Journal of Computational and Applied Mathematics 453 (2025) 116142

Contents lists available at ScienceDirect

Journal of Computational and Applied Mathematics

journal homepage: www.elsevier.com/locate/cam

Gaussian Markov Random Fields over graphs of paths and high relative accuracy

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ARTICLE INFO

MSC:
15A09
65F05

Keywords:
Gaussian Markov random field
High relative accuracy
Totally positive matrices

ABSTRACT

The present paper presents some results that allow us to perform with High Relative Accuracy linear algebra operations with correlation and covariance matrices of Gaussian Markov Random Fields over graphs of paths. Some numerical experiments are carried out showing the computational benefits of this approach.

1. Introduction

A (discrete-time) Markov Chain [1] is a stochastic model in which the value observed at a certain period of time depends only on the value observed at the previous period of time. Markov Randoms Fields [2] arise in the context of spatio-temporal modelling as a natural generalization of Markov Chains in which the time index is substituted by a graph. In case the joint distribution of a Markov Random Field is multivariate Gaussian, then we are dealing with a Multivariate Gaussian Markov Random Field (GMRF) [3]. All these types of models have been used successfully in a wide range of applications. For instance, one can find GMRFs in disease control [4] and image recognition [5].

From a different perspective, linear algebra operations with covariance matrices are commonplace in statistics. For instance, Principal Component Analysis (PCA) [6] is a popular multivariate technique that can be used with the purpose of data reduction and that is based on the identification of the eigenvalues of the (sample) covariance matrix. As another example, it is quite typical in statistical simulation to generate a random vector in which the components are dependent from another random vector in which the components are independent. Quite conveniently, this latter random vector can be simulated easily (see, e.g., [7]) if the covariance matrix of the former random vector is factorized as the product of a positive semi-definite matrix and its transpose.

In this paper, we explore conditions under which some linear algebra operations with covariance matrices can be carried out with High Relative Accuracy (HRA), meaning that the relative error of the computations is of the order of machine precision. More specifically, we will follow the direction started by Koev [8] and others authors (see, for instance, [9,10]) in which different algorithms for performing linear algebra operations with HRA were presented for nonsingular totally positive matrices, assuming that their bidiagonal factorizations can be obtained with HRA. For this purpose, we bring to the attention the results presented in [11], where different conditions under which the covariance matrix or the inverse of the covariance matrix of a GMRF are totally positive, thus allowing us to use the algorithms proposed by Koev.

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https://doi.org/10.1016/j.cam.2024.116142
Received 31 July 2023; Received in revised form 27 June 2024
Available online 17 July 2024

The remainder of the paper is structured as follows. Firstly, we introduce some basic notions on GMRFs in Section 2 and some auxiliary results on totally positive matrices in Section 3. Section 4 provides the bidiagonal decomposition of a correlation matrix of a GMRF over a graph of paths with natural ordering and provides some results regarding HRA for linear algebra operations with such correlation matrix, whereas these results are extended to covariance matrices in Section 5. Some numerical experiments supporting the use of HRA algorithms over classical ones are shown in Section 6. We end with some conclusions and discussions on future work in Section 7.

2. Gaussian Markov random fields

In probability theory and statistics [12], the covariance matrix of a random vector plays an important role; for instance, in the study of the scale of a multivariate random vector and in the study of the interactions between the components of a multivariate random vector. Formally, given a random vector $\vec{X} = (X_1, \dots, X_n)$ of dimension n, the covariance matrix $\Sigma = (\Sigma_{i,j})_{1\leq i,j\leq n}$ of $\vec{X}$ is defined as:

$$E\left(\left(\vec{X} - E(\vec{X})\right)\left(\vec{X} - E(\vec{X})\right)^T\right),$$

where $E(\cdot)$ denotes the expected value vector of a random vector. The entries of the covariance matrix Σ are thus such that, for any $i, j \in \{1, \dots, n\}$:

$$\Sigma_{i,j} = \mathrm{Cov}(X_i, X_j) = E(X_i\, X_j) - E(X_i)\, E(X_j).$$

The covariance matrix is always symmetric and positive semi-definite [13]. Formally, an $n \times n$ matrix $M = (M_{i,j})_{1\leq i,j\leq n}$ is called symmetric if $M_{i,j} = M_{j,i}$, for any $i, j \in \{1, \dots, n\}$. An $n \times n$ symmetric (real) matrix is called positive semi-definite if $\mathbf{x}^T M \mathbf{x} \geq 0$, for any $\mathbf{x} \in \mathbb{R}^n$.

In some cases, the scales of the components of the multivariate random distribution are not of interest and we only want to study the interaction between said components. In such case, we are only interested in the so-called correlation matrix, which is the matrix resulting from rescaling the covariance matrix such that all its diagonal entries are equal to one. Formally, the correlation matrix $S = (S_{i,j})_{1\leq i,j\leq n}$ of the random vector $\vec{X}$ is defined as:

$$S = A^{-1}\, \Sigma A^{-1},$$

where $A = (A_{i,j})_{1\leq i,j\leq n}$ is the diagonal matrix such that $A_{i,i} = \sqrt{\Sigma_{i,i}}$, for any $i \in \{1, \dots, n\}$. As a result, the entries of the correlation matrix S are such that, for any $i, j \in \{1, \dots, n\}$:

$$S_{i,j} = \frac{\Sigma_{i,j}}{\sqrt{\Sigma_{i,i}\, \Sigma_{j,j}}}.$$

The value $S_{i,j}$ is oftentimes referred to as Pearson's correlation coefficient between X_i and X_j.

Covariance and correlation matrices are very important in a particular type of random vectors: Gaussian random vectors. In particular, Gaussian random vectors are parameterized by a mean vector $\vec{\mu}$ and a covariance matrix Σ, resulting in the following probability density function [12]:

$$f(\vec{x}) = \frac{1}{\sqrt{(2\pi)^n |\Sigma|}} \exp\left(-\frac{(\vec{x} - \vec{\mu})^T \Sigma^{-1} (\vec{x} - \vec{\mu})}{2}\right),$$

for any $\vec{x} \in \mathbb{R}^n$.

Linear algebra operations with covariance and correlation matrices are used in many practical applications [14–16]. Therefore, the development of efficient and accurate numerical methods to deal with the computation of eigenvalues and the inverse matrix is of key interest to the field of statistics. In this direction, GMRFs are a particular type of multivariate Gaussian distribution in which the dependence structure is linked to a simple undirected graph and for which such efficient and accurate numerical methods may be developed under some circumstances that will be discussed later on in the present manuscript.

We recall that a simple undirected graph $G = (V, E)$ (see [17]) is a couple formed by a finite set V, called the set of nodes, and a set E of subsets of V, each of these subsets being of cardinality 2, called the set of edges. If $\{i, j\} \in E$, the nodes i and j are said to be adjacent. The degree of incidence of a node $i \in V$ is the number of nodes that are adjacent to i. A graph is said to be connected if, given any two nodes, there exists a sequence of adjacent nodes that starts in one of the nodes and ends in the other one. A subset of nodes is said to be a connected component if every two nodes in the subset are connected and the subset is maximal with respect to this property [17]. A path graph is a graph in which any connected component consists of a unique node or has two nodes with degree of incidence 1 and the rest have degree of incidence 2.

A GMRF over a graph $G = (V, E)$ is a Gaussian random vector $\vec{X}$ for which each component of the vector is associated with a node in V and such that, if $\{i, j\} \notin E$ with $i \neq j$, then X_i and X_j are conditionally independent given the value of all other variables [3]. From an algebraic point of view, a GMRF can be characterized by zeros in the inverse of the covariance matrix, as formalized in the following key theorem [18].

Theorem 2.1. *Let $G = (V, E)$ be a graph with $V = \{1, 2, \dots, n\}$ and $\vec{X}$ be a random vector with multivariate Gaussian distribution and covariance matrix Σ. It holds that $\vec{X}$ is a GMRF over G if and only if:*

$$\{i, j\} \notin E \quad \Longrightarrow \quad \left(\Sigma^{-1}\right)_{i,j} = 0.$$

As discussed in [3], computations concerning GMRFs become simpler when the inverse of the covariance matrix is sparse, i.e., most of its entries are zero. In this direction, throughout this paper we will deal with GMRFs over a graph of paths with natural ordering [11], which are a type of GMRF with a very sparse inverse covariance matrix.

Definition 2.1. Let $G = (V, E)$ with $V = \{1, \dots, n\}$ be a graph such that any connected component is a path graph. If for any $i, j \in V$ with $i < j$ and $\{i, j\} \in E$ it holds that $j - i = 1$, then G is called a graph of paths with natural ordering.

As discussed in [11], there is a close connection between GMRFs over a graph of paths with natural ordering and a prominent type of matrices called totally positive matrices. The following section is dedicated to recalling some auxiliary results on totally positive matrices.

3. Auxiliary results on totally positive matrices

A minor of a matrix A of dimension $n \times n$ is the determinant of a submatrix of A. In particular, the minor of A associated with the indices $\{i_1, \dots, i_k\}$ and $\{j_1, \dots, j_k\}$, denoted by $A_{\{i_1,\dots,i_k\},\{j_1,\dots,j_k\}}$, is the determinant of the $k \times k$ submatrix of A containing the rows associated with the indices $i_1, \dots, i_k$ and the columns associated with the indices $j_1, \dots, j_k$. A matrix is called nonsingular if its determinant is nonzero and is called totally positive [19,20] if every minor is non-negative. In particular, a nonsingular totally positive matrix is a matrix that is nonsingular and totally positive.

Neville elimination [21] is an alternative procedure to Gaussian elimination that allows us to produce zeros in a column of a matrix by adding to each row an appropriate multiple of the previous one. When performing Neville elimination, one may need to permute some of the rows and columns of the matrix. Interestingly, when dealing with nonsingular totally positive matrices, it is not necessary to permute rows or columns [21], therefore we will simply ignore the permutation of rows and columns when explaining the Neville elimination procedure right after.

For a nonsingular totally positive matrix, $T = (T_{i,j})_{1 \le i,j \le n}$, the Neville elimination leads to a sequence of matrices:

$$T = T^{(1)} \to T^{(2)} \to \cdots \to T^{(n)} = U,$$

where $U = (U_{i,j})_{1 \le i,j \le n}$ is an upper triangular matrix. Formally, the matrix $T^{(k+1)} = \left(T_{i,j}^{(k+1)}\right)_{1 \le i,j \le n}$ can be obtained from $T^{(k)} = \left(T_{i,j}^{(k)}\right)_{1 \le i,j \le n}$ as follows [21]:

$$T_{i,j}^{(k+1)} = \begin{cases} T_{i,j}^{(k)} - \dfrac{T_{i,k}^{(k)}}{T_{i-1,k}^{(k)}} T_{i-1,j}^{(k)}, & \text{if } k+1 \le i \le n,\ k \le j \le n \text{ and } T_{i-1,k}^{(k)} \neq 0, \\ T_{i,j}^{(k)}, & \text{otherwise.} \end{cases}$$

This procedure can be expressed as a product of matrices $E_i(\alpha)$, with $2 \le i \le n$, which have all the diagonal entries equal to 1, the $(i, i-1)$-entry equal to α and the rest of its entries equal to 0 (see [22]). It is also important to notice that $E_i(\alpha)^{-1} = E_i(-\alpha)$.

The quantities $p_{ij} = T_{i,j}^{(j)}$ are referred to as the pivots of the Neville elimination [21]. The multipliers m_{ij} $(1 \le j < i \le n)$ of the Neville elimination are defined as follows [21]:

$$m_{i,j} = \begin{cases} \dfrac{T_{i,j}^{(j)}}{T_{i-1,j}^{(j)}} = \dfrac{p_{i,j}}{p_{i-1,j}}, & \text{if } p_{i-1,j} \neq 0, \\ 0, & \text{otherwise.} \end{cases} \tag{1}$$

We finish the section by introducing the notion of complete Neville elimination of an $n \times n$ matrix T (see [21]). This procedure consists of firstly performing Neville elimination of T until one obtains the upper triangular matrix U, and, subsequently, performing the Neville elimination of U^T (the transpose of U). This procedure leads to a diagonal matrix $D = (D_{i,j})_{1 \le i,j \le n}$. The multipliers associated with the Neville elimination of U^T will be denoted as $\tilde{m}_{i,j}$. As discussed in page 116 of [23], these multipliers $\tilde{m}_{i,j}$ coincide with the multipliers obtained when performing the Neville elimination of T^T. As a result, if the initial matrix is symmetric, it then holds that

$$m_{i,j} = \tilde{m}_{i,j}, \quad 1 \le j < i \le n. \tag{2}$$

Remark 3.1. Observe that, when the complete Neville elimination is performed, the diagonal entries of U coincide with the diagonal entries of D, that is, $U_{i,i} = D_{i,i}$ with $i \in \{1, \dots, n\}$.

The following result is a straightforward consequence of Eqs. (1) and (2) and of Theorem 3.1 in [21].

Theorem 3.1. *A symmetric matrix T is nonsingular totally positive if and only if the complete Neville elimination of T can be performed without rows or columns exchanges, the diagonal pivots of the Neville elimination of T are positive and the multipliers of the Neville elimination of T are non-negative.*

From Eq. (2) and Theorem 4.2 in [23], the following result holds.

Theorem 3.2. *Any symmetric nonsingular totally positive matrix T admits a bidiagonal decomposition of the form:*

$$T = F_{n-1} \dots F_1 D F_1^T \dots F_{n-1}^T, \tag{3}$$

where D is a diagonal matrix with positive diagonal entries $D_{i,i} = p_{i,i}$, with $i \in \{1, \dots, n\}$, and each F_i has the following structure:

$$F_i = \begin{pmatrix} 1 & & & & & & & \\ 0 & 1 & & & & & & \\ & \ddots & \ddots & & & & & \\ & & 0 & 1 & & & & \\ & & & m_{i+1,1} & 1 & & & \\ & & & & \ddots & \ddots & & \\ & & & & & m_{n,n-i} & 1 \end{pmatrix},$$

where $p_{i,i}$ are the diagonal pivots of the Neville elimination of T, and $m_{i,j}$ are the multipliers of the Neville elimination of T.

Bearing in mind the results of [24] concerning the bidiagonal decomposition of a matrix, the following notation is introduced.

Definition 3.1. Let T be a symmetric nonsingular totally positive matrix expressed as the product $T = F_{n-1} \dots F_1 D F_1^T \dots F_{n-1}^T$ given in Theorem 3.2. The bidiagonal decomposition of T, denoted as $BD(T)$, is the $n \times n$ matrix defined as:

$$BD(T)_{i,j} = \begin{cases} m_{i,j}, & \text{if } i > j, \\ m_{j,i}, & \text{if } i < j, \\ p_{i,i}, & \text{if } j = i. \end{cases}$$

4. High relative accuracy and the correlation matrix of a Gaussian Markov random field over a graph of paths with natural ordering

In this section, we provide the bidiagonal decomposition of the correlation matrix associated with an n-dimensional GMRF over a graph of paths with natural ordering. Next, we show that, under certain conditions (namely non-negative/non-positive correlations between adjacent variables), several operations related to the correlation matrix may be carried out with HRA. We recall that HRA means that the relative errors of the computations are of the order of machine precision, independently of the size of the matrix condition number.

4.1. Bidiagonal decomposition of the correlation matrix of a Gaussian Markov random field over a graph of paths with natural ordering

The following result (see [25]) describes the entries of a correlation matrix over a graph of paths with natural ordering.

Lemma 4.1. *Let $\vec{X}$ be an n-dimensional GMRF over a graph of paths with natural ordering. Given Pearson's correlation coefficients between adjacent variables, denoted by $\rho_{1,2}, \dots, \rho_{n-1,n}$, the correlation matrix $S = (S_{i,j})_{1 \le i,j \le n}$ is obtained as follows:*

$$S_{i,j} = S_{j,i} = \prod_{k=j}^{i-1} \rho_{k,k+1},$$

for any $i, j \in \{1 \dots, n\}$ such that $i \ge j$.

Remark 4.1. Since 1 is the identity element for multiplication, the product of the elements of an empty set is always 1, thus $\prod_{k=k_1}^{k_2} \rho_{k,k+1} = 1$ if $k_2 < k_1$.

The next theorem provides the bidiagonal decomposition of the correlation matrix of a GMRF over a graph of paths with natural ordering.

Theorem 4.1. *Let $\vec{X}$ be an n-dimensional GMRF over a graph of paths with natural ordering. Given Pearson's correlation coefficients between adjacent variables, denoted by $\rho_{1,2}, \dots, \rho_{n-1,n}$, the bidiagonal decomposition $BD(S)_{1 \le i,j \le n}$ of the correlation matrix $S = (S_{i,j})_{1 \le i,j \le n}$ is the following:*

$$BD(S)_{i,j} = \begin{cases} 1, & \text{if } i = j = 1, \\ 1 - \rho_{i-1,i}^2, & \text{if } i = j > 1, \\ \rho_{i-1,i}, & \text{if } j = 1 \text{ and } i > 1, \\ \rho_{j-1,j}, & \text{if } i = 1 \text{ and } j > 1, \\ 0, & \text{else.} \end{cases}$$

Proof. Let us obtain the bidiagonal decomposition in the form of Eq. (3) by performing Neville elimination. We will make zeros below the main diagonal, starting from the last row.

From Lemma 4.1, it follows that $S_{n,j}$, with $j < n$, is such that:

$$S_{n,j} = \prod_{k=j}^{n-1} \rho_{k,k+1} = \rho_{n-1,n} \prod_{k=j}^{n-2} \rho_{k,k+1} = \rho_{n-1,n}\, S_{n-1,j}.$$

Therefore, it is clear that the entries below the diagonal that are located in the last row can be vanished by subtracting to the last row the $(n-1)$th row multiplied by $m_{n,1} = \rho_{n-1,n}$ (see Eq. (1)).

This procedure can be repeated $n-1$ times, subtracting to the ith row, the $(i-1)$th row multiplied by $m_{i,1} = \rho_{i-1,i}$ in the order $i = n, \dots, 2$. Each step corresponds to a matrix $E_i(-\rho_{i-1,i})$.

In this way, we have obtained an upper triangular matrix U that can be expressed as

$$U = S^{(n)} = S^{(2)} = \left(\prod_{i=2}^{n} E_i(-\rho_{i-1,1}) \right) S^{(1)} = \left(\prod_{i=2}^{n} E_i(-\rho_{i-1,1}) \right) S\,. \tag{4}$$

Note that $m_{i,j} = 0$ for any $2 \le j < i < n$.

The matrix U satisfies that $U_{1,j} = S_{1,j}$, for any $j \in \{1, \dots, n\}$. In addition, $U_{i,j} = S_{i,j} - \rho_{i-1,i} S_{i-1,j}$ if $1 < i \le j \le n$.

Next, the Neville elimination of U^T is carried out, obtaining at the end of the process a diagonal matrix $D = (D_{i,j})_{1 \le i,j \le n}$.

Note that the diagonal entries of D coincide with the diagonal entries of U (see Remark 3.1). These values are the following ones:

$$D_{1,1} = U_{1,1} = S_{1,1} = 1\,,$$
$$D_{i,i} = U_{i,i} = S_{i,i} - \rho_{i-1,i} S_{i-1,i} = 1 - \rho_{i-1,i}^2\,,$$

for any $i \in \{2, \dots, n\}$.

Taking into account the previous results and Eq. (4), we obtain:

$$\prod_{i=2}^{n} E_i(-\rho_{i-1,1}) S \prod_{i=2}^{n} E_{n-i+2}(-\rho_{i-1,1})^T = D.$$

In conclusion, and considering that $E_i(-\rho_{i-1,1})^{-1} = E_i(\rho_{i-1,1})$, we have the bidiagonal decomposition of matrix S in the form of Eq. (3), as follows:

$$S = \prod_{i=2}^{n} E_i(\rho_{i-1,1}) D \prod_{i=2}^{n} E_{n-i+2}(\rho_{i-1,1})^T.$$

Finally, we just need to use Definition 3.1 to obtain $BD(S)$ and the proof is complete. □

Remark 4.2. In fact, the bidiagonal decomposition of S has the following form:

$$BD(S) = \begin{pmatrix} 1 & \vec{v}^T \\ \vec{v} & D \end{pmatrix}$$

where $\vec{v} = (\rho_{1,2}, \dots, \rho_{n-1,n})$ and D is a diagonal matrix fulfilling $D_{i,i} = 1 - \rho_{i,i+1}^2$ for any $i \in \{1, \dots, n-1\}$.

In the following, we provide a simple example of the bidiagonal decomposition of a correlation matrix.

Example 4.1. Consider the case $n = 3$, in which the correlation matrix has the following structure:

$$S = \begin{pmatrix} 1 & \rho_{1,2} & \rho_{1,2}\rho_{2,3} \\ \rho_{1,2} & 1 & \rho_{2,3} \\ \rho_{1,2}\rho_{2,3} & \rho_{2,3} & 1 \end{pmatrix}.$$

The procedure detailed in the proof of Theorem 4.1 is the following.

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -\rho_{2,3} & 1 \end{pmatrix} \begin{pmatrix} 1 & \rho_{1,2} & \rho_{1,2}\rho_{2,3} \\ \rho_{1,2} & 1 & \rho_{2,3} \\ \rho_{1,2}\rho_{2,3} & \rho_{2,3} & 1 \end{pmatrix} = \begin{pmatrix} 1 & \rho_{1,2} & \rho_{1,2}\rho_{2,3} \\ \rho_{1,2} & 1 & \rho_{2,3} \\ 0 & 0 & 1 - \rho_{2,3}^2 \end{pmatrix},$$

$$\begin{pmatrix} 1 & 0 & 0 \\ -\rho_{1,2} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -\rho_{2,3} & 1 \end{pmatrix} \begin{pmatrix} 1 & \rho_{1,2} & \rho_{1,2}\rho_{2,3} \\ \rho_{1,2} & 1 & \rho_{2,3} \\ \rho_{1,2}\rho_{2,3} & \rho_{2,3} & 1 \end{pmatrix} = \begin{pmatrix} 1 & \rho_{1,2} & \rho_{1,2}\rho_{2,3} \\ 0 & 1 - \rho_{1,2}^2 & \rho_{2,3}(1 - \rho_{1,2}^2) \\ 0 & 0 & 1 - \rho_{2,3}^2 \end{pmatrix} =: U\,.$$

Next, we carry out the Neville elimination of U^T or, equivalently, the Neville elimination of U by columns.

$$U \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & -\rho_{2,3} \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & \rho_{1,2} & 0 \\ 0 & 1 - \rho_{1,2}^2 & 0 \\ 0 & 0 & 1 - \rho_{2,3}^2 \end{pmatrix},$$

$$U\begin{pmatrix}1&0&0\\0&1&-\rho_{2,3}\\0&0&1\end{pmatrix}\begin{pmatrix}1&-\rho_{1,2}&0\\0&1&0\\0&0&1\end{pmatrix}=\begin{pmatrix}1&0&0\\0&1-\rho_{1,2}^2&0\\0&0&1-\rho_{2,3}^2\end{pmatrix}=:D\,.$$

In summary, we can write:

$$S=\begin{pmatrix}1&0&0\\0&1&0\\0&\rho_{2,3}&1\end{pmatrix}\begin{pmatrix}1&0&0\\\rho_{1,2}&1&0\\0&0&1\end{pmatrix}\begin{pmatrix}1&0&0\\0&1-\rho_{1,2}^2&0\\0&0&1-\rho_{2,3}^2\end{pmatrix}\begin{pmatrix}1&\rho_{1,2}&0\\0&1&0\\0&0&1\end{pmatrix}\begin{pmatrix}1&0&0\\0&1&\rho_{2,3}\\0&0&1\end{pmatrix}.$$

Therefore, the bidiagonal decomposition of S is as follows:

$$BD(S)=\begin{pmatrix}1&\rho_{1,2}&\rho_{2,3}\\\rho_{1,2}&1-\rho_{1,2}^2&0\\\rho_{2,3}&0&1-\rho_{2,3}^2\end{pmatrix}.$$

4.2. The case of non-negative Pearson's correlation coefficients between adjacent variables

As a result of Theorem 4.1, a necessary and sufficient condition for the correlation matrix of a GMRF over a graph of paths with natural ordering to be totally positive is that all Pearson's correlation coefficients between adjacent variables are non-negative. This result was already proven in Theorem 3.1 in [11].

Theorem 4.2. *Let $\vec{X}$ be an n-dimensional GMRF over a graph of paths with natural ordering. The correlation matrix is totally positive if and only if all Pearson's correlation coefficients between adjacent variables are non-negative.*

A sufficient condition to guarantee that we can perform an algorithm with HRA is the condition of No Inaccurate Cancellation (NIC) (see [26]). An algorithm fulfils the NIC condition if it does not subtract non-initial data. Note that operations such as sums of numbers of the same sign, multiplications, divisions, subtractions of initial data and even square roots may be used (see page 89 of [26]).

The following theorem shows that, under the hypotheses of Theorem 4.2, many linear algebra operations can be performed with the corresponding correlation matrices with HRA. These linear algebra operations include the calculation of the eigenvalues of a correlation matrix (which coincide with the singular values because a correlation matrix is symmetric).

Theorem 4.3. *Let $\vec{X}$ be an n-dimensional GMRF over a graph of paths with natural ordering. If the correlation matrix S is nonsingular, all Pearson's correlation coefficients between adjacent variables are non-negative, then $BD(S)$ can be computed with HRA, as well as the eigenvalues of S, the inverse of S and the solution of the linear system of equations ($S\vec{x}=\vec{b}$), with vector $\vec{b}$ with alternate signs ($b_ib_{i+1}\leq 0$ for any $i\in\{1,\dots,n-1\}$).*

Proof. If Pearson's correlation coefficients between adjacent variables $\rho_{i,i+1}$ ($1\leq i\leq n-1$) are non-negative, it follows from Theorem 4.2 that the correlation matrix S is totally positive. Using the equality $1-x^2=(1+x)(1-x)$, all the elements of the bidiagonal decomposition given by Theorem 4.1, are given by sums, products and subtractions of initial data, therefore we know the $BD(S)$ to HRA. Since S is also nonsingular, the algorithms proposed in [8] and the algorithm TNInverseExpand in [10] (to compute S^{-1}) obtain with HRA the eigenvalues of S, the inverse S^{-1} of S and also the solution of the linear system of equations ($S\vec{x}=\vec{b}$), with vector $\vec{b}$ with alternate signs. □

The previous result requires that the correlation matrix S is nonsingular. Considering the bidiagonal decomposition of S given in Theorem 4.1, we have that the nonsingularity of S depends on the nonsingularity of the diagonal matrix D, where the diagonal entries are 1 (if $i=1$) and $1-\rho_{i-1,i}^2$ (if $i\in\{2,\dots,n\}$). Therefore, S (or, equivalently, D) is nonsingular if and only if $|\rho_{i-1,i}|<1$, for any $i\in\{2,\dots,n\}$.

Remark 4.3. In the proof of Theorem 4.1, when performing an elementary step of Neville elimination to produce a zero entry in the first column, all entries of its row to the left of the diagonal entry also become null. Therefore, making zeros in the first column already transforms the matrix into an upper triangular matrix. In consequence, this process of obtaining the bidiagonal decomposition of an $n\times n$ correlation matrix can be performed in $O(n^2)$ elementary operations.

4.3. The case of non-positive Pearson's correlation coefficients between adjacent variables

In this subsection, we study the case in which Pearson's correlation coefficients between adjacent variables are non-positive, in contrast to the case studied in the previous section in which these coefficients were non-negative. As discussed in Theorem 3.1 in [11], the fact that all correlations between adjacent variables of a GMRF over a graph of paths with natural ordering are non-positive is a necessary and sufficient condition for assuring that the inverse of the correlation matrix is totally positive (rather than the correlation matrix itself, as in the case of non-negative correlations).

Proposition 4.1. *Let $\vec{X}$ be an n-dimensional GMRF over a graph of paths with natural ordering. The inverse of the correlation matrix is totally positive if and only if all Pearson's correlation coefficients between adjacent variables are non-positive.*

We shall take advantage of the previous result by using $BD((S^{-1})^{\#})$ in order to compute with HRA the eigenvalues of S. For that purpose, we firstly need to introduce the concept of conversion of a matrix (see page 171 of [19]).

Definition 4.1. Given an $n\times n$ matrix $A=(A_{i,j})_{1\leq i,j\leq n}$, the conversion of matrix A, denoted by $A^{\#}$, is the matrix whose entries $A^{\#}_{i,j}$ are given by $A_{n-i+1,n-j+1}$, with $i,j\in\{1,\dots,n\}$.

Interestingly, the conversion of a given matrix can be obtained by using the backward identity matrix. Let P_n be the $n\times n$ backward identity matrix, whose entry at the ith row and jth column, with $i,j\in\{1,\dots,n\}$, is defined as:

$$\begin{cases} 1, & \text{if } i+j=n+1,\\ 0, & \text{otherwise}. \end{cases}$$

It holds that $A^{\#}=P_nAP_n$.

Note that left-multiplication of an $n\times n$ matrix A by the backward identity matrix P_n is equivalent to reordering the rows of A such that the kth row in A becomes the $(n-k+1)$th row in P_nA. An analogous result, but reordering the columns of A rather than the rows, follows when we consider the right-multiplication of A by the backward identity matrix P_n, where the kth column in A becomes the $(n-k+1)$th column in AP_n.

Theorem 4.4. *Let $\vec{X}$ be an n-dimensional GMRF over a graph of paths with natural ordering. If the correlation matrix S is nonsingular, all Pearson's correlation coefficients between adjacent variables are non-positive, then $BD(S)$ can be computed with HRA, as well as the eigenvalues of S.*

Proof. Using the equality $1-x^2=(1+x)(1-x)$, all the elements of the bidiagonal decomposition given by Theorem 4.1, are given by sums, products and subtractions of initial data, therefore we know the $BD(S)$ to HRA. In fact, $BD(S)$ also gives the LDU factorization (with L a lower triangular matrix with unit diagonal, D a nonsingular diagonal matrix and U an upper triangular matrix with unit diagonal) of the nonsingular matrix S because, by the uniqueness of the LDU factorization of a nonsingular matrix, if we know its bidiagonal decomposition in the form of Eq. (3), then we have $L=F_{n-1}\dots F_1$ and $U=L^T$.

Since S^{-1} is the inverse of the correlation matrix of a GMRF over a graph of paths with natural ordering, it is tridiagonal (see Definition 2.7 and Remark 3.1 in [11]). Therefore, the LDU factorization of S^{-1} satisfies that the lower and upper triangular matrices of the factorization are bidiagonal and that $U=L^T$. Clearly, the same property holds for $(S^{-1})^{\#}$.

Taking into account that $(P_n)^{-1}=P_n$, $(AB)^{\#}=A^{\#}B^{\#}$ and since $S=LDL^T$, we can write

$$\begin{aligned}(S^{-1})^{\#} &= ((LDL^T)^{-1})^{\#}\\ &= ((L^T)^{-1})^{\#}(D^{-1})^{\#}(L^{-1})^{\#}\\ &= \tilde{L}\tilde{D}\tilde{L}^T,\end{aligned}\tag{5}$$

where $\tilde{L}=(U^{-1})^{\#}$ is the bidiagonal lower triangular matrix with unit diagonal and $\tilde{D}=(D^{-1})^{\#}$ is the nonsingular diagonal matrix of the LDU factorization of $(S^{-1})^{\#}$. Observe that $\tilde{L}\tilde{D}\tilde{L}^T$ also gives the bidiagonal decomposition of $(S^{-1})^{\#}$ in the form of Eq. (3).

Therefore, we have a bidiagonal decomposition of $(S^{-1})^{\#}$. By Proposition 4.1, S^{-1} is totally positive, and, therefore, $(S^{-1})^{\#}$ is also totally positive. In fact, the off-diagonal entries of the bidiagonal matrix $(L^{-1})^{\#}$ are the numbers opposite in sign to Pearson's correlation coefficients, and, therefore, are non-negative. Therefore, we have $BD((S^{-1})^{\#})$ with HRA and so the algorithm proposed in [8] computes the eigenvalues of $(S^{-1})^{\#}$ to HRA. Note that S^{-1} and $(S^{-1})^{\#}$ have the same eigenvalues, because they are similar matrices. Therefore, we know the eigenvalues of S^{-1} to HRA and also the eigenvalues of S, which are their inverses. □

Remark 4.4. Under the hypotheses of Theorem 4.4 we can also assure HRA for calculating the inverse S^{-1} and for solving a linear system of equations ($S\vec{x}=\vec{b}$), with vector $\vec{b}$ with constant sign ($b_ib_{i+1}\geq 0$ for any $i\in\{1,\dots,n-1\}$). In fact, the proof of Theorem 4.4 provides the bidiagonal factorization of $(S^{-1})^{\#}$ in Eq. (5), with all factors non-negative. So we can obtain $(S^{-1})^{\#}=\tilde{L}\tilde{D}\tilde{U}$ without subtractions. Thus we can get S^{-1} from $(S^{-1})^{\#}$ with HRA. Finally, for the system of linear equations $S\vec{x}=\vec{b}$ we obtain $x=S^{-1}\vec{b}$. Since S^{-1} is TP by Proposition 4.1 we can calculate the value $\vec{x}=S^{-1}b$ without subtractions and so with HRA.

5. High relative accuracy and the covariance matrix of a Gaussian Markov random field over a graph of paths with natural ordering

Correlation matrices are widely used in some applications in which the scale of the different components should not be taken into account and only the relations between the components are important. For example, this is the case of Principal Component Analysis (PCA) [6], which is highly influenced by the scale of the different components and, thus, each of the components should be standardized before the application of PCA. However, in statistics, one mostly deals with covariance matrices rather than with correlation matrices. We devote this section to generalize Theorems 4.3 and 4.4 for covariance matrices.

Given a covariance matrix Σ, the associated correlation matrix S is obtained by scaling its rows and columns by multiplying from the left and from the right by a diagonal matrix A with non-negative entries, i.e., $\Sigma=ASA$. Therefore, a covariance matrix is totally positive if and only if the associated correlation matrix is totally positive (see [11]).

Theorem 5.1. *Let $\vec{X}$ be an n-dimensional GMRF over a graph of paths with natural ordering.*

- *The covariance matrix is totally positive if and only if all Pearson's correlation coefficients between adjacent variables are non-negative.*
- *The inverse of the covariance matrix is totally positive if and only if all Pearson's correlation coefficients between adjacent variables are non-positive.*

Moreover, it is possible to link the bidiagonal decomposition of S with the bidiagonal decomposition of Σ quite straightforwardly. For this purpose, we firstly need to proof the following result.

Lemma 5.1. *Let $T = (T_{i,j})_{1\leq i,j\leq n}$ be a matrix that admits the following bidiagonal decomposition $T = L_n \dots L_1 D U_1 \dots U_n$ and $A = (A_{i,j})_{1\leq i,j\leq n}$ be a nonsingular diagonal matrix with non-negative entries. The bidiagonal decomposition of ATA is the following:*

$$ATA = \tilde{L}_n \dots \tilde{L}_1 \tilde{D} \tilde{U}_1 \dots \tilde{U}_n.$$

where $\tilde{D} = ADA$ and, for any $i \in \{1, \dots, n\}$, $\tilde{L}_i = AL_iA^{-1}$ and $\tilde{U}_i = A^{-1}U_iA$.

Proof. Clearly, we have a decomposition of ATA:

$$\begin{aligned}\tilde{L}_n \dots \tilde{L}_1 \tilde{D} \tilde{U}_1 \dots \tilde{U}_n &= \left(AL_nA^{-1}\right) \dots \left(AL_1A^{-1}\right)(ADA)\left(A^{-1}U_1A\right) \dots \left(A^{-1}U_nA\right)\\ &= AL_n \dots L_1 D U_1 \dots U_nA = ATA\,.\end{aligned}$$

In addition, $\left(\tilde{L}_i\right)_{j,k} = \left(L_i\right)_{j,k} \frac{A_{j,j}}{A_{k,k}}$. for any $i, j, k \in \{1, \dots, n\}$, therefore $\tilde{L}_i$ is a lower bidiagonal matrix having null elements in the same positions as L_i and with all diagonal entries equal to 1 for any $i \in \{1, \dots, n\}$. Similarly, $\tilde{U}_i$ is an upper bidiagonal matrix having null elements in the same positions as U_i and with all diagonal entries equal to 1 for any $i \in \{1, \dots, n\}$. Finally, $\tilde{D} = ADA$ is a diagonal matrix with non-negative diagonal entries. Thus, it is concluded that $\tilde{L}_n \dots \tilde{L}_1 \tilde{D} \tilde{U}_1 \dots \tilde{U}_n$ is a bidiagonal decomposition of ATA. □

The latter result is of interest to the present paper when we consider $T = S$ and $ATA = \Sigma$. In such a way, it is possible to extend the results obtained for correlation matrices to covariance matrices.

Theorem 5.2. *Let $\vec{X}$ be an n-dimensional GMRF over a graph of paths with natural ordering. If the covariance matrix Σ is nonsingular, Pearson's correlation coefficients between adjacent variables are of the same sign and $\Sigma_{i,i}$ for all i are given, then the eigenvalues of Σ can be computed with HRA, as well as Σ^{-1}, and the solution of the linear system of equations ($\Sigma\vec{x} = \vec{b}$), with vector $\vec{b}$ with alternate (constant) sign for the case of non-negative (non-positive) Pearson's correlation coefficients.*

Proof. Let S be the correlation matrix such that $\Sigma = ASA$, with A being a nonsingular diagonal matrix with non-negative entries. We separate the case of non-negative and non-positive Pearson's correlation coefficients.

- Non-negative correlations: From Lemma 5.1, the bidiagonal decomposition of Σ can be expressed as:

  $$\Sigma = \left(AL_nA^{-1}\right) \dots \left(AL_1A^{-1}\right)(ADA)\left(A^{-1}U_1A\right) \dots \left(A^{-1}U_nA\right),$$

  where $S = L_n \dots L_1 D U_1 \dots U_n$ is the bidiagonal decomposition of S, which can be computed with HRA due to Theorem 4.3. In addition, the multiplication by a non-negative diagonal matrix can be performed with HRA, thus the bidiagonal decomposition of Σ can be computed with HRA. Therefore, the algorithms proposed in [8] and in [10] compute with HRA the eigenvalues of Σ, Σ^{-1} and also the solution of linear system of equations ($\Sigma x = b$), with vector b with alternate signs.
- Non-positive correlations: The matrix Σ^{-1} is totally positive as a consequence of Lemma 5.1, as well as the matrix $(\Sigma^{-1})^{\#}$. In particular, we can express $(\Sigma^{-1})^{\#}$ as:

  $$\begin{aligned}(\Sigma^{-1})^{\#} &= P_n\Sigma^{-1}P_n = P_nA^{-1}S^{-1}A^{-1}P_n = P_nA^{-1}P_nP_nS^{-1}P_nP_nA^{-1}P_n\\ &= (A^{-1})^{\#}(S^{-1})^{\#}(A^{-1})^{\#}\,.\end{aligned}$$

  The bidiagonal decomposition of $(S^{-1})^{\#}$ can be computed with HRA, as discussed in the proof of Theorem 4.4. Therefore, due to Lemma 5.1 and reasoning in the same manner as in the case of non-negative Pearson's correlation coefficients, the bidiagonal decomposition of $(\Sigma^{-1})^{\#}$ can be performed with HRA. Note that the eigenvalues of $(\Sigma^{-1})^{\#}$ and Σ^{-1} coincide and, therefore, the eigenvalues of Σ can be computed with HRA just by inverting the ones of $(\Sigma^{-1})^{\#}$. For all other computations, it suffices to consider similar arguments as those in Remark 4.4. □

6. Numerical results

The theoretical results presented in the latter sections state that some linear algebra operations such as the computation of eigenvalues or the inversion of the covariance matrix of a GMRF over a path graph with natural ordering and Pearson's correlation coefficients between adjacent variables of the same sign can be computed with HRA. In this section, we present some numerical experiments that compare the routines included in the package `TNTool` [8,24,27] with the ones implemented in Matlab [28].

Table 1
Eigenvalues and relative error of the function `eig` from Matlab and the `TNEigenValues` routine for a covariance matrix of a GMRF over a graph of paths.

λ	e_{Matlab}	e_{HRA}
829.3977282	$6.85358 \cdot 10^{-16}$	$1.37072 \cdot 10^{-16}$
2.305512952	$3.85241 \cdot 10^{-16}$	0
0.475753414	$4.24717 \cdot 10^{-15}$	$2.33361 \cdot 10^{-16}$
0.272038611	$4.08112 \cdot 10^{-16}$	$8.16225 \cdot 10^{-16}$
0.128908647	$2.77752 \cdot 10^{-14}$	0
0.081036698	$3.69907 \cdot 10^{-14}$	$3.42506 \cdot 10^{-16}$
0.05315597	$1.56646 \cdot 10^{-14}$	$3.91615 \cdot 10^{-16}$
0.04047131	$1.11101 \cdot 10^{-13}$	$8.57261 \cdot 10^{-16}$
0.02337366	$2.11222 \cdot 10^{-13}$	$7.4217 \cdot 10^{-16}$
0.021173508	$1.39115 \cdot 10^{-13}$	$3.27716 \cdot 10^{-16}$
0.018288115	$6.20353 \cdot 10^{-14}$	$5.69131 \cdot 10^{-16}$
0.010478701	$1.00156 \cdot 10^{-13}$	$1.65548 \cdot 10^{-16}$
0.007793824	$1.15528 \cdot 10^{-12}$	$2.22577 \cdot 10^{-16}$
0.006356334	$6.95927 \cdot 10^{-15}$	$1.22811 \cdot 10^{-15}$
0.005521986	$2.29957 \cdot 10^{-13}$	$3.14148 \cdot 10^{-16}$
0.005269281	$8.88879 \cdot 10^{-15}$	$4.93822 \cdot 10^{-16}$
0.002673709	$3.50356 \cdot 10^{-14}$	$3.24404 \cdot 10^{-16}$
0.002287389	$6.56004 \cdot 10^{-14}$	$3.79193 \cdot 10^{-16}$
0.001335167	$4.32003 \cdot 10^{-14}$	0
0.000902647	$1.22156 \cdot 10^{-13}$	0

6.1. Computation of eigenvalues

We compare the accuracy in the computation of the eigenvalues made by the `TNEigenValues` routine [27], which computes the eigenvalues starting from the bidiagonal decomposition of a totally positive matrix, and by the conventional eigenvalue algorithm of LAPACK [29] (as implemented by `eig` in Matlab). In particular, both methods are compared with the eigenvalues obtained by MATHEMATICA [30] with 60 significant digits. In all the experiments, Pearson's correlation coefficients close to either 1 or -1 have been considered, since the condition number of the correlation/covariance matrix increases with the absolute value of the coefficients. This behaviour is due to the fact that, if the correlation is strong, the random vector tends to distribute over a one-dimensional axis, implying that all but one eigenvalue of its correlation/covariance matrix are close to 0. It is expected that the behaviour of the usual method of Matlab has a bad relative accuracy when the condition number increases, whereas the `TNEigenValues` routine stills maintain a good relative accuracy.

Firstly, a 20×20 covariance matrix of a GMRF over a graph of paths was generated randomly. The correlation coefficients were selected randomly with uniform distribution over the interval $[0.999, 1)$ and the variances were selected randomly with uniform distribution over the interval $[1, 10]$. The eigenvalues of the generated covariance matrix as well as the relative errors for both Matlab and `TNEigenValues` given are presented in Table 1. As can be seen, the relative errors for the Matlab routine increase for smaller eigenvalues.

We have also compared both procedures for other correlation and covariance matrices of different sizes, considering both non-negative and non-positive correlations between adjacent variables. In Fig. 1, the maximum relative error among all the eigenvalues when $\rho = \pm 0.999$ and n ranges from 10 to 50 is represented. For the cases of covariance matrices, the covariance has been chosen such that $\Sigma_{i,i} = i^2$ with $i \in \{1, \ldots, n\}$. It is shown that the HRA procedure with the routine `TNEigenValues` has a relative error two orders of magnitude smaller than the usual procedure considering the function `eig` from Matlab for all the considered cases. Additional experiments with matrices of dimension 100 led to similar experimental results, without a significant increase of the relative error for the function `eig`. This is mainly because the condition number of the correlation/covariance matrix does not increase greatly as the dimension of the matrix increases. For instance, if $\rho = 0.999$ and the variance is constant, the condition number of the associated matrix is 3.97×10^4 if $n = 20$ and 1.99×10^5 if $n = 100$.

In addition, the maximum relative error among all eigenvalues has been represented with respect to the condition number of the associated matrix. The dimension of the matrix was fixed to 20, and the absolute value of the Pearson's correlation coefficient was chosen among $\rho = 1 - 10^p$ with $p = \{1, \ldots, 9\}$, causing the condition number to increase as p increases. As it can be seen in Fig. 2, increasing the condition number of the matrix makes the relative accuracy of the usual method from Matlab to decrease. On the contrary, computations with HRA always exhibit a small relative error, independently of the condition number of the associated matrix. For instance, in the case of correlation matrices with non-negative correlation coefficients, the relative error of the Matlab function is 3.56×10^{-15} for a condition number of 3.97×10^5, which increases to 1.29×10^{-6} for a condition number of 3.99×10^{10}. The HRA method has, for all the cases, a relative error below 2×10^{-15}.

6.2. Computation of the inverse matrix

We compare the accuracy in the computation of the inverse matrix made by the `TNInverseExpand` routine [27], which computes the inverse matrix given the bidiagonal decomposition of the matrix to invert, and the usual inversion algorithm (as implemented by `inv` in Matlab).

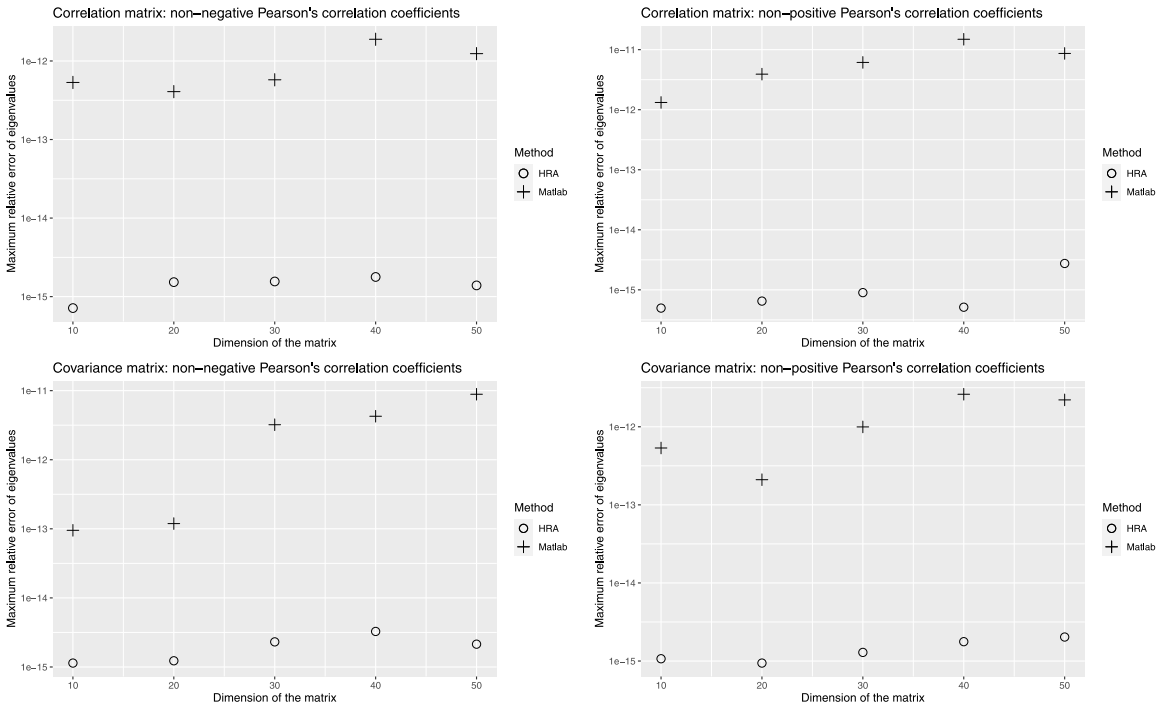

Fig. 1. Maximum relative error in the computation of the eigenvalues by the function `eig` from Matlab and the `TNEigenValues` routine for matrices of different dimension.

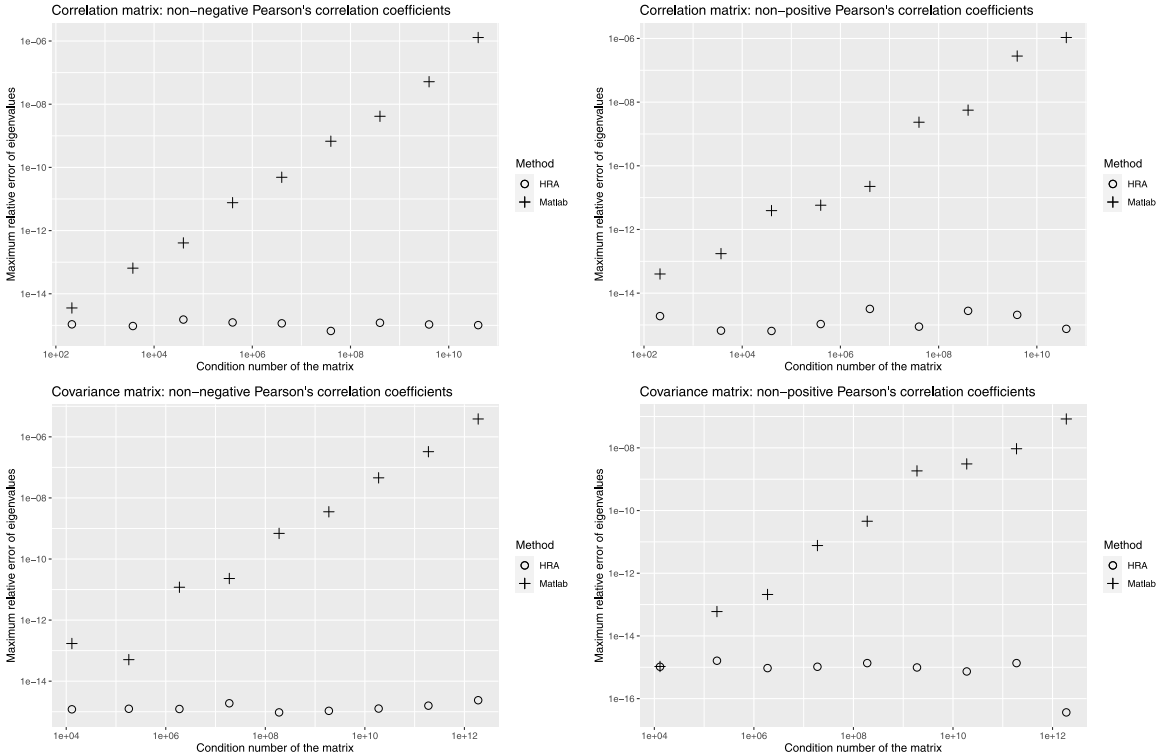

Fig. 2. Maximum relative error in the computation of the eigenvalues by the function `eig` from Matlab and the `TNEigenValues` routine for matrices of different condition number.

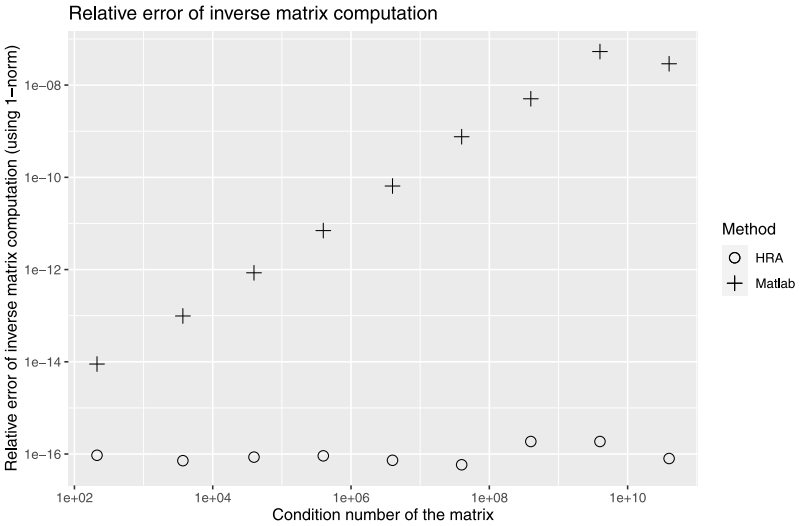

Fig. 3. Relative error in the computation of the inverse matrix by the function `inv` from Matlab and the `TNInverseExpand` routine for matrices of different condition number.

In case all Pearson's correlation coefficients between adjacent nodes are constant, the expression of the exact solution is known, since the correlation matrix coincides with a Kac–Murdock–Szegö matrix [31].

Proposition 6.1 ([31]). *Let S be a matrix defined by $S_{i,j} = \rho^{|i-j|}$ for any $i, j \in \{1, \dots, n\}$, with $\rho \in [-1, 1] \backslash \{0\}$. It follows that S^{-1} is characterized by the following expression.*

- $\left(S^{-1}\right)_{1,1} = \left(S^{-1}\right)_{n,n} = \frac{1}{1-\rho^2}$,
- $\left(S^{-1}\right)_{i,i} = \frac{1+\rho^2}{1-\rho^2}$, *if* $i \in \{2, \dots, n-1\}$,
- $\left(S^{-1}\right)_{i,j} = \left(S^{-1}\right)_{j,i} = \frac{-\rho}{1-\rho^2}$, *if* $i, j \in \{1, \dots, n\}$, *if* $i + 1 = j$,
- $\left(S^{-1}\right)_{i,j} = 0$, *otherwise.*

By considering the latter expression, the inverse matrix of the correlation/covariance matrix of a GMRF over a graph of paths may be obtained with 60 significant digits by using MATHEMATICA. Therefore, the accuracy of both functions `inv` and `TNInverseExpand` may be measured by means of the 1-norm for matrices, defined as $\|A\|_1 = \max_{1 \le j \le n} \sum_{i=1}^{n} |A_{ij}|$. More specifically, the difference of the matrix obtained by using MATHEMATICA and those obtained by using, respectively, the functions `inv` and `TNInverseExpand` needs to be computed.

Setting the dimension of the correlation/covariance matrix to 20 and varying Pearson's correlation coefficient as $\rho = 1 - 10^p$ with $p = \{1, \dots, 9\}$, causing the condition number to increase as p increases, we obtain the relative errors shown in Fig. 3. It can be seen that, as the condition number of the matrix to be inverted increases, the accuracy of the results given by the function `inv` decreases. On the contrary, the results given by the HRA procedure have a smaller relative error, regardless of the condition number of the matrix to be inverted.

7. Conclusions and future work

In this paper, we have presented techniques for performing with HRA some linear algebra operations with correlation/covariance matrices of GMRF over graphs of paths with natural ordering in which the correlations between adjacent variables in the graph were either non-positive or non-negative. It should be borne in mind that all results are immediately extended to GMRF over graphs of paths (not necessarily with natural ordering) by simply reindexing the random vector with respect to a natural ordering.

Future work will aim at generalizing the present results to GMRF over different graphs that admit a totally positive covariance matrix. Unfortunately, in this more general case, a closed-form expression for the bidiagonal decomposition of the correlation/covariance matrix is not yet known.

In addition, another interesting problem is to apply these methods to covariance matrices derived from data. In this direction, it is necessary to construct statistical estimators of distributions that fulfil the conditions given by Theorem 5.2, since they do not exist in the current literature.

Data availability

No data was used for the research described in the article.

Acknowledgements

This research was partially supported through the Spanish research grants PID2022-138569NB-I00 (MCIU/AEI), PID2022-139886NB-I00 (MCIU/AEI), PID2022-140585NB-I00 (MICIU/AEI/10.13039/501100011033 and "FEDER/UE") and RED2022-134176-T (MCI/AEI), Gobierno de Aragón (E41_23R), and Principado de Asturias (Programa Severo Ochoa, BP21042).

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