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Null spaces of correlation matrices

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Abstract

Let **R** be the real numbers and $\mathbf{R}^n$ the vector space of all column vectors of length n. Let $\mathscr{C}_n$ be the convex set of all real correlation matrices of size n. If V is a subspace of $\mathbf{R}^n$ of dimension k, we consider the face F_V of $\mathscr{C}_n$ consisting of all $A \in \mathscr{C}_n$ such that $V \subset \mathscr{N}(A)$, i.e., $AV = \mathbf{0}$. If F_V is nonempty, we say that V is realizable. We give complete geometric descriptions of F_V in the cases $k = 1, n = 4$, and $k = 2, n = 5$. For $k = 2, n = 5$, we provide a simple algebraic method for describing F_V.

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1. Introduction

Let A be a real symmetric matrix of size n. We say that A is a *correlation matrix* if A is positive semidefinite and every main diagonal entry is 1. Let $\mathscr{C}_n$ be the set of all correlation matrices of size n. It is known that $\mathscr{C}_n$ is a compact convex set. The extreme points of $\mathscr{C}_n$ are not fully determined, but the vertices are known [10]. (A vertex of a convex set K is an extreme point having a full dimensional normal cone; the normal cone of a boundary point x_0 consists of all normals to supporting hyperplanes for K at x_0.) The vertices of $\mathscr{C}_n$ consist exactly of the 2^{n-1} correlation matrices of rank 1. In the study of the structure of $\mathscr{C}_n$, the following problem is of interest. Suppose that V is a subspace of $\mathbf{R}^n$ of dimension k. When is V contained

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in the null space of some correlation matrix? This question has been fully answered in [5] for $k = 1$, but for higher dimensions the problem is unsolved. To motivate the discussion, put

$$F_V = \{A \in \mathscr{C}_n : AV = \mathbf{0}\},$$

and for $v \in V$,

$$F_v = \{A \in \mathscr{C}_n : Av = \mathbf{0}\}.$$

Then F_V is a face of $\mathscr{C}_n$. Furthermore, all faces of $\mathscr{C}_n$ are of the form F_V for some subspace V of $\mathbf{R}^n$ (see [11]). If we know the faces of $\mathscr{C}_n$, we have a good idea of the structure. Thus, we would like to have a geometric description of F_V. For $n = 3$, a complete pictorial description of the faces of $\mathscr{C}_3$ is available in [10]. There is some discussion of this problem in [11]. For other literature on $\mathscr{C}_n$, its faces and extreme points (see, e.g., [7,9,12]).

The structure of F_V is well understood if $n = 3$ [10] or $k = n - 1$ or $n - 2$ [8]. In this paper, we will give a full geometric description of F_V in the case $k = 1, n = 4$, and $k = 2, n = 5$.

2. Preliminary definitions and results

Definition 2.1. Let $v \in \mathbf{R}^n$. We say that $v = (v_1, \ldots, v_n)^{\mathrm{T}}$ is *balanced* (as in [10] or [11]) if for every $i = 1, \ldots, n$,

$$|v_i| \leqslant \sum_{j \neq i} |v_j|.$$

It is easy to check that any null vector of a correlation matrix is balanced. In fact, the converse is true [5]. If v is balanced, then there is a correlation matrix $A \in \mathscr{C}_n$ such that $Av = \mathbf{0}$.

Definition 2.2. Let V be a subspace of $\mathbf{R}^n$. We say that V is *balanced* if every vector in V is balanced. We say that V is *realizable* if there is an $A \in \mathscr{C}_n$ such that $Av = \mathbf{0}$ for all $v \in V$ (write $AV = \mathbf{0}$).

Clearly any realizable subspace must be balanced. It is also clear from [5] that the converse is true for $\dim V = 1$. But it is false for $\dim V > 1$. Before proving this, we present a method for constructing balanced subspaces (Proposition 2.3). We thank one of the referees for pointing this result out to us, and a resulting simplification in the proof of Theorem 2.4.

Recall that a seminorm on $\mathbf{R}^k$ is a function $N : \mathbf{R}^k \to \mathbf{R}$ with the properties $N(cx) = |c|N(x)$ for each $c \in \mathbf{R}$, $x \in \mathbf{R}^k$ and $N(x + y) \leqslant N(x) + N(y)$ for all $x, y \in \mathbf{R}^k$.

Proposition 2.3. *Let $x_1, \ldots, x_n$ be N-unit vectors in $\mathbf{R}^k$ (i.e., $N(x_1) = \cdots = N(x_n) = 1$) and let X be the k-by-n matrix whose columns are $x_1, \ldots, x_n$. Then $\mathcal{N}(X)$, the null space of X, is balanced.*

Proof. Let $v \in \mathcal{N}(X)$. Then

$$\sum_{j=1}^{n} v_j x_j = 0; \quad \text{thus } v_i x_i = -\sum_{j \neq i} v_j x_j, \quad i = 1, \ldots, n.$$

It follows that

$$|v_i| = N(v_i x_i) = N\left(-\sum_{j \neq i} v_j x_j \right) \leqslant \sum_{j \neq i} N(v_j x_j) = \sum_{j \neq i} |v_j|.$$

Thus the null space of X is balanced. $\square$

Theorem 2.4. *Let $n \geqslant 4$ be given. Then for every integer k, $2 \leqslant k \leqslant n-2$, there exists a subspace $V \subset \mathbf{R}^n$ of dimension k such that V is balanced but not realizable.*

Proof. First we verify the result for $k = n - 2$. Let

$$u = (1, 0, -1, 1, \ldots, 1), \quad w = (0, 1, 1, \ldots, 1)$$

be row vectors of length n. Let B be the submatrix whose rows are u and w and let $V = \mathcal{N}(B)$. Then $\dim V = n - 2$. For each column x of B, $\|x\|_\infty = 1$. Since $\|\cdot\|_\infty$ is a norm on $\mathbf{R}^2$, V is balanced by Proposition 2.3.

Now we show that V is not realizable. Suppose that A is a correlation matrix such that $AV = \mathbf{0}$. We may factor A as $A = C^{\mathrm{T}} C$ where the columns of C are unit vectors in the $\|\cdot\|_2$ norm. Then $\mathcal{N}(C) = \mathcal{N}(A)$, so $V \subseteq \mathcal{N}(C)$. The vectors

$$y = (1, -1, 1, 0, \ldots, 0)^{\mathrm{T}} \quad \text{and} \quad z = (1, 1, 0, -1, 0, \ldots, 0)^{\mathrm{T}}$$

are orthogonal to u and v; thus each is in V and hence in $\mathcal{N}(C)$. Let $c_1, \ldots, c_4$ be the first four columns of C. Since $Cy = Cz = 0$, we have $c_3 = c_2 - c_1$ and $c_4 = c_1 + c_2$. Since all c_j are unit vectors, a simple calculation shows that $\frac{1}{2} = c_1 \cdot c_2 = -\frac{1}{2}$, a contradiction. Therefore V is not realizable.

Now suppose that $k < n - 2$. Construct a k-dimensional subspace W of $\mathbf{R}^{k+2}$ which is balanced but not realizable. Then append $n - k - 2$ zeros in W to produce a subspace V of dimension k in $\mathbf{R}^n$. Clearly, V is balanced. If V were realizable, and A were a correlation matrix such that $AV = \mathbf{0}$, then $A[1, \ldots, k+2]$ would be a correlation matrix which kills W. This contradiction completes the proof. $\square$

Remark 2.5. The example for the case $k = 2$, $n = 4$ was provided by Laurent [8].

Suppose that v and w are balanced vectors in $\mathbf{R}^n$. If there is no common position where both coordinates of v and w are nonzero, then it is clear that $\mathrm{Span}\{v, w\}$ is balanced. We can extend this a little as the following result shows.

Lemma 2.6. *Let* $v = (v_1, \ldots, v_r, 0, \ldots, 0)^{\mathrm{T}}$ *and let* $w = (0, \ldots, 0, w_r, \ldots, w_n)^{\mathrm{T}}$ *be balanced vectors. Then* $\mathrm{Span}\{v, w\}$ *is balanced.*

Proof. Let $z = av + bw$. Then

$$\begin{aligned}
|z_1| = |av_1| &\leqslant |a| \sum_{i=2}^{r} |v_i| \\
&= \sum_{i=2}^{r-1} |av_i| + |av_r + bw_r| + |av_r| - |av_r + bw_r| \\
&\leqslant \sum_{i=2}^{r-1} |av_i| + |av_r + bw_r| + |bw_r| \\
&\leqslant \sum_{i=2}^{r-1} |av_i| + |av_r + bw_r| + |b| \sum_{i=r+1}^{n} |w_i| \\
&= \sum_{i=2}^{r-1} |z_i| + |z_r| + \sum_{i=r+1}^{n} |z_i| = \sum_{i=2}^{n} |z_i|.
\end{aligned}$$

A similar argument holds for $|z_2|, \ldots, |z_n|$, except $|z_r|$. But

$$\begin{aligned}
|z_r| = |av_r + bw_r| &\leqslant |a||v_r| + |b||w_r| \\
&\leqslant |a| \sum_{i=1}^{r-1} |v_i| + |b| \sum_{i=r+1}^{n} |w_i| = \sum_{i \neq r} |z_i|,
\end{aligned}$$

which completes the proof. □

Definition 2.7. Let $v = (v_1, \ldots, v_n)^{\mathrm{T}} \in \mathbf{R}^n$. Following [10], we define the *gap* of v by

$$\mathrm{gap}(v) = \min_{S \subset \{1,\ldots,n\}} \left| \sum_{i \in S} v_i - \sum_{i \notin S} v_i \right|.$$

Remark 2.8. Note that $\mathrm{gap}(v) = 0$ is equivalent to the existence of a vector $u \in \{-1, 1\}^n$ such that $u^{\mathrm{T}} v = \mathbf{0}$ which occurs if and only if $(uu^{\mathrm{T}})v = \mathbf{0}$. Since each rank 1 correlation matrix is of the form uu^{T}, $u \in \{-1, 1\}^n$, we observe that F_v contains a rank one matrix if and only if $\mathrm{gap}(v) = 0$.

As we shall see, the rank one correlation matrices that annihilate v play an important role in analyzing the structure of F_v. It is clear that $\mathscr{C}_n$ is invariant under similarity by a permutation matrix or a diagonal orthogonal matrix. Thus, in studying F_v, we may assume that for $v = (v_1, \ldots, v_n)^{\mathrm{T}}$, we have $v_1 = 1 \geqslant v_2 \geqslant \cdots \geqslant v_n \geqslant 0$.

For $n = 3, 4$, it is easy to see which vectors have gap zero. If $v = (1, a, b)^{\mathrm{T}}$, $1 \geqslant a \geqslant b \geqslant 0$, then $\mathrm{gap}(v) = 0$ if and only if

(i) $1 = a + b$, $b > 0$, or
(ii) $a = 1$, $b = 0$.

In case (i), F_v consists of the single rank one matrix

$$\begin{bmatrix} 1 & -1 & -1 \\ -1 & 1 & 1 \\ -1 & 1 & 1 \end{bmatrix}.$$

In case (ii), F_v consists of all matrices of the form

$$\begin{bmatrix} 1 & -1 & x \\ -1 & 1 & -x \\ x & -x & 1 \end{bmatrix}, \quad -1 \leqslant x \leqslant 1,$$

and thus contains two rank one matrices. The reason we have two rank one matrices in case (ii) is that $\mathrm{gap}(1, 1, 0)^{\mathrm{T}} = 0$ for both $S = \{1\}$ and $S = \{1, 3\}$ (as well as their complements). To make this more precise, consider the following definition.

Definition 2.9. For each $v = (v_1, \ldots, v_n)^{\mathrm{T}} \in \mathbf{R}^n$ with $\mathrm{gap}(v) = 0$, define

$$m_v = \frac{1}{2}\left|\left\{S \subset \{1, \ldots, n\} : \sum_{i \in S} v_i - \sum_{i \neq S} v_i = 0\right\}\right|. \tag{2.1}$$

It is evident that m_v equals the number of rank 1 matrices in F_v. (The 1/2 is in the formula because the roles of S and the complement of S can be switched without producing an additional rank one correlation matrix that kills v.)

Now consider $n = 4$. Suppose $v = (1, a, b, c)^{\mathrm{T}}$, $1 \geqslant a \geqslant b \geqslant c \geqslant 0$. Then if $\mathrm{gap}(v) = 0$, one of the following equations must hold:

(i) $1 - a - b - c = 0$,
(ii) $1 - a - b + c = 0$,
(iii) $1 - a + b - c = 0$,
(iv) $1 + a - b - c = 0$,
(v) $1 - a + b + c = 0$.

These equations yield six different cases, which are summarized in the following table. To distinguish cases, all coordinates are taken to lie in (0, 1) unless otherwise specified.

$(1, a, b, c)^{\mathrm{T}}$	Number of rank one matrices
$(1, 1, 0, 0)^{\mathrm{T}}$	4
$(1, a, 1-a, 0)^{\mathrm{T}}$	2
$(1, 1, 1, 1)^{\mathrm{T}}$	3
$(1, 1, b, b)^{\mathrm{T}}$	2
$(1, a, b, 1-a-b)^{\mathrm{T}}$	1
$(1, a, b, a+b-1)^{\mathrm{T}}$	1

In the following section, we will give a more explicit description of F_v. We conclude this section with a few more useful results.

Lemma 2.10. *Let A be a symmetric matrix of size n. Assume that the entries of A are in $R = F[x_1, \ldots, x_t]$, where F is a field. Suppose that $v_1, \ldots, v_r$ are linearly independent vectors in F^n and that $Av_j = \mathbf{0}$, $j = 1, \ldots, r$, for all $x_1, \ldots, x_t$. Let*

$$C_{n-r}(A)$$

be the $(n-r)$th compound matrix of A. Then there is a nonzero polynomial $q(x_1, \ldots, x_t)$ in R such that

$$C_{n-r}(A) = q(x_1, \ldots, x_t)B,$$

where $B \in M_n(F)$, i.e., B is a constant matrix.

Proof. If the rank of A is less than $n-r$, then $C_{n-r}(A)$ must be zero and the result is obvious. Otherwise, the problem is invariant under left or right multiplication of A by permutation matrices, so we will assume that the leading entry in $C_{n-r}(A)$ is nonzero. Since A is symmetric, so is $C_{n-r}(A)$. Moreover, the rank of $C_{n-r}(A)$ must be one (see [13, p. 117–121]). It follows that the column space of $C_{n-r}(A)$ is spanned by the first column of $C_{n-r}(A)$. Denote this first column by $(p_1, \ldots, p_k)^{\mathrm{T}}$, where $k = \binom{n}{n-r}$. Then the (i, j) entry in $C_{n-r}(A)$ must be

$$\frac{p_i p_j}{p_1}.$$

Now suppose that $p_j \neq 0$. Since $C_{n-r}(A)$ kills a $(k-1)$-dimensional subspace of F^k, the null space of $C_{n-r}(A)$ must contain a vector with nonzero coordinates in positions 1 and j and zeros elsewhere. Thus $p_j = sp_1$, where $s \in F$ and this proves the result with $q(x_1, \ldots, x_t) = p_1$. $\square$

Lemma 2.11. *Suppose $A = (1-t)B_1 + tB_2$, $0 < t < 1$ where A, B_1, B_2 are positive semidefinite. Then*

(i) $\mathcal{N}(A) \subset \mathcal{N}(B_i)$, $i = 1, 2$.
(ii) $\operatorname{rank} B_i \leqslant \operatorname{rank} A$, $i = 1, 2$.

Proof. (i) Let $x \in \mathcal{N}(A)$. Then $0 = x^{\mathrm{T}}Ax = (1-t)x^{\mathrm{T}}B_1x + tx^{\mathrm{T}}B_2x$. Since $x^{\mathrm{T}}B_ix \geqslant 0$, $i = 1, 2$, $x^{\mathrm{T}}B_1x = x^{\mathrm{T}}B_2x = 0$. Thus $B_1^{1/2}x = B_2^{1/2}x = 0$, so $B_1x = B_2x = 0$. Then $x \in \mathcal{N}(B_i)$, $i = 1, 2$.

(ii) By (i) the nullity of B_i is greater than or equal to the nullity of A, so rank $B_i \leqslant$ rank A, $i = 1, 2$. □

Our next result is a special kind of matrix completion problem. For additional information on positive semidefinite completions (see [2,14]).

Theorem 2.12. *Let*

$$P = \begin{bmatrix} 1 & b^{\mathrm{T}} \\ b & B \end{bmatrix}, \quad \text{and} \quad Q = \begin{bmatrix} B & c \\ c^{\mathrm{T}} & 1 \end{bmatrix}$$

be correlation matrices of size $n-1$. Suppose that

$$\begin{bmatrix} 1 \\ w \end{bmatrix} \in \mathcal{N}(P), \quad \text{and} \quad \begin{bmatrix} z \\ 1 \end{bmatrix} \in \mathcal{N}(Q).$$

Let $q = -b^{\mathrm{T}}z$, and let

$$A = \begin{bmatrix} 1 & b^{\mathrm{T}} & q \\ b & B & c \\ q & c^{\mathrm{T}} & 1 \end{bmatrix}.$$

Then A is a correlation matrix of size n with rank A = rank P. *Moreover*,

$$\begin{bmatrix} 1 \\ w \\ 0 \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} 0 \\ z \\ 1 \end{bmatrix} \in \mathcal{N}(A).$$

Proof. By the definition of q,

$$\begin{bmatrix} 1 & b^{\mathrm{T}} & q \end{bmatrix} \begin{bmatrix} 0 \\ z \\ 1 \end{bmatrix} = 0,$$

and

$$\begin{bmatrix} 0 \\ z \\ 1 \end{bmatrix} \in \mathcal{N}\left(\begin{bmatrix} b & B & c \\ q & c^{\mathrm{T}} & 1 \end{bmatrix}\right).$$

Consequently,

$$\begin{bmatrix} 0 \\ z \\ 1 \end{bmatrix} \in \mathcal{N}(A).$$

It follows that

$$\begin{bmatrix} q \\ c \\ 1 \end{bmatrix}$$

is a linear combination of the columns of

$$\begin{bmatrix} b^{\mathrm{T}} \\ B \\ c^{\mathrm{T}} \end{bmatrix}.$$

Thus by the symmetry of A, $[q \quad c^{\mathrm{T}} \quad 1]$ is a linear combination of the rows of $[b \quad B \quad c]$. But

$$\begin{bmatrix} 1 \\ w \\ 0 \end{bmatrix} \in \mathscr{N}([\,b \quad B \quad c\,]),$$

so

$$[\,q \quad c^{\mathrm{T}} \quad 1\,] \begin{bmatrix} 1 \\ w \\ 0 \end{bmatrix} = 0.$$

Therefore,

$$\begin{bmatrix} 1 \\ w \\ 0 \end{bmatrix} \in \mathscr{N}(A).$$

Since the last row (column) of A is a linear combination of the preceding rows (columns) of A,

$$\operatorname{rank} A = \operatorname{rank} P.$$

Therefore the number of nonzero eigenvalues of A must be the same as the number of nonzero eigenvalues of P. But P is positive semidefinite. Thus the number of nonzero eigenvalues of P is the number of positive eigenvalues of P, which by interlacing is less than or equal to the number of positive eigenvalues of A. Hence A is positive semidefinite and a correlation matrix. □

The following lemma is a simple exercise; thus we omit the proof.

Lemma 2.13. *Let $v = (a, b, c)^{\mathrm{T}}$ be balanced, with $abc \neq 0$. Then there is exactly one correlation matrix A such that $Av = \mathbf{0}$.*

We also need the following column inclusion result (see [1,6]).

Lemma 2.14. *Let*

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

be a positive semidefinite matrix. Then each column of C is in the column space of B.

3. Main results and proofs

We now proceed to describe the set F_v for $n = 4$. Let

$$A = \begin{bmatrix} 1 & r & s & t \\ r & 1 & u & y \\ s & u & 1 & x \\ t & y & x & 1 \end{bmatrix}, \quad A(1) = \begin{bmatrix} 1 & u & y \\ u & 1 & x \\ y & x & 1 \end{bmatrix},$$

and let $v = [1, a, b, c]^{\mathrm{T}}$.

Lemma 3.1. *Let (x, y) be one of the points*

$$(1, 1), \quad (1, -1), \quad (-1, 1), \quad (-1, -1).$$

Assume that $v \in \mathcal{N}(A)$ and that $\det A(1) \geqslant 0$. *Then A is a rank* 1 *correlation matrix.*

Proof. We have

$$\begin{aligned} \det A(1) &= 1 + 2uxy - u^2 - x^2 - y^2 \\ &= -1 + 2xyu - u^2 = -(1 - xyu)^2 \geqslant 0. \end{aligned}$$

Thus $u = 1/xy = xy$. Then $A(1) = ww^{\mathrm{T}}$, for $w = [1, xy, y]^{\mathrm{T}}$, so $A(1)$ is a rank 1 correlation matrix. Since $Av = \mathbf{0}$ and A is symmetric, the first column (row) of A is a linear combination of the following columns (rows). Thus $\operatorname{rank}(A) = 1$ also. By interlacing, the nonzero eigenvalue of A is positive, so A is a rank 1 correlation matrix. $\square$

Written out, the equation $Av = 0$ is:

$$\begin{bmatrix} 1 & r & s & t \\ r & 1 & u & y \\ s & u & 1 & x \\ t & y & x & 1 \end{bmatrix} \begin{bmatrix} 1 \\ a \\ b \\ c \end{bmatrix} = 0.$$

Assume from now on that $ab \neq 0$. The equation $Av = \mathbf{0}$ gives a set of four linear equations in the unknowns r, s, t, u, x, y. Letting x, y be the free variables and solving for r, s, t, u we find that the matrix A has the parametric form [11] given by

$$A(x, y) = \begin{bmatrix} 1 & \frac{-a^2+b^2+c^2-1}{2a} + \frac{bcx}{a} & \frac{a^2-b^2+c^2-1}{2b} + \frac{acy}{b} & -c - ay - bx \\ \frac{-a^2+b^2+c^2-1}{2a} + \frac{bcx}{a} & 1 & \frac{1-a^2-b^2-c^2}{2ab} - \frac{cy}{b} - \frac{cx}{a} & y \\ \frac{a^2-b^2+c^2-1}{2b} + \frac{acy}{b} & \frac{1-a^2-b^2-c^2}{2ab} - \frac{cy}{b} - \frac{cx}{a} & 1 & x \\ -c - ay - bx & y & x & 1 \end{bmatrix}. \tag{3.1}$$

Necessarily $A(x, y)$ is singular for all $x, y \in R$. Before analyzing $A(x, y)$ in detail, we begin with an example. This example is a degenerate case for which F_v contains three matrices of rank one.

Example 3.2. $a = b = c = 1$.

Then $A(x, y)$ becomes:

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

In order that A be a correlation matrix it is necessary that $|x|, |y| \leqslant 1$, and $-1-x-y \geqslant -1$. Then (x, y) must lie in the triangle T determined by the lines $x + y = 0$, $x = -1$, $y = -1$.

The vertices of T are $(1, -1)$, $(-1, 1)$, $(-1, -1)$. Substituting in A above, we see that each of these three points gives rise to a rank one correlation matrix. (Note that we could have arrived at the same conclusion by applying Lemma 3.1.) Since each point (x, y) in T is a convex combination of the vertices of T, each corresponding matrix, $A(x, y)$ is a convex combination of rank one correlation matrices, and hence is also a correlation matrix. Therefore, there is a one-to-one correspondence between T and F_v.

We now apply Lemma 2.10 to the general $A(x, y)$ with $n = 4$, $k = 1$. (We have replaced r with k to avoid notational problems.) Upon calculating the $(1, 1)$ entry of $C_3(A)$, we find that

$$\begin{aligned} q(x, y) = {} & -(1/4a^2b^2)(1 + 4y^2a^2b^2 + 4c^2x^2b^2 + 4c^2y^2a^2 + 4c^3xb \\ & + 4c^3ya + 4b^3cx + 4a^3cy - 4cya - 4cxb + 12c^2xyab \\ & + c^4 + 8cy^2a^2xb + 8cx^2b^2ya + a^4 + b^4 + 2a^2c^2 + 2b^2c^2 \\ & + 4x^2a^2b^2 + 4b^2cya + 4b^3xya + 4a^2cxb + 4a^3xyb \\ & - 2a^2b^2 - 4xyab - 2a^2 - 2b^2 - 2c^2). \end{aligned} \tag{3.2}$$

For convenience, we replace $q(x, y)$ with a scalar multiple:

$$\begin{aligned} p(x, y) = {} & 8cb^2ax^2y + 8ca^2bxy^2 + 4a^2b^2x^2 + 4c^2b^2x^2 + 4b^3axy \\ & + 4a^3bxy + 12c^2abxy - 4abxy + 4a^2b^2y^2 + 4c^2a^2y^2 \\ & + 4c^3bx + 4b^3cx + 4a^2cbx - 4cbx - 4cay + 4b^2cay \\ & + 4a^3cy + 4c^3ay + 1 + b^4 + 2a^2c^2 + 2b^2c^2 + a^4 \\ & - 2a^2b^2 + c^4 - 2a^2 - 2b^2 - 2c^2. \end{aligned} \tag{3.3}$$

Note that $p(x, y) \leqslant 0$ if $A(x, y) \in F_v$.

Definition 3.3. Let B be the unit square $\{(x, y) \in R^2 : -1 \leqslant x, y \leqslant 1\}$.

The following is an immediate consequence of Lemma 3.1.

Corollary 3.4. *If $p(x, y)$ vanishes at one of the four corners of B, the corresponding matrix $A(x, y)$ is a rank 1 correlation matrix.*

We now show that the boundary of F_v is determined by the polynomial p inside B.

Definition 3.5. Let $B_v = \{(x, y) \in B : A(x, y) \in F_v\}$.

Theorem 3.6. *A point (x_0, y_0) is on ∂B_v if and only if $(x_0, y_0) \in B$ and $p(x_0, y_0) = 0$.*

Proof. First, suppose (x_0, y_0) is on ∂B_v. Then by definition, $(x_0, y_0) \in B$. Since $A(x_0, y_0)$ is positive semidefinite, we have $p(x_0, y_0) \leqslant 0$. Suppose $p(x_0, y_0) < 0$. Then $A(x_0, y_0)[\{2, 3, 4\}]$ is positive definite so $|x_0|, |y_0| < 1$. But then $A(x, y)[\{2, 3, 4\}]$ is positive definite for (x, y) sufficiently close to (x_0, y_0), and therefore, $A(x, y) \in F_v$ for (x, y) sufficiently close to (x_0, y_0) implying that (x_0, y_0) is in the interior of B_v, a contradiction. Consequently, $p(x_0, y_0) = 0$.

Now suppose $(x_0, y_0) \in B$ and $p(x_0, y_0) = 0$. There are two cases:

I. If (x_0, y_0) is a corner of B, then $A(x_0, y_0)$ is a rank one correlation matrix. Thus, $(x_0, y_0) \in B_v$, and since $B_v \subset B$, (x_0, y_0) is on ∂B_v.

II. (x_0, y_0) is not a corner of B. By Lemma 2.10 with $n = 4$, $r = 1$, rank $A(x_0, y_0) \leqslant 2$. Now either $|x_0| < 1$ or $|y_0| < 1$. Without loss of generality, say $|x_0| < 1$, Then

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

is positive definite, so $A(x_0, y_0)$ has two positive eigenvalues by interlacing. Thus $A(x_0, y_0)$ is positive semidefinite and $(x_0, y_0) \in B_v$. But if (x_0, y_0) is in the interior of B_v, then the points (x, y) sufficiently close to (x_0, y_0) are on a line containing (x_0, y_0) and are in B_v. By Lemma 2.11, rank $A(x, y) \leqslant 2$ at all such points. Then $p(x, y)$ vanishes identically in a neighborhood of (x_0, y_0), which is impossible. Therefore, (x_0, y_0) is on ∂B_v. $\square$

Theorem 3.6 shows that finding the boundary of F_v reduces to finding where the plane cubic algebraic curve $p(x, y)$ vanishes. We now look at a second example.

Example 3.7. $a = 1, b = 0.5, c = 0.5$.

In this case, we have the equation under Fig. 1 for the cubic curve. The plot of this equation shows (see Corollary 3.4) that there are two rank one correlation matrices on ∂B_v, and hence there is a straight line as a component.

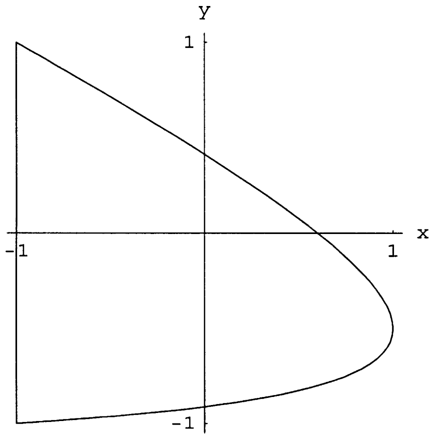


Fig. 1. $(1+x)(xy+1.25x+2y^2+y-0.75)=0$.

More generally, substituting $a=1$, $c=b$ into $p(x,y)$ we obtain the polynomial

$$4b^2(1+x)(2bxy+x+b^2x+2y^2+2by-1+b^2).$$

The two factors on the right hand side are the two components of the curve and intersect at the two left corners of B, so by Corollary 3.4, these correspond to rank 1 correlation matrices. These intersection points are singular points of $p(x,y)$ defined as follows.

Definition 3.8. A singular point (x_0, y_0) of $p(x,y)$ is a point simultaneously satisfying the equations:

$$p(x,y)=0, \quad p_x(x,y)=0, \quad p_y(x,y)=0.$$

As we shall see, each singular point of $p(x,y)$ corresponds to a rank 1 correlation matrix in F_v. In Example 3.2 there are three singular points and in Example 3.7 there are two. We shall show that in all other cases in the following theorem, there is at most one singular point, and generically there are zero.

Theorem 3.9. *Let $v=(1,a,b,c)^{\mathrm{T}}$ with $1 \geqslant a \geqslant b \geqslant c \geqslant 0$. Assume that there is at least one rank one matrix associated with ∂B_v, i.e.,* gap$(v)=0$. *If $v=(1,1,0,0)^{\mathrm{T}}$, then F_v is essentially $\mathscr{C}_3$. If $v=(1,a,1-a,0)^{\mathrm{T}}$, $a \neq 1$, then F_v is a line segment. In all other cases, ∂B_v is the intersection of a plane cubic algebraic curve with B. The singularities of this curve occur where the curve meets the vertices of B, and correspond to rank one correlation matrices. The nature of this intersection is described by the following table. Once again, note that all coordinates of v lie in* $(0,1)$ *unless otherwise specified.*

v	∂B_v
$(1, 1, 1, 1)^{\mathrm{T}}$	*A right triangle with vertices at three corners of B*
$(1, 1, b, b)^{\mathrm{T}}$	*A line segment connecting two corners of B and a quadratic curve passing through those two corners*
$(1, a, b, 1-a-b)^{\mathrm{T}}$	*An isolated point* $(1, 1)$
$(1, a, b, a+b-1)^{\mathrm{T}}$	*Part of a cubic curve with a node at* $(-1, -1)$, *the only corner of B that the curve meets*

Remark 3.10. Theorem 3.9 shows that there is a one-to-one correspondence between each singular point and each rank one correlation matrix in F_v. In particular, for $c > 0$, if $a \neq 1$ or $b \neq c$, there can be at most one rank one correlation matrix in F_v. Also, each rank two correlation matrix in F_v corresponds to a zero of $p(x, y)$ (and thus a point on ∂B_v) which is not a singular point. Each rank three correlation matrix in F_v corresponds to a point at which $p(x, y) < 0$, i.e., an interior point of B_v.

Proof of theorem 3.9. Let $v = (1, 1, 0, 0)^{\mathrm{T}}$. Let C be any 3×3 correlation matrix. Extend C to a 4×4 correlation matrix A with the requirement that the second row (and second column) be the negative of the first. Then A has the form

$$\begin{bmatrix} 1 & -1 & -r & -s \\ -1 & 1 & r & s \\ -r & r & 1 & t \\ -s & s & t & 1 \end{bmatrix}$$

and this completely describes F_v.

Now let $v = (1, a, 1-a, 0)^{\mathrm{T}}$, $a < 1$. By Lemma 2.13 $A[1, 2, 3]$ is uniquely determined and in fact must be

$$\begin{bmatrix} 1 & -1 & -1 \\ -1 & 1 & 1 \\ -1 & 1 & 1 \end{bmatrix}.$$

It follows from Lemma 2.14 that any 4×4 correlation matrix A such that $Av = \mathbf{0}$ must have the form

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

where $-1 \leqslant x \leqslant 1$. Thus F_v is a line segment.

We now assume that $c > 0$, and then find those a, b, c which allow singular points. Taking partial derivatives we find

$$\begin{aligned} p_x = {} & 16cb^2axy + 8ca^2by^2 + 8b^2a^2x + 8c^2b^2x + 4a^3by + 4ab^3y \\ & - 4aby + 12c^2aby + 4c^3b + 4b^3c + 4a^2cb - 4cb, \end{aligned} \tag{3.4}$$

and

$$p_y = 8cb^2ax^2 + 16ca^2bxy + 4a^3bx + 4b^3ax - 4abx + 12c^2abx \\ + 8c^2a^2y + 8a^2b^2y + 4c^3a + 4b^2ca + 4a^3c - 4ca. \tag{3.5}$$

We use resultants [4, pp. 71–73] to find the common zeros of p, p_x, p_y. We consider p, p_y as polynomials of degree 2 and 1 in y. Their resultant is the 3×3 matrix R with rows,

$$\left[8a^2cbx + 4a^2c^2 + 4a^2b^2 \quad 16a^2cbx + 8a^2c^2 + 8a^2b^2 \quad 0\right],$$

$$\left[8cb^2ax^2 + 4a^3bx + 12c^2abx - 4abx + 4b^3ax - 4ca + 4a^3c + 4c^3a \right.\\ + 4cb^2a \quad 8cb^2ax^2 + 4a^3bx + 12c^2abx - 4abx + 4b^3ax - 4ca \\ \left. + 4a^3c + 4c^3a + 4cb^2a \quad 16a^2cbx + 8a^2c^2 + 8a^2b^2\right],$$

and

$$\left[4c^2b^2x^2 + 4a^2b^2x^2 + 4b^3cx + 4c^3bx + 4a^2cbx - 4cbx + 2a^2c^2 + 2b^2c^2 \right.\\ + 1 + b^4 + c^4 - 2a^2b^2 + a^4 - 2a^2 - 2b^2 - 2c^2 \quad 0 \quad 8cb^2ax^2 + 4a^3bx \\ \left. + 12c^2abx - 4abx + 4b^3ax - 4ca + 4a^3c + 4c^3a + 4cb^2a\right].$$

Then

$$\det R = -64b^2a^4(x-1)(x+1)(2cbx + c^2 + b^2) \\ \times (2cbx - 1 + 2a - a^2 + c^2 + b^2)(2cbx - 1 - 2a - a^2 + c^2 + b^2) \tag{3.6}$$

vanishes at any common zero of p and p_y.

We consider its five possible zeros in turn.

I. If $x = 1$, then substituting in $p_y = 0$ gives

$$y_1 = -\frac{b^2 + 2cb - 1 + a^2 + c^2}{2\,(b+c)\,a}.$$

II. Substituting $x = -1$ into $p_y = 0$ gives

$$y_2 = \frac{b^2 - 2cb - 1 + a^2 + c^2}{2\,(-c+b)\,a}.$$

III. Substituting $x_3 = -(c^2 + b^2)/2cb$ into $p_y = 0$ gives

$$-\frac{2a(-c+b)(b+c)(-1+a)(1+a)}{c} = 0.$$

IV. Substituting $x_4 = (1 - 2a + a^2 - c^2 - b^2)/2cb$ into $p_y = 0$ gives

$$y_4 = -\frac{a^2 - 2a + 1 - b^2 + c^2}{2c(-1+a)}.$$

V. Substituting $x_5 = (1 + 2a + a^2 - c^2 - b^2)/2cb$ into $p_y = 0$ gives

$$y_5 = -\frac{a^2 + 2a + 1 - b^2 + c^2}{2c\,(1 + a)}.$$

First consider case III. In order for $p_y = 0$ we must have $a = 1$ or $c = b$. Suppose $a = 1$. Substituting $a = 1$, $x_3 = -(c^2 + b^2)/2cb$ into $p(x, y) = 0$ yields

$$\frac{(-c + b)^2\,(b + c)^2}{c^2} = 0,$$

so $c = b$. We have already treated this case in Examples 3.2 and 3.7. There are three singular points if $a = b = c = 1$ and two if $a = 1 > b = c$. In either case these are corners of B.

Now suppose $c = b$. Then $x_3 = -1$. Substituting these into $p(x, y) = 0$ yields $(-1 + a)^2(1 + a)^2 = 0$ so $a = 1$. This is identical to the previous case.

We now substitute each of I, II, IV, V into $p_x = 0$.

I.

$$-\frac{2b^2(a + 1 + c + b)(1 + a - c - b)(a - 1 + c + b)(a - 1 - c - b)}{(b + c)^2} = 0.$$

This can occur if $a = b = c = 1$ or $c = 1 - a - b$. We have already treated the first possibility.

Therefore we suppose that $c = 1 - a - b$. Then $y_1 = 1$ and we have a singularity at $(1, 1)$. Consider the first row $[1\ \ a_{12}\ \ a_{13}\ \ a_{14}]$ of the correlation matrix A. Then

$$0 = 1 + a_{12}a + a_{13}b + a_{14}(1 - a - b) \geqslant 1 - a - b - (1 - a - b) = 0.$$

so the first row must be $[1\ \ -1\ \ -1\ \ -1]$. It follows also that $a_{23} = 1$ and F_v consists of the unique matrix

$$\begin{bmatrix} 1 & -1 & -1 & -1 \\ -1 & 1 & 1 & 1 \\ -1 & 1 & 1 & 1 \\ -1 & 1 & 1 & 1 \end{bmatrix}.$$

We now show that $(1, 1)$ is an isolated point on the curve $p(x, y) = 0$. Let $A(x, y)$ be the generic symmetric matrix with all ones on the main diagonal that kills v. There are two ways we can find $p(x, y)$ for $c = 1 - a - b$. One is to substitute directly into Eq. (3.3) as we did in the paragraph following Example 3.7. A second way is to substitute $c = 1 - a - b$ in any 3×3 submatrix of $A(x, y)$. By Lemma 2.10, the determinant of this submatrix is a constant multiple of $p(x, y)$. We will utilize both methods in this paper and illustrate both in this proof. Using the second here, we put $c = 1 - a - b$ in $\det A(x, y)[2, 3, 4]$ and obtain

$$\begin{vmatrix} 1 & \frac{-a^2-b^2+a+b-ab-ya+ya^2+yab-xb+xba+xb^2}{ab} & y \\ \frac{-a^2-b^2+a+b-ab-ya+ya^2+yab-xb+xba+xb^2}{ab} & 1 & x \\ y & x & 1 \end{vmatrix},$$

which we set equal to zero. Since $p(x, y)$ contains no x^3 or y^3 term, we may solve for y in terms of x using the quadratic formula and in the solution we obtain the following formula for the discriminant:

$$b^3(x+1)(x-1)^2(b+a-1)(bxa+2a-ab+b^2x-bx+b-b^2).$$

In this case, the only rank one correlation matrix that kills v requires that $x = y = 1$. When $x = 1$, the factors in the discriminant other than $(x-1)^2$ become

$$b^3(2)(-c)(2a),$$

which is always negative. Therefore, for values of x near 1, we cannot get any values for y. It follows that $(1, 1)$ must be an isolated point on the curve.

II.

$$\frac{2b^2(a+1+c-b)(a+1-c+b)(a-1+c-b)(a-1-c+b)}{(-c+b)^2} = 0.$$

This can occur if $a = 1$, $b = c$ which we have already treated, or if $c = a + b - 1$. In the latter case $y_2 = -1$ also. Before treating this case, we consider cases IV and V.

IV.

$$\frac{2ba(a-1+c-b)(a-1-c+b)(a-1+c+b)(a-1-c-b)}{c(-1+a)^2} = 0.$$

This can occur in three ways, two of which $a = 1$, $c = b$ and $c = 1 - a - b$ we have already considered. The third is $c = a + b - 1$, which also occurs in II. In this case $x_4 = y_4 = -1$ so this turns out to be the same singular point as in II.

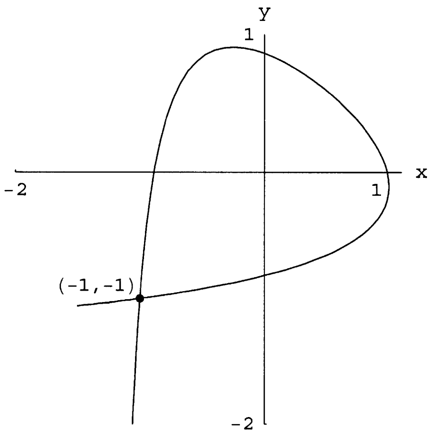
V.

$$-\frac{2ba(a+1-c+b)(a+1+c+b)(1+a-c-b)(a+1+c-b)}{c(1+a)^2} = 0.$$

This occurs only if $1 + a = b + c$, i.e. if $a = b = c = 1$ which we considered above.

To conclude our discussion of singular points, it remains to consider the case $c = a + b - 1$. To illuminate this discussion, we first consider a special case.

Example 3.11. Let $v = (4, 3, 2, 1)^{\mathrm{T}}$. (For convenience, we do not normalize the first coordinate.) Clearly only one rank one correlation matrix kills v, corresponding to $(-1, -1)$, the only singularity. Note that the curve can be tangent to other points on B.



$$-\tfrac{35}{64}+\tfrac{5}{8}x^2-\tfrac{3}{32}y-\tfrac{1}{16}x+\tfrac{45}{64}y^2+\tfrac{9}{16}y^2x+\tfrac{3}{8}yx^2=0.$$

Note that the singular point $(-1,-1)$ is a node for this v. We show that this is always the case. Substituting $c=a+b-1$ into $\frac{1}{4}p(x,y)$ gives the polynomial

$$\begin{aligned}
&2b^2a^2x^2y+2b^3ax^2y-2b^2ax^2y+2b^2a^2xy^2+2a^3bxy^2-2a^2bxy^2\\
&+b^2x^2+2b^3ax^2+b^4x^2+2a^2b^2x^2-2b^3x^2-2b^2ax^2+4a^3bxy\\
&+2abxy+6a^2b^2xy-6a^2bxy+4b^3axy-6ab^2xy+a^2y^2-2a^2by^2\\
&-2a^3y^2+2a^2b^2y^2+a^4y^2+2a^3by^2+2a^3bx+2abx-4a^2bx-4b^3x\\
&+4b^3ax-6b^2ax+4a^2b^2x+2b^2x+2b^4x+2a^2y+2a^4y-4b^2ay\\
&+4a^2b^2y+2b^3ay+4a^3by+2aby-6a^2by-4a^3y+2a^2b^2-2b^3\\
&-4a^2b+b^2+2b^3a+a^2-2a^3+2ba-4b^2a+2a^3b+a^4+b^4.
\end{aligned}\tag{3.7}$$

To analyze the singularity, we translate it to the origin by replacing x by $u-1$, and y by $v-1$ (not the same v as in F_v), keeping only the quadratic terms. The result is

$$q(u,v)=b^2(1-b)^2u^2+2ab(1-a-b-ab)uv+a^2(1-a)^2v^2.$$

The discriminant of this quadratic form is $16a^3b^3(a+b-1)=16a^3b^3c\neq 0$. So there are two tangent lines to the curve at the singular point and it follows that the singularity must be a node.

Finally, substituting $x=y=-1$, $c=a+b-1$ into $A(x,y)$ we obtain the rank one correlation matrix

$$\begin{bmatrix} 1 & -1 & -1 & 1\\ -1 & 1 & 1 & -1\\ -1 & 1 & 1 & -1\\ 1 & -1 & -1 & 1 \end{bmatrix}.$$

This concludes the proof. □

Remark 3.12. If the curve $p(x, y) = 0$ crosses the boundary of B, it must do so at a corner. Otherwise, by continuity, points on the curve sufficiently close to the crossing point would represent rank 2 correlation matrices, a contradiction, since x or y would have modulus larger than 1.

Theorem 3.13. *Let v be as in Theorem* 3.9 *and balanced. Assume that ∂B_v has no singularities, i.e.,* $\text{gap}(v) \neq 0$. *If $v = (1, a, b, 0)^{\mathrm{T}}$, then ∂B_v is an ellipse tangent to B at four points. If $v = (1, a, b, c)^{\mathrm{T}}$, $c > 0$, then ∂B_v is a smooth topological component (in the Euclidean topology) of an irreducible plane algebraic curve.*

Proof. Let $v = (1, a, b, 0)^{\mathrm{T}}$ with $1 \geqslant a \geqslant b > 0$ be balanced, so that $a + b > 1$. We want to describe the boundary of F_v, the face of the correlation matrices that kill v. Now the generic matrix $A(x, y)$ of F_v can be parameterized as follows:

$$\begin{bmatrix} 1 & r & s & -ay-bx \\ r & 1 & t & y \\ s & t & 1 & x \\ -ay-bx & y & x & 1 \end{bmatrix}.$$

By Lemma 2.13 r, s, and t are uniquely determined. Since $a + b > 1$, none of them is ± 1. Since

$$\det A[2, 3, 4] = 1 + 2txy - x^2 - y^2 - t^2,$$

$p(x, y) = 0$ is the equation of an ellipse. Note that if we set $x = 1$, this forces $y = t$ and if $x = -1$, then $y = -t$. A similar statement holds if we choose $y = \pm 1$. By Remark 3.12 the ellipse ∂B_v is tangent to B at the four points $(\pm 1, \pm t)$ and $(\pm t, \pm 1)$.

Now consider $v = (1, a, b, c)^{\mathrm{T}}$, $c > 0$. It follows from (3.3) that the curve $p(x, y) = 0$ is cubic with no x^3 or y^3 term. If $p(x, y)$ reduced, one component would be a straight line. If this line does not intersect the square B, then all boundary points of B_v lie on a quadratic curve and because B_v is bounded this curve must be an ellipse. But then $p(x, y)$ must have x^3 and y^3 terms, a contradiction. If the line does intersect B, it must also cross the boundary of B. By Remark 3.12, it must do so at a corner. By Lemma 3.1, $A(x_0, y_0)$ is a rank 1 correlation matrix forcing $\text{gap}(v) = 0$, a contradiction. Therefore, $p(x, y)$ is irreducible and ∂B_v is a topological component of $p(x, y) = 0$. $\square$

The following example will illustrate the first possibility.

Take $v = \frac{1}{4}(4, 3, 2, 0)^{\mathrm{T}}$. Any correlation matrix that kills v must have the form (for suitable x, y)

$$\begin{bmatrix} 1 & -7/8 & -11/16 & z \\ -7/8 & 1 & 1/4 & y \\ -11/16 & 1/4 & 1 & x \\ z & y & x & 1 \end{bmatrix}.$$

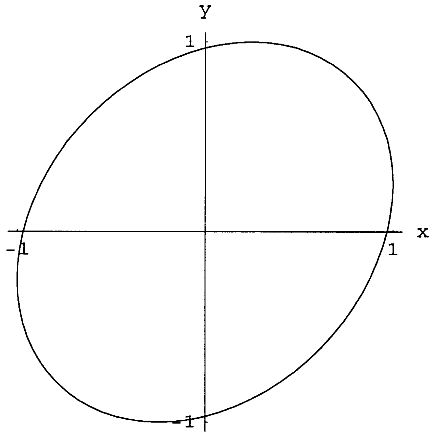


Fig. 2. $\frac{15}{16} - y^2 + \frac{1}{2}xy - x^2 = 0$.

Note that $\det A[2, 3, 4] = \frac{15}{16} - y^2 + \frac{1}{2}xy - x^2$. If we set this quadratic polynomial equal to zero, we get an ellipse. Moreover, it is easy to see that the points of tangency to B of the ellipse are $(1, \frac{1}{4})$, $(-1, -\frac{1}{4})$, $(\frac{1}{4}, 1)$ and $(-\frac{1}{4}, -1)$. Fig. 2 shows the plot.

Remark 3.14. For $k = 1$, $n = 4$, a description of these faces is given in [11]. We point out a minor error at the end of the paper about faces of dimension 2. The paragraph following Eq. (6.3) on page 546 says that the boundary of these faces is described by a polynomial of degree less than or equal to 2. As we have seen above, the boundary is given by the polynomial $p(x, y)$, which is generically of degree 3. The description we have given of these two dimensional faces is also more detailed and complete.

We will use the information for the case $k = 1$, $n = 4$ to develop the case $k = 2$, $n = 5$. Let v, w be linearly independent vectors in $\mathbf{R}^5$. If there is a common component zero, then we are in the 4×4 case, so assume that v and w have no common zero component. Then by taking suitable permutations and linear combinations of v and w, we may assume that they have the form

$$v = (1, a, b, c, 0)^{\mathrm{T}}, \quad w = (0, d, e, f, 1)^{\mathrm{T}}.$$

Assume that $1 \geqslant a \geqslant b \geqslant c \geqslant 0$, and set $v_1 = (1, a, b, c)^{\mathrm{T}}$, $w_1 = (d, e, f, 1)^{\mathrm{T}}$. Let $V = \operatorname{Span}\{v, w\}$, so that

$$F_V = \{A \in \mathscr{C}_5 : Av = Aw = \mathbf{0}\}.$$

If either v or w is not balanced, V is not realizable ($F_V = \emptyset$), so we will assume that both vectors are balanced. Even so, as we saw in Section 2, it is still possible that V

may not be realizable. We wish to discuss a process for determining the geometric structure of F_V. For convenience, put

$$G_V = \{\text{symmetric } A\text{: } a_{ii} = 1,\ i = 1, \ldots, 5, \text{ and } Av = Aw = \mathbf{0}\}.$$

Before we discuss the general method, we first eliminate some cases where additional coordinates of v_1 or w_1 are zero.

Theorem 3.15. *Suppose that* $v = (1, 1, 0, 0, 0)^{\mathrm{T}}$. *Then* F_V *is in* 1–1 *correspondence with* F_{w_1}.

Proof. Let S be any 4×4 correlation matrix such that $Sw_1 = \mathbf{0}$. Then, as in the first part of the proof of Theorem 3.9, we extend S to a unique correlation matrix in F_V. □

Theorem 3.16. *Let* $v = (1, a, b, 0, 0)^{\mathrm{T}}$, *and* $w = (0, 0, e, f, 1)^{\mathrm{T}}$ *be balanced vectors with* $abef \neq 0$. *Then* V *is realizable.*

Proof. Note from Lemma 2.6 that V is already balanced. By Lemma 2.13 any matrix A which kills both v and w has $A[1, 2, 3]$ and $A[3, 4, 5]$ uniquely determined and both are in $\mathscr{C}_3$. We now assert that such a matrix A can be chosen in F_V. Designate the $(2, 4)$ and $(4, 2)$ entry to be y. If we require $AV = \mathbf{0}$, then a calculation shows that every other entry must be linear in y, i.e., G_V can be parameterized with one variable. Thus we will denote G_V by $A(y)$. Now we examine

$$A(y)[2, 3, 4] = \begin{bmatrix} 1 & \alpha & y \\ \alpha & 1 & \beta \\ y & \beta & 1 \end{bmatrix},$$

where $|\alpha|, |\beta| \leqslant 1$. Let $p(y) = \det A[2, 3, 4]$. By Lemma 2.10, $C_3(A(y)) = p(y)B$, and we can take $p(y) = \det A[2, 3, 4]$. Note that $p(y)$ is quadratic in y and that the discriminant of $p(y)$ is $4(1 - \alpha^2)(1 - \beta^2)$. Thus both roots of $p(y)$ are real. Let y_0 be a root of $p(y)$. Then $C_3(A(y_0)) = 0$, so rank $A(y_0) \leqslant 2$. There are two cases:

(i) Either $|\alpha| < 1$ or $|\beta| < 1$. Then either

$$\begin{bmatrix} 1 & \alpha \\ \alpha & 1 \end{bmatrix} \quad \text{or} \quad \begin{bmatrix} 1 & \beta \\ \beta & 1 \end{bmatrix}$$

has two positive eigenvalues. By interlacing, $A(y_0)$ is a rank 2 correlation matrix in F_V.

(ii) Both $|\alpha|$ and $|\beta|$ are 1. Then by the same calculation as in the proof of Lemma 3.1, $y_0 = \alpha\beta$ and $A(y_0)[2, 3, 4]$ is a rank 1 correlation matrix. Because $|\beta| = |y_0| = 1$, and $\det A(y_0)[2, 3, 4] = 0$, by Lemma 3.1 $A(y_0)[1, 2, 3, 4]$ is a rank 1 correlation matrix. A similar argument using $|\alpha| = |y_0| = 1$ shows that $A(y_0)[2, 3, 4, 5]$ is a rank 1 correlation matrix. By Theorem 2.12, $A(y_0)$ is a rank 1 correlation matrix with v and w in its null space. Therefore V is realizable. □

We now discuss the general case. Recall that

$$G_V = \{\text{symmetric } A : a_{ii} = 1,\ i = 1, \ldots 5,\ \text{ and } Av = Aw = \mathbf{0}\}.$$

Clearly G_V is the solution set to a system of ten linear equations in ten unknowns, and $F_V \subset G_V$. If v and w have at most one common non-zero coordinate, then V is realizable by Theorem 3.15 or Theorem 3.16. Otherwise, we may assume that $abde \neq 0$. Recall that

$$A[1, 2, 3, 4]v_1 = \mathbf{0} = A[2, 3, 4, 5]w_1. \tag{3.8}$$

Let y and x be, respectively, the $(2, 4)$ and $(3, 4)$ entries of A. Recalling the discussion following Lemma 3.1, we see that the equation $A[1, 2, 3, 4]v_1 = \mathbf{0}$ determines the $(2, 3)$ entry of A and that this entry is linear in x and y. Call this entry $L(x, y)$. Similarly the equation $A[2, 3, 4, 5]w_1 = \mathbf{0}$ determines the $(2, 3)$ entry of A as a linear function of x and y which we call $M(x, y)$. We then have the following three possibilities for G_V.

Theorem 3.17. *Let $G_V, A, v_1, w_1, L(x, y), M(x, y)$ be as in the previous paragraph. Then*

(a) *G_V is empty if the equation $L(x, y) = M(x, y)$ is inconsistent.*
(b) *G_V can be expressed as a 1-parameter matrix $A(x)$ (or $A(y)$) depending linearly on x if $L(x, y) = M(x, y)$ is the equation of a straight line.*
(c) *G_V can be expressed as a two parameter matrix $A(x, y)$ depending linearly on x and y if $L(x, y) = M(x, y)$ for all x and y.*

Proof. (a) Having $L(x, y) = M(x, y)$ be inconsistent implies that the Eqs. (3.8) are inconsistent, so G_V is empty.

(b) Write $L(x, y) = M(x, y)$ as $rx + sy + t = 0$. Then either $r \neq 0$ or $s \neq 0$. We assume that $s \neq 0$. (The argument for $r \neq 0$ is similar.) Then in order for the Eqs. (3.8) to be consistent we must have $y = -(rx/s) - (t/s)$. Let $f(x) = -(rx/s) - (t/s)$. Then $L(x, f(x)) = M(x, f(x))$ identically. The Eqs. (3.8) also determine the $(1, 2)$, $(1, 3)$, $(1, 4)$ and $(2, 5)$, $(3, 5)$, $(4, 5)$ entries of A as linear functions of x and y. Replace each y with $f(x)$. Then these entries become linear functions of x. Finally, as in the proof of Theorem 2.12, the equations $Av = Aw = \mathbf{0}$ determine the $(1, 5)$ entry of A uniquely, which must be a linear function of x. This completes the proof of (b).

(c) Since $L(x, y) = M(x, y)$ identically, the Eqs. (3.8) are consistent for all x and y, and they determine the $(1, 2)$, $(1, 3)$, $(1, 4)$, $(2, 3)$, $(2, 5)$, $(3, 5)$, $(4, 5)$ entries of A as linear functions of x and y. Then again, the equations $Ax = Ay = \mathbf{0}$ determine the $(1, 5)$ entry of A uniquely as a function of x and y. □

We now develop a theorem similar to Theorem 3.17 for F_V. We will need the following modification of Definition 3.5.

Definition 3.18. Let $B_V = \{(x, y) \in B : A \in F_V\}$.

(a) If $L(x, y) = M(x, y)$ for all x and y, let

$$B_{v_1} = \{(x, y) \in B : A(x, y)[1, 2, 3, 4] \in F_{v_1}\},$$
$$B_{w_1} = \{(x, y) \in B : A(x, y)[2, 3, 4, 5] \in F_{w_1}\}.$$

(b) If $L(x, y) = M(x, y)$ is the equation of a nonvertical line, let

$$C_{v_1} = \{x \in [-1, 1] : A(x)[1, 2, 3, 4] \in F_{v_1}\},$$
$$C_{w_1} = \{x \in [-1, 1] : A(x)[2, 3, 4, 5] \in F_{w_1}\}.$$

Note that the equations in part (a) of this definition are also meaningful in the case that $L(x, y) = M(x, y)$ is the equation of a line as long as we understand that there is no 5×5 matrix $A(x, y)$ in this case, just two 4×4 matrices determined as in the beginning of Section 3. Also note that by convexity and continuity, both C_{v_1} and C_{w_1} are closed intervals.

Theorem 3.19. *Let the notation be as in the discussion above. Assume that v, w are balanced. Then*

(i) *if $L(x, y) = M(x, y)$ is inconsistent, V is not realizable, i.e., F_V is empty.*
(ii) *if $L(x, y) = M(x, y)$ for all x, y, $B_V = B_{v_1} = B_{w_1}$.*
(iii) *if $L(x, y) = M(x, y)$ is the equation of a non-vertical line, V is realizable if and only if $C_{v_1} \cap C_{w_1}$ is nonempty. If we let $C_{v_1} \cap C_{w_1} = [s, t]$, then F_V is the line segment $\{A(x) : s \leqslant x \leqslant t\}$. (Similar statements apply if $L(x, y) = M(x, y)$ is a vertical line.) Moreover, $(s, f(s))$ and $(t, f(t))$ are in $\partial B_{v_1} \cap \partial B_{w_1}$.*

Proof. (i) Since $F_V \subset G_V$, and G_V is empty in this case, F_V is empty.

(ii) Let $(x, y) \in B_{v_1}$. Then $A(x, y)[1, 2, 3, 4] \in F_{v_1}$, so $A(x, y)[2, 3, 4]$ is also a correlation matrix. Since $A(x, y)[2, 3, 4, 5]w_1 = \mathbf{0}$, rank $A[2, 3, 4, 5] =$ rank $A[2, 3, 4]$. Then $A[2, 3, 4, 5]$ is also a correlation matrix. By Theorem 2.12, $A(x, y)$ is also a correlation matrix and $(x, y) \in B_V$. Therefore, $B_{v_1} \subset B_V$. But trivially, $B_V \subset B_{v_1}$. Thus $B_{v_1} = B_V$ and similarly $B_{w_1} = B_V$.

(iii) If V is realizable, then $A(x) \in F_V$ for some $x \in [-1, 1]$. Then $A(x)[1, 2, 3, 4] \in F_{v_1}$ and $A(x)[2, 3, 4, 5] \in F_{w_1}$, so $C_{v_1} \cap C_{w_1}$ is nonempty. If $C_{v_1} \cap C_{w_1}$ is nonempty, it follows from Theorem 2.12 that $A(x) \in F_V$, so V is realizable. Repeating this argument shows that $\{A(x) : s \leqslant x \leqslant t\} = F_V$.

In order to verify the final statement, consider the left-hand endpoint s of $C_{v_1} \cap C_{w_1}$. Then s is a left-hand endpoint of either C_{v_1} or C_{w_1}, say C_{v_1}. The fact that $A(x) \in G_V$ for all x implies that rank $A(x)[1, 2, 3, 4] \leqslant 3$ for all x. If rank $A(s)[1, 2, 3, 4] = 3$, then $A(s)[1, 2, 3, 4]$ has three positive eigenvalues, and so does $A(s - \varepsilon)[1, 2, 3, 4]$ for $\varepsilon > 0$ sufficiently small. Then $A(s - \varepsilon)[1, 2, 3, 4] \in F_{v_1}$, a contradiction. Therefore, rank $A(s)[1, 2, 3, 4] \leqslant 2$. If we now regard $A[1, 2, 3, 4]$ as a linear function of both x and y as in the discussion following Lemma 3.1, we have $\operatorname{rank} A(s, f(s))[1, 2, 3, 4] \leqslant 2$. By Remark 3.10, $(s, f(s))$ is a zero of $p(x, y)$ and a point on ∂B_{v_1}. Recall that $p(x, y)$ is a multiple of $\det A(x, y)[2, 3, 4]$. Thus $\det A(s, f(s))[2, 3, 4] = 0$. If we instead take the underlying matrix to be $A(x, y)[2, 3, 4, 5] \in F_{w_1}$, and define $\hat{p}(x, y)$ to be a multiple of $\det A(x, y)[2, 3, 4]$, in that matrix, then $\hat{p}(s, f(s)) = 0$ (though $\hat{p} \neq p$ in general). Applying Theorem 3.6 with a suitable permutation similarity to $A(x, y)[2, 3, 4, 5]$, we conclude that $(s, f(s))$ is also a point on ∂B_{w_1}. Similarly, $(t, f(t)) \in \partial B_{v_1} \cap \partial B_{w_1}$. This completes the proof. □

The generic case, part (iii) of Theorem 3.19 gives a geometric description of F_V. It is a line segment with endpoints in $\partial B_{v_1} \cap \partial B_{w_1}$. By Bezout's Theorem [3], this intersection could have as many as nine points. Thus, if we separately find ∂B_{v_1} and ∂B_{w_1} and then their points of intersection, we have insufficient information to determine which are the endpoints of F_V. In the next section we will produce a number of illustrative examples.

Theorem 3.19(iii) gives one criterion that V be realizable. We conclude this section by giving a simple algebraic criterion.

Theorem 3.20. *Assume that $L(x, y) = M(x, y)$ is the equation of a line, where $L(x, y)$, $M(x, y)$, $A(x)$ (or $A(y)$) are as in the discussion above. Let*

$$g(x) = \det A(x)[2, 3, 4],$$

a polynomial of degree $\leqslant 3$. Find its roots.

(i) *If there is a root $x_0 \in (-1, 1)$, $A(x_0)$ is a rank 2 correlation matrix and F_V is nonempty.*
(ii) *If $x_0 = \pm 1$, is a root, then $A(x_0)$ is a correlation matrix if and only if $|f(x_0)| \leqslant 1$. Its rank is 2 if $|f(x_0)| < 1$ and is 1 if $|f(x_0)| = 1$.*
(iii) *If all roots of g lie outside $[-1, 1]$, then F_V is empty.*

Proof. (i) Suppose x_0 is a root of g in $(-1, 1)$. Then $A(x_0)[2, 3, 4]$ is singular and $A(x_0)[3, 4]$ is positive definite. Therefore, $A(x_0)[2, 3, 4]$ is a rank 2 correlation matrix. It follows from the form of v_1 and w_1 that

$$\operatorname{rank} A(x_0)[1, 2, 3, 4] = \operatorname{rank} A(x_0)[2, 3, 4] = \operatorname{rank} A(x_0)[2, 3, 4, 5].$$

Therefore, $A(x_0)[1, 2, 3, 4]$ and $A(x_0)[2, 3, 4, 5]$ are rank 2 correlation matrices and it follows from Theorem 2.12 that $A(x_0)$ is a rank 2 correlation matrix.

(ii) Suppose $x_0 = \pm 1$ is a root of $g(x)$. If $|f(x_0)| > 1$, then

$$A(x_0)[2, 3, 4] = \begin{bmatrix} 1 & L(x_0, f(x_0)) & f(x_0) \\ L(x_0, f(x_0)) & 1 & x_0 \\ f(x_0) & x_0 & 1 \end{bmatrix}$$

is not a correlation matrix and hence neither is $A(x_0)$.

If $|f(x_0)| < 1$, we repeat the argument in (i) to show that $A(x_0)$ is a rank 2 correlation matrix.

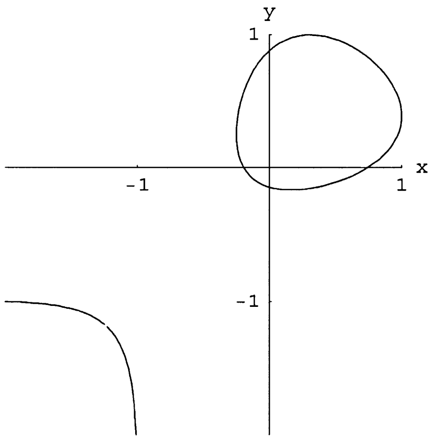
If $|f(x_0)| = 1$, it follows from Lemma 3.1 that $A(x_0)[1, 2, 3, 4]$ and $A(x_0)[2, 3, 4, 5]$ are rank 1 correlation matrices and from Theorem 2.12 that $A(x_0)$ is a rank 1 correlation matrix.

(iii) Suppose F_V is nonempty. In Theorem 3.19(iii), $(s, f(s)) \in \partial B_{v_1}$, which means that $|s| \leqslant 1$ and $p(s, f(s)) = 0$. Since $g(s) = \det A(s)[2, 3, 4]$ is a multiple of $p(s, f(s))$, $g(s) = 0$ and thus g has a root in $[-1, 1]$. □

4. Illustrative examples

In this section, we will provide some plots to illustrate some of the ideas. In most cases, we are plotting only ∂B_v. We display a scalar multiple of the polynomial $p(x, y)$ whose zero set is the curve we illustrate. In some cases, as in Figs. 1 and 2 and the next example, we are plotting just one curve with $k = 1$, $n = 4$. In the others, we have $k = 2$, $n = 5$, and there are two curves as well as the line determined in Theorem 3.19.

Example 4.1. Here we let $v = (5, 3, 2, 1)^{\mathrm{T}}$. (Once again, we do not normalize the first coordinate of v.) Since $\mathrm{gap}(v) \neq 0$, F_v has no rank one matrices; thus ∂B_v is smooth. Observe part of another topological component of the curve which must be outside of B.



$$\frac{23}{144} - \frac{10}{9}x^2 + \frac{11}{12}y + \frac{11}{18}x + \frac{3}{2}yx - \frac{5}{4}y^2 - y^2x - \frac{2}{3}yx^2 = 0.$$

The rest of our illustrations involve $k = 2$, $n = 5$. We obtain the pictures by plotting the zero set of the product of the two cubic polynomials corresponding to ∂B_{v_1}

and ∂B_{w_1} and the linear function $L(x, y) - M(x, y) = 0$. In some cases, we have chosen some of the coordinates of v or w to be negative. This is strictly for convenience. The following example is one in which F_V is empty. The two curves ∂B_{v_1} and ∂B_{w_1} have non-empty intersection in B. However, the line $L(x, y) - M(x, y) = 0$ misses B.

Example 4.2. Let $v = \frac{1}{3}(3, 3, 2, 1, 0)^{\mathrm{T}}$, and $w = \frac{1}{4}(0, 1, 2, 2, -4)^{\mathrm{T}}$. Put $V = \mathrm{Span}\{v, w\}$. The curves and line are plotted simultaneously. The illustration shows that B_V is empty even though the two cubic curves meet. Observe that the line $L(x, y) - M(x, y) = 0$ meets B only at $(1, 1)$. In this example, we outline some of the calculations.

$$\begin{bmatrix} 3 & -3 & -2 & -1 \end{bmatrix} \begin{bmatrix} 1 & m & n & p \\ m & 1 & l & y \\ n & l & 1 & x \\ p & y & x & 1 \end{bmatrix} \begin{bmatrix} 3 \\ 3 \\ 2 \\ 1 \end{bmatrix} = -5 - 12l - 6y - 4x = 0.$$

Hence $l = -\frac{5}{12} - \frac{1}{2}y - \frac{1}{3}x$.

$$\det \begin{bmatrix} 1 & -\frac{5}{12} - \frac{1}{2}y - \frac{1}{3}x & y \\ -\frac{5}{12} - \frac{1}{2}y - \frac{1}{3}x & 1 & x \\ y & x & 1 \end{bmatrix}$$

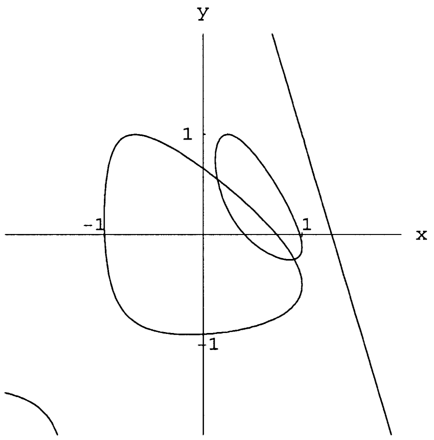
$$= \frac{119}{144} - \frac{10}{9}x^2 - \frac{5}{12}y - \frac{5}{18}x - \frac{7}{6}yx - \frac{5}{4}y^2 - y^2x - \frac{2}{3}yx^2.$$

$$\begin{bmatrix} 1 & 2 & 2 & 4 \end{bmatrix} \begin{bmatrix} 1 & l & y & r \\ l & 1 & x & s \\ y & x & 1 & t \\ r & s & t & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \\ 2 \\ -4 \end{bmatrix} = -7 + 4l + 4y + 8x = 0.$$

Hence $l = \frac{7}{4} - y - 2x$.

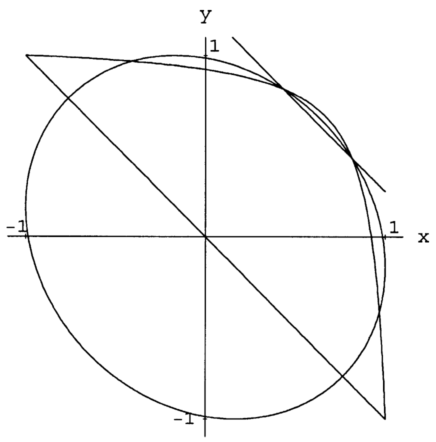
$$\det \begin{bmatrix} 1 & \frac{7}{4} - y - 2x & y \\ \frac{7}{4} - y - 2x & 1 & x \\ y & x & 1 \end{bmatrix}$$

$$= -\frac{33}{16} - 5x^2 + \frac{7}{2}y + 7x - \frac{1}{2}yx - 2y^2 - 2y^2x - 4yx^2.$$



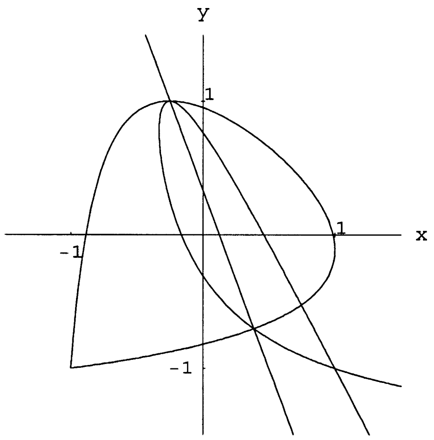
$$\left(-\tfrac{33}{16} - 5x^2 + \tfrac{7}{2}y + 7x - \tfrac{1}{2}yx - 2y^2 - 2y^2x - 4yx^2\right)$$
$$\times \left(\tfrac{119}{144} - \tfrac{10}{9}x^2 - \tfrac{5}{12}y - \tfrac{5}{18}x - \tfrac{7}{6}yx - \tfrac{5}{4}y^2 - y^2x - \tfrac{2}{3}yx^2\right)\left(y - \tfrac{13}{3} + \tfrac{10}{3}x\right) = 0.$$

Example 4.3. Let $V = \operatorname{Span}\{v, w\}$, where $v = \frac{1}{3}(3, 3, 1, 0, 0)^{\mathrm{T}}$, $w = (0, -3, -3, 2, 2)^{\mathrm{T}}$. By Theorems 3.9 and 3.13, ∂B_{v_1} is an ellipse and ∂B_{w_1} will be determined by a line and a quadratic curve (in this case a hyperbola). Note that the intersection of the two curves consists of six points, the maximum allowed by Bezout's Theorem. We give the polynomial but not the calculations. The second factor is clearly that of the ellipse and the last that of the line $L(x, y) = M(x, y)$. Observe that F_V is nonempty and is clearly a line segment.



$$\left(-\tfrac{13}{9}y^2 + \tfrac{4}{3}x + \tfrac{4}{3}y - \tfrac{26}{9}xy - \tfrac{13}{9}x^2 + \tfrac{4}{3}x^2y + \tfrac{4}{3}xy^2\right)$$
$$\times \left(\tfrac{35}{36} - y^2 - \tfrac{1}{3}xy - x^2\right)\left(-\tfrac{5}{6} + \tfrac{2}{3}x + \tfrac{2}{3}y\right) = 0.$$

Example 4.4. Let $V = \mathrm{Span}\{v, w\}$, where $v = \frac{1}{4}(4, 3, 2, 1, 0)^{\mathrm{T}}$, $w = \frac{1}{4}(0, 1, 2, 3, 4)^{\mathrm{T}}$. Note that both ∂B_{v_1} and ∂B_{w_1} have nodes, but in different locations. In this case F_V is a line.



$$\left(\tfrac{3}{4} - 10x^2 + \tfrac{3}{2}y + 3x - 8xy - \tfrac{13}{4}y^2 - 3y^2x - 6yx^2\right)$$
$$\times\left(\tfrac{35}{36} - \tfrac{10}{9}x^2 + \tfrac{1}{6}y + \tfrac{1}{9}x - \tfrac{5}{4}y^2 - y^2x - \tfrac{2}{3}yx^2\right)\left(x - \tfrac{1}{8} + \tfrac{3}{8}y\right) = 0.$$

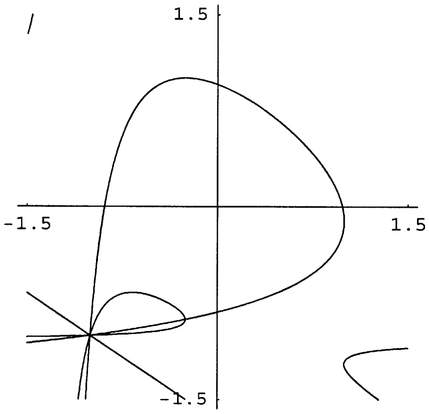
We continue with this example to illustrate Theorem 3.20, using algebraic means to find the endpoints of the line segment illustrated above. To be on the straight line, we must have $x = \frac{1}{8}(1 - 3y)$. We substitute this value for x in $A(x, y)[2, 3, 4]$ and compute the determinant, obtaining

$$\det\begin{bmatrix} 1 & \frac{1}{6} - \frac{1}{2}y - \frac{1}{3}\left(\frac{1}{8}(1-3y)\right) & y \\ \frac{1}{6} - \frac{1}{2}y - \frac{1}{3}\left(\frac{1}{8}(1-3y)\right) & 1 & \frac{1}{8}(1-3y) \\ y & \frac{1}{8}(1-3y) & 1 \end{bmatrix}$$
$$= \frac{31}{32} + \frac{7}{32}y - \frac{47}{32}y^2 + \frac{9}{32}y^3.$$

The roots of this polynomial are 1, $\frac{19}{9} \pm \frac{8}{9}\sqrt{10}$, two of which are $\leqslant 1$ in absolute value. This yields the endpoints of the line segment to be $(-\frac{1}{4}, 1)$, and approximately $(0.3875, -0.7)$ as the illustration above will confirm.

Example 4.5. Here we will have the two cubic curves with a common node. There are other points of intersection in B but F_V has only one matrix, namely at the node. Let $v = \frac{1}{4}(4, 3, 2, 1, 0)^{\mathrm{T}}$, $w = (0, 3, 2, 4, 1)^{\mathrm{T}}$. Note that there is a common rank one correlation matrix in F_V. In fact, F_V is a single point. We will give the plot and illustrate again the algebraic process of Theorem 3.20.

The polynomial and its plot is



$$\left(-\tfrac{40}{9}-\tfrac{25}{9}x^2-\tfrac{28}{3}y-\tfrac{56}{9}x-10yx-5y^2-4y^2x-\tfrac{8}{3}yx^2\right)$$
$$\times\left(\tfrac{35}{36}-\tfrac{10}{9}x^2+\tfrac{1}{6}y+\tfrac{1}{9}x-\tfrac{5}{4}y^2-y^2x-\tfrac{2}{3}yx^2\right)\left(-x-\tfrac{5}{2}-\tfrac{3}{2}y\right)=0.$$

From the equation above, we see that the line is given by $x=-\frac{5}{2}-\frac{3}{2}y$. We compute

$$\begin{aligned}
&\det A(x,y)[2,3,4]\\
&=\det\begin{bmatrix} 1 & -\frac{7}{3}-2y-\frac{4}{3}\left(-\frac{5}{2}-\frac{3}{2}y\right) & y \\ -\frac{7}{3}-2y-\frac{4}{3}\left(-\frac{5}{2}-\frac{3}{2}y\right) & 1 & -\frac{5}{2}-\frac{3}{2}y \\ y & -\frac{5}{2}-\frac{3}{2}y & 1 \end{bmatrix}\\
&=-\frac{25}{4}-\frac{25}{2}y-\frac{25}{4}y^2.
\end{aligned}$$

The roots are both -1, yielding $(-1,-1)$ as the only point on ∂B_V.

Remark 4.6. Consider the case $k=2$, $n=5$. Suppose that V turns out not to be realizable. Of course it is still possible that V could be balanced. Is it possible to look at the relative positions of ∂B_{v_1}, ∂B_{w_1}, and the line $L(x,y)=M(x,y)$ to determine if V is balanced?

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