

# Conditional independence between two variables given any conditioning subset implies block diagonal covariance matrix for multivariate Gaussian distributions

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## Abstract

Let  $x = (x_{\mathbb{V}})$  be a multivariate Gaussian variable with covariance matrix  $\Sigma$ . For  $i$  and  $j$  in  $\mathbb{V}$ , we show that if the conditional covariance between  $x_i$  and  $x_j$  given any conditioning set  $\mathbb{K} \subset \mathbb{V} \setminus \{i, j\}$  is equal to zero, then  $\Sigma$  is block diagonal and  $i$  and  $j$  belong to two different blocks.

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## 1. Introduction

As pointed out by Dawid (1998), the concept of conditional independence is believed to be the fundamental knowledge in the process of scientific inference. For multivariate Gaussian variables, conditional independence is quantified by conditional covariance. Investigation of such coefficients have led to a better characterization of interactions between variables, in particular through the use of conditional independence graphs (Whittaker, 1990; Lauritzen, 1996; Edwards, 2000). Marginal correlation coefficients have also been examined through covariance graphs (Kauermann, 1996; Edwards, 2000). It would be interesting to generalize these approaches by simultaneously considering *all possible* conditional covariances for a given pair of variables. For instance, consider the case of a three-dimensional Gaussian variable  $x = (x_1, x_2, x_3)$  with covariance matrix  $\Sigma$ . If  $\text{Corr}[x_1, x_2|x_3] = 0$ , then  $\text{Corr}[x_1, x_2] = \text{Corr}[x_1, x_3] \cdot \text{Corr}[x_2, x_3]$  (Wermuth, 1976; Whittaker, 1990, Proposition 2.6.5). If one furthermore has  $\text{Corr}[x_1, x_2] = 0$ , it directly comes out that either  $\text{Corr}[x_1, x_3] = 0$  or  $\text{Corr}[x_2, x_3] = 0$ . In other words, the following yields:

$$\{\text{Corr}[x_1, x_2] = 0 \text{ and } \text{Corr}[x_1, x_2|x_3] = 0\} \Rightarrow \Sigma \text{ is block diagonal.}$$

To our knowledge, no generalization of such a result has been shown yet. This paper is a first step in this direction. We prove a result that demonstrates how this approach can inform us regarding the global pattern of interaction and shed light into the structure of the variables.

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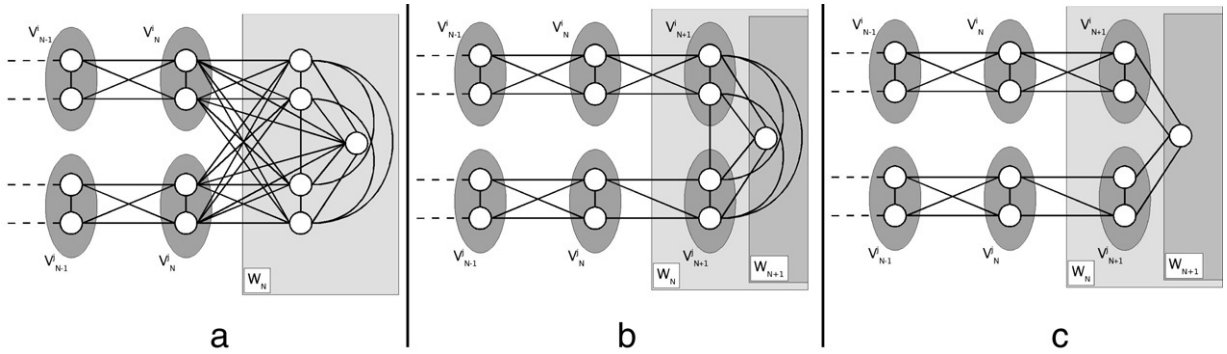


Fig. 1. Sketch of proof. From an original partitioning of  $\mathbb{V}$  into  $\{\mathbb{V}_0^i, \dots, \mathbb{V}_N^i, \mathbb{V}_0^j, \dots, \mathbb{V}_N^j, \mathbb{W}_N\}$  (a), we proceed as follows. We first show that for all elements of  $\mathbb{W}_N$  there can be no marginal covariance with both  $\mathbb{V}_N^i$  and  $\mathbb{V}_N^j$ . We then partition  $\mathbb{W}_N$  into elements that covariate with  $\mathbb{V}_N^i$  (gathered in  $\mathbb{V}_{N+1}^i$ ), elements that covariate with  $\mathbb{V}_N^j$  (gathered in  $\mathbb{V}_{N+1}^j$ ), and elements that covariate with neither (gathered in  $\mathbb{W}_{N+1}$ ) (b). Last, we show that elements of  $\mathbb{V}_{N+1}^i$  and  $\mathbb{V}_{N+1}^j$  must have zero marginal covariance (c).

**2. Main theorem**

Let  $\mathbb{V}$  be a finite set and  $x = x_{\mathbb{V}} = (x_v)_{v \in \mathbb{V}}$  be a multivariate Gaussian variable indexed on  $\mathbb{V}$  with covariance matrix  $\Sigma$ .

**Theorem 1.** *Let  $i$  and  $j$  be two elements of  $\mathbb{V}$  and further assume that  $x_i$  and  $x_j$  are conditionally independent given any set of remaining variables, i.e.,*

$$\forall \mathbb{K} \subset \mathbb{V} \setminus \{i, j\} \quad \text{Cov}[x_i, x_j | x_{\mathbb{K}}] = 0. \tag{1}$$

*Then  $\Sigma$  is block diagonal and  $i$  and  $j$  belong to two different blocks.*

Sole consideration of marginal and/or partial covariance is not sufficient to provide this result, for there exist covariance matrices that are not block diagonal while including variables for which  $\text{Cov}[x_i, x_j] = 0$  and/or  $\text{Cov}[x_i, x_j | x_{\mathbb{V} \setminus \{i, j\}}] = 0$ .

This result can be established by successive examination of conditional independence constraints (see Fig. 1 for a graphical sketch of proof). First,  $\text{Corr}[x_i, x_j] = 0$  and, hence,  $\Sigma_{i,j} = 0$ . We also have  $\text{Cov}[x_i, x_j | x_{\mathbb{K}}] = 0$  for any  $k \in \mathbb{V} \setminus \{i, j\}$ . Since  $\Sigma_{i,j} = 0$ , the general formula for conditional covariance (Anderson, 1958, p. 28) simplifies to

$$\text{Cov}[x_i, x_j | x_{\mathbb{K}}] = - \frac{\Sigma_{i,k} \Sigma_{k,j}}{\Sigma_{k,k}}.$$

For  $\text{Cov}[x_i, x_j | x_{\mathbb{K}}]$  to be equal to zero, we must then have  $\Sigma_{i,k} \Sigma_{k,j} = 0$ , i.e., either  $\Sigma_{i,k} = 0$  or  $\Sigma_{j,k} = 0$ . This line of reasoning being valid for any  $k \notin \{i, j\}$ , it is possible to separate  $\mathbb{V} \setminus \{i, j\}$  into three sets:  $\mathbb{V}_1^i$  such that  $\Sigma_{i,k} \neq 0$  and  $\Sigma_{j,k} = 0$  for  $k \in \mathbb{V}_1^i$ ;  $\mathbb{V}_1^j$  such that  $\Sigma_{i,k} = 0$  and  $\Sigma_{j,k} \neq 0$  for  $k \in \mathbb{V}_1^j$ ; and  $\mathbb{W}_1$  such that  $\Sigma_{i,k} = 0$  and  $\Sigma_{j,k} = 0$  for  $k \in \mathbb{W}_1$ . Let then be  $\mathbb{K} = \{k, l\}$  with  $k \in \mathbb{V}_1^i$  and  $l \in \mathbb{V}_1^j$ .  $\text{Cov}[x_i, x_j | x_{\mathbb{K}}]$  is given by (see Eq. (A.1))

$$\text{Cov}[x_i, x_j | x_{\mathbb{K}}] = - \sum_{a,b \in \mathbb{K}} (\Sigma_{i \cup j, \mathbb{K}})_{i,a} \frac{(-1)^{\text{pos}_{\mathbb{K}}(a) + \text{pos}_{\mathbb{K}}(b)} \det[\Sigma_{\mathbb{K} \setminus \{b\}, \mathbb{K} \setminus \{a\}}]}{\det[\Sigma_{\mathbb{K}, \mathbb{K}}]} (\Sigma_{\mathbb{K}, i \cup j})_{b,j},$$

where  $\text{pos}_{\mathbb{K}}(a)$  stands for the position of  $a$  in  $\mathbb{K}$ . Since  $k \in \mathbb{V}_1^i$  and  $l \in \mathbb{V}_1^j$ , we have  $\Sigma_{i,l} = \Sigma_{j,k} = 0$  and  $\text{Cov}[x_i, x_j | x_{\mathbb{K}}]$  boils down to

$$\text{Cov}[x_i, x_j | x_{\mathbb{K}}] = \frac{\Sigma_{i,k} \Sigma_{k,l} \Sigma_{l,j}}{\Sigma_{k,k} \Sigma_{l,l} - \Sigma_{k,k}^2}.$$

Since we must also have  $\text{Cov}[x_i, x_j | x_{\mathbb{K}}] = 0$  according to our hypothesis, this equation leads to  $\Sigma_{k,l} = 0$ , given that  $\Sigma_{i,k}$  and  $\Sigma_{j,l}$  are different from zero. Elements of  $\mathbb{V}_1^i$  (resp.  $\mathbb{V}_1^j$ ) have hence a zero marginal correlation to both  $j$  (resp.  $i$ ) and all elements of  $\mathbb{V}_1^j$  (resp.  $\mathbb{V}_1^i$ ).

We then proceed by induction. Assume that there exist  $2(N + 1)$  subsets  $\mathbb{V}_n^i$  and  $\mathbb{V}_n^j$ , with  $n = 0, \dots, N$ , and one set  $\mathbb{W}_N$  of  $\mathbb{V}$  such that

- $\mathbb{V}_0^i = \{i\}$  and  $\mathbb{V}_0^j = \{j\}$ ;
- $\{\mathbb{V}_0^i, \dots, \mathbb{V}_N^i, \mathbb{V}_0^j, \dots, \mathbb{V}_N^j, \mathbb{W}_N\}$  is a partition of  $\mathbb{V}$ .
- nonzero marginal correlations can only be found between  $\mathbb{V}_{n-1}^i$  and  $\mathbb{V}_n^i$ , between  $\mathbb{V}_{n-1}^j$  and  $\mathbb{V}_n^j$ , or between  $\mathbb{W}_N$  and  $\{\mathbb{V}_N^i, \mathbb{V}_N^j\}$ .
- all marginal correlations between  $\mathbb{V}_{n-1}^i$  and  $\mathbb{V}_n^i$ , as well as between  $\mathbb{V}_{n-1}^j$  and  $\mathbb{V}_n^j$  are different from zero.

Since we proved that  $\Sigma_{i,j} = 0$ ,  $\Sigma_{i,l} = 0$  for  $l \in \mathbb{V}_1^j$ ,  $\Sigma_{j,k} = 0$  for  $k \in \mathbb{V}_1^i$ ,  $\Sigma_{k,l} = 0$  for  $(k, l) \in \mathbb{V}_1^i \times \mathbb{V}_1^j$  and constructed  $\mathbb{V}_1^i$  and  $\mathbb{V}_1^j$  so that  $\Sigma_{i,k} \neq 0$  for  $k \in \mathbb{V}_1^i$  and  $\Sigma_{j,l} \neq 0$  for  $l \in \mathbb{V}_1^j$ , the assumption holds for  $N = 1$ . We now assume that it also holds for a given  $N \geq 1$ . If  $\mathbb{W}_N$  is empty, then the process stops. Otherwise, the first step consists of setting  $\mathbb{K} = \{k_1, l_1, \dots, k_N, l_N, m\}$ , with  $(k_n, l_n) \in \mathbb{V}_n^i \times \mathbb{V}_n^j$  for  $n = 1 \dots, N$ , and  $m \in \mathbb{W}_N$ . Given the assumption of independence between  $x_i$  and  $x_j$ , we must have  $\text{Cov}[x_i, x_j | x_{\mathbb{K}}] = 0$ . This conditional covariance coefficient is equal to (cf. Eq. (A.2))

$$\frac{\Sigma_{i,k_1} \Sigma_{j,l_1} \left[ \prod_{n=1, \dots, N-1} \Sigma_{k_n, k_{n+1}} \Sigma_{l_n, l_{n+1}} \right] \Sigma_{k_N, m} \Sigma_{l_N, m}}{\det [\Sigma_{\mathbb{K}, \mathbb{K}}]}$$

and is equal to zero if and only if  $\Sigma_{k_N, m} \Sigma_{l_N, m} = 0$ , since, by construction all  $\Sigma_{k_n, k_{n+1}}$  and  $\Sigma_{l_n, l_{n+1}}$  are different from zero. It is then possible to separate  $\mathbb{W}_N$  into three sets:  $\mathbb{V}_{N+1}^i$  such that  $\Sigma_{k_N, m} \neq 0$  and  $\Sigma_{l_N, m} = 0$  for all  $m \in \mathbb{V}_{N+1}^i$ ;  $\mathbb{V}_{N+1}^j$  such that  $\Sigma_{k_N, m} = 0$  and  $\Sigma_{l_N, m} \neq 0$  for all  $m \in \mathbb{V}_{N+1}^j$ ; and  $\mathbb{W}_{N+1}$  such that  $\Sigma_{k_N, m} = \Sigma_{l_N, m} = 0$  for all  $m \in \mathbb{W}_{N+1}$ . It now remains to prove that we have  $\Sigma_{k,l} = 0$  for  $(k, l) \in \mathbb{V}_{N+1}^i \times \mathbb{V}_{N+1}^j$ . To this aim, set  $\mathbb{K} = \{k_1, l_1, \dots, k_{N+1}, l_{N+1}\}$  with  $(k_n, l_n) \in \mathbb{V}_n^i \times \mathbb{V}_n^j$  for  $n = 1 \dots, N + 1$ . Since  $x_i$  and  $x_j$  are independent, we must have  $\text{Cov}[x_i, x_j | x_{\mathbb{K}}] = 0$ . This quantity being equal to (see Eq. (A.3))

$$\text{Cov}[x_i, x_j | x_{\mathbb{K}}] = \frac{\Sigma_{i,k_1} \Sigma_{j,l_1} \left[ \prod_{n=1, \dots, N} \Sigma_{k_n, k_{n+1}} \Sigma_{l_n, l_{n+1}} \right] \Sigma_{k_{N+1}, l_{N+1}}}{\det [\Sigma_{\mathbb{K}, \mathbb{K}}]}$$

it is equal to zero if and only if  $\Sigma_{k_{N+1}, l_{N+1}} = 0$ . The assumption is therefore also valid for  $N + 1$ .

The sequence  $(\mathbb{W}_N)$  is of decreasing cardinal.  $\mathbb{V}$  being a finite set, there exists a step  $N_0$  for which  $\mathbb{W}_{N_0}$  is empty: the process ends there. Set  $\mathbb{V}^i = \{\mathbb{V}_0^i, \dots, \mathbb{V}_{N_0}^i\}$  and  $\mathbb{V}^j = \{\mathbb{V}_0^j, \dots, \mathbb{V}_{N_0}^j\}$ .  $\{\mathbb{V}^i, \mathbb{V}^j\}$  is hence a partition of  $\mathbb{V}$  for which there exists no marginal correlation between an element of  $\mathbb{V}^i$  and an element of  $\mathbb{V}^j$ . Consequently, the covariance matrix of  $x$  has the following structural form:

$$\begin{pmatrix} \Sigma_{\mathbb{V}^i, \mathbb{V}^i} & 0 \\ 0 & \Sigma_{\mathbb{V}^j, \mathbb{V}^j} \end{pmatrix},$$

thereby proving the theorem.

### 3. Discussion and perspectives

In this paper, we considered  $x = x_{\mathbb{V}} = (x_v)_{v \in \mathbb{V}}$  a multivariate Gaussian variable with covariance matrix  $\Sigma$ . For  $i$  and  $j$  in  $\mathbb{V}$ , we showed that if the conditional covariance between  $x_i$  and  $x_j$  given any conditioning set  $\mathbb{K} \subset \mathbb{V} \setminus \{i, j\}$  is equal to zero, then  $\Sigma$  is block diagonal and  $i$  and  $j$  belonged to two different blocks. Note that the converse of this theorem is straightforward. Indeed, if one considers that the covariance matrix  $\Sigma$  is block diagonal, then any conditional covariance between variables belonging to two different blocks is equal to zero according to Eq. (A.1).

Theorem 1 shows that, for multivariate Gaussian variables, there is a clear separation between two variables  $x_i$  and  $x_j$  that are independent with regard to any conditioning subset, and that this separation also applies to all other

variables, which are either “with”  $x_i$  or “with”  $x_j$ . Consequently, their effect can be analyzed independently in one block of variables or the other.

Interestingly, this result nicely relates two distinct properties of Gaussian distributions. The block diagonal property of the covariance matrix is clearly a global feature of Gaussian probability distributions. By contrast, the relationship of “complete independence” (i.e., conditioned on all subsets) is rather a local description and characterization of the interaction structure between variables, since the definition gives a particular role to  $x_i$  and  $x_j$ . This perspective differs from the common approach, where one usually sets a “level” of conditioning (marginal for covariance graphs, partial for conditional independence graphs) and then varies the two variables on which correlation is calculated. In this “dual” approach, the definition does not so much depend on the conditioning set than on the variables whose conditional covariance we examine. We mainly focus on the independence pattern that can be exhibited with a single pair of variables and its potential implications onto the global structure. We believe that there is much to gain by analyzing variables from this perspective and hope to be able to provide further results along the same lines in the near future.

**Acknowledgment**

We are in debt to an anonymous referee for pointing out that the result exposed here is well known for three-dimensional Gaussian variables.

**Appendix. Calculation of  $\text{Cov}[x_i, x_j | x_{\mathbb{K}}]$**

The conditional covariance between  $i$  and  $j$  given  $\mathbb{K}$  reads (Anderson, 1958, p. 28)

$$\text{Cov}[x_i, x_j | x_{\mathbb{K}}] = \Sigma_{i,j} - \sum_{a,b \in \mathbb{K}} (\Sigma_{i \cup j, \mathbb{K}})_{i,a} \left[ (\Sigma_{\mathbb{K}, \mathbb{K}})^{-1} \right]_{a,b} (\Sigma_{\mathbb{K}, i \cup j})_{b,j}.$$

Calculating  $(\Sigma_{\mathbb{K}, \mathbb{K}})^{-1}$  from the adjoint matrix (Horn and Johnson, 1999) yields for  $\text{Cov}[x_i, x_j | x_{\mathbb{K}}]$ :

$$\text{cov}[x_i, x_j | x_{\mathbb{K}}] = \Sigma_{i,j} - \sum_{a,b \in \mathbb{K}} (\Sigma_{i \cup j, \mathbb{K}})_{i,a} \frac{(-1)^{\text{pos}_{\mathbb{K}}(a) + \text{pos}_{\mathbb{K}}(b)} \det[\Sigma_{\mathbb{K} \setminus \{b\}, \mathbb{K} \setminus \{a\}}]}{\det[\Sigma_{\mathbb{K}, \mathbb{K}}]} (\Sigma_{\mathbb{K}, i \cup j})_{b,j}, \tag{A.1}$$

where  $\text{pos}_{\mathbb{K}}(a)$  stands for the position of  $a$  in  $\mathbb{K}$ . From now on, we also assume that there exist  $2(N + 1) + 1$  subsets of  $\mathbb{V}$ , namely  $\mathbb{V}_n^i, \mathbb{V}_n^j$ , with  $n = 0, \dots, N$ , and  $\mathbb{W}_N$ , respecting the conditions detailed on page 3.

First, for  $N \geq 1$ , set  $\mathbb{K} = \{k_1, l_1, \dots, k_N, l_N, m\}$ ,  $k_n \in \mathbb{V}_n^i$  and  $l_n \in \mathbb{V}_n^j$  for  $n = 1 \dots, N$ , and  $m \in \mathbb{W}_N$ . By construction, only elements in  $\mathbb{V}_1^i$  (resp.  $\mathbb{V}_1^j$ ) have nonzero marginal covariance with  $i$  (resp.  $j$ ). Consequently, the sum in Eq. (A.1) can be simplified into

$$\Sigma_{i,k_1} \frac{(-1)^{\text{pos}_{\mathbb{K}}(a) + \text{pos}_{\mathbb{K}}(b)} \det[\Sigma_{\mathbb{K} \setminus \{l_1\}, \mathbb{K} \setminus \{k_1\}}]}{\det[\Sigma_{\mathbb{K}, \mathbb{K}}]} \Sigma_{j,l_1}.$$

Given the definition of  $\mathbb{K}$ ,  $\Sigma_{\mathbb{K}, \mathbb{K}}$ ,  $\Sigma_{\mathbb{K} \setminus \{l_1\}, \mathbb{K} \setminus \{k_1\}}$ , and the determinant of the latter matrix respectively read

$$\Sigma_{\mathbb{K}, \mathbb{K}} = \begin{pmatrix} \Sigma_{k_1, k_1} & 0 & \Sigma_{k_1, k_2} & 0 & 0 & 0 & 0 & \dots & 0 \\ 0 & \Sigma_{l_1, l_1} & 0 & \Sigma_{l_1, l_2} & 0 & 0 & 0 & & \\ \Sigma_{k_1, k_2} & 0 & \Sigma_{k_2, k_2} & 0 & \Sigma_{k_2, k_3} & 0 & 0 & & \vdots \\ 0 & \Sigma_{l_1, l_2} & 0 & \Sigma_{l_2, l_2} & 0 & \Sigma_{l_2, l_3} & 0 & & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & & 0 & \Sigma_{l_{N-1}, l_N} & 0 & \Sigma_{l_{N-1}, l_{N-1}} & 0 & \Sigma_{l_{N-1}, l_{N-1}} & 0 \\ \vdots & & 0 & 0 & \Sigma_{k_{N-1}, k_N} & 0 & \Sigma_{k_N, k_N} & 0 & \Sigma_{k_N, m} \\ & & 0 & 0 & 0 & \Sigma_{l_{N-1}, l_N} & 0 & \Sigma_{l_N, l_N} & \Sigma_{l_N, m} \\ 0 & \dots & 0 & 0 & 0 & 0 & \Sigma_{k_N, m} & \Sigma_{l_N, m} & \Sigma_{m, m} \end{pmatrix},$$

$$\Sigma_{\mathbb{K} \setminus \{l_1\}, \mathbb{K} \setminus \{k_1\}} = \begin{pmatrix} 0 & \Sigma_{k_1, k_2} & 0 & 0 & 0 & 0 & 0 & \dots & 0 \\ 0 & \Sigma_{k_2, k_2} & 0 & \Sigma_{k_2, k_3} & 0 & 0 & 0 & & \\ \Sigma_{l_1, l_2} & 0 & \Sigma_{l_2, l_2} & 0 & \Sigma_{l_2, l_3} & 0 & 0 & & \vdots \\ 0 & \Sigma_{k_2, k_3} & 0 & \Sigma_{k_3, k_3} & 0 & \Sigma_{k_3, k_4} & 0 & & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & & 0 & \Sigma_{l_{N-1}, l_N} & 0 & \Sigma_{l_{N-1}, l_{N-1}} & 0 & \Sigma_{l_{N-1}, l_{N-1}} & 0 \\ \vdots & & 0 & 0 & \Sigma_{k_{N-1}, k_N} & 0 & \Sigma_{k_N, k_N} & 0 & \Sigma_{k_N, m} \\ & & 0 & 0 & 0 & \Sigma_{l_{N-1}, l_N} & 0 & \Sigma_{l_N, l_N} & \Sigma_{l_N, m} \\ 0 & \dots & 0 & 0 & 0 & 0 & \Sigma_{k_N, m} & \Sigma_{l_N, m} & \Sigma_{m, m} \end{pmatrix},$$

and

$$\det [\Sigma_{\mathbb{K} \setminus \{l_1\}, \mathbb{K} \setminus \{k_1\}}] = -\Sigma_{k_1, k_2} \det (\Sigma_{\mathbb{K} \setminus \{l_1, k_1\}, \mathbb{K} \setminus \{k_1, k_2\}}).$$

We also have

$$\Sigma_{\mathbb{K} \setminus \{l_1, k_1\}, \mathbb{K} \setminus \{k_1, k_2\}} = \begin{pmatrix} 0 & 0 & \Sigma_{k_2, k_3} & 0 & 0 & 0 & 0 & \dots & 0 \\ \Sigma_{l_1, l_2} & \Sigma_{l_2, l_2} & 0 & \Sigma_{l_2, l_3} & 0 & 0 & 0 & & \\ 0 & 0 & \Sigma_{k_3, k_3} & 0 & \Sigma_{k_3, k_4} & 0 & 0 & & \vdots \\ 0 & \Sigma_{l_2, l_3} & 0 & \Sigma_{l_3, l_3} & 0 & \Sigma_{l_3, l_4} & 0 & & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & & 0 & \Sigma_{l_{N-1}, l_N} & 0 & \Sigma_{l_{N-1}, l_{N-1}} & 0 & \Sigma_{l_{N-1}, l_{N-1}} & 0 \\ \vdots & & 0 & 0 & \Sigma_{k_{N-1}, k_N} & 0 & \Sigma_{k_N, k_N} & 0 & \Sigma_{k_N, m} \\ & & 0 & 0 & 0 & \Sigma_{l_{N-1}, l_N} & 0 & \Sigma_{l_N, l_N} & \Sigma_{l_N, m} \\ 0 & \dots & 0 & 0 & 0 & 0 & \Sigma_{k_N, m} & \Sigma_{l_N, m} & \Sigma_{m, m} \end{pmatrix},$$

and, hence,

$$\det (\Sigma_{\mathbb{K} \setminus \{l_1, k_1\}, \mathbb{K} \setminus \{k_1, k_2\}}) = -\Sigma_{l_1, l_2} \det (\Sigma_{\mathbb{K} \setminus \{l_1, k_1, l_2\}, \mathbb{K} \setminus \{k_1, l_1, k_2\}}).$$

This leads to

$$\det [\Sigma_{\mathbb{K} \setminus \{l_1\}, \mathbb{K} \setminus \{k_1\}}] = \Sigma_{k_1, k_2} \Sigma_{l_1, l_2} \det (\Sigma_{\mathbb{K} \setminus \{l_1, k_1, l_2\}, \mathbb{K} \setminus \{k_1, l_1, k_2\}}),$$

with

$$\Sigma_{\mathbb{K} \setminus \{l_1, k_1, l_2\}, \mathbb{K} \setminus \{k_1, k_2, l_1\}} = \begin{pmatrix} 0 & \Sigma_{k_2, k_3} & 0 & 0 & 0 & 0 & 0 & \dots & 0 \\ 0 & \Sigma_{k_3, k_3} & 0 & \Sigma_{k_3, k_4} & 0 & 0 & 0 & & \\ \Sigma_{l_2, l_3} & 0 & \Sigma_{l_3, l_3} & 0 & \Sigma_{l_3, l_4} & 0 & 0 & & \vdots \\ 0 & \Sigma_{l_3, l_4} & 0 & \Sigma_{k_4, k_4} & 0 & \Sigma_{k_4, k_5} & 0 & & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & & 0 & \Sigma_{l_{N-1}, l_N} & 0 & \Sigma_{l_{N-1}, l_{N-1}} & 0 & \Sigma_{l_{N-1}, l_{N-1}} & 0 \\ \vdots & & 0 & 0 & \Sigma_{k_{N-1}, k_N} & 0 & \Sigma_{k_N, k_N} & 0 & \Sigma_{k_N, m} \\ & & 0 & 0 & 0 & \Sigma_{l_{N-1}, l_N} & 0 & \Sigma_{l_N, l_N} & \Sigma_{l_N, m} \\ 0 & \dots & 0 & 0 & 0 & 0 & \Sigma_{k_N, m} & \Sigma_{l_N, m} & \Sigma_{m, m} \end{pmatrix},$$

which is of the same form as  $\Sigma_{\mathbb{K} \setminus \{l_1\}, \mathbb{K} \setminus \{k_1\}}$ . Consequently, a similar calculation shows that

$$\det (\Sigma_{\mathbb{K} \setminus \{l_1, k_1, l_2\}, \mathbb{K} \setminus \{k_1, l_1, k_2\}}) = \Sigma_{k_2, k_3} \Sigma_{l_2, l_3} \det (\Sigma_{\mathbb{K} \setminus \{l_1, k_1, l_2, k_2, l_3\}, \mathbb{K} \setminus \{k_1, l_1, k_2, l_2, k_3\}}),$$

and, by induction, one can hence easily show that, for all  $n \geq 2$ ,

$$\det \left( \Sigma_{\mathbb{K} \setminus \{l_1, k_1, \dots, l_{n-1}, k_{n-1}, l_n\}}, \mathbb{K} \setminus \{k_1, l_1, \dots, k_{n-1}, l_{n-1}, k_n\} \right) = \Sigma_{k_n, k_{n+1}} \Sigma_{l_n, l_{n+1}} \det \left( \Sigma_{\mathbb{K} \setminus \{l_1, k_1, \dots, l_n, k_n, l_{n+1}\}}, \mathbb{K} \setminus \{k_1, l_1, \dots, k_n, l_n, k_{n+1}, l_{n+1}\} \right).$$

We hence obtain that

$$\det \left[ \Sigma_{\mathbb{K} \setminus \{l_1\}}, \mathbb{K} \setminus \{k_1\} \right] = \det \left( \Sigma_{\mathbb{K} \setminus \{l_1, k_1, \dots, k_{N-2}, l_{N-2}, l_{N-1}\}}, \mathbb{K} \setminus \{k_1, l_1, \dots, k_{N-2}, l_{N-2}, k_{N-1}\} \right) \prod_{n=1, \dots, N-2} \Sigma_{k_n, k_{n+1}} \Sigma_{l_n, l_{n+1}},$$

where the matrix whose determinant is calculated is equal to

$$\Sigma_{\mathbb{K} \setminus \{l_1, k_1, \dots, k_{N-2}, l_{N-2}, l_{N-1}\}}, \mathbb{K} \setminus \{k_1, l_1, \dots, k_{N-2}, l_{N-2}, k_{N-1}\} = \Sigma_{\{k_{N-1}, k_N, l_n, m\}, \{l_{N-1}, k_N, l_N, m\}} = \begin{pmatrix} 0 & \Sigma_{k_{N-1}, k_N} & 0 & 0 \\ 0 & \Sigma_{k_N, k_N} & 0 & \Sigma_{k_N, m} \\ \Sigma_{l_{N-1}, l_N} & 0 & \Sigma_{l_N, l_N} & \Sigma_{l_N, m} \\ 0 & \Sigma_{k_N, m} & \Sigma_{l_N, m} & \Sigma_{m, m} \end{pmatrix}.$$

The determinant of this matrix can be obtained by a similar argument as previously developed:

$$\begin{aligned} \det \left( \Sigma_{\{k_{N-1}, k_N, l_n, m\}, \{l_{N-1}, k_N, l_N, m\}} \right) &= -\Sigma_{k_{N-1}, k_N} \begin{vmatrix} 0 & 0 & \Sigma_{k_N, m} \\ \Sigma_{l_{N-1}, l_N} & \Sigma_{l_N, l_N} & \Sigma_{l_N, m} \\ 0 & \Sigma_{l_N, m} & \Sigma_{m, m} \end{vmatrix} \\ &= \Sigma_{k_{N-1}, k_N} \Sigma_{l_{N-1}, l_N} \begin{vmatrix} 0 & \Sigma_{k_N, m} \\ \Sigma_{l_N, m} & \Sigma_{m, m} \end{vmatrix} \\ &= -\Sigma_{k_{N-1}, k_N} \Sigma_{l_{N-1}, l_N} \Sigma_{k_N, m} \Sigma_{l_N, m}. \end{aligned}$$

We finally have

$$\det \left[ \Sigma_{\mathbb{K} \setminus \{l_1\}}, \mathbb{K} \setminus \{k_1\} \right] = \Sigma_{k_N, m} \Sigma_{l_N, m} \prod_{n=1, \dots, N-1} \Sigma_{k_n, k_{n+1}} \Sigma_{l_n, l_{n+1}},$$

and, in conclusion, for  $\mathbb{K} = \{k_1, l_1, \dots, k_N, l_N, m\}$ , we obtain for  $\text{Cov} [x_i, x_j | x_{\mathbb{K}}]$

$$\frac{\Sigma_{i, k_1} \left[ \prod_{n=1, \dots, N-1} \Sigma_{k_n, k_{n+1}} \right] \Sigma_{k_N, m} \cdot \Sigma_{j, l_1} \left[ \prod_{n=1, \dots, N-1} \Sigma_{l_n, l_{n+1}} \right] \Sigma_{l_N, m}}{\det \left[ \Sigma_{\mathbb{K}, \mathbb{K}} \right]} \tag{A.2}$$

The second case is rather similar to the first one. Set  $\mathbb{K} = \{k_1, l_1, \dots, k_{N+1}, l_{N+1}\}$ , with  $N \geq 1$ ,  $k_n \in \mathbb{V}_n^i$  and  $l_n \in \mathbb{V}_n^j$  for  $n = 1 \dots, N + 1$ . The previous line of reasoning can be applied in this case too, except that  $\Sigma_{\mathbb{K} \setminus \{l_1, k_1, \dots, l_{N-1}\}}, \mathbb{K} \setminus \{k_1, l_1, \dots, k_{N-1}\}$  reads

$$\Sigma_{\{k_{N-1}, k_N, l_N, k_{N+1}, l_{N+1}\}, \{l_{N-1}, k_N, l_N, k_{N+1}, l_{N+1}\}} = \begin{pmatrix} 0 & \Sigma_{k_{N-1}, k_N} & 0 & 0 & 0 \\ 0 & \Sigma_{k_N, k_N} & 0 & \Sigma_{k_N, k_{N+1}} & 0 \\ \Sigma_{l_{N-1}, l_N} & 0 & \Sigma_{l_N, l_N} & 0 & \Sigma_{l_N, l_{N+1}} \\ 0 & \Sigma_{k_N, k_{N+1}} & 0 & \Sigma_{k_{N+1}, k_{N+1}} & \Sigma_{k_{N+1}, l_{N+1}} \\ 0 & 0 & \Sigma_{l_N, l_{N+1}} & \Sigma_{k_{N+1}, l_{N+1}} & \Sigma_{l_N, l_N} \end{pmatrix},$$

leading to a determinant of  $\Sigma_{\mathbb{K} \setminus \{l_1, k_1, \dots, l_{N-1}\}}, \mathbb{K} \setminus \{k_1, l_1, \dots, k_{N-1}\}$  equal to

$$\begin{aligned} &= -\Sigma_{k_{N-1}, k_N} \begin{vmatrix} 0 & 0 & \Sigma_{k_N, k_{N+1}} & 0 \\ \Sigma_{l_{N-1}, l_N} & \Sigma_{l_N, l_N} & 0 & \Sigma_{l_N, l_{N+1}} \\ 0 & 0 & \Sigma_{k_{N+1}, k_{N+1}} & \Sigma_{k_{N+1}, l_{N+1}} \\ 0 & \Sigma_{l_N, l_{N+1}} & 0 & \Sigma_{l_N, l_N} \end{vmatrix} \\ &= \Sigma_{k_{N-1}, k_N} \Sigma_{l_{N-1}, l_N} \begin{vmatrix} 0 & \Sigma_{k_N, k_{N+1}} & 0 \\ 0 & \Sigma_{k_{N+1}, k_{N+1}} & \Sigma_{k_{N+1}, l_{N+1}} \\ \Sigma_{l_N, l_{N+1}} & 0 & \Sigma_{l_N, l_N} \end{vmatrix} \end{aligned}$$

$$\begin{aligned}
&= -\Sigma_{k_{N-1}, k_N} \Sigma_{l_{N-1}, l_N} \Sigma_{k_N, k_{N+1}} \begin{vmatrix} 0 & \Sigma_{k_{N+1}, l_{N+1}} \\ \Sigma_{l_N, l_{N+1}} & \Sigma_{l_N, l_N} \end{vmatrix} \\
&= \Sigma_{k_{N-1}, k_N} \Sigma_{l_{N-1}, l_N} \Sigma_{k_N, k_{N+1}} \Sigma_{l_N, l_{N+1}} \Sigma_{k_{N+1}, l_{N+1}}.
\end{aligned}$$

Finally,  $\text{Cov}[x_i, x_j | x_{\mathbb{K}}]$  reads

$$\frac{\Sigma_{i, k_1} \left[ \prod_{n=1, \dots, N} \Sigma_{k_n, k_{n+1}} \right] \cdot \Sigma_{j, l_1} \left[ \prod_{n=1, \dots, N} \Sigma_{l_n, l_{n+1}} \right] \cdot \Sigma_{k_{N+1}, l_{N+1}}}{\det[\Sigma_{\mathbb{K}, \mathbb{K}}]}. \tag{A.3}$$

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