of the conditions in Table 1.*

*Furthermore, for each of the above quadruples the number of singular points and the location of each are listed in Table 2.*

Singular points occur in some instances in which  $\det A(x, y)$  does not factor, which follows from the results in the next section.

## 7. Rank

If  $(x_0, y_0)$  is a boundary point of the PSD completion region  $R$ , then  $\text{rank } A(x_0, y_0) \leq 3$ . In particular, this occurs if  $R = \{(x_0, y_0)\}$ , a single point. If  $\text{rank } A(x_0, y_0) \leq 2$ , then  $(x_0, y_0)$  satisfies (22) and (23) and so by (18) we have:

Table 2

$(a, b, c, d)$	#	Singular Points			
$(0, 0, 0, 0)$	4	$(1, 1), (1, -1), (-1, 1), (-1, -1)$			
$a \neq 0, \pm 1$	3				
$(a, a, a, a)$		$(1, 1), (1, 2a^2 - 1), (2a^2 - 1, 1)$			
$(a, -a, a, -a)$		$(-1, -1), (1 - 2a^2, -1), (-1, 1 - 2a^2)$			
$(a, a, -a, -a)$		$(1, -1), (1, 1 - 2a^2), (2a^2 - 1, -1)$			
$(a, -a, -a, a)$		$(-1, 1), (1 - 2a^2, 1), (-1, 2a^2 - 1)$			
$ a ,  b ,  c  \neq 1$ $ b ,  c  \neq  a $	2				
$(a, b, a, b)$		$(ab \pm \sqrt{(1 - a^2)(1 - b^2)}, ab \mp \sqrt{(1 - a^2)(1 - b^2)})$			
$(a, b, -a, -b)$		$(ab \pm \sqrt{(1 - a^2)(1 - b^2)}, -ab \pm \sqrt{(1 - a^2)(1 - b^2)})$			
$(a, b, b, a)$		$(ab \pm \sqrt{(1 - a^2)(1 - b^2)}, 1)$			
$(a, b, -b, -a)$		$(ab \pm \sqrt{(1 - a^2)(1 - b^2)}, -1)$			
$(a, a, c, c)$		$(1, ac \pm \sqrt{(1 - a^2)(1 - c^2)})$			
$(a, -a, c, -c)$		$(-1, -ac \pm \sqrt{(1 - a^2)(1 - c^2)})$			
$(a, b, c, d)$	#	Singular Points	$(a, b, c, d)$	#	Singular Points
$(1, b, 1, b)$	1	$(b, b)$	$(a, 1, a, 1)$	1	$(a, a)$
$(-1, b, -1, b)$		$(-b, -b)$	$(a, -1, a, -1)$		$(-a, -a)$
$(1, b, -1, -b)$		$(b, -b)$	$(a, 1, -a, -1)$		$(a, -a)$
$(-1, b, 1, -b)$		$(-b, b)$	$(a, -1, -a, 1)$		$(-a, a)$
$(a, 1, 1, a)$		$(a, 1)$	$(1, b, b, 1)$		$(b, 1)$
$(a, -1, -1, a)$		$(-a, 1)$	$(-1, b, b, -1)$		$(-b, 1)$
$(a, 1, -1, -a)$		$(a, -1)$	$(1, b, -b, -1)$		$(b, -1)$
$(a, -1, 1, -a)$		$(-a, -1)$	$(-1, b, -b, 1)$		$(-b, -1)$
$(1, 1, c, c)$		$(1, c)$	$(a, a, 1, 1)$		$(1, a)$
$(-1, -1, c, c)$		$(1, -c)$	$(a, a, -1, -1)$		$(1, -a)$
$(1, -1, c, -c)$		$(-1, -c)$	$(a, -a, 1, -1)$		$(-1, -a)$
$(-1, 1, c, -c)$		$(-1, c)$	$(a, -a, -1, 1)$		$(-1, a)$

**Proposition 5.** *If  $A(x_0, y_0)$  is PSD with rank 1 or 2, then  $(x_0, y_0)$  is a singular point of the completion region  $R$ .*

The converse of Proposition 5 is false as can be seen from the example

$$A(x, y) = \begin{bmatrix} 1 & a & x & 1 \\ a & 1 & a & y \\ x & a & 1 & a \\ 1 & y & a & 1 \end{bmatrix}, \quad -\frac{1}{2} < a < 1.$$

The completion region  $R$  is the point  $(a, a)$ , and furthermore

$$\frac{\partial}{\partial x} \det A(a, a) = \frac{\partial}{\partial y} \det A(a, a) = 0,$$

so  $(a, a)$  is a singular point of  $R$ . But,  $\det A(a, a)[1, 2, 3] = (1 - a)^2(1 + 2a) \neq 0$ , so  $\text{rank } A(a, a) = 3$ .

Nevertheless, Proposition 5 enables us to identify many instances of singular points.

In this section we determine all quadruples  $(a, b, c, d)$  for which there is a PSD completion of rank at most 2, a question of much interest in its own right. We will show that this can occur in three ways: either there is a unique PSD completion, or the determinant factors, or the completion region contains a unique rank 2 PSD completion but it is not a single point. The first two cases are not mutually exclusive; however, in the third case the determinant does not factor and this gives new instances of singular points other than those in the last section.

In order to identify the  $(a, b, c, d)$  for which there is a PSD completion of rank at most 2, we first recall a result from [2, pp. 9–10].

**Lemma 3.** *Let  $0 \leq \alpha, \beta, \gamma \leq \pi$ . Then the matrix*

$$B = \begin{bmatrix} 1 & \cos \alpha & \cos \gamma \\ \cos \alpha & 1 & \cos \beta \\ \cos \gamma & \cos \beta & 1 \end{bmatrix}$$

is PSD if and only if

$$\alpha \leq \beta + \gamma, \quad \beta \leq \alpha + \gamma, \quad \gamma \leq \alpha + \beta, \quad \alpha + \beta + \gamma \leq 2\pi. \tag{39}$$

Furthermore,  $B$  is singular if and only if one of these inequalities is an equality.

Let  $0 \leq \alpha, \beta, \gamma, \delta \leq \pi$ , and let

$$C = \begin{bmatrix} 1 & \cos \alpha & ? & \cos \delta \\ \cos \alpha & 1 & \cos \beta & ? \\ ? & \cos \beta & 1 & \cos \gamma \\ \cos \delta & ? & \cos \gamma & 1 \end{bmatrix}.$$

At this point it is useful to restate Proposition 3 in terms of  $\alpha, \beta, \gamma, \delta$ . The equality in (10) becomes

$$|\cos \alpha \cos \beta - \cos \gamma \cos \delta| = \sin \alpha \sin \beta + \sin \gamma \sin \delta,$$

which is equivalent to

$$\cos \alpha \cos \beta \pm \sin \alpha \sin \beta = \cos \gamma \cos \delta \mp \sin \gamma \sin \delta.$$

Therefore,

$$\cos(\alpha - \beta) = \cos(\gamma + \delta) \text{ or } \cos(\alpha + \beta) = \cos(\gamma - \delta).$$

The first equality occurs if and only if either

$$\alpha - \beta = \gamma + \delta, \quad \beta - \alpha = \gamma + \delta, \quad \alpha - \beta + \gamma + \delta = 2\pi,$$

or

$$\beta - \alpha + \gamma + \delta = 2\pi,$$

and the second occurs if and only if

$$\alpha + \beta = \gamma - \delta, \quad \alpha + \beta = \delta - \gamma, \quad \alpha + \beta + \gamma - \delta = 2\pi,$$

or

$$\alpha + \beta + \delta - \gamma = 2\pi.$$

Therefore, the equality in (10) occurs if and only if one of the following hold:

$$\alpha = \beta + \gamma + \delta, \quad \beta + \gamma + \delta = 2\pi + \alpha,$$

$$\beta = \alpha + \gamma + \delta, \quad \alpha + \gamma + \delta = 2\pi + \beta,$$

$$\gamma = \alpha + \beta + \delta, \quad \alpha + \beta + \delta = 2\pi + \gamma,$$

$$\delta = \alpha + \beta + \gamma, \quad \alpha + \beta + \gamma = 2\pi + \delta.$$

This also shows that the equality in (10) is in fact symmetric in  $a, b, c, d$ . We could also substitute in the inequality in (10), but it is more instructive to derive a different equivalent condition in terms of  $\alpha, \beta, \gamma, \delta$ . Suppose  $|a| = 1$ , i.e.,  $\alpha = 0$  or  $\pi$ . Then the matrix

$$\begin{bmatrix} 1 & \pm 1 & ? & \cos \delta \\ \pm 1 & 1 & \cos \beta & ? \\ ? & \cos \beta & 1 & \cos \gamma \\ \cos \delta & ? & \cos \gamma & 1 \end{bmatrix}$$

has a PSD completion if and only if

$$\begin{bmatrix} 1 & \pm 1 & \pm \cos \beta & \cos \delta \\ \pm 1 & 1 & \cos \beta & \pm \cos \delta \\ \pm \cos \beta & \cos \beta & 1 & \cos \gamma \\ \cos \delta & \pm \cos \delta & \cos \gamma & 1 \end{bmatrix}$$

is PSD, i.e., if and only if

$$\begin{bmatrix} 1 & \cos \beta & \cos \delta \\ \cos \beta & 1 & \cos \gamma \\ \cos \delta & \cos \gamma & 1 \end{bmatrix}$$

is PSD for  $\alpha = 0$  and

$$\begin{bmatrix} 1 & \cos \beta & -\cos \delta \\ \cos \beta & 1 & \cos \gamma \\ -\cos \delta & \cos \gamma & 1 \end{bmatrix} = \begin{bmatrix} 1 & \cos \beta & \cos(\pi - \delta) \\ \cos \beta & 1 & \cos \gamma \\ \cos(\pi - \delta) & \cos \gamma & 1 \end{bmatrix}$$

is PSD for  $\alpha = \pi$ . The matrix for  $\alpha = 0$  is PSD if and only if

$$\beta \leq \gamma + \delta, \quad \gamma \leq \beta + \delta, \quad \delta \leq \beta + \gamma,$$

and

$$\beta + \gamma + \delta \leq 2\pi$$

by Lemma 3. Since  $\alpha = 0$ , we may write these as

$$\alpha + \beta \leq \gamma + \delta, \quad \alpha + \gamma \leq \beta + \delta, \quad \alpha + \delta \leq \beta + \gamma, \quad \alpha + \beta + \gamma + \delta \leq 2\pi.$$

The matrix for  $\alpha = \pi$  is PSD if and only if

$$\beta \leq \gamma + \pi - \delta, \quad \gamma \leq \beta + \pi - \delta, \quad \pi - \delta \leq \beta + \gamma,$$

and

$$\beta + \gamma + \pi - \delta \leq 2\pi,$$

or if and only if

$$\beta + \delta \leq \alpha + \gamma, \quad \gamma + \delta \leq \alpha + \beta, \quad 2\pi \leq \alpha + \beta + \gamma + \delta, \quad \beta + \gamma \leq \alpha + \delta.$$

The analogs of these inequalities for  $\beta = 0$  or  $\pi$ ,  $\gamma = 0$  or  $\pi$ , and  $\delta = 0$  or  $\pi$  are clear. Thus, we have;

**Proposition 6.** *The matrix*

$$C = \begin{bmatrix} 1 & \cos \alpha & ? & \cos \delta \\ \cos \alpha & 1 & \cos \beta & ? \\ ? & \cos \beta & 1 & \cos \gamma \\ \cos \delta & ? & \cos \gamma & 1 \end{bmatrix}$$

has a unique PSD completion if and only if

(a) *one of the following hold:*

$$\begin{aligned} \alpha &= \beta + \gamma + \delta, & \beta + \gamma + \delta &= 2\pi + \alpha, \\ \beta &= \alpha + \gamma + \delta, & \alpha + \gamma + \delta &= 2\pi + \beta, \\ \gamma &= \alpha + \beta + \delta, & \alpha + \beta + \delta &= 2\pi + \gamma, \\ \delta &= \alpha + \beta + \gamma, & \alpha + \beta + \gamma &= 2\pi + \delta, \end{aligned} \tag{40}$$

or

(b)  $\{\alpha, \beta, \gamma, \delta\} \cap \{0, \pi\} \neq \emptyset$ , and if  $\alpha = 0(\pi)$ , all of the following hold:

$$\begin{aligned} \alpha + \beta &\leq (\geq) \gamma + \delta, & \alpha + \gamma &\leq (\geq) \beta + \delta, \\ \alpha + \delta &\leq (\geq) \beta + \gamma, & \alpha + \beta + \gamma + \delta &\leq (\geq) 2\pi, \end{aligned}$$

while if  $\beta = 0$  or  $\pi$ ,  $\gamma = 0$  or  $\pi$ , or  $\delta = 0$  or  $\pi$ , analogous inequalities are required to hold.

**Corollary 1.** *If one of the equalities in (40) hold, then C has a unique PSD completion  $\hat{C}$  and,  $\text{rank}(\hat{C}) \leq 2$ .*

**Proof.** Assume that one of the equalities on the left-hand side of (40) holds. Without loss of generality, say



$$\delta = \alpha + \beta + \gamma.$$

Let

$$M(\theta, \phi) = \begin{bmatrix} 1 & \cos \alpha & \cos \theta & \cos(\alpha + \beta + \gamma) \\ \cos \alpha & 1 & \cos \beta & \cos \phi \\ \cos \theta & \cos \beta & 1 & \cos \gamma \\ \cos(\alpha + \beta + \gamma) & \cos \phi & \cos \gamma & 1 \end{bmatrix}$$

be the unique PSD completion of  $C$ . Using Lemma 3,  $M(\theta, \phi)[1, 2, 3]$  is PSD only if  $\theta \leq \alpha + \beta$  and  $M(\theta, \phi)[1, 3, 4]$  is PSD only if  $\theta + \gamma \geq \alpha + \beta + \gamma$ , and hence,  $\theta = \alpha + \beta$ . Similarly, by Lemma 3 again,  $M(\theta, \phi)[2, 3, 4]$  and  $M(\theta, \phi)[1, 2, 4]$  are PSD only if  $\phi = \beta + \gamma$ . Thus  $M(\alpha + \beta, \beta + \gamma)$  is the unique PSD completion of  $C$ . By Lemma 3, all the  $3 \times 3$  principal minors are 0. Also,  $M(\alpha + \beta, \beta + \gamma)$  is singular because the completion region is a single point. Thus,  $\text{rank } M(\alpha + \beta, \beta + \gamma) \leq 2$ .

A similar argument shows that the unique PSD completion of  $C$  has rank at most 2 if  $\alpha + \beta + \gamma = 2\pi + \delta$ . In this case,  $\theta = 2\pi - \alpha - \beta$  and  $\phi = 2\pi - \beta - \gamma$ . By the symmetry of equations (40), this concludes the proof.  $\square$

We now find necessary and sufficient conditions on  $\alpha, \beta, \gamma, \delta$  such that the matrix  $C$  has a PSD completion of rank at most 2. We will make use of two observations. Let

$$C(\theta, \phi) = \begin{bmatrix} 1 & \cos \alpha & \cos \theta & \cos \delta \\ \cos \alpha & 1 & \cos \beta & \cos \phi \\ \cos \theta & \cos \beta & 1 & \cos \gamma \\ \cos \delta & \cos \phi & \cos \gamma & 1 \end{bmatrix}, \tag{41}$$

with  $0 \leq \theta, \phi \leq \pi$ .

**Observation 2.** Rank  $C(\theta, \phi) \leq 2$  if and only if

$$\det \begin{bmatrix} 1 & \cos \alpha & \cos \theta \\ \cos \alpha & 1 & \cos \beta \\ \cos \theta & \cos \beta & 1 \end{bmatrix} = 0, \quad \det \begin{bmatrix} 1 & \cos \theta & \cos \delta \\ \cos \theta & 1 & \cos \gamma \\ \cos \delta & \cos \gamma & 1 \end{bmatrix} = 0, \tag{42}$$

$$\det \begin{bmatrix} 1 & \cos \beta & \cos \phi \\ \cos \beta & 1 & \cos \gamma \\ \cos \phi & \cos \gamma & 1 \end{bmatrix} = 0, \quad \det \begin{bmatrix} 1 & \cos \alpha & \cos \delta \\ \cos \alpha & 1 & \cos \phi \\ \cos \delta & \cos \phi & 1 \end{bmatrix} = 0 \tag{43}$$

and  $\det C(\theta, \phi) = 0$ .

**Observation 3.** We have rank  $C(\theta, \phi) \leq 2$  if and only if  $C(\theta, \phi)$  is the Gram matrix of four unit vectors  $\{\vec{u}_1, \vec{u}_2, \vec{u}_3, \vec{u}_4\}$  in  $\mathbb{R}^2$ ; i.e.,  $c_{ij} = \langle \vec{u}_i, \vec{u}_j \rangle$ ,  $1 \leq i, j \leq 4$ .

By Lemma 3, (42) is satisfied if and only if  $\theta$  satisfies one equation from the left and one equation from the right of (44), below:

$$\left. \begin{array}{l} \alpha + \beta \\ \alpha - \beta \\ -\alpha + \beta \\ 2\pi - \alpha - \beta \end{array} \right\} = \theta = \left\{ \begin{array}{l} \gamma + \delta \\ \gamma - \delta \\ -\gamma + \delta \\ 2\pi - \gamma - \delta \end{array} \right. \quad (44)$$

There are 16 cases which give the following 12 possible linear relations between  $\alpha$ ,  $\beta$ ,  $\gamma$  and  $\delta$ :

$$\delta = \alpha + \beta + \gamma, \quad \gamma = \alpha + \beta + \delta, \quad \beta = \alpha + \gamma + \delta, \quad \alpha = \beta + \gamma + \delta \quad (45)$$

$$\begin{array}{l} 2\pi + \delta = \alpha + \beta + \gamma, \quad 2\pi + \gamma = \alpha + \beta + \delta, \\ 2\pi + \beta = \alpha + \gamma + \delta, \quad 2\pi + \alpha = \beta + \gamma + \delta \end{array} \quad (46)$$

and

$$\begin{array}{l} \alpha + \beta = \gamma + \delta, \quad \alpha + \gamma = \beta + \delta, \\ \alpha + \delta = \beta + \gamma, \quad \alpha + \beta + \gamma + \delta = 2\pi. \end{array} \quad (47)$$

Thus, a necessary condition for  $C$  to have a PSD completion of rank at most 2 is that at least one of the 12 equations in (45), (46) and (47) holds. We now investigate whether this is also a sufficient condition, and furthermore, describe the completion region for each possibility that can occur.

Comparing the equations in (45) and (46) with Corollary 1, we have a unique PSD completion of rank  $\leq 2$  in these cases. So it remains to consider those cases where none of the equations in (45), (46) holds. We begin with the following elementary fact.

**Observation 4.** *If rank  $C(\theta, \phi) \leq 2$  and none of the equations in (45) and (46) holds, then  $0 < \alpha, \beta, \gamma, \delta < \pi$ .*

**Proof.** By way of contradiction, suppose one of  $\alpha, \beta, \gamma, \delta$  is 0 or  $\pi$ . Without loss of generality, let it be  $\alpha$ . First suppose  $\alpha = 0$ . Then, by Observation 3, the two unit vectors  $\vec{u}_1$  and  $\vec{u}_2$  are identical and we have one of the diagrams in Fig. 6(a), i.e., either

$$\beta = \alpha + \gamma + \delta, \quad \delta = \alpha + \beta + \gamma, \quad \gamma = \alpha + \beta + \delta,$$

or

$$\beta + \gamma + \delta = 2\pi + \alpha,$$

a contradiction. Suppose  $\alpha = \pi$ . Then we have one of the diagrams in Fig. 6(b), i.e.,

$$\alpha = \beta + \gamma + \delta, \quad \alpha + \beta + \delta = 2\pi + \gamma, \quad \alpha + \gamma + \beta = 2\pi + \delta,$$

or

$$\alpha + \delta + \gamma = 2\pi + \beta,$$

a contradiction.  $\square$

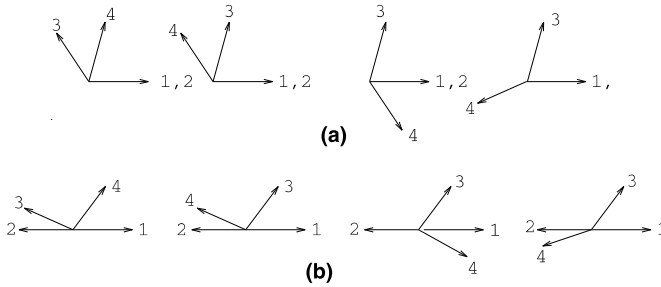


Fig. 6. Possible configurations of unit vectors.

The matrix

$$\begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

shows that the hypothesis  $\text{rank } C(\theta, \phi) \leq 2$  cannot be omitted.

We now consider the four equations in (47). There are two cases:

- I. Two of the equations in (47) hold simultaneously. There are  $\binom{4}{2} = 6$  possibilities.
- II. Exactly one of the four equations in (47) holds.

Consider Case I. The first possibility is that  $\alpha + \beta = \gamma + \delta$  and  $\alpha + \gamma = \beta + \delta$ . Then  $\alpha + \beta - \gamma = \alpha + \gamma - \beta$ , so  $\beta = \gamma$  and  $\alpha = \delta$ . Considering the remaining five possibilities, we arrive at Table 3. The second and third columns in this table give, respectively, the possible quadruples  $(\alpha, \beta, \gamma, \delta)$  and  $(a, b, c, d)$  satisfying the corresponding equations in the first column.

Note that these six cases are the same as those in Tables 1 and 2 for which  $\det A(x, y)$  factors and there are generically two singular points. We shall see that each of these singular points gives rise to a rank 2 PSD completion. For the first case in Table 3, the determinant factors into cubic and linear polynomials and for the second case, the determinant factors into two quadratic polynomials. Since each of cases 3–6 of Table 3 also gives one of these two factorizations, it suffices to just consider the possibilities for the first and second cases.

Suppose we have the first case  $(\alpha, \beta, \beta, \alpha)$ ,  $0 < \alpha, \beta < \pi$ . Provided  $\beta \neq \alpha$  and  $\beta \neq \pi - \alpha$ , we have exactly two rank 2 PSD completions,

$$\begin{bmatrix} 1 & \cos \alpha & \cos(\alpha + \beta) & \cos \alpha \\ \cos \alpha & 1 & \cos \beta & 1 \\ \cos(\alpha + \beta) & \cos \beta & 1 & \cos \beta \\ \cos \alpha & 1 & \cos \beta & 1 \end{bmatrix},$$

Table 3.

Eq. (47)	$(\alpha, \beta, \gamma, \delta)$	$(a, b, c, d)$
$\alpha + \beta = \gamma + \delta$ $\alpha + \gamma = \beta + \delta$	$(\alpha, \beta, \beta, \alpha)$ $0 < \alpha, \beta < \pi$	$(a, b, b, a)$ $ a ,  b  < 1$
$\alpha + \beta = \gamma + \delta$ $\alpha + \delta = \beta + \gamma$	$(\alpha, \beta, \alpha, \beta)$ $0 < \alpha, \beta < \pi$	$(a, b, a, b)$ $ a ,  b  < 1$
$\alpha + \beta = \gamma + \delta$ $\alpha + \beta + \gamma + \delta = 2\pi$	$(\alpha, \pi - \alpha, \gamma, \pi - \gamma)$ $0 < \alpha, \gamma < \pi$	$(a, -a, c, -c)$ $ a ,  c  < 1$
$\alpha + \gamma = \beta + \delta$ $\alpha + \delta = \beta + \gamma$	$(\alpha, \alpha, \gamma, \gamma)$ $0 < \alpha, \gamma < \pi$	$(a, a, c, c)$ $ a ,  c  < 1$
$\alpha + \gamma = \beta + \delta$ $\alpha + \beta + \gamma + \delta = 2\pi$	$(\alpha, \beta, \pi - \alpha, \pi - \beta)$ $0 < \alpha, \beta < \pi$	$(a, b, -a, -b)$ $ a ,  b  < 1$
$\alpha + \delta = \beta + \gamma$ $\alpha + \beta + \gamma + \delta = 2\pi$	$(\alpha, \beta, \pi - \beta, \pi - \alpha)$ $0 < \alpha, \beta < \pi$	$(a, b, -b, -a)$ $ a ,  b  < 1$

$$\begin{bmatrix} 1 & \cos \alpha & \cos(\alpha - \beta) & \cos \alpha \\ \cos \alpha & 1 & \cos \beta & 1 \\ \cos(\alpha - \beta) & \cos \beta & 1 & \cos \beta \\ \cos \alpha & 1 & \cos \beta & 1 \end{bmatrix}.$$

By Proposition 5,  $(\cos(\alpha + \beta), 1)$  and  $(\cos(\alpha - \beta), 1)$  are singular points of the completion region; Theorem 1 then implies that there can be no other rank 2 PSD completions. The second graph in Fig. 5 is an example of this case, and the two sharp points on the boundary yield the two rank 2 PSD completions above.

If  $\beta = \alpha \neq \frac{1}{2}\pi$ , then we have the case  $(\alpha, \alpha, \alpha, \alpha)$ ,  $\alpha \notin \{0, \frac{1}{2}\pi, \pi\}$ , with the three rank 2 PSD completions,

$$\begin{bmatrix} 1 & \cos \alpha & 1 & \cos \alpha \\ \cos \alpha & 1 & \cos \alpha & 1 \\ 1 & \cos \alpha & 1 & \cos \alpha \\ \cos \alpha & 1 & \cos \alpha & 1 \end{bmatrix}, \quad \begin{bmatrix} 1 & \cos \alpha & 1 & \cos \alpha \\ \cos \alpha & 1 & \cos \alpha & \cos 2\alpha \\ 1 & \cos \alpha & 1 & \cos \alpha \\ \cos \alpha & \cos 2\alpha & \cos \alpha & 1 \end{bmatrix}, \quad \begin{bmatrix} 1 & \cos \alpha & \cos 2\alpha & \cos \alpha \\ \cos \alpha & 1 & \cos \alpha & 1 \\ \cos 2\alpha & \cos \alpha & 1 & \cos \alpha \\ \cos \alpha & 1 & \cos \alpha & 1 \end{bmatrix}. \tag{48}$$

Since there are exactly three singular points in this case by Theorem 1, as before there can be no other rank 2 PSD completions. The third graph in Fig. 5 illustrates this case and the three ‘corners’ yield the three rank 2 PSD completions in (48).

If  $\beta = \pi - \alpha \neq \frac{1}{2}\pi$ , we now have the case  $(\alpha, \pi - \alpha, \pi - \alpha, \alpha)$ ,  $\alpha \notin \{0, \frac{1}{2}\pi, \pi\}$ , with the three rank 2 PSD completions,

$$\begin{aligned} & \begin{bmatrix} 1 & \cos \alpha & -1 & \cos \alpha \\ \cos \alpha & 1 & -\cos \alpha & 1 \\ -1 & -\cos \alpha & 1 & -\cos \alpha \\ \cos \alpha & 1 & -\cos \alpha & 1 \end{bmatrix}, \\ & \begin{bmatrix} 1 & \cos \alpha & -1 & \cos \alpha \\ \cos \alpha & 1 & -\cos \alpha & \cos 2\alpha \\ -1 & -\cos \alpha & 1 & -\cos \alpha \\ \cos \alpha & \cos 2\alpha & -\cos \alpha & 1 \end{bmatrix}, \\ & \begin{bmatrix} 1 & \cos \alpha & -\cos 2\alpha & \cos \alpha \\ \cos \alpha & 1 & -\cos \alpha & 1 \\ -\cos 2\alpha & -\cos \alpha & 1 & -\cos \alpha \\ \cos \alpha & 1 & -\cos \alpha & 1 \end{bmatrix}. \end{aligned} \tag{49}$$

Finally, if  $\beta = \alpha = \frac{1}{2}\pi$ , we have the case  $a = b = c = d = 0$  with four rank 2 PSD completions, corresponding to the four corners of the square  $S$ :

$$\begin{aligned} & \begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{bmatrix}, \begin{bmatrix} 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & 1 \\ -1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{bmatrix}, \\ & \begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & -1 \\ 1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \end{bmatrix}, \begin{bmatrix} 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \\ -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \end{bmatrix}. \end{aligned} \tag{50}$$

It remains to consider the second case  $(\alpha, \beta, \alpha, \beta)$ ,  $0 < \alpha, \beta < \pi$ . Provided  $\beta \neq \alpha$  and  $\beta \neq \pi - \alpha$ , we have exactly two rank 2 PSD completions,

$$\begin{bmatrix} 1 & \cos \alpha & \cos(\alpha + \beta) & \cos \beta \\ \cos \alpha & 1 & \cos \beta & \cos(\alpha - \beta) \\ \cos(\alpha + \beta) & \cos \beta & 1 & \cos \alpha \\ \cos \beta & \cos(\alpha - \beta) & \cos \alpha & 1 \end{bmatrix}$$

and

$$\begin{bmatrix} 1 & \cos \alpha & \cos(\alpha - \beta) & \cos \beta \\ \cos \alpha & 1 & \cos \beta & \cos(\alpha + \beta) \\ \cos(\alpha - \beta) & \cos \beta & 1 & \cos \alpha \\ \cos \beta & \cos(\alpha + \beta) & \cos \alpha & 1 \end{bmatrix}.$$

The first graph in Fig. 5 is an example of this case and the ‘corners’ of the lens shaped region yield these two rank 2 PSD completions.

If  $\beta = \alpha \neq \frac{1}{2}\pi$ , we have the case  $(\alpha, \alpha, \alpha, \alpha)$  and the same three rank 2 PSD completions as in (48). If  $\beta = \pi - \alpha \neq \frac{1}{2}\pi$ , we have the case  $(\alpha, \pi - \alpha, \alpha, \pi - \alpha)$  which has three rank 2 PSD completions that are sign similar to those of (49). Finally, if  $\beta = \alpha = \frac{1}{2}\pi$ , we have the same four rank 2 PSD completions as in (50).

We have now established a one-to-one correspondence between each rank 2 PSD completion of any quadruple  $(\alpha, \beta, \gamma, \delta)$  occurring in Table 3 and the singular points associated with the quadruple  $(a, b, c, d)$  in Table 2 excluding those rows with exactly one singular point. Each of those rows admits a unique PSD completion of rank at most 2. This yields a partial converse to Proposition 5.

**Proposition 7.** *Let  $(a, b, c, d)$  be a quadruple for which  $A(x, y)$  has a PSD completion and  $\det A(x, y)$  factors. If  $(x_0, y_0)$  is a singular point of the completion region  $R$ , then  $\text{rank } A(x_0, y_0) \leq 2$ .*

We now consider Case II in which we assume none of the equations in (45) and (46) holds and exactly one equation in (47) holds. Thus, none of the cases in Table 3 occurs. Also, in order to have a rank 2 PSD completion, we must have  $0 < \alpha, \beta, \gamma, \delta < \pi$  by Observation 4. Thus, by Table 1 in Theorem 1, we are in a case in which  $\det A(x, y)$  does not factor. By Lemma 2, there is at most one singular point in the completion region. So by Proposition 5, there is at most one rank 2 PSD completion of  $A(x, y)$ . We now show that there is a rank 2 completion in each of these cases.

(i) Assume  $\alpha + \beta = \gamma + \delta$ . Without loss of generality, we may assume  $\alpha$  is the largest of  $\alpha, \beta, \gamma, \delta$ . Note that the largest is unique, for if  $\gamma = \alpha$ , then  $\delta = \beta$ , which is one of the cases in Table 3, and similarly if  $\delta = \alpha$ ; if  $\beta = \alpha$ , then  $\delta = \gamma = \alpha$ , in which case we get  $(\alpha, \alpha, \alpha, \alpha)$ , which is a special case of  $(\alpha, \alpha, \gamma, \gamma)$ , the fourth case in Table 3. So,  $\alpha > \gamma, \delta$  and  $\beta < \gamma, \delta$ . Also,  $\alpha + \beta \neq \pi$ , or else  $\alpha + \beta + \gamma + \delta = 2\pi$ , and we again have one of the cases in Table 3.

We now use Observation 3. We arrange four unit vectors as indicated by Fig. 7 so that  $\alpha, \beta, \gamma, \delta$  are the angles between the first and second, second and third, third and fourth, first and fourth vectors, respectively. This can be done since  $\alpha + \beta = \gamma + \delta$ .

Since  $\theta$  is the angle between the first and third vectors, either  $\theta = \alpha + \beta$  or else  $\theta = 2\pi - \alpha - \beta$ . Also, since  $\phi$  is the angle between the second and fourth vectors,  $\phi = \gamma - \beta$ . It follows that

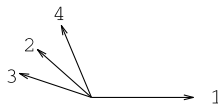


Fig. 7.  $\alpha + \beta = \gamma + \delta$ .

$$C(\theta, \phi) = \begin{bmatrix} 1 & \cos \alpha & \cos(\alpha + \beta) & \cos \delta \\ \cos \alpha & 1 & \cos \beta & \cos(\gamma - \beta) \\ \cos(\alpha + \beta) & \cos \beta & 1 & \cos \gamma \\ \cos \delta & \cos(\gamma - \beta) & \cos \gamma & 1 \end{bmatrix}$$

is a PSD completion of rank 2 which is necessarily unique. By Proposition 6 it is not the only PSD completion.

The fourth graph in Fig. 5 is an example of this case with  $(\alpha, \beta, \gamma, \delta) = (\frac{3}{4}\pi, \frac{1}{6}\pi, \frac{2}{3}\pi, \frac{1}{4}\pi)$ . The unique sharp point on the boundary is  $(\cos \frac{11}{12}\pi, \cos \frac{1}{2}\pi) \approx (-0.966, 0)$ .

(ii)  $\alpha + \delta = \beta + \gamma$ . Similar to (i),  $\beta + \gamma \neq \pi$ , and we may assume  $\alpha < \beta$ ,  $\gamma$  and  $\beta, \gamma < \delta$ . Then, as in (i), we may orient four unit vectors in  $\mathbb{R}^2$  as in Fig. 8, from which we conclude that  $\theta = \beta - \alpha$  and either  $\phi = \beta + \gamma$  or else  $\phi = 2\pi - \beta - \gamma$ . Then  $C(\theta, \phi)$  is the unique PSD completion of rank 2. Moreover, just as in (i), it is not the only PSD completion.

(iii)  $\alpha + \gamma = \beta + \delta$ . Then  $\alpha + \gamma \neq \pi$  and we may assume  $\beta < \alpha$ ,  $\gamma$  and  $\alpha, \gamma < \delta$ . We may again orient four unit vectors in  $\mathbb{R}^2$  as shown in Fig. 9. Consequently,  $\theta = \alpha - \beta$ ,  $\phi = \gamma - \beta$ , and again there is a unique PSD completion of rank 2. Again this is not the only PSD completion.

(iv)  $\alpha + \beta + \gamma + \delta = 2\pi$ . Without loss of generality, we assume  $\alpha$  is the largest. Then  $\alpha \geq \frac{1}{2}\pi$ . If  $\alpha = \frac{1}{2}\pi$ , then  $\beta = \gamma = \delta = \frac{1}{2}\pi$ , hence all four equations in (47) hold simultaneously, a contradiction. So,  $\alpha > \frac{1}{2}\pi$ . Moreover,  $\alpha + \beta \neq \pi$ , or else  $\alpha + \beta = \gamma + \delta$  and two equations in (47) hold. Then, we may orient four unit vectors in  $\mathbb{R}^2$  as in Fig. 10, from which it follows that  $\theta = \alpha + \beta$  or  $\theta = 2\pi - \alpha - \beta$ , and

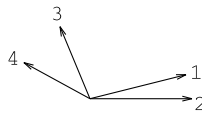


Fig. 8.  $\alpha + \delta = \beta + \gamma$ .

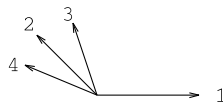


Fig. 9.  $\alpha + \gamma = \beta + \delta$ .

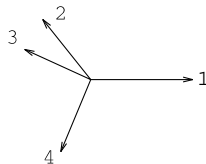


Fig. 10.  $\alpha + \beta + \gamma + \delta = 2\pi$ .

$\phi = \beta + \gamma$  or  $\phi = 2\pi - \beta - \gamma$ . Again there is a unique PSD completion of rank 2, and as before it is not the only PSD completion.

We now summarize all of the above results in Theorem 2.

**Theorem 2.** *Let  $0 \leq \alpha, \beta, \gamma, \delta \leq \pi$  and let*

$$C = \begin{bmatrix} 1 & \cos \alpha & ? & \cos \delta \\ \cos \alpha & 1 & \cos \beta & ? \\ ? & \cos \beta & 1 & \cos \gamma \\ \cos \delta & ? & \cos \gamma & 1 \end{bmatrix}.$$

Also, let  $A(x, y)$  be the matrix in (8) with  $a = \cos \alpha$ ,  $b = \cos \beta$ ,  $c = \cos \gamma$  and  $d = \cos \delta$ . Then  $C$  has a PSD completion of rank  $\leq 2$  if and only if at least one of the following 12 equations holds.

$$\begin{aligned} \alpha &= \beta + \gamma + \delta, & 2\pi + \alpha &= \beta + \gamma + \delta, \\ \beta &= \alpha + \gamma + \delta, & 2\pi + \beta &= \alpha + \gamma + \delta, \\ \gamma &= \alpha + \beta + \delta, & 2\pi + \gamma &= \alpha + \beta + \delta, \\ \delta &= \alpha + \beta + \gamma, & 2\pi + \delta &= \alpha + \beta + \gamma, \end{aligned} \tag{51}$$

$$\begin{aligned} \alpha + \beta &= \gamma + \delta, \\ \alpha + \gamma &= \beta + \delta, \\ \alpha + \delta &= \beta + \gamma, \\ \alpha + \beta + \gamma + \delta &= 2\pi. \end{aligned} \tag{52}$$

Furthermore, one of the following three mutually exclusive cases occurs.

1. If any of the equations in (51) holds, then  $C$  has a unique PSD completion and its rank is at most 2.
2. If any of the six relations
  - (i)  $\gamma = \alpha, \delta = \beta$ ,
  - (ii)  $\delta = \alpha, \gamma = \beta$ ,
  - (iii)  $\beta = \alpha, \delta = \gamma$ ,
  - (iv)  $\alpha + \gamma = \pi = \beta + \delta$ ,
  - (v)  $\alpha + \delta = \pi = \beta + \gamma$ ,
  - (vi)  $\alpha + \beta = \pi = \gamma + \delta$

holds, but none of the equations in (51) holds, then there are two, three or four PSD completions of  $C$  with rank at most 2. Furthermore, there is a one-to-one correspondence between these completions and the singular points of the completion region, and  $\det A(x, y)$  factors as indicated in Table 1.

3. If exactly one of the equations in (52) holds, but none of the equations in (51) holds, then  $\det A(x, y)$  is irreducible and  $C$  has exactly one PSD completion of



rank at most 2. This completion necessarily corresponds to a singular point of the completion region, which is not a single point.

Theorem 2 gives necessary and sufficient conditions on the parameters  $\alpha, \beta, \gamma, \delta$  so that  $C$  has a PSD completion of rank at most 2. One may only want to know whether or not a PSD completion of rank 1 or 2 of the partial PSD matrix  $A(x, y)$  in (8) is possible, and not the nature of all such completions. This can be reduced to just checking whether or not the entries  $a, b, c, d$  satisfy a polynomial equation.

**Observation 5.** A necessary condition that  $A(x, y)$ , given by (8), has a PSD completion of rank at most 2 is that the ordered quadruple  $(a, b, c, d)$  must satisfy

$$a^4 + b^4 + c^4 + d^4 - 2a^2b^2 - 2a^2c^2 - 2a^2d^2 - 2b^2c^2 - 2b^2d^2 - 2c^2d^2 + 8abcd - 4a^3bcd - 4ab^3cd - 4abc^3d - 4abcd^3 + 4a^2b^2c^2 + 4a^2b^2d^2 + 4a^2c^2d^2 + 4b^2c^2d^2 = 0. \tag{53}$$

**Proof.** Suppose there is a point  $(x, y)$  in  $R$  such that the matrix  $A(x, y)$  has rank 1 or 2. Then in particular we have

$$\det \begin{bmatrix} 1 & a & x \\ a & 1 & b \\ x & b & 1 \end{bmatrix} = \det \begin{bmatrix} 1 & x & d \\ x & 1 & c \\ d & c & 1 \end{bmatrix} = 0. \tag{54}$$

But, (54) holds if and only if

$$1 - a^2 - b^2 - x^2 + 2abx = 0 = 1 - c^2 - d^2 - x^2 + 2cdx,$$

if and only if

$$x = ab \pm \sqrt{(1 - a^2)(1 - b^2)} = cd \pm \sqrt{(1 - c^2)(1 - d^2)},$$

and it can be shown with some algebra that one of these four equalities holds if and only if (53) holds.  $\square$

We conjecture that (53) is also a sufficient condition so that  $A(x, y)$  has a PSD completion of rank at most 2.

### 8. Concluding remarks

If a PD completion of a partial PD matrix  $A$  exists, then from [4] there is a unique PD completion  $A_c$ , called the determinant maximizing completion, whose determinant is maximal among all PD completions of  $A$ . Furthermore,  $A_c^{-1}$  has zeros in those positions corresponding to the unspecified entries in  $A$ . From the elementary cases of the PSD completion region of  $A(x, y)$  that we mentioned in Section 4, it may appear that this determinant maximizing completion  $A_c$  occurs at the centroid of the PSD region. We show that this is not necessarily true.

For example, consider  $A(x, y)$  in (8) with  $a = b = c = d = 1/\sqrt{2}$ . According to Table 1,

$$\det A(x, y) = (xy + x + y - 1)(x - 1)(y - 1)$$

and there are three singular points for the PSD completion region, namely  $(1, 1)$ ,  $(1, 0)$  and  $(0, 1)$  (the third graph in Fig. 5 illustrates a similar case with  $a = .5$ ). The PSD region is bounded above by  $f(x) = 1$ , below by  $g(x) = (1 - x)/(1 + x)$  and from the right by the line  $x = 1$ .

Let  $M_x$  and  $M_y$  be the moments about the  $x$ -axis and  $y$ -axis, respectively. Then

$$M_y = \int_0^1 x \left( 1 - \frac{1-x}{1+x} \right) dx = 2 \ln 2 - 1$$

and

$$\text{Area} = \int_0^1 \left( 1 - \frac{1-x}{1+x} \right) dx = 2 - 2 \ln 2.$$

By symmetry,  $\bar{y} = \bar{x}$ , so the centroid is

$$(\bar{x}, \bar{y}) = \left( \frac{2 \ln 2 - 1}{2 - 2 \ln 2}, \frac{2 \ln 2 - 1}{2 - 2 \ln 2} \right)$$

The PSD completion region is not empty in this case, so there is a unique determinant maximizing completion  $A_c = A(x_0, y_0)$ . Since  $\det A(x_0, y_0) = \det A(y_0, x_0)$ , we must have  $y_0 = x_0$ . Then  $(A_c^{-1})_{13} = 0$ , so

$$\begin{aligned} \det A[\{2, 3, 4\}|\{1, 2, 4\}](x_0, x_0) &= \det \begin{bmatrix} \frac{1}{\sqrt{2}} & 1 & x_0 \\ x_0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & x_0 & 1 \end{bmatrix} \\ &= (x_0 - 1)(x_0^2 + x_0 - 1) = 0 \end{aligned}$$

Since  $x_0 = 1$  yields a PSD completion with determinant 0, then we must have

$$x_0 = \frac{-1 + \sqrt{5}}{2} \neq \bar{x}.$$

So, the determinant maximizing completion

$$A_c = A \left( \frac{-1 + \sqrt{5}}{2}, \frac{-1 + \sqrt{5}}{2} \right) \neq A(\bar{x}, \bar{y}).$$

It is of great interest to obtain information about the PSD completion region for partial PSD matrices associated with more complex nonchordal graphs. We give one example to illustrate how the above results can be applied. Let  $G$  be the graph  $K_{2,m}$ , shown in Fig. 11, and let

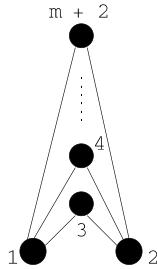


Fig. 11.  $K_{2,m}$ .

$$A = \begin{bmatrix} 1 & ? & a_{13} & \dots & \dots & a_{1n} \\ ? & 1 & a_{23} & \dots & \dots & a_{2n} \\ a_{13} & a_{23} & 1 & ? & \dots & ? \\ \vdots & \vdots & ? & 1 & \dots & ? \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{1n} & a_{2n} & ? & ? & \dots & 1 \end{bmatrix}$$

be a real partial PSD matrix of order  $n = m + 2$  whose graph is  $K_{2,m}$ . Note that  $K_{2,m}$  is missing  $k = \binom{m}{2} + 1$  edges. Let  $R_A \subseteq \mathbb{R}^k$  be the PSD completion region of  $A$ . Note also that there are  $(k - 1)$  4-cycles in  $K_{2,m}$ , namely  $12ij$  where  $\{i, j\} \subseteq \{3, \dots, m + 2\}$ .

Let  $x$  be the unspecified entry in the first row and second column, and for each  $\{i, j\} \subseteq \{3, \dots, m + 2\}$ ,  $i < j$ , let  $y_{ij}$  be the unspecified entry in row  $i$  and column  $j$  of  $A$ . For each such  $i, j$  let

$$A(x, y_{ij}) = \begin{bmatrix} 1 & x & a_{1i} & a_{1j} \\ x & 1 & a_{2i} & a_{2j} \\ a_{1i} & a_{2i} & 1 & y_{ij} \\ a_{1j} & a_{2j} & y_{ij} & 1 \end{bmatrix}$$

be the principal submatrix of  $A$ , with two unspecified entries  $x, y_{ij}$ , associated with the induced 4-cycle  $12ij$  of  $K_{2,m}$ . Let  $R_{A_{ij}}$  be the real PSD completion region of  $A(x, y_{ij})$ . Then if

$$(x, y_{34}, y_{35}, \dots, y_{n-1,n}) \in R_A,$$

then necessarily

$$(x, y_{ij}) \in R_{A_{ij}}$$

for all  $\{i, j\} \subseteq \{3, \dots, m + 2\}$ ,  $i < j$ . In other words, the projection of  $R_A$  onto the  $x, y_{ij}$ -plane is contained in  $R_{A_{ij}}$  for  $3 \leq i < j \leq m$ ; so the complicated region  $R_A$  can be investigated in terms of these more elementary regions, each of which is the completion region for a 4-cycle.

The PSD completion region  $R$  of the matrix  $A(x, y)$  given in (8) exhibits many interesting properties as detailed above. However, there are still a number of interesting open questions concerning  $R$ . One that seems very difficult is the “inverse PSD completion problem”: given a convex subset  $K$  of the square  $S$ , is there a quadruple  $(a, b, c, d)$  such that the completion region  $R$  of  $A(x, y)$  is  $K$ . Our work enables us to eliminate many sets from consideration, for example any  $K$  with 5 or more sharp points on its boundary. However, if  $K$  is a given set with a smooth boundary, it remains unclear whether or not  $K$  can be such a completion region. To this end it would be helpful to determine interesting characteristics of  $R$  in the absence of singular points. We believe that Theorem 2 describes all occurrences of singular points for nontrivial completion regions, but this has not been proved. A further question of interest is whether the theory of algebraic curves can give useful information in other instances of the PSD completion problem.

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