

A parameterization of positive definite matrices in terms of partial correlation vines

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Abstract

We present a parameterization of the class PD(n) of positive definite $n \times n$ matrices using regular vines and partial correlations. Using a bijection from $(-1, 1)^{\binom{n}{2}} \rightarrow C(n)$, ($C(n)$ is the class of $n \times n$ correlation matrices) with a clear probabilistic interpretation (Bedford and Cooke [8]), we suggest a new approach to various problems involving positive definiteness.

Keywords: correlation, tree dependence, positive definite matrix, matrix completion.

1 Introduction

Positive (semi) definiteness is an important property of square matrices. There are algorithms for testing positive definiteness such as the Choleski decomposition or algorithms based on finding eigenvalues of a matrix. We propose to study positive definiteness using partial correlations [4] in conjunction with a new structure which we call a regular vine [1], [8]. A symmetric real ($n \times n$) matrix with off-diagonal elements in the interval $(-1, 1)$ and with "1"s on the main diagonal is called a *proto correlation matrix*. For a given $n \times n$ proto correlation matrix we consider regular vines. A vine is a set of trees such that the edges of the tree T_i are nodes of the tree T_{i+1} and all trees have the maximum number of edges. A vine is regular if two edges of T_i are joined by an edge of T_{i+1} only if these edges share a common node in T_i . A regular vine is called canonical if each tree T_i has a unique node of degree $n - i$ (precise definitions are given in Section 3). In total there are $\binom{n}{2} 2^{n-2}$ partial correlations. Partial correlations can be assigned to the edges of a regular vine such that conditioning and conditioned sets of the vine and partial correlations coincide (see Section 3). There are $\binom{n}{2}$ edges in a regular vine on n elements; hence $\binom{n}{2}$ of the $\binom{n}{2} 2^{n-2}$ partial correlations are selected in this way. It turns out that these partial correlations are algebraically independent and uniquely determine the correlation matrix. In fact, a regular vine may be used to construct a bijection from $(-1, 1)$ to the set of correlation matrices. (see Theorem 3.2).

This relationship can be used to specify dependence in high dimensional distributions [2] but also to decide whether a proto correlation matrix is positive definite. This algorithm can be also used to transform a non-positive definite matrix into a positive definite matrix. With the new algorithm these alterations have a clear probabilistic interpretation. This approach can be useful where a high dimensional correlation matrix should be specified (e.g. dependent Monte Carlo simulations), or when correlations are inferred from noisy physical measurements¹. In complex problems many entries in the correlation matrix may be unspecified, and this partially specified

¹This arises e.g. in structural mechanics when correlations are inferred from vibration modes

matrix must be extended to a positive definite matrix. We present preliminary results for the matrix completion problem using canonical vine partial correlation specifications. In particular, we present effective procedures for deciding whether a partially specified matrix can be extended to a positive definite matrix for certain non-chordal graphs [5], [6], [3], [9], [10].

This paper is organized as follows. In the Section 2 we present definition of partial correlations in terms of partial regression coefficients. In Section 3 we introduce vines and present definitions and theorems showing relationship between vines and positive definite matrices. Section 4 contains an algorithm for testing positive definiteness of a matrix using the canonical vine. The relationship between the new algorithm and known matrix theory results is also shown. In Section 5 repairing violation of positive definiteness is given and finally in Section 6 the algorithm solving the completion problem for special cases is presented.

2 Partial correlations

Let us consider variables X_i with zero mean and standard deviations σ_i , $i = 1, \dots, n$. Let the numbers $b_{1n;2,\dots,n-1}, \dots, b_{n-1n;1,\dots,n-2}$ minimize

$$E \left((b_{1n;2,\dots,n-1}X_1 - b_{2n;1,3,\dots,n-1}X_2 - \dots - b_{n-1n;1,\dots,n-2}X_{n-1} - X_n)^2 \right);$$

then the *partial correlations* are defined as (Yule and Kendall [4]):

$$\rho_{n,n-1;1,\dots,n-2} = \text{sgn}(b_{n,n-1;1,\dots,n-2}) (b_{n,n-1;1,\dots,n-2}b_{n-1,n;1,\dots,n-2})^{\frac{1}{2}}, \text{ etc.}$$

Partial correlations can be computed from correlations with the following recursive formula:

$$\rho_{n-1,n;1,\dots,n-2} = \frac{\rho_{n,n-1;1,\dots,n-3} - \rho_{n-2,n;1,\dots,n-3} \cdot \rho_{n-2,n-1;1,\dots,n-3}}{\sqrt{1 - \rho_{n-2,n;1,\dots,n-3}^2} \sqrt{1 - \rho_{n-2,n-1;1,\dots,n-3}^2}}. \quad (1)$$

All partial correlations can be computed from the correlations by iterating the above equation. In general it can be written as follows:

Let X_i, \dots, X_n be random variables, and let i, j, k be set of distinct indices and let C be a (possibly empty) set of indices disjoint from $\{i, j, k\}$. The *partial correlation of X_i and X_j given $\{X_k, \cup\{X_h|h \in C\}\}$* is

$$\rho_{ij;kC} = \frac{\rho_{ij;C} - \rho_{ik;C} \rho_{jk;C}}{\sqrt{1 - \rho_{ik;C}^2} \sqrt{1 - \rho_{jk;C}^2}}; \quad \rho_{ik;C} < 1, \rho_{jk;C} < 1. \quad (2)$$

where $\rho_{ij} = \rho(X_i, X_j)$.

If $\rho_{ik;C}^2 = 1$ or $\rho_{jk;C}^2 = 1$, then $\rho_{ij;kC}$ is not defined.

If X_1, \dots, X_n follow a joint normal distribution with variance covariance matrix of full rank, then partial correlations correspond to conditional correlations. The relationship between partial correlations and conditional correlations is studied in Kurowicka and Cooke [2].

3 Vines

Definition 3.1 (Tree) $T = (N, E)$ is a tree with nodes N and edges E if E is a subset of unordered pairs of N with no cycle and there is a path between each pair of nodes. That is, there does not exist a sequence a_1, \dots, a_k ($k > 2$) of elements of N such that

$$\{a_1, a_2\} \in E, \dots, \{a_{k-1}, a_k\} \in E, \{a_k, a_1\} \in E$$

and for any $a, b \in N$ there exists a sequence c_2, \dots, c_{k-1} of elements of N such that

$$\{a, c_2\} \in E, \{c_2, c_3\} \in E, \dots, \{c_{k-1}, b\} \in E.$$

Definition 3.2 (Regular vine) V is a regular vine on n elements if

1. $V = (T_1, \dots, T_{n-1})$
2. T_1 is a tree with nodes $N_1 = \{1, \dots, n\}$, and edges E_1 ;
for $i = 2, \dots, n-1$ T_i is a tree with nodes $N_i = E_{i-1}$.
3. (**proximity**) for $i = 2, \dots, n-1$, $\{a, b\} \in E_i$, $\#a\Delta b = 2$ where Δ denotes the symmetric difference. In other words, if a and b are nodes of T_i connected by an edge, where $a = \{a_1, a_2\}$, $b = \{b_1, b_2\}$, then exactly one of the a_i equals one of the b_i .

Definition 3.3 (Constraint set)

1. For $j \in E_i$, $i \leq n-1$ the subset $U_j(k)$ of $E_{i-k} = N_{i-k+1}$ is defined by

$$U_j(k) = \{e \mid \exists e_{i-(k-1)} \in e_{i-(k-2)} \in \dots \in j, e \in e_{i-(k-1)}\}$$
is called the **k-fold union**² of j ; $k = 1, \dots, i$
 $U_j^* = U_j(i)$ is the **complete union** of j , that is, the subset of $\{1, \dots, n\}$ reachable from j by the membership relation.
If $a \in N_1$ then $U_a^* = \emptyset$.
 $U_j(1) = \{j_1, j_2\} = j$.
By definition we write $U_j(0) = \{j\}$.
2. For $i = 1, \dots, n-1$, $e_i \in E_i$, if $e_i = \{j, k\}$ then the **conditioning set** associated with e_i is

$$D_{e_i} = U_j^* \cap U_k^*$$

and the **conditioned sets** associated with e_i are

$$C_{e_i, j} = U_j^* \setminus D_{e_i}; C_{e_i, k} = U_k^* \setminus D_{e_i}.$$

3. The **constraint set** for V is

$$CV = \{D_{e_i}, C_{e_i, j}, C_{e_i, k} \mid e_i \in E_i; e_i = \{j, k\}, i = 1, \dots, n-1\}.$$

Note that for $e \in E_1$, the conditioning set is empty.

For $e_i \in E_i$, $i \leq n-1$, $e_i = \{j, k\}$ we have $U_{e_i}^* = U_j^* \cup U_k^*$.

We present below two examples of a regular vines on 5 elements with conditioned and conditioning sets. We use the regular vine in Figure 2 to illustrate Definition 3.3.

We get

$$\begin{aligned} T_1 &= (N_1, E_1), \quad N_1 = \{1, 2, \dots, 5\}, \quad E_1 = \{\{1, 2\}, \{1, 3\}, \{1, 4\}, \{1, 5\}\}; \\ T_2 &= (N_2, E_2), \quad N_2 = E_1, \quad E_2 = \{\{\{1, 2\}, \{1, 3\}\}, \{\{1, 2\}, \{1, 4\}\}, \{\{1, 2\}, \{1, 5\}\}\}; \\ &\vdots \end{aligned}$$

The complete union of $j = \{1, 2\}$ is $U_j^* = \{1, 2\}$ and for $k = \{1, 3\}$, $U_k^* = \{1, 3\}$. Hence the conditioning set of the edge $e = \{\{1, 2\}, \{1, 3\}\}$ in T_2 is $D_e = U_j^* \cap U_k^* = \{1, 2\} \cap \{1, 3\} = \{1\}$. The conditioned sets are $C_{e, j} = U_j^* \setminus D_e = \{1, 2\} \setminus \{1\} = \{2\}$ and $C_{e, k} = U_k^* \setminus D_e = \{1, 3\} \setminus \{1\} = \{3\}$. The dotted edge of T_2 between $\{1, 2\}$ and $\{1, 3\}$ in Figure 2 is denoted $2, 3|1$, which gives the elements of the conditioned sets $\{2\}, \{3\}$ before ”|” and conditioning set $\{1\}$ after ”|”.

²The 1-fold union of a set is the set of elements i.e. the set itself, the 2-fold union is the set of elements of elements, etc.

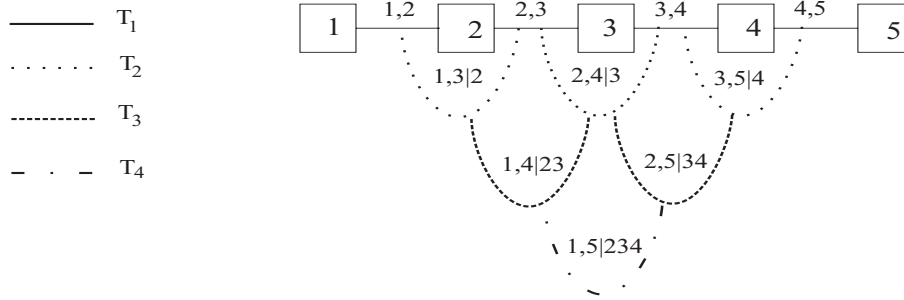


Figure 1. A regular vine on 5 elements showing conditioned and conditioning sets.

Definition 3.4 (Canonical vine) A regular vine is called a canonical vine if each tree T_i has a unique node of degree $n - i$. The node with maximal degree in T_1 is the root.

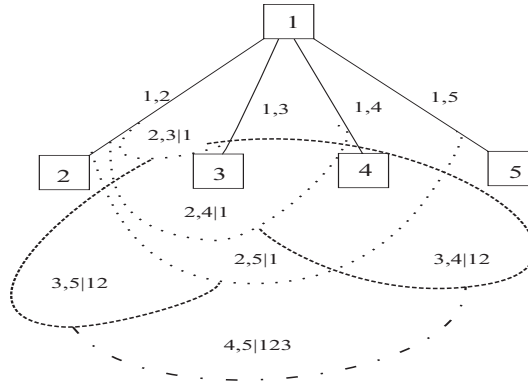


Figure 2. A canonical vine on 5 elements.

For regular vines the structure of the constraint set is particularly simple, as shown by the following lemmata [1].

Lemma 3.1 Let V be a regular vine on n elements, and let $j \in E_i$. Then

$$\#U_j(k) = 2\#U_j(k-1) - \#U_j(k-2); k = 2, 3, \dots \quad (3)$$

Proof. For $e_h \in U_j(k-1)$ write $e_h = \{e_{h,1}, e_{h,2}\}$ and consider the lexicographical ordering of the names $e_{h,c}, c = 1, 2$. There are $2k$ names in this ordering. $U_j(k)$ is the number of names in the ordering, diminished by the number of names which refer to an element which is already named earlier in the ordering. By regularity, for every element in $U_j(k-2)$, there is exactly one name in the lexicographical ordering which denotes an element previously named in the ordering. Hence (3) holds. \square

Lemma 3.2 Let V be a regular vine on n elements, and let $j \in E_i$. Then

$$\#U_j(k) = k + 1; k = 0, 1, \dots, i. \quad (4)$$

Proof. The statement clearly holds for $k = 0, k = 1$. By the proximity property it follows immediately that it holds for $k = 2$. Suppose (4) holds up to $k - 1$. Then $\#U_j(k-1) = k$. By Lemma 3.1

$$\#U_j(k) = 2\#U_j(k-1) - \#U_j(k-2).$$

With the induction hypothesis we conclude

$$\#U_j(k) = 2k - (k - 1) = k + 1. \quad \square$$

Lemma 3.3 *If V is a regular vine on n elements then for all $i = 1, \dots, n - 1$, and all $e_i \in E_i$, the conditioned sets associated with e_i are singletons, $\#U_{e_i}^* = i + 1$, and $\#D_{e_i} = i - 1$.*

Proof. Let $e_i \in E_i$ and $e_i = \{j, k\}$. By Lemma 3.2 $\#U_{e_i}^* = i + 1$. Let $D = U_j^* \cap U_k^*$ and $C = U_j^* \Delta U_k^*$. It suffices to show that $\#C = 2$. We get

$$i + 1 = \#D + \#C \quad (5)$$

and

$$2i = \#U_j^* + \#U_k^* = \#C + 2\#D. \quad (6)$$

When we divide (6) by 2 and subtract from (5) then

$$\#C = 2.$$

Hence $\#(U_j^* \setminus D) = 1$, $\#(U_k^* \setminus D) = 1$ and $\#D = i - 1$. \square

Lemma 3.4 *Let V be a regular vine, and suppose for $j, k \in E_i$, $U_j^* = U_k^*$, then $j = k$.*

Proof. We claim that $U_j(x + 1) = U_k(x + 1)$ implies $U_j(x) = U_k(x)$. In any tree, the number of edges between y vertices is less or equal to $y - 1$. $\#U_j(x + 1) = x + 2$ and $U_j(x + 1) \subseteq N_{i-x}$, so in tree T_{i-x} the number of edges between the nodes in $U_j(x + 1)$ is less then or equal to $x + 1$. $\#U_j(x) = x + 1 = \#U_k(x)$, so both of these sets must consist of the $x + 1$ possible edges between the nodes of T_{i-x} that are in $U_j(x + 1) = U_k(x + 1)$. Hence $U_j(x) = U_k(x)$. Since $U_j^* = U_k^*$, that is $U_j(i) = U_k(i)$, repeated application of this result produces $U_j(1) = U_k(1)$, that is, $j = k$. \square

Lemma 3.5 *If the conditioned sets of edges i, j in a regular vine are equal, then $i = j$.*

Proof. Suppose i and j have the same conditioned sets. By Lemma 3.3 the conditioned sets are singletons, say $\{a\}, \{b\}, a \in N, b \in N$. Let D_i respectively D_j be the conditioning sets of edges i and j . Then in the tree T_1 there is a path from a to b through the nodes in D_i , and also a path from a to b through the nodes in D_j . If $D_i \neq D_j$, then there must be a cycle in the edges E_1 , but this is impossible since T_1 is a tree. It follows that $D_i = D_j$, and from Lemma 3.4 it follows that $i = j$. \square

Definition 3.5 (Partial correlation specification) *A partial correlation specification for a regular vine is an assignment of values in $(-1, 1)$ to each edge of the vine.*

The edges in a regular vine may be associated with a set of partial correlations in the following way:

for $i = 1, \dots, n - 1$, with $e \in E_i, e = \{j, k\}$ we associate

$$\rho_{C_{e,j}C_{e,k};D_e}.$$

From Lemma 3.3 it follows that the sets $C_{e,j}$ and $C_{e,k}$ are singletons, and by definition their intersection with D_e is empty. For tree T_1 , the conditioning sets D_e are empty and the partial correlations are just the ordinary correlations. The *order* of a partial correlation is the cardinality of the conditioning set. Hence this association involves $(n - 1)$ partial correlations of order zero, $(n - 2)$ of order one, \dots and one of order $(n - 2)$. In total there are

$$\sum_{j=1}^{n-1} j = \binom{n}{2}$$

edges in a regular vine and the same number of partial correlations associated with the edges of a regular vine. Since the conditioned sets of each edge must be distinct, it follows that each pair of indices appears once as conditioned variables in a regular vine.

The following theorem shows that the correlations are uniquely determined by the partial correlations on a regular vine.

Theorem 3.1 *Let X_1, \dots, X_n and Y_1, \dots, Y_n be random variables satisfying the same partial correlation vine specification. Then for $i \neq j$*

$$\rho(X_i, X_j) = \rho(Y_i, Y_j).$$

Proof. It suffices to show that the the correlations $\rho_{ij} = \rho(X_i, X_j)$ can be calculated from the partial correlations specified by the vine. Proof is by induction on the number of elements n . The basic case ($n = 2$) is trivial. Assume the theorem holds for $i = 2, \dots, n-1$. For a regular vine over n elements the tree T_{n-1} has one edge, say $e = \{j, k\}$. By Lemma 3.3, $\#D_e = n-2$. Re-indexing the variables X_1, \dots, X_n if necessary, we may assume that

$$\begin{aligned} C_{e,j} &= U_j^* \setminus D_e = X_{n-1}, \\ C_{e,k} &= U_k^* \setminus D_e = X_n, \\ U_j^* &= \{1, \dots, n-1\} \\ U_k^* &= \{1, \dots, n-2, n\} \\ D_e &= \{1, \dots, n-2\}. \end{aligned}$$

The correlations over U_j^* and U_k^* are determined by the induction step. It remains to determine the correlation $\rho_{n-1,n}$. The left hand side of

$$\rho_{n-1,n;1\dots n-2} = \frac{\rho_{n-1,n;1\dots n-3} - \rho_{n-2,n;1\dots n-3}\rho_{n-2,n-1;1\dots n-3}}{\sqrt{1 - \rho_{n-2,n-1;1\dots n-3}^2}\sqrt{1 - \rho_{n-2,n-1;1\dots n-3}^2}} \quad (7)$$

is determined by the vine specification. The terms

$$\rho_{n-2,n-1;1\dots n-3}, \rho_{n-2,n;1\dots n-3}$$

are determined by the induction hypohese. It follows that we can solve the above equation for $\rho_{n-1,n;1\dots n-3}$, and write

$$\rho_{n-1,n;1\dots n-3} = \frac{\rho_{n-1,n;1\dots n-4} - \rho_{n-3,n-1;1\dots n-4}\rho_{n-3,n;1\dots n-4}}{\sqrt{1 - \rho_{n-3,n-1;1\dots n-4}^2}\sqrt{1 - \rho_{n-3,n;1\dots n-4}^2}}$$

Proceeding in this manner, we eventually find

$$\rho_{n-1,n;1} = \frac{\rho_{n-1,n} - \rho_{1n-1}\rho_{1n}}{\sqrt{1 - \rho_{1n-1}^2}\sqrt{1 - \rho_{1n}^2}}$$

This equation may now be solved for $\rho_{n-1,n}$. \square

The Lemmas 3.6, 3.7 and 3.8 below will be used in matrix completion problem in Section 6. The following lemma shows that $\rho_{n-1,n;1\dots n-2}$ can be chosen arbitrarily in (7) and the resulting system could be solved for $\rho_{n-1,n}$. This idea is the basis for the proof of Theorem 3.2 below.

Lemma 3.6 *If $z, x, y \in (-1, 1)$, then also $w \in (-1, 1)$, where*

$$w = z\sqrt{(1-x^2)(1-y^2)} + xy.$$

Proof. We substitute $x = \cos \alpha, y = \cos \beta$, and use

$$\begin{aligned} 1 - \cos^2 \alpha &= \sin^2 \alpha; \\ \cos \alpha \cos \beta &= \frac{\cos(\alpha - \beta) + \cos(\alpha + \beta)}{2}; \\ \sin \alpha \sin \beta &= \frac{\cos(\alpha - \beta) - \cos(\alpha + \beta)}{2}; \end{aligned}$$

and find

$$z \left| \frac{\cos(\alpha - \beta) - \cos(\alpha + \beta)}{2} \right| + \frac{\cos(\alpha - \beta) + \cos(\alpha + \beta)}{2} = w.$$

Write this as

$$z \left| \frac{a - b}{2} \right| + \frac{a + b}{2} = w;$$

where $a, b \in (-1, 1)$. As the left hand side is linear in z , its extreme values must occur when $z = 1$ or $z = -1$. It is easy to check that in these cases, $w \in (-1, 1)$. \square

In the next lemma we will see that it is always possible to find a single unknown variable on the right hand side of equation (2) such that the left hand side will lie in the interval $(-1, 1)$.

Lemma 3.7 *Let $w, y \in (-1, 1)$, $x \in (-1, 1)$ and*

$$z = \frac{w - xy}{\sqrt{(1-x^2)(1-y^2)}} \tag{8}$$

then

$$z \in (-1, 1) \Leftrightarrow x \in I_z, \quad I_z \neq \emptyset, \quad I_z = (\underline{x}, \bar{x}) \cap (-1, 1)$$

where

$$\begin{aligned} \underline{x} &= yw - \sqrt{(1-y^2)(1-w^2)} \\ \bar{x} &= yw + \sqrt{(1-y^2)(1-w^2)}. \end{aligned}$$

Proof. It suffices to find the solution of the following inequality

$$(w - xy)^2 < (1 - x^2)(1 - y^2)$$

which is equivalent to

$$x^2 - 2wyx + w^2 + y^2 - 1 < 0. \tag{9}$$

We get

$$\begin{aligned} \Delta &= 4w^2y^2 - 4w^2 - 4y^2 + 4 \\ &= 4(1 - y^2)(1 - w^2). \end{aligned}$$

Since $y, w \in (-1, 1)$ then $\Delta > 0$ and inequality (9) has always a solution with

$$x \in \left(yw - \sqrt{(1-y^2)(1-w^2)}; yw + \sqrt{(1-y^2)(1-w^2)} \right) = I_x$$

Since $w, y \in (-1, 1)$ then $wy \in (-1, 1)$. We want also $x \in (-1, 1)$ so we get

$$I_z = I_x \cap (-1, 1) \tag{10}$$

which is always non-empty. \square

Remark 3.1 *Similar considerations hold if we change the role of w and x in (8). Then we obtain that we can always find w such that $z \in (-1, 1)$. This solution belongs to the following non-empty interval*

$$I = \left(xy - \sqrt{(1-x^2)(1-y^2)}; xy + \sqrt{(1-x^2)(1-y^2)} \right) \cap (-1, 1).$$

Lemma 3.8 *Let $w \in (-1, 1)$ and let z be given by (8).*

$$z \in (-1, 1) \Leftrightarrow (x, y) \in A(w)$$

where

$$A(w) = \left\{ (x, y) : \frac{(y - wx)^2}{1 - w^2} + x^2 < 1 \right\}. \quad (11)$$

Proof. It suffices to find points $(x, y) \in (-1, 1)^2$ such that

$$(w - xy)^2 < (1 - x^2)(1 - y^2)$$

therefore we test when the function

$$\begin{aligned} g(x, y) &= (w - xy)^2 - (1 - x^2)(1 - y^2) \\ &= x^2 + y^2 - 2wxy + w^2 - 1 \\ &= x^2(1 - w^2) + (y - xw)^2 - (1 - w^2) \end{aligned}$$

is less than zero.

It is easy to notice that $g(x, y)$ is less than zero if $(x, y) \in A(w)$. \square

Remark 3.2 *Note that point $(0, 0)$ always belongs to $A(w)$.*

In [8] the following is proved:

Theorem 3.2 *For any regular vine on n elements there is a one to one correspondence between the set of $n \times n$ positive definite correlation matrices and the set of partial correlation specifications for the vine.*

The above theorem shows that all assignments of the numbers between -1 and 1 to the edges of a regular vine are consistent and all correlation matrices can be obtained this way. This relationship can be used in constructing high dimensional distributions realizing a given correlation matrix. It can be also used to determine whether a proto correlation matrix is positive definite simply by calculating partial correlations assigned to the edges of regular vine (see Section 4).

4 Positive definiteness

If A is an $n \times n$ symmetric matrix with positive numbers on the main diagonal, we may transform A to a matrix $\overline{A} = DAD$ where

$$d_{ij} = \begin{cases} \frac{1}{\sqrt{a_{ii}}} & \text{if } i = j \\ 0 & \text{otherwise.} \end{cases}$$

Thus

$$\overline{a_{ij}} = \frac{a_{ij}}{\sqrt{a_{ii}a_{jj}}}. \quad (12)$$

\bar{A} has "1"-s on the main diagonal. Since it is known that \bar{A} is positive definite if and only if all principle submatrices are positive definite then we can restrict our further considerations to the matrices which after transformation (12) have all $\bar{a}_{ij} \in (-1, 1)$ where $i \neq j$. The matrix with all off-diagonal elements from the interval $(-1, 1)$ and with "1"-s on the main diagonal is called *proto correlation matrix*. It is well known that A is positive definite ($A \succ 0$) if and only if \bar{A} is positive definite.

In order to check positive definiteness of the matrix \bar{A} we will use the partial correlation specification for the canonical vine. Because of the one-to one correspondence between partial correlation specifications on a regular vine and positive definite matrices given in Theorem 3.2, it is enough to check whether all partial correlations from the partial correlation specification on the vine are in the interval $(-1, 1)$ to decide that \bar{A} is positive definite .

We illustrate this algorithm for 5×5 proto correlation matrix given by

$$\begin{bmatrix} 1 & \rho_{12} & \rho_{13} & \rho_{14} & \rho_{15} \\ \rho_{21} & 1 & \rho_{23} & \rho_{24} & \rho_{25} \\ \rho_{31} & \rho_{32} & 1 & \rho_{34} & \rho_{35} \\ \rho_{41} & \rho_{42} & \rho_{43} & 1 & \rho_{45} \\ \rho_{51} & \rho_{52} & \rho_{53} & \rho_{54} & 1 \end{bmatrix}$$

For this matrix we will consider the canonical vine on 5 variables.

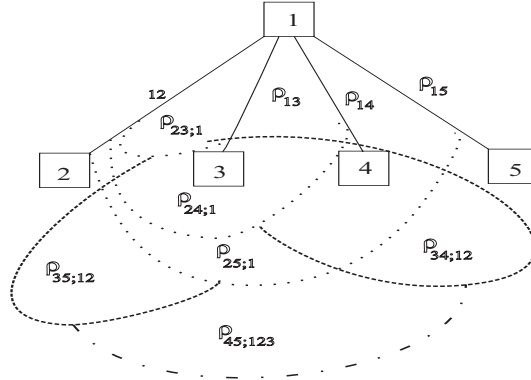


Figure 3. Partial correlation specification for a canonical vine on 5 variables with root 1.

In the first tree we have to read correlations from the matrix \bar{A} . For the second tree we will use formula (2) and calculate the following correlations:

$$\rho_{23;1}, \rho_{24;1}, \rho_{25;1}.$$

To calculate correlations $\rho_{34;12}, \rho_{35;12}$ with the formula (2), we will also have to calculate $\rho_{34;1}$ and $\rho_{35;1}$. Similarly, to calculate $\rho_{45;123}$ we will need $\rho_{45;12}$ and $\rho_{45;1}$.

In general we must calculate using formula (2)

$$\begin{aligned} \binom{n-1}{2} & \text{ partial correlations of the first order} \\ \binom{n-2}{2} & \text{ partial correlations of the second order} \\ & \vdots \\ \binom{n-(n-2)}{2} & \text{ partial correlations of the (n-2) order.} \end{aligned}$$

Hence in order to verify positive definiteness of the matrix \bar{A} we have to calculate

$$\sum_{k=1}^{n-2} \binom{n-k}{2} = \frac{(n-2)(n-1)n}{6} < \frac{n^3}{6}$$

partial correlations using formula (2).

Example 1

Let us consider the matrix

$$A = \begin{bmatrix} 25 & 12 & -7 & 0.5 & 18 \\ 12 & 9 & -1.8 & 1.2 & 6 \\ -7 & -1.8 & 4 & 0.4 & -6.4 \\ 0.5 & 1.2 & 0.4 & 1 & -0.4 \\ 18 & 6 & -6.4 & -0.4 & 16 \end{bmatrix}$$

and transform A to proto correlation matrix using formula (12). Then we get

$$\bar{A} = \begin{bmatrix} 1 & 0.8 & -0.7 & 0.1 & 0.9 \\ 0.8 & 1 & -0.3 & 0.4 & 0.5 \\ -0.7 & -0.3 & 1 & 0.2 & -0.8 \\ 0.1 & 0.4 & 0.2 & 1 & -0.1 \\ 0.9 & 0.5 & -0.8 & -0.1 & 1 \end{bmatrix}.$$

Since

$$\begin{aligned} \begin{bmatrix} \rho_{23;1} & \rho_{24;1} & \rho_{25;1} \\ \rho_{34;1} & \rho_{35;1} & \rho_{45;1} \end{bmatrix} &= \begin{bmatrix} 0.6068, & 0.5360, & -0.8412 \\ 0.3800, & -0.5461, & 0.0281 \end{bmatrix} \\ \begin{bmatrix} \rho_{34;12} & \rho_{35;12} & \rho_{45;12} \end{bmatrix} &= \begin{bmatrix} 0.0816, & -0.0830, & 0.0351 \end{bmatrix} \\ \begin{bmatrix} \rho_{45;123} \end{bmatrix} &= \begin{bmatrix} 0.0351 \end{bmatrix} \end{aligned}$$

are all between $(-1, 1)$, it follows that, \bar{A} and A are positive definite.

We now show the relationship between above procedure of testing positive definiteness and a test procedure based on the Schur complement.

Theorem 4.1 (Schur complement)

Suppose that symmetric matrix M is partitioned as

$$M = \begin{bmatrix} X & Y \\ Y^T & Z \end{bmatrix}$$

where X, Z are square. Then

$$M \succ 0 \Leftrightarrow X \succ 0 \text{ and } Z - Y^T X^{-1} Y \succ 0.$$

Let A be an $n \times n$ proto correlation matrix partitioned in the following way

$$A = \begin{bmatrix} X_k & Y_k \\ Y_k^T & Z_k \end{bmatrix}$$

where X is $k \times k, 1 \leq k \leq n - 2$ and Z $n - k \times n - k$ matrix.

We introduce the following notation:

$A_{;12\dots k}$: matrix of the k -th order partial correlations with conditioned set $\{12\dots k\}$.³

If M is a square matrix with positive elements on the main diagonal then let \bar{M} denote the matrix M transformed to proto correlation matrix using transformation (12).

³Note that $A_{;12\dots n-2} = \begin{bmatrix} 1 & \rho_{n,n-1;12\dots n-2} \\ \rho_{n,n-1;12\dots n-2} & 1 \end{bmatrix}$.

Theorem 4.2

$$A \succ 0 \Leftrightarrow \forall_{1 \leq k \leq n-2} \overline{(Z_k - Y_k^T X_k^{-1} Y_k)} = A_{;12\dots k}.$$

Proof. The proof is by iteration with respect to k . For $k = 1$ we get

$$A = \begin{bmatrix} X_1 & Y_1 \\ Y_1^T & Z_1 \end{bmatrix}$$

where

$$X_1 = [1], \quad Y_1 = [\rho_{12} \ \rho_{13} \ \dots \ \rho_{1n}], \quad Z_1 = \begin{bmatrix} 1 & \rho_{23} & \rho_{24} & \dots & \rho_{2n} \\ \rho_{23} & 1 & \rho_{34} & \dots & \rho_{3n} \\ \dots & \dots & \dots & \dots & \dots \\ \rho_{2,n-1} & \rho_{3,n-1} & \dots & 1 & \rho_{n-1,n} \\ \rho_{2n} & \rho_{3n} & \dots & \dots & 1 \end{bmatrix}.$$

Since certainly $X_1 \succ 0$, then by Theorem 4.1

$$A \succ 0 \text{ if and only if } Z_1 - Y_1^T X_1^{-1} Y_1 \succ 0.$$

We get

$$\widetilde{A}_{;1} = Z_1 - Y_1^T X_1^{-1} Y_1 = \begin{bmatrix} 1 - \rho_{12}^2 & \rho_{23} - \rho_{12}\rho_{13} & \dots & \rho_{2n} - \rho_{12}\rho_{1n} \\ \rho_{23} - \rho_{12}\rho_{13} & 1 - \rho_{13}^2 & \dots & \rho_{3n} - \rho_{13}\rho_{1n} \\ \dots & \dots & \dots & \dots \\ \rho_{2n} - \rho_{12}\rho_{1n} & \rho_{3n} - \rho_{13}\rho_{1n} & \dots & 1 - \rho_{1n}^2 \end{bmatrix}$$

Since A is a proto correlation matrix then $\rho_{ij} \in (-1, 1)$ where $i, j = 1, 2, \dots, n$ and $i \neq j$. Hence all elements on the main diagonal of $\widetilde{A}_{;1}$ are positive so the transformation (12) can be applied. After transformation $\widetilde{A}_{;1}$ will be of the form

$$\begin{bmatrix} 1 & \frac{\rho_{23} - \rho_{12}\rho_{13}}{\sqrt{(1-\rho_{12}^2)(1-\rho_{13}^2)}} & \dots & \dots & \frac{\rho_{2n} - \rho_{12}\rho_{1n}}{\sqrt{(1-\rho_{12}^2)(1-\rho_{1n}^2)}} \\ \frac{\rho_{23} - \rho_{12}\rho_{13}}{\sqrt{(1-\rho_{12}^2)(1-\rho_{13}^2)}} & 1 & \dots & \dots & \frac{\rho_{3n} - \rho_{13}\rho_{1n}}{\sqrt{(1-\rho_{13}^2)(1-\rho_{1n}^2)}} \\ \dots & \dots & \dots & \dots & \dots \\ \frac{\rho_{2,n-1} - \rho_{12}\rho_{1,n-1}}{\sqrt{(1-\rho_{12}^2)(1-\rho_{1,n-1}^2)}} & \frac{\rho_{3,n-1} - \rho_{13}\rho_{1,n-1}}{\sqrt{(1-\rho_{13}^2)(1-\rho_{1,n-1}^2)}} & \dots & 1 & \frac{\rho_{n-1,n} - \rho_{1,n-1}\rho_{1n}}{\sqrt{(1-\rho_{1,n-1}^2)(1-\rho_{1n}^2)}} \\ \frac{\rho_{2n} - \rho_{12}\rho_{1n}}{\sqrt{(1-\rho_{12}^2)(1-\rho_{1n}^2)}} & \frac{\rho_{3n} - \rho_{13}\rho_{1n}}{\sqrt{(1-\rho_{13}^2)(1-\rho_{1n}^2)}} & \dots & \dots & 1 \end{bmatrix}$$

which by formula (2) is equal to $A_{;1}$. Hence $A \succ 0$ if and only if $A_{;1} \succ 0$.

If any element of the first row of $A_{;1}$ is not in $(-1, 1)$ then A and $A_{;1}$ are not positive definite.⁴ If all elements of the first row of $A_{;1}$ are in $(-1, 1)$ we can apply the above steps with $A_{;1}$ in the role of A . Let $A_{;1}(i, j)$ denote the (i, j) element of $A_{;1}$. The result of applying Theorem 4.1 and transformation (12) to $A_{;1}$ yields a matrix with off-diagonal elements (i, j) , $i, j = 2, 3, \dots, n$

$$\frac{A_{;1}(i, j) - A_{;1}(2, i)A_{;1}(2, j)}{\sqrt{(1 - A_{;1}^2(2, i))(1 - A_{;1}^2(2, j))}}.$$

By the recursive formula (2), this is equal to

$$\rho_{ij;12}$$

so $A_{;12}$ is the matrix of second order partial correlations. The proof is completed by repeating the above argument. If the elements of $A_{;12\dots k}$ are not in $(-1, 1)$ then A is not positive definite and the argument terminates; otherwise we compute $A_{;12\dots n-2}$ and conclude that A is positive definite. \square

⁴Note that this is equivalent to checking if all correlations in the second tree in the canonical partial correlation vine are in $(-1, 1)$.

Corollary 4.1

$$\begin{aligned}
A \succ 0 &\Leftrightarrow [\rho_{12} \in (-1, 1), \dots, \rho_{1n} \in (-1, 1) \text{ and } A_{;1} \succ 0] \\
&\Leftrightarrow [\rho_{23;1} \in (-1, 1), \dots, \rho_{2n;1} \in (-1, 1) \text{ and } A_{;12} \succ 0] \\
&\vdots \\
&\Leftrightarrow [\rho_{n-2,n-1;1\dots n-3} \in (-1, 1), \rho_{n-2,n;1\dots n-3} \in (-1, 1) \text{ and } A_{;12\dots n-2} \succ 0] \\
&\Leftrightarrow \rho_{n,n-1;12\dots n-2} \in (-1, 1).
\end{aligned}$$

5 Repairing violations of positive definiteness

In physical applications it often happens that correlations are estimated by noisy procedures. It may thus arise that the measured matrix is not positive definite. If we want to use this matrix we must change it to get a positive definite matrix which is as close as possible to the measured matrix.

Partial correlation specifications on a regular vine can be used to alter a non-positive definite matrix A so as to obtain a positive definite matrix B . If the matrix is not positive definite then there exists at least one element in the partial correlation specification of the canonical vine which is not in the interval $(-1, 1)$. We will change the value of that element and recalculate partial correlations on the vine using the following algorithm:

for $1 \leq s \leq n - 2$, $j = s + 2, s + 3, \dots, n$

$$\rho_{s+1,j;12\dots s} \notin (-1, 1) \rightarrow \rho_{s+1,j;12\dots s} := V(\rho_{s+1,j;12\dots s})$$

where $V(\rho_{s+1,j;12\dots s}) \in (-1, 1)$ is the altered value of $\rho_{s+1,j;12\dots s}$.

Recalculate partial correlations of lower order as follows:

$$\begin{aligned}
V(\rho_{s+1,j;1\dots t-1}) &= V(\rho_{s+1,j;1\dots t}) \sqrt{(1 - \rho_{t,s+1;1\dots t-1}^2)(1 - \rho_{s+1,j;1\dots t-1}^2)} \\
&\quad + \rho_{t,s+1;1\dots t-1} \rho_{s+1,j;1\dots t-1},
\end{aligned} \tag{13}$$

where $t = s, s - 1, \dots, 1$.

Theorem 5.1 *The following hold:*

- a. *all recalculated partial correlations are in the interval $(-1, 1)$,*
- b. *changing the value of the partial correlation on the vine leads to changing only one correlation in the matrix and doesn't effect correlations which were already changed.*
- c. *there is a linear relationship between altered value of partial correlation and correlation with the same conditioned set in the proto correlation matrix,*
- d. *this method always produces a positive definite matrix.*

Proof.

- a. This condition follows directly from Lemma 3.6.
- b. The condition (b) is a result of observation that changing the value of the correlation $\rho_{s+1,j;12\dots s}$ in the above algorithm leads to recalculate correlations of the lower order but only with the same indices before ";", that is, $s + 1, j$.

- c. Since $\rho_{s+1,j;12\dots t-1}$ is linear in $\rho_{s+1,j;12\dots t}$ for all $t = s, s-1, \dots, 1$ the linear relationship between $\rho_{s+1,j}$ and $\rho_{s+1,j;12\dots s}$ follows by substitution.
- d. Applying the above algorithm whenever a partial correlation outside the interval $(-1, 1)$ is found, we eventually obtain that all partial correlations in partial correlation specification on the vine are in $(-1, 1)$, that is, the altered matrix is positive definite. \square

From the statement (c) of Theorem 5.1 we can obtain the following result.

Corollary 5.1 *If*

$$|\rho_{s+1,j;12\dots s} - V(\rho_{s+1,j;12\dots s})^{(1)}| < |\rho_{s+1,j;12\dots s} - V(\rho_{s+1,j;12\dots s})^{(2)}|$$

then

$$|\rho_{s+1,j} - \rho_{s+1,j}^{(1)}| < |\rho_{s+1,j} - \rho_{s+1,j}^{(2)}|.$$

where $V(\rho_{s+1,j;12\dots s})^{(1)}$ and $V(\rho_{s+1,j;12\dots s})^{(2)}$ are two different choices of $V(\rho_{s+1,j;12\dots s})$ in 13

Let us consider following example:

Example 2

Let

$$A = \begin{bmatrix} 1 & -0.6 & -0.8 & 0.5 & 0.9 \\ -0.6 & 1 & 0.6 & -0.4 & -0.4 \\ -0.8 & 0.6 & 1 & 0.1 & -0.5 \\ 0.5 & -0.4 & 0.1 & 1 & 0.7 \\ 0.9 & -0.4 & -0.5 & 0.7 & 1 \end{bmatrix}.$$

We get $\rho_{34;12} = 1.0420$ hence A is not positive definite.

Since $\rho_{34;12} > 1$ then we will change its value to $V(\rho_{34;12}) = 0.9$ and recalculate lower order correlations

$$V(\rho_{34;1}) = V(\rho_{34;12})\sqrt{(1 - \rho_{23;1}^2)(1 - \rho_{24;1}^2)} + \rho_{23;1}\rho_{24;1}$$

and

$$V(\rho_{34}) = V(\rho_{34;1})\sqrt{(1 - \rho_{13}^2)(1 - \rho_{14}^2)} + \rho_{13}\rho_{14}$$

This way we will get for our example $V(\rho_{34;1}) = 0.9623$ and finally the new value in the proto correlation matrix $V(\rho_{34}) = 0.0293$. Next we will apply the same algorithm to verify that this altered matrix is positive definite. We obtained matrix

$$B = \begin{bmatrix} 1 & -0.6 & -0.8 & 0.5 & 0.9 \\ -0.6 & 1 & 0.6 & -0.4 & -0.4 \\ -0.8 & 0.6 & 1 & 0.0293 & -0.5 \\ 0.5 & -0.4 & 0.0293 & 1 & 0.7 \\ 0.9 & -0.4 & -0.5 & 0.7 & 1 \end{bmatrix}$$

which is positive definite. Note that only cell (3,4) is altered.

Remark 5.1 *In Example 2 we could choose new value of the correlation $\rho_{34;12}$, that is, $V(\rho_{34;12})$ as 0.99 then the altered value of correlation ρ_{34} is 0.0741. If we change $\rho_{34;12}$ to 0.999 then we calculate that ρ_{34} is 0.0786 but in this case we obtain that $\rho_{45;123}$ is equal -1.6224. If we change this value to -0.999 we calculate $\rho_{45} = 0.7052$.*

Remark 5.2 *Note that the choice of vine has a significant effect on the resulting altered matrix. The canonical vine favors entries in the first row. They are not changed. The changes are greater the further we go from the first row. Hence when fixing a matrix one should rearrange variables to have the most reliable entries in the first row.*

6 Completion problem

In this section we apply the canonical vine to the completion problem. First, however, we quote the known results of the completion problem which can be found in [5], [6], [3], [9], [10]. The following definitions are taken from Laurent [6]. We define the set of correlation matrices $\mathcal{E}_{n \times n}$ as follows:

$$\mathcal{E}_{n \times n} = \{X = (x_{ij}) \text{ symmetric } n \times n \mid X \succeq 0, x_{ii} = 1 \text{ for all } i = 1, 2, \dots, n\}.$$

Let $G = (N, E)$ be a graph where $N = \{1, 2, \dots, n\}$. G is simple i.e. has no loops or parallel edges. We define the set \mathcal{E}_n as a projection of $\mathcal{E}_{n \times n}$ on the subspace R^E indexed by the edge set of G

$$\mathcal{E}_n(G) = \{x \in R^E \mid \exists A = (a_{ij}) \in \mathcal{E}_{n \times n} \text{ such that } a_{ij} = x_{ij} \text{ for all } (i, j) \in E\}.$$

The sets $\mathcal{E}_{n \times n}$ and $\mathcal{E}_n(G)$ are called *eliptopes*.

Let $G = (N, E)$ be a graph. Given a subset $U \subseteq N$, $G(U)$ denotes the subgraph of G induced by U , with node set U and with edge set $\{(u, v) \in E \mid u, v \in U\}$. One says that U is a *clique* in G when $G(U)$ is a complete graph.

Suppose X has diagonal entries 1, and let $x = (x_{ij})_{ij \in E} \in R^E$ denote the vector whose components are specified entries of X . Let G denote the graph with edge set E .

Definition 6.1

X is completable if $x \in \mathcal{E}_n(G)$.

Clique condition

$$x \in \mathcal{E}_n(G) \Rightarrow$$

For every clique K in G , the projection x_K of x on the edge set of K belongs to $\mathcal{E}_k(K)$. (14)

The clique condition is also described by saying that every fully specified principal submatrix is positive definite, and a matrix with this property is called partial positive definite. It is shown in [7] that every partial positive definite matrix whose graph is G can be completed to a positive definite matrix if and only if G is *chordal* (graph G is said to be *chordal* if every cycle of G with length ≥ 4 has a chord; a *chord* of the cycle C is an edge joining two nonconsecutive nodes of C).

Since every vector $x \in \mathcal{E}(G)$ has all entries in the interval $[-1, 1]$, we can find

$$a_e = \frac{\arccos x_e}{\pi} \in [0, 1] \text{ for every } e \in E.$$

Cycle condition

$$x \in \mathcal{E}(G) \Rightarrow a = (a_e)_{e \in E} \text{ satisfies condition}$$

$$\sum_{e \in F} a_e - \sum_{e \in C \setminus F} a_e \leq |F| - 1 \quad (15)$$

for C a cycle in G, F ⊆ C with |F| odd.

The conditions (14) and (15) are necessary but in general not sufficient. As noted, (14) is sufficient for chordal graphs.

The condition (15) is sufficient for the cycles and *series-parallel* graphs i.e. graphs with no K_4 -*minors*⁵ [10], [6].

These two conditions taken together suffice for describing eliptope $\mathcal{E}_n(G)$ for the graphs called *cycle completable* [9] i.e. chordal graphs, series-parallel graphs and their *clique sums* (where *clique sum* of graphs $G_1 = (N_1, E_1)$ and $G_2 = (N_2, E_2)$ is a graph $G = (N_1 \cup N_2, E_1 \cup E_2)$ such that the set $K = N_1 \cap N_2$ induces a clique (possibly empty) in both G_1 and G_2 and there is no edge between a node of $N_1 \setminus K$ and node of $N_2 \setminus K$).

Now we present the solution of the completion problem for the special cases of graphs using partial correlation specification of a canonical vine; the root node is always chosen to be 1. We shall see that verifying the relevant conditions for completability simultaneously gives the set of completions.

In the cases below we consider only symmetric matrices so only upper part is shown and unspecified entries in this matrix are indicated by "□".

Case 1

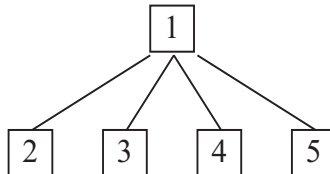
We have the following partial proto correlation matrix which needs to be completed

$$\begin{bmatrix} 1 & \rho_{12} & \rho_{13} & \rho_{14} & \cdots & \rho_{1,k+1} & \rho_{1,k+2} & \cdots & \rho_{1n} \\ & 1 & \rho_{23} & \rho_{24} & \cdots & \rho_{2,k+1} & \rho_{2,k+2} & \cdots & \rho_{2n} \\ & & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ & & & & 1 & \rho_{k,k+1} & \rho_{k,k+2} & \cdots & \rho_{k,n} \\ & & & & & 1 & \square & \cdots & \square \\ & & & & & & \cdots & \cdots & \cdots \\ & & & & & & & 1 & \square \\ & & & & & & & & 1 \\ & & & & & & & & & 1 \end{bmatrix}$$

In this case all entries in rows k+1 to n are not specified. For $n = 5$ and $k = 1$ this corresponds to the graph in Figure 4.

Since all correlations from the rows 1 to k are given we can calculate all partial correlations in canonical vine specifications up to (k - 1)-th order.

Assigning the remaining partial correlations of order k to n - 2 in the canonical vine any value from the interval (-1,1), we can specify all empty cells recalculating partial correlations using the algorithm (13). In this case the matrix can be completed if and only if all partial correlations of order less than k are in the interval (-1, 1). Hence we must evaluate formula (2) $\sum_{j=k+1}^{n-1} \left[\binom{j}{2} - \binom{n-k}{2} \right]$ times.



⁵A graph H is said to be *minor* of the graph G if H can be obtained from G by repeatedly deleting and/or contracting edges and deleting isolated nodes. *Deleting* an edge e in graph G means discarding it from the edge set of G . *Contracting* edge $e = uv$ means identifying both end nodes of e and discarding multiple edges and loops if some are created during the identification of u and v .

Figure 4. Chordal graph corresponding to Case 1 with $n=5$ and $k=1$.

Case 2

a:

$$\begin{bmatrix} 1 & \rho_{12} & \rho_{13} & \cdots & \rho_{1,k+1} & \rho_{1,k+2} & \rho_{1,k+3} & \rho_{1,k+4} & \cdots & \rho_{1n} \\ & 1 & \rho_{23} & \cdots & \rho_{2,k+1} & \rho_{2,k+2} & \rho_{2,k+3} & \rho_{2,k+4} & \cdots & \rho_{2n} \\ & & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ & & & 1 & \rho_{k,k+1} & \rho_{k,k+2} & \rho_{k,k+3} & \rho_{k,k+4} & \cdots & \rho_{k,n} \\ & & & & 1 & \rho_{k+1,k+2} & \square & \rho_{k+1,k+4} & \cdots & \rho_{k+1,n} \\ & & & & & 1 & \rho_{k+2,k+3} & \rho_{k+2,k+4} & \cdots & \rho_{k+2,n} \\ & & & & & & 1 & \square & \cdots & \square \\ & & & & & & & \cdots & \cdots & \cdots \\ & & & & & & & 1 & \square & \square \\ & & & & & & & & 1 & \square \\ & & & & & & & & & 1 \end{bmatrix}$$

In this case all entries in rows $k+3$ to n and entry $(k+1,k+3)$ are unspecified. For $n=4$ and $k=1$ this case corresponds to the graph on Figure 5 (left). We can calculate all partial correlations of order less than k and all of order k except $\rho_{k+1,k+3;1\dots k}$. If all these partial correlations are in the interval $(-1, 1)$ then the matrix can be completed. To find $\rho_{k+1,k+3}$ we choose a value of $\rho_{k+1,k+3;1\dots k}$ which belongs to the non-empty interval $I_{k+2,k+3;1\dots k+1}$ ⁶ given by (10) and then calculate $\rho_{k+1,k+3}$ using algorithm (13). Similar solutions are obtained when the empty cell in row $k+1$ occupies any other position except position $(k+1, k+2)$.

b:

$$\begin{bmatrix} 1 & \rho_{12} & \rho_{13} & \cdots & \rho_{1,k+1} & \rho_{1,k+2} & \rho_{1,k+3} & \rho_{1,k+4} & \cdots & \rho_{1n} \\ & 1 & \rho_{23} & \cdots & \rho_{2,k+1} & \rho_{2,k+2} & \rho_{2,k+3} & \rho_{2,k+4} & \cdots & \rho_{2n} \\ & & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ & & & 1 & \rho_{k,k+1} & \rho_{k,k+2} & \rho_{k,k+3} & \rho_{k,k+4} & \cdots & \rho_{k,n} \\ & & & & 1 & \square & \square & \rho_{k+1,k+4} & \cdots & \rho_{k+1,n} \\ & & & & & 1 & \rho_{k+2,k+3} & \rho_{k+2,k+4} & \cdots & \rho_{k+2,n} \\ & & & & & & 1 & \square & \cdots & \square \\ & & & & & & & \cdots & \cdots & \cdots \\ & & & & & & & 1 & \square & \square \\ & & & & & & & & 1 & \square \\ & & & & & & & & & 1 \end{bmatrix}$$

The difference with Case a is that additionally entry $(k+1,k+2)$ is omitted. For $n=4$ and $k=1$ this corresponds to the graph on Figure 5 (right). In contrast to Case 2a the partial correlation $\rho_{k+1,k+2;1\dots k}$, which cannot be calculated now, appears in every correlation of order $k+1$. To find values for correlations $\rho_{k+1,k+2}$ and $\rho_{k+1,k+3}$, we must first choose $\rho_{k+1,k+2;1\dots k}$ such that all correlations of order $k+1$ except $\rho_{k+1,k+3;1\dots k+1}$ are in $(-1,1)$. Hence

$$\rho_{k+1,k+2;1\dots k} \in I_{k+1,k+2;1\dots k} = I_{k+2,k+4;1\dots k+1} \cap I_{k+2,k+5;1\dots k+1} \cap \cdots \cap I_{k+2,n;1\dots k+1}.$$

Next given this value of $\rho_{k+1,k+2;1\dots k}$, the value of $\rho_{k+1,k+3;1\dots k}$ can be found. In this case the matrix can be completed if all correlations which can be computed are in $(-1, 1)$ and if the interval $I_{k+1,k+2;1\dots k}$ is not empty.

⁶We write $I_{k+1,k+2;1\dots k}$ instead of $I_{\rho_{k+1,k+2;1\dots k}}$.

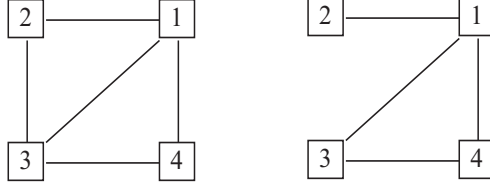


Figure 5. Chordal graphs corresponding to Case 2a (left) and Case 2b (right) with $n=4$ and $k=1$.

Case 3

This case is an example of non-chordal graph with one cycle with length 4.

$$\begin{bmatrix} 1 & \rho_{12} & \rho_{13} & \cdots & \rho_{1,k+1} & \rho_{1,k+2} & \rho_{1,k+3} & \rho_{1,k+4} & \cdots & \rho_{1n} \\ & 1 & \rho_{23} & \cdots & \rho_{2,k+1} & \rho_{2,k+2} & \rho_{2,k+3} & \rho_{2,k+4} & \cdots & \rho_{2n} \\ & & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ & & & 1 & \rho_{k,k+1} & \rho_{k,k+2} & \rho_{k,k+3} & \rho_{k,k+4} & \cdots & \rho_{k,n} \\ & & & & 1 & \rho_{k+1,k+2} & \square & \rho_{k+1,k+4} & \cdots & \rho_{k+1,n} \\ & & & & & 1 & \rho_{k+2,k+3} & \square & \cdots & \rho_{k+2,n} \\ & & & & & & 1 & \rho_{k+3,k+4} & \cdots & \rho_{k+3,n} \\ & & & & & & & \cdots & \cdots & \cdots \\ & & & & & & & 1 & \square & \square \\ & & & & & & & & 1 & \square \\ & & & & & & & & & 1 \end{bmatrix}$$

We can see that rows $k+3$ to n and entries $(k+1,k+3)$ and $(k+2,k+4)$ are unspecified. For $k=1$ and $n=5$ this corresponds to the graph on Figure 6 (left). In this case we can calculate all partial correlations of order less than k and all of order k except $\rho_{k+1,k+3;12\dots k}$ and $\rho_{k+2,k+4;12\dots k}$. Using Lemma 3.7 we choose $\rho_{k+1,k+3;12\dots k}$ belonging to the intersection

$$I_{k+1,k+3;12\dots k} = I_{k+2,k+3;12\dots k+1} \cap I_{k+3,k+4;1\dots k+1}$$

of two intervals such that $\rho_{k+2,k+3;12\dots k+1}$ and $\rho_{k+3,k+4;1\dots k+1}$ are in $(-1, 1)$ if this intersection is non-empty. We next can find possible solutions for $\rho_{k+3,k+4;12\dots k+1}$ such that $\rho_{k+3,k+4;12\dots k+2}$ is in $(-1, 1)$. Recalculating correlations using formula (13) we can fill empty cells in the cycle. In this case the matrix can be completed if all correlations which can be calculated are in $(-1, 1)$ and if $I_{k+1,k+3;1\dots k}$ is not empty. If the intersection of $I_{k+2,k+3;1\dots k+1}$ and $I_{k+3,k+4;1\dots k+1}$ is empty then this matrix cannot be completed (see Example 5).

Remark 6.1 We notice that the procedure of finding correlation $\rho_{k+1,k+3;12\dots k}$ which belongs to the interval $I_{k+1,k+3;12\dots k}$ allows us to choose a chord in this circuit. In this way, Case 3 can be reduced to the previous cases where chordal graphs were considered.

In Section 3 of [10] the completion problem for a cycle was solved. The approach used in [10] consist of solving a system of equations which is equivalent to (16). In Case 4 we present this approach in terms of partial correlation specification on a vine.

Case 4

In this case we show the general solution of the completion problem for the cycle of length n ($n \geq 4$). The following matrix corresponds to the cycle of length n (The cycle of length 6 is presented on Figure 6 (right))

$$\begin{bmatrix} 1 & \rho_{12} & \square & \square & \cdots & \square & \rho_{1n} \\ & 1 & \rho_{23} & \square & \cdots & \square & \square \\ & & \cdots & \cdots & \cdots & \cdots & \cdots \\ & & & 1 & \rho_{n-3,n-2} & \square & \square \\ & & & & 1 & \rho_{n-2,n-1} & \square \\ & & & & & 1 & \rho_{n-1,n} \\ & & & & & & 1 \end{bmatrix}$$

We have to choose correlations $\rho_{13}, \rho_{14}, \dots, \rho_{1n-1}$ such that by Lemma 3.7 and Lemma 3.8 the following system is satisfied

$$\left\{ \begin{array}{ll} \rho_{13} & \in I_{23;1} \\ (\rho_{13}, \rho_{14}) & \in A(\rho_{34}) \\ (\rho_{14}, \rho_{15}) & \in A(\rho_{45}) \\ \dots & \dots \\ (\rho_{1,n-2}, \rho_{1,n-1}) & \in A(\rho_{n-2,n-1}) \\ \rho_{1,n-1} & \in I_{n-1,n;1} \end{array} \right. \quad (16)$$

where $I_{23;1}$ denotes $I_{\rho_{23;1}}$.

If we can solve (16) then this matrix can be completed. We complete our matrix with the algorithm presented below:

$$\begin{aligned} \rho_{34;12} \in (-1, 1) &\Leftrightarrow \rho_{24;1} \in I_{34;12} \Rightarrow \rho_{24} \text{ can be calculated with (13)} \\ \rho_{35;12} \in (-1, 1) &\Leftrightarrow \rho_{25;1} \in I_{35;12} \Rightarrow \rho_{25} \text{ can be calculated} \\ &\dots \\ \rho_{n-1,n;12} \in (-1, 1) &\Leftrightarrow \rho_{2n;1} \in I_{n-1n;12} \Rightarrow \rho_{2n} \text{ can be calculated} \\ \rho_{45;123} \in (-1, 1) &\Leftrightarrow \rho_{35;12} \in I_{45;123} \Rightarrow \rho_{35;1} \text{ and next } \rho_{35} \text{ can be calculated} \\ &\dots \\ \rho_{n-1,n;123} \in (-1, 1) &\Leftrightarrow \rho_{3n;12} \in I_{n-1,n;123} \Rightarrow \rho_{3n;1} \text{ and next } \rho_{3n} \text{ can be calculated} \\ &\dots \\ \rho_{n-1,n;12\dots n-2} \in (-1, 1) &\Leftrightarrow \rho_{n-2n;12\dots n-3} \in I_{n-1,n;12\dots n-2} \Rightarrow \rho_{n-2,n;12\dots n-4} \\ &\text{and next } \rho_{n-2,n;12\dots n-4}, \dots, \rho_{n-2,n} \text{ can be calculated} \end{aligned}$$

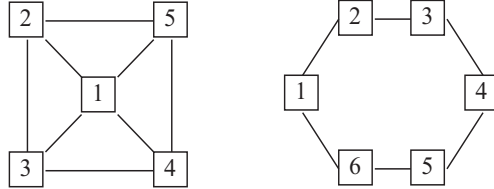


Figure 6. Graphs corresponding to Case 3 (left) with $k=1, n=5$ and Case 4 (right) with $n=6$.

Case 5

In this case we consider wheel on n ($n \geq 4$) elements (a *wheel* on n elements is a graph composed of a circuit C on $n - 1$ nodes together with an additional node adjacent to all nodes of C).

The following matrix corresponds to the wheel of length n

$$\begin{bmatrix} 1 & \rho_{12} & \rho_{13} & \rho_{14} & \rho_{15} & \dots & \dots & \rho_{1,n-1} & \rho_{1n} \\ & 1 & \rho_{23} & \square & \square & \dots & \dots & \square & \rho_{2n} \\ & & 1 & \rho_{34} & \square & \dots & \dots & \square & \square \\ & & & \dots & \dots & \dots & \dots & \dots & \dots \\ & & & & & 1 & \rho_{n-3,n-2} & \square & \square \\ & & & & & & 1 & \rho_{n-2,n-1} & \square \\ & & & & & & & 1 & \rho_{n-1,n} \\ & & & & & & & & 1 \end{bmatrix}.$$

This case can be reduced to the Case 5 by applying Theorem 4.1. If correlations $\rho_{k,k+1;1}$ for

$k = 2, 3, \dots, n - 1$ and $\rho_{2n;1}$ are in $(-1,1)$ then the following matrix needs to be completed

$$\begin{bmatrix} 1 & \rho_{23;1} & \square & \square & \dots & \square & \rho_{2n;1} \\ & 1 & \rho_{34;1} & \square & \dots & \square & \square \\ & & \dots & \dots & \dots & \dots & \dots \\ & & & & 1 & \rho_{n-2,n-1;1} & \square \\ & & & & & 1 & \rho_{n-1,n;1} \\ & & & & & & 1 \end{bmatrix}.$$

Remark 6.2 Note that it is shown in [10] that the wheel on n ($n \geq 5$) elements is not cycle completable.

Remark 6.3 To our knowledge Case 5 is the first method for completing the wheel. Methods of completing chordal graphs and cycles have been previously presented in [7] and [10].

Example 4

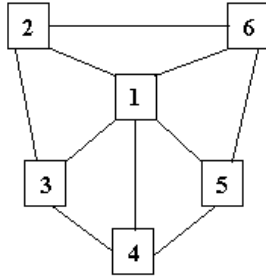


Figure 5. A wheel on 6 elements.

The following matrix corresponds to a wheel on 6 elements

$$\begin{bmatrix} 1 & \rho_{12} & \rho_{13} & \rho_{14} & \rho_{15} & \rho_{16} \\ & 1 & \rho_{23} & \square & \square & \rho_{26} \\ & & 1 & \rho_{34} & \square & \square \\ & & & 1 & \rho_{45} & \square \\ & & & & 1 & \rho_{56} \\ & & & & & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0.8 & 0.1 & -0.3 & 0.5 & -0.4 \\ & 1 & 0 & \square & \square & -0.1 \\ & & 1 & -0.6 & \square & \square \\ & & & 1 & -0.7 & \square \\ & & & & 1 & 0.2 \\ & & & & & 1 \end{bmatrix}.$$

We can calculate

$$[\rho_{23;1}, \rho_{26;1}, \rho_{34;1}, \rho_{45;1}, \rho_{56;1}] = [-0.1340, 0.4001, -0.6005, -0.6658, 0.5040].$$

We must choose correlations $\rho_{24;1}$ and $\rho_{25;1}$ such that the system similar to (16) is satisfied. Since $\rho_{24;1} \in I_{34;12} = (-0.7119, 0.8729)$ and $\rho_{25;1} \in I_{56;12} = (-0.5899, 0.9932)$ then we can choose $\rho_{24;1} = \rho_{25;1} = 0$. Hence $\rho_{34;12} = -0.6060$, $\rho_{45;12} = -0.6658$ and $\rho_{56;12} = 0.5499$. (Note that $\rho_{45;12}$ depends on $\rho_{24;1}$ and $\rho_{25;1}$. Hence we must choose these correlations such that also $\rho_{45;12} \in (-1, 1)$. If it is not possible then this graph cannot be completed.)

Now we can find $\rho_{35;12} \in I_{45;123} = (-0.1900, 0.9970)$. Let us choose $\rho_{35;12} = 0$ then $\rho_{45;123} = -0.8370$ and $\rho_{36;12} \in I_{56;123} = (-0.8352, 0.8352)$. Hence we can also take $\rho_{36;12} = 0$ then $\rho_{56;123} =$

0.5499. Finally we get $\rho_{46;123} \in I_{56;1234} = (-0.9173, -0.0032)$. We take for instance $\rho_{46;123} = -0.5$ and now we can recalculate all correlations using algorithm 13.

$$\begin{aligned}
\rho_{24;1} = 0 &\Rightarrow \rho_{24} = \rho_{12}\rho_{14} = -0.24 \\
\rho_{25;1} = 0 &\Rightarrow \rho_{25} = \rho_{12}\rho_{15} = 0.4 \\
\rho_{35;12} = 0 &\Rightarrow \rho_{35;1} = \rho_{23;1}\rho_{25;1} = 0 \\
&\Rightarrow \rho_{35} = \rho_{13}\rho_{15} = 0.05 \\
\rho_{36;12} = 0 &\Rightarrow \rho_{36;1} = \rho_{23;1}\rho_{26;1} = -0.0536 \\
&\Rightarrow \rho_{36} = \rho_{36;1}\sqrt{(1 - \rho_{13}^2)(1 - \rho_{16}^2)} + \rho_{13}\rho_{16} = -0.0889 \\
\rho_{46;123} = -0.5 &\Rightarrow \rho_{46;12} = -0.3977 \Rightarrow \rho_{46;1} = -0.3645 \Rightarrow \rho_{46} = -0.1987.
\end{aligned}$$

We obtain that the matrix

$$\begin{bmatrix}
1 & 0.8 & 0.1 & -0.3 & 0.5 & -0.4 \\
& 1 & 0 & -0.24 & 0.4 & -0.1 \\
& & 1 & -0.6 & 0.05 & -0.0889 \\
& & & 1 & -0.7 & -0.1987 \\
& & & & 1 & 0.2 \\
& & & & & 1
\end{bmatrix}$$

is positive definite.

Example 5

Let us consider the following matrix

$$\begin{bmatrix}
1 & \rho_{12} & \rho_{13} & \rho_{14} & \rho_{15} \\
& 1 & \rho_{23} & \square & \rho_{25} \\
& & 1 & \rho_{34} & \square \\
& & & 1 & \rho_{45} \\
& & & & 1
\end{bmatrix} = \begin{bmatrix}
1 & 0.7 & -0.3 & 0.2 & 0.5 \\
& 1 & -0.8 & \square & 0.7 \\
& & 1 & 0.6 & \square \\
& & & 1 & 0.9 \\
& & & & 1
\end{bmatrix}$$

which corresponds to the Case 3 with $n=5$ and $k=1$. We can calculate

$$[\rho_{23;1}, \rho_{25;1}, \rho_{34;1}, \rho_{45;1}] = [-0.8661, 0.5659, 0.7061, 0.9428].$$

Now following the procedure presented in Case 3 we must choose correlation $\rho_{24;1}$ such that it belong to the intersection of $I_{34;12}$ and $I_{45;12}$. We get however that

$$\begin{aligned}
I_{34;12} &= (-0.9655, -0.2576), \\
I_{45;12} &= (0.2587, 0.8084).
\end{aligned}$$

Hence the intersection is empty. From this we conclude that this matrix cannot be completed.

General solution strategy

We consider a practicable strategy for finding a completion of an incomplete proto correlation matrix, if such a solution exists. The following matrix is given (assumed to be symmetric)

$$\begin{bmatrix}
1 & \rho_{12} & \rho_{13} & \dots & \rho_{1,n-1} & \rho_{1n} \\
\rho_{21} & 1 & \rho_{23} & \dots & \rho_{2,n-1} & \rho_{2n} \\
\rho_{31} & \rho_{32} & 1 & \dots & \rho_{3,n-1} & \rho_{3n} \\
\dots & \dots & \dots & \dots & \dots & \dots \\
\rho_{n-1,1} & \rho_{n-1,2} & \rho_{n-1,3} & \dots & 1 & \rho_{n-1,n} \\
\rho_{n1} & \rho_{n2} & \rho_{n3} & \dots & \rho_{n,n-1} & 1
\end{bmatrix}.$$

First, we remark that by Lemma 3.7 we know that if the matrix is completable, then the set of solutions is open. Some of the entries ρ_{ij} are not specified. We first order the rows and columns to obtain a maximal bottom right triangle above the diagonal with unspecified elements. If all unspecified cells appear in this triangle, then the choices of values for the partial correlations whose conditioned sets correspond with the empty cells is unconstrained (case 1). Any choice yields a completion under (2). If there is an unspecified cell (i, j) such that some (i, k) is specified, $k > j$, then the choice of partial correlations $\rho_{ij;1\dots i-1}$ is constrained. The different ways in which these are constrained are illustrated in the cases above. In general, we can say that for all unspecified cells in the i -th row, $\rho_{ij;1\dots i-1}$ must be chosen such that all partial correlations $\rho_{kj;1\dots i}$, $k > i$ are in $(-1, 1)$.

Define $C_k = \{j \in \{k+1, \dots, n\} | \rho_{kj} \text{ unspecified}\}$ and $D_j = \{k \in \{j+1, \dots, n\} | \rho_{kj} \text{ specified}\}$. To choose values for ρ_{1j} , $j \in C_1$ we must solve a system such that all correlations of the first order $\rho_{kj;1}$ are in the interval $(-1, 1)$, where $k \in D_j$, using Lemma 3.7 and/or Lemma 3.8. (If the system has no solutions, the matrix is not completable.) If this system has solutions then we can fill all empty cells in the first row and the values of $\rho_{kj;1}$ are fixed. Next we repeat the same operation for the unspecified elements in the second row ρ_{2j} , $j \in C_2$. We must solve a system such that all correlations of the second order $\rho_{kj;12}$ where $k \in D_j$ are in the interval $(-1, 1)$. If this system has solutions we obtain partial correlations of the first order $\rho_{2j;1}$. If this system has no solutions, we return to C_1 and choose another solution, re-fixing the values of $\rho_{kj;1}$. If the matrix is completable, we can find a solution for C_1 which allows us to fix values for C_2 in finitely many steps. We continue in this way through row n . Of course this strategy is not an effective procedure for deciding whether or not a given incomplete matrix is completable. The issue of decidability of real closed fields is not addressed in this paper.

7 Conclusions

We have explained the use of partial correlation specifications on a canonical vine in various problems regarding positive definiteness of proto correlation matrices. One attractive feature is that the steps in the algorithms acquire a probabilistic interpretation through the notion of partial correlations. We note, however, that they cannot apply to problems involving positive semidefiniteness. Indeed, the denominators in (2) must be non-zero and this implies that all partial correlations must be greater than -1 and less than 1. The speed of these algorithms appears to be comparable to that of previous algorithms.

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