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RESEARCH ARTICLE

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Total positivity and high relative accuracy for several classes of Hankel matrices

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Summary
Gramian matrices with respect to inner products defined for Hilbert spaces supported on bounded and unbounded intervals are represented through a bidiagonal factorization. It is proved that the considered matrices are strictly totally positive Hankel matrices and their catalecticant determinants are also calculated. Using the proposed representation, the numerical resolution of linear algebra problems with these matrices can be achieved to high relative accuracy. Numerical experiments are provided, and they illustrate the excellent results obtained when applying the theoretical results.

KEYWORDS
bidiagonal decompositions, Gramian matrices, Hankel matrices, high relative accuracy, totally positive matrices

1 | INTRODUCTION

A Hankel matrix (also called catalecticant matrix) is a square matrix, in which each ascending skew-diagonal from left to right is constant. Under certain conditions, Hankel matrices are strictly totally positive, that is, all their minors are positive (cf. sect. 4.6 of Reference 1). The determinant of a Hankel matrix is called Hankel (or catalecticant) determinant. Hankel determinants have important applications in random matrix theory. In Reference 2, Hankel determinants of mass matrices $A = (a_{i,j})_{1\le i,j\le n+1}$, with

$$a_{i,j} = \int_0^\infty t^{i+j-2} u(t)\, dt,$$

are computed asymptotically for weight functions $u(t)$ supported in a semi-infinite interval. For finite intervals, this type of Hankel determinants have been considered in References 3,4.

In Numerical Linear Algebra, Hilbert matrices

$$H_n = \left(\frac{1}{i+j-1}\right)_{1\le i,j\le n}, \quad n \in \mathbb{N},$$

are well-known Hankel matrices. Their inverses and determinants have explicit formulas, however they are very ill-conditioned for moderate values of their dimension. Therefore, they can be used to test numerical algorithms and see how they perform on ill-conditioned or nearly singular matrices. The determinant of the $n \times n$ Hilbert matrix H_n is

$$\det\ H_n = \frac{p_n^4}{p_{2n}}, \quad p_n := \prod_{k=1}^{n-1} k!,$$

(see Reference 5) which goes to zero very quickly as the dimension n increases. In fact, the determinant of H_n is practically zero for $n > 5$ and then, most numerical algorithms would conclude that H_n is singular.

Hilbert matrices can be considered as Gramian (mass) matrices of polynomial monomial bases on $[0, 1]$ and belong to the class of totally positive matrices, whose minors are nonnegative (see References 6,7). Totally positive matrices can be expressed in terms of bidiagonal matrices (see References 8,9). As we shall see in this paper, the mentioned factorization provides an explicit expression for the determinant of totally positive matrices. Furthermore, in References 6,7, this factorization is used to obtain an appropriated representation of Hilbert matrices allowing to derive algorithms to high relative accuracy for the resolution of relevant linear algebra problems, such as the computation of their singular values or inverses. Excellent results have also been obtained when dealing with Gramian matrices of other bases, such as Poisson and Bernstein bases on the interval $[0, 1]$ and bases $\{t^i e^{\lambda t}\}$ (see References 10, 11 and 7, respectively).

During the last years, the design of algorithms adapted to the structure of totally positive matrices, allowing the accurate resolution of linear algebra problems independently of their classical condition numbers has attracted the interest of many researchers (see References 7,10–30). It is very important to achieve algorithms to high relative accuracy because their relative errors will have the order of the machine precision and will not be drastically affected by the dimension or conditioning of the considered matrices. It is well known that algorithms avoiding inaccurate cancelations, that is, requiring the computation of multiplications, divisions, additions of numbers with the same sign, can be performed to high relative accuracy (see p. 52 in Reference 17). Moreover, if the floating-point arithmetic is well-implemented the subtraction of initial data can also be allowed without losing high relative accuracy (see p. 53 in Reference 17).

This paper provides many examples of strictly totally positive Hankel matrices and catalecticant determinants. In turn, these matrices can lead to new strictly totally positive matrices, since in addition to the ordinary product (see theorem 3.1 of Reference 31) the Hadamard product of strictly totally positive Hankel matrices is also a strictly totally positive Hankel matrix (cf. sect. 4.10 of Reference 1). In particular, Gramian matrices of several polynomial and exponential bases with respect to inner products supported on bounded and unbounded intervals are considered. By means of Neville elimination, their total positivity is analyzed and a bidiagonal factorization of the considered matrices and their inverses is derived. Let us observe that the bidiagonal factorization of Gramian matrices can be considered for the accurate resolution of the linear system of normal equations when approximating in the least-squares sense. On the other hand, many degree reduction methods also require an inversion of these matrices, and they will become more efficient if the matrix inverses are explicitly expressed.

In order to make this paper as self-contained as possible, Section 2 recalls basic concepts and results on total positivity, Neville elimination and high relative accuracy that will be crucial to derive factorizations and procedures to achieve computations to high relative accuracy with the considered Gramian matrices. Section 3 focuses on Gramian matrices of monomial bases with respect to several inner products defined on compact intervals. On the other hand, Section 4 deals with fundamental solution sets of differential equations and inner products defined for Hilbert spaces on unbounded intervals. Gramian matrices of even power bases are also analyzed in Section 5. Finally, the performed numerical experimentation is illustrated in Section 6.

2 | BASIC ASPECTS ON TOTAL POSITIVITY, NEVILLE ELIMINATION AND HIGH RELATIVE ACCURACY

Let us suppose that U is an $(n + 1)$-dimensional Hilbert space of functions under an inner product $\langle \cdot, \cdot \rangle$. Given linearly independent functions $v_0, \dots, v_n$ in U, the corresponding Gramian matrix is the symmetric matrix $G = (g_{i,j})_{1 \le i,j \le n+1}$ with

$$g_{i,j} := \langle v_{i-1}, v_{j-1} \rangle, \quad 1 \le i, j \le n + 1.$$

A real value $y \neq 0$ is said to be computed to high relative accuracy (HRA) whenever the obtained $\widetilde{y}$ satisfies

$$\frac{|y-\widetilde{y}|}{|y|} < ku,$$

where u is the unit round-off (or machine precision) and $k > 0$ is a constant, which does not depend on the arithmetic precision.

As explained in the Introduction, bidiagonal factorizations are very useful to achieve computations to high relative accuracy with totally positive matrices. As we are going to see, the Neville elimination provides a representation of this class of matrices that can lead to algorithms with high relative accuracy for the computation of their eigenvalues, singular values or inverses (cf. References 8,9,32).

The essence of the Neville elimination procedure is to make zeros in a column of a given matrix $A \in \mathbb{R}^{(n+1)\times(n+1)}$ by adding to each row an appropriate multiple of the previous one. In every major step, the Neville elimination calculates a matrix $A^{(k+1)}$, $k = 1, 2, \dots, n$, from the matrix $A^{(k)}$, previously obtained, with $A^{(1)} := A$. In more detail, $A^{(k+1)}$ is computed from $A^{(k)}$ according to the following formula

$$a_{i,j}^{(k+1)} := \begin{cases} a_{i,j}^{(k)}, & \text{if } 1 \leq i \leq k, \\ a_{i,j}^{(k)} - \frac{a_{i,k}^{(k)}}{a_{i-1,k}^{(k)}} a_{i-1,j}^{(k)}, & \text{if } k+1 \leq i,j \leq n+1, \text{ and } a_{i-1,j}^{(k)} \neq 0, \\ a_{i,j}^{(k)}, & \text{if } k+1 \leq i \leq n+1, \text{ and } a_{i-1,k}^{(k)} = 0. \end{cases} \tag{1}$$

The process finishes when $U := A^{(n+1)}$ is an upper triangular matrix. The entry

$$p_{i,j} := a_{i,j}^{(j)}, \quad 1 \leq j \leq i \leq n+1, \tag{2}$$

is the (i,j) pivot and $p_{i,i}$ is called the i-th diagonal pivot of the Neville elimination of A. If all the pivots are nonzero, they can be expressed, in terms of minors with consecutive columns, as follows:

$$p_{i,1} = a_{i,1}, \ 1 < i \leq n+1,$$
$$p_{i,j} = \frac{\det A[i-j+1, \dots, i|1, \dots, j]}{\det A[i-j+1, \dots, i-1|1, \dots, j-1]}, \ 1 < j \leq i \leq n+1,$$

(see lemma 2.6 of Reference 32). The Neville elimination of A can be done without row exchanges if all the pivots are nonzero. Then, the value

$$m_{i,j} := a_{i,j}^{(j)}/a_{i-1,j}^{(j)} = p_{i,j}/p_{i-1,j}, \quad 1 \leq j < i \leq n+1, \tag{3}$$

is called the (i,j) multiplier.

The complete Neville elimination of A consists of performing the Neville elimination to obtain the upper triangular matrix $U = A^{(n+1)}$ and next, the Neville elimination of the lower triangular matrix U^T.

A matrix is said to be totally positive or TP if all its minors are nonnegative and strictly totally positive or STP if all its minors are positive (see Reference 31). A given matrix A is STP (resp. nonsingular TP) if and only if its complete Neville elimination can be performed without row and column exchanges, the multipliers of the Neville elimination of A and A^T are positive (resp. nonnegative), and the diagonal pivots of the Neville elimination of A are positive (see theorem 4.1, corollary 5.5 of Reference 32 and the arguments of p. 116 of Reference 9).

In Reference 9, it is shown that a nonsingular totally positive matrix $A \in \mathbb{R}^{(n+1)\times(n+1)}$ can be decomposed as follows,

$$A = F_n F_{n-1} \cdots F_1 D G_1 G_2 \cdots G_n, \tag{4}$$

where $F_i \in \mathbb{R}^{(n+1)\times(n+1)}$ (respectively, $G_i \in \mathbb{R}^{(n+1)\times(n+1)}$), $i = 1, \dots, n$, are the totally positive, lower (respectively, upper) triangular bidiagonal matrices of the following form

$$F_i = \begin{pmatrix} 1 & & & & & \\ & \ddots & & & & \\ & & 1 & & & \\ & & m_{i+1,1} & 1 & & \\ & & & \ddots & \ddots & \\ & & & & m_{n+1,n+1-i} & 1 \end{pmatrix}, \quad G_i^T = \begin{pmatrix} 1 & & & & & \\ & \ddots & & & & \\ & & 1 & & & \\ & & \widetilde{m}_{i+1,1} & 1 & & \\ & & & \ddots & \ddots & \\ & & & & \widetilde{m}_{n+1,n+1-i} & 1 \end{pmatrix}, \tag{5}$$

and D is a diagonal matrix whose diagonal entries are $p_{i,i} > 0, i = 1, \dots, n+1$. The diagonal elements $p_{i,i}$ are the diagonal pivots of the Neville elimination of A. Moreover, the elements $m_{i,j}$ and $\widetilde{m}_{i,j}$ are the multipliers of the Neville elimination of A and A^T, respectively.

The transpose of A is also totally positive and, using the factorization (4), can be written as follows

$$A^T = G_n^T G_{n-1}^T \cdots G_1^T D F_1^T F_2^T \cdots F_n^T.$$

If, in addition, A is symmetric, then we can deduce that $G_i = F_i^T$, $i = 1, \dots, n$, and then

$$A = F_n F_{n-1} \cdots F_1 D F_1^T F_2^T \cdots F_n^T. \tag{6}$$

Using theorem 2.2 of Reference 28, the inverse matrix A^{-1} can also be factorized as product of bidiagonal matrices,

$$A^{-1} = \widehat{G}_1 \widehat{G}_2 \cdots \widehat{G}_n D^{-1} \widehat{F}_n \widehat{F}_{n-1} \cdots \widehat{F}_1, \tag{7}$$

where $\widehat{F}_i \in \mathbb{R}^{(n+1)\times(n+1)}$ (respectively, $\widehat{G}_i \in \mathbb{R}^{(n+1)\times(n+1)}$), $i = 1, \dots, n$, are the lower (respectively, upper) triangular bidiagonal matrices whose off-diagonal entries can also be obtained from the multipliers $m_{i,j}$ and $\widetilde{m}_{i,j}$ of the Neville elimination as follows

$$\widehat{F}_i = \begin{pmatrix} 1 & & & & & \\ & \ddots & & & & \\ & & 1 & & & \\ & & -m_{i+1,i} & 1 & & \\ & & & \ddots & \ddots & \\ & & & & -m_{n+1,i} & 1 \end{pmatrix}, \quad \widehat{G}_i^T = \begin{pmatrix} 1 & & & & & \\ & \ddots & & & & \\ & & 1 & & & \\ & & -\widetilde{m}_{i+1,i} & 1 & & \\ & & & \ddots & \ddots & \\ & & & & -\widetilde{m}_{n+1,i} & 1 \end{pmatrix}. \tag{8}$$

Under certain conditions, the factorizations (4) and (7) are unique and in Reference 12 more general classes of matrices admitting this bidiagonal factorization were obtained. Moreover, the previous bidiagonal decompositions can be represented in a compact matricial form by means of $BD(A) = (BD(A)_{i,j})_{1\le i,j\le n+1}$, with

$$BD(A)_{i,j} := \begin{cases} m_{i,j}, & \text{if } i > j, \\ p_{i,i}, & \text{if } i = j, \\ \widetilde{m}_{j,i}, & \text{if } i < j, \end{cases} \tag{9}$$

(see Reference 19).

If $BD(A)$ can be obtained to high relative accuracy, then the MATLAB functions `TNEigenValues`, `TNSingularValues`, `TNInverseExpand` and `TNSolve` available in the software library `TNTool` in Reference 33 take as input argument $BD(A)$ and compute to high relative accuracy the eigenvalues and singular values of A, the inverse matrix A^{-1} (using the algorithm presented in Reference 28) and even the solution of linear systems $Ax = b$, for vectors b with alternating signs.

The following auxiliary result can easily be proved and will be useful in next sections.

Lemma 1. *Let $\alpha > 0$ and $A \in \mathbb{R}^{(n+1)\times(n+1)}$ be a nonsingular totally positive matrix whose factorization (4) is*

$$A = F_n F_{n-1} \cdots F_1 D G_1 G_2 \cdots G_n.$$

Then, the factorization (4) of the scaled matrix $\tilde{A} := \alpha A$ is

$$\widetilde{A} = F_n F_{n-1} \cdots F_1 \widetilde{D} G_1 G_2 \cdots G_n,$$

where $\widetilde{D} = \alpha D$. Then

$$BD(\widetilde{A})_{i,j} := \begin{cases} BD(A)_{i,j}, & \text{if } i \neq j, \\ \alpha BD(A)_{i,i}, & \text{if } i = j, \end{cases} \tag{10}$$

Proof. The result follows taking into account that $\alpha F_i = F_i \alpha$, $i = 1, \ldots, n$. ■

Let us notice that, taking into account the diagonal and bidiagonal structure of the matrix factors in (4), the determinant of nonsingular totally positive matrices can be expressed as the product of the diagonal pivots of their Neville elimination. This fact is stated in the following result that we shall use in forthcoming sections to derive Hankel (or catalecticant) determinants.

Lemma 2. *Let $A \in \mathbb{R}^{(n+1)\times(n+1)}$ be a nonsingular totally positive matrix. Then,*

$$\det\ A = \prod_{i=1}^{n+1} p_{i,i}, \tag{11}$$

where $p_{i,i}$ are the diagonal pivots of the Neville elimination of A given by (2).

Proof. Let $A = F_n \cdots F_1 D G_1 \cdots G_n$ the factorization (4) of A. Since $\det\ G_i = \det\ F_i = 1$, $i = 1, \ldots, n$, we have $\det\ A = \det\ D = \prod_{i=1}^{n+1} p_{i,i}$. ■

In the following sections we are going to use the following generalization of combinatorial numbers. Given $\alpha \in \mathbb{R}$ and $n \in \mathbb{N}$,

$$\binom{\alpha}{n} := \frac{\alpha(\alpha-1)\cdots(\alpha-n+1)}{n!}, \quad \binom{\alpha}{\alpha-n} := \binom{\alpha}{n}. \tag{12}$$

It can be checked that these combinatorial numbers satisfy the following useful identities

$$\frac{\alpha}{n}\binom{\alpha-1}{n-1} = \binom{\alpha}{n}, \quad \frac{\alpha-n}{n}\binom{\alpha-1}{n-1} = \binom{\alpha-1}{n}, \quad \frac{\alpha}{\alpha-n+1}\binom{\alpha-1}{n-1} = \binom{\alpha}{n-1}. \tag{13}$$

3 | GRAMIAN MATRICES OF MONOMIAL BASES ON COMPACT INTERVALS

Let $\mathbf{P}^n(I)$ be the $(n+1)$-dimensional linear space formed by all polynomials in the variable t defined on a real interval I and whose degree is not greater than n, that is, $\mathbf{P}^n(I) := \text{span}\{1, t, \ldots, t^n\}$, $t \in I$. It is well known that $\mathbf{P}^n([0,1])$ is a Hilbert space under the inner product

$$\langle p, q \rangle := \int_0^1 p(t)q(t)\ dt. \tag{14}$$

The $(n+1)\times(n+1)$ Gramian matrix of the power basis $(1, \ldots, t^n)$ with respect to (14) is:

$$H_{n+1} := \left(\int_0^1 t^{i+j-2}\ dt\right)_{1\le i,j\le n+1} = \left(\frac{1}{i+j-1}\right)_{1\le i,j\le n+1}. \tag{15}$$

The matrix H_{n+1} is called Hilbert matrix. Note that $H_{n+1} = (H_{i,j})_{1\le i,j\le n+1}$ is a Hankel matrix because it has constant values along its antidiagonals, that is,

$$H_{i,j} = H_{i+k,j-k}, \quad k = 1, \ldots ,j-i, \quad i < j.$$

It is well known that Hilbert matrices are strictly totally positive. The factorization (4) of H_{n+1} can be accurately computed in $O(n^2)$ time (see formulae (3.6) of sect. 3 of Reference 19). Moreover, in Reference 7, the pivots and the multipliers of the Neville elimination of H_{n+1} are explicitly derived.

In this section we shall generalize Hilbert matrices, by considering Gramian matrices of monomial bases $(1, \ldots , t^n)$, $n \in \mathbb{N}$, with respect to more general inner products defined on compact intervals.

First, let us generalize (14) by introducing a Chebyshev-type weight $w(t) = t^a(1-t)^b$ as follows

$$\langle u, v\rangle_{a,b} := \int_0^1 t^a(1-t)^b u(t)v(t)\, dt. \tag{16}$$

For any $a, b > -1$, $\mathbf{P}^n([0, 1])$ is a Hilbert space under the inner product (16). The Gramian matrix of $(1, \ldots , t^n)$ with respect to (16) is the symmetric matrix $G_n^{(a,b)} = (G_{i,j}^{(a,b)})_{1\le i,j\le n+1}$, such that

$$G_{i,j}^{(a,b)} := \int_0^1 t^{a+i+j-2}(1-t)^b\, dt = \beta(a+i+j-1, b+1), \quad 1 \le i,j \le n+1, \tag{17}$$

where β is the well-known Euler Beta function. We shall say that the matrix (17) is a Chebyshev Gramian matrix. Note that $G_n^{(a,b)}$ is a Hankel matrix.

The following result provides explicit expressions for the diagonal pivots and multipliers of the Neville elimination of the Chebyshev Gramian matrices and then, their bidiagonal factorization (4). As a consequence, the analysis of their total positivity will also be performed.

Theorem 1. *For any $a, b > -1$, the diagonal pivots and multipliers of the Neville elimination of the Chebyshev Gramian matrix $G_n^{(a,b)}$ in (17) satisfy*

$$p_{1,1} = \beta(a+1, b+1), \quad p_{i+1,i+1} = \frac{i(a+i)(b+i)(a+b+i)}{(a+b+2i)^2(a+b+2i-1)(a+b+2i+1)}\, p_{i,i}, \quad 1 \le i \le n. \tag{18}$$

$$m_{i,j} = \widetilde{m}_{i,j} = \frac{(a+i-1)(a+b+i-1)}{(a+b+i+j-1)(a+b+i+j-2)}, \quad 1 \le j < i \le n+1. \tag{19}$$

Proof. Let $G^{(k)} = (G_{i,j}^{(k)})_{1\le i,j\le n+1}$, $k = 1, \ldots , n+1$, be the matrices obtained after $k-1$ steps of the Neville elimination of $G_n^{(a,b)}$, with $G^{(1)} := G_n^{(a,b)}$. We are going to see that

$$G_{i,j}^{(k)} = \frac{\binom{j-1}{k-1}}{\binom{a+b+i+k-2}{k-1}}\beta(a+i+j-k, b+k), \quad 1 \le i,j \le n+1, \tag{20}$$

by induction on k and considering the generalization of combinatorial numbers (12). For $k = 1$, equality (20) is deduced from (17). Now, let us suppose that (20) holds for some $k \in \{1, \ldots , n\}$. Then, taking into account the following properties of Euler Gamma and Beta functions

$$\beta(x, y) = \frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)}, \quad \Gamma(x+1) = x\Gamma(x), \tag{21}$$

we can write

$$\frac{G_{i,k}^{(k)}}{G_{i-1,k}^{(k)}} = \frac{(a+i-1)(a+b+i-1)}{(a+b+i+k-1)(a+b+i+k-2)}.$$

Note that $G_{i,j}^{(k+1)}$ is obtained as explained in (1) and then,

$$G_{i,j}^{(k+1)} = G_{i,j}^{(k)} - \frac{(a+i-1)(a+b+i-1)}{(a+b+i+k-1)(a+b+i+k-2)} G_{i-1,j}^{(k)}. \tag{22}$$

Now, defining

$$\widetilde{G}_{i,j}^{(k+1)} := \frac{\binom{a+b+i+k-2}{k-1}}{\binom{j-1}{k-1}} G_{i,j}^{(k+1)},$$

and using (13), (20), (21) and (22), the following identities are obtained

$$\begin{aligned}
\widetilde{G}_{i,j}^{(k+1)} &= \beta(a+i+j-k-1, b+k)\left(\frac{a+i+j-k-1}{a+b+i+j-1} - \frac{a+i-1}{a+b+i+k-1}\right) \\
&= \beta(a+i+j-k-1, b+k)\frac{(b+k)(j-k)}{(a+b+i+j-1)(a+b+i+k-1)} \\
&= \frac{(j-k)}{(a+b+i+k-1)}\beta(a+i+j-k-1, b+k+1)
\end{aligned}$$

and, finally,

$$G_{i,j}^{(k+1)} = \frac{\binom{j-1}{k}}{\binom{a+b+i+k-1}{k}} \beta(a+i+j-k-1, b+k+1), \tag{23}$$

confirming formula (20) for $k+1$.

By (2) and (20), the pivots $p_{i,j}$ of the Neville elimination of $G_n^{(a,b)}$ satisfy

$$p_{i,j} = G_{i,j}^{(j)} = \frac{1}{\binom{a+b+i+j-2}{j-1}} \beta(a+i, b+j), \quad 1 \le j \le i \le n+1, \tag{24}$$

and, for $i = j$, we have

$$p_{i,i} = \frac{1}{\binom{a+b+2i-2}{i-1}} \beta(a+i, b+i), \quad i = 1, \dots, n+1. \tag{25}$$

Using (25), it can be checked that

$$p_{1,1} = \beta(a+1, b+1), \quad \frac{p_{i+1,i+1}}{p_{i,i}} = \frac{i(a+i)(b+i)(a+b+i)}{(a+b+2i)^2(a+b+2i-1)(a+b+2i+1)}, \quad i = 1, \dots, n,$$

and so, (18) is confirmed.

Finally, using (3) and (24), the multipliers of the Neville elimination can be written as in (19). Taking into account that $G_n^{(a,b)}$ is a symmetric matrix, we conclude that $\widetilde{m}_{i,j} = m_{i,j}$, $1 \le j < i \le n+1$ (see (6)). ∎

Taking into account formula (25) for the diagonal pivots, we can derive an explicit expression for the Hankel determinant $\det G_n^{(a,b)}$.

Corollary 1. *Let $a, b > -1$ and $G_n^{(a,b)}$ be the Chebyshev Gramian matrix in (17). Then*

$$\det G_n^{(a,b)} = \prod_{i=1}^{n+1} \frac{\beta(a+i, b+i)}{\binom{a+b+2i-2}{i-1}}.$$

Furthermore, a simple inspection of the sign of the pivots and multipliers of the Neville elimination given in Theorem 1, provides the values of a and b guaranteeing the total positivity of Chebyshev Gramian matrices (see Section 2). In addition, (18) can be used in order to find the following sufficient conditions for obtaining the bidiagonal decompositions (and so, the remaining linear algebra calculations) to high relative accuracy.

Corollary 2. *For any $a, b > -1$ such that $a + b > -1$, the Chebyshev Gramian matrix $G_n^{(a,b)}$ in (17) is STP. In addition, if $\Gamma(a+1)$, $\Gamma(b+1)$ and $\Gamma(a+b+2)$ can be evaluated to high relative accuracy, then $G_n^{(a,b)}$ and its inverse matrix can also be computed to high relative accuracy.*

Given a compact interval $I = [t_0, t_1]$, we can also consider the basis $(1, t - t_0, \ldots, (t - t_0)^n)$ of $\mathbf{P}^n(I)$. The following result generalizes Theorem 1, deriving the bidiagonal factorization (4) of the Gramian matrix of this basis, with respect to the inner product defined by

$$\langle u, v\rangle_{a,b} := \int_{t_0}^{t_1} (t - t_0)^a (t_1 - t)^b u(t) v(t)\, dt, \tag{26}$$

with $a, b > -1$ to guarantee integrability.

Theorem 2. *The diagonal pivots and multipliers of the Neville elimination of the Gramian matrix $\widetilde{G}_n^{(a,b)}$ of the basis $(1, t - t_0, \ldots, (t - t_0)^n)$ with respect to the inner product (26) satisfy*

$$\begin{aligned} p_{1,1} &= (t_1 - t_0)^{a+b+1} \beta(a+1, b+1),\\ p_{i+1,i+1} &= (t_1 - t_0)^2 \frac{i(a+i)(b+i)(a+b+i)}{(a+b+2i)^2(a+b+2i-1)(a+b+2i+1)}\, p_{i,i}, \quad 1 \le i \le n,\\ m_{i,j} = \widetilde{m}_{i,j} &= (t_1 - t_0) \frac{(a+i-1)(a+b+i-1)}{(a+b+i+j-1)(a+b+i+j-2)}, \quad 1 \le j < i \le n+1. \end{aligned}$$

Given $a, b > -1$ such that $a + b > -2$, $\widetilde{G}_n^{(a,b)}$ is STP. If, in addition, $\Gamma(a+1)$, $\Gamma(b+1)$ and $\Gamma(a+b+2)$ can be evaluated to high relative accuracy, then $\widetilde{G}_n^{(a,b)}$, its inverse matrix and their respective bidiagonal decompositions can also be computed to high relative accuracy.

Proof. Using the change of variable $t = (\tau - t_0)/(t_1 - t_0)$, we can write

$$\begin{aligned} \widetilde{G}_{i,j}^{(a,b)} &= \int_{t_0}^{t_1} (\tau - t_0)^{i+j+a-2} (t_1 - \tau)^b\, d\tau = (t_1 - t_0)^{i+j+a+b-1} \int_0^1 t^{i+j+a-2} (1 - t)^b\, dt\\ &= (t_1 - t_0)^{i+j+a+b-1} G_{i,j}^{(a,b)}, \quad 1 \le i, j \le n+1, \end{aligned} \tag{27}$$

where $\widetilde{G}_n^{(a,b)} = (\widetilde{G}_{i,j}^{(a,b)})_{1 \le i,j \le n+1}$ and $G_n^{(a,b)} = (G_{i,j}^{(a,b)})_{1 \le i,j \le n+1}$ is the Gramian matrix (17). Then

$$\widetilde{G}_{i,j}^{(a,b)} = (t_1 - t_0)^{i+j+a+b-1} G_{i,j}^{(a,b)} \tag{28}$$

Since $(t_1 - t_0)^{i+j+a+b-1} > 0$ and, under the considered conditions, $G_n^{(a,b)}$ is strictly totally positive (see Corollary 2), we conclude that $\widetilde{G}_n^{(a,b)}$ is also a strictly totally positive matrix. Taking into account formulae (25) and (19) for the diagonal pivots and multipliers of the Neville elimination of $G_n^{(a,b)}$, we deduce from Lemma 1 that the entries of $BD(\widetilde{G}_n^{(a,b)})$ are described by (27). Analyzing the sign of the entries of $BD(\widetilde{G}_n^{(a,b)})$, the result follows. ∎

By Theorem 2, the decomposition (4) of $\widetilde{G}_n^{(a,b)}$ and (7) of $(\widetilde{G}_n^{(a,b)})^{-1}$, can be stored by means of $BD(\widetilde{G}_n^{(a,b)}) = (BD(\widetilde{G}_n^{(a,b)})_{i,j})_{1 \le i,j \le n+1}$, with

$$BD(\widetilde{G}_n^{(a,b)})_{i,j} := \begin{cases} (t_1 - t_0) \frac{(a+i-1)(a+b+i-1)}{(a+b+i+j-1)(a+b+i+j-2)}, & \text{if } i > j,\\ (t_1 - t_0)^{a+b+2i-1} \frac{1}{\binom{a+b+2i-2}{i-1}} \beta(a+i, b+i), & \text{if } i = j,\\ (t_1 - t_0) \frac{(a+j-1)(a+b+j-1)}{(a+b+i+j-1)(a+b+i+j-2)}, & \text{if } i < j. \end{cases} \tag{29}$$

4 | GRAMIAN MATRICES ON UNBOUNDED INTERVALS

In this section, we are going to consider the system of functions

$$(e^{\lambda t}, te^{\lambda t}, \dots, t^n e^{\lambda t}), \quad \lambda \in \mathbb{R}, \tag{30}$$

which forms a fundamental solution set of the differential equation

$$y^{(n)} + a_{n-1}y^{(n-1)} + \cdots + a_1 y' + a_0 y = 0,$$

with the characteristic equation $F(t) = (t-\lambda)^n = 0$. Clearly, the basis (30) becomes the polynomial monomial basis for $\lambda = 0$. In Reference 34, the relevance and interesting applications to spectral and Lyapunov stability theory of their Wronskian and Gramian matrices is illustrated. In Reference 7, it is shown that for $\lambda < 0$ the Gramian matrix of (30) with respect to the inner product

$$\langle f, g\rangle := \int_0^{+\infty} f(t)g(t)\, dt, \tag{31}$$

is strictly totally positive and its bidiagonal factorization (4) is obtained.

In this section we shall consider the more general inner product obtained with generalized Laguerre weights $w(t) = t^a e^{-t}$,

$$\langle u, v\rangle_a := \int_0^{\infty} t^a e^{-t} u(t)v(t)\, dt, \quad a > -1. \tag{32}$$

For $\lambda < 1/2$, the Gramian matrix of the basis (30) with respect to (32) is the symmetric matrix $G_n^{(a,\lambda)} = \left(G_{i,j}^{(a,\lambda)}\right)_{1\le i,j\le n+1}$ with

$$G_{i,j}^{(a,\lambda)} := \langle t^{i-1}e^{\lambda t}, t^{j-1}e^{\lambda t}\rangle = \int_0^{+\infty} t^{a+i+j-2} e^{(2\lambda-1)t}\, dt,$$

for $1 \le i,j \le n+1$. By means of the change of variable $\tau := -(2\lambda - 1)t$, we have

$$G_{i,j}^{(a,\lambda)} = \int_0^{+\infty} t^{a+i+j-2} e^{(2\lambda-1)t}\, dt = \frac{1}{(1-2\lambda)^{a+i+j-1}} \int_0^{+\infty} \tau^{a+i+j-2} e^{-\tau}\, dt = \frac{1}{(1-2\lambda)^{a+i+j-1}} \Gamma(a+i+j-1). \tag{33}$$

Clearly, $G_n^{(a,\lambda)}$ is a Hankel matrix. We shall say that $G_n^{(a,\lambda)}$ is a Laguerre Gramian matrix.

The following result derives the pivots and multipliers of the Neville elimination of the Laguerre Gramian matrix $G_n^{(a,\lambda)}$ and then, its bidiagonal factorization (4).

Theorem 3. *Given $a > -1$ and $\lambda < 1/2$, the diagonal pivots and multipliers of the Neville elimination of the Laguerre Gramian matrix $G_n^{(a,\lambda)}$ described by (33) satisfy*

$$p_{1,1} = \frac{1}{(1-2\lambda)^{a+1}} \Gamma(a+1), \quad p_{i+1,i+1} = \frac{i(a+i)}{(1-2\lambda)^2} p_{i,i}, \quad 1 \le i \le n, \tag{34}$$

$$m_{i,j} = \widetilde{m}_{i,j} = \frac{a+i-1}{1-2\lambda}, \quad 1 \le j < i \le n+1. \tag{35}$$

Proof. Let $G^{(k)} = (G_{i,j}^{(k)})_{1\le i,j\le n+1}$, $k = 1, \dots, n+1$, be the matrices obtained after $k-1$ steps of the Neville elimination of $G_n^{(a,\lambda)}$, with $G^{(1)} := G_n^{(a,\lambda)}$. By induction on k, we are going to see that

$$G_{i,j}^{(k)} = (k-1)! \binom{j-1}{k-1} \frac{\Gamma(a+i+j-k)}{(1-2\lambda)^{a+i+j-1}}, \quad 1 \le i,j \le n+1. \tag{36}$$

By (33), equality (36) readily follows for $k = 1$. Now, assuming that (36) holds for some $k \in \{1, \dots, n\}$ and taking into account that $\Gamma(x+1) = x\Gamma(x)$, we can write

$$\frac{G_{i,k}^{(k)}}{G_{i-1,k}^{(k)}} = \frac{1}{1-2\lambda}\frac{\Gamma(a+i)}{\Gamma(a+i-1)} = \frac{a+i-1}{1-2\lambda}. \tag{37}$$

The element $G_{i,j}^{(k+1)}$ is obtained as explained in (1). Then, defining

$$\widetilde{G}_{i,j}^{(k+1)} := \frac{(1-2\lambda)^{a+i+j-1}}{(k-1)!\binom{j-1}{k-1}} G_{i,j}^{(k+1)},$$

and using (21), (37) and (36), we can write

$$\widetilde{G}_{i,j}^{(k+1)} = \Gamma(a+i+j-k) - (a+i-1)\Gamma(a+i+j-k-1) = (j-k)\Gamma(a+i+j-k-1),$$

and, finally,

$$G_{i,j}^{(k+1)} = k!\binom{j-1}{k}\frac{\Gamma(a+i+j-k-1)}{(1-2\lambda)^{a+i+j-1}},$$

which corresponds to formula (36) for $k+1$.

Now, by (2) and (36), the pivots $p_{i,j}$ of the Neville elimination of $G_n^{(a,\lambda)}$ satisfy

$$p_{i,j} = G_{i,j}^{(j)} = (j-1)!\frac{\Gamma(a+i)}{(1-2\lambda)^{a+i+j-1}}, \tag{38}$$

for $1 \le j \le i \le n+1$. The diagonal pivots are obtained for $i = j$,

$$p_{i,i} = (i-1)!\frac{\Gamma(a+i)}{(1-2\lambda)^{a+2i-1}}, \quad 1 \le i \le n+1. \tag{39}$$

Then, it can easily be checked that

$$p_{1,1} = \frac{\Gamma(a+1)}{(1-2\lambda)^{a+1}}, \quad \frac{p_{i+1,i+1}}{p_{i,i}} = \frac{i!}{(i-1)!}\frac{1}{(1-2\lambda)^2}\frac{\Gamma(a+i+1)}{\Gamma(a+i)} = \frac{i(a+i)}{(1-2\lambda)^2},$$

for $i = 1, \dots, n$ and so, (34) holds. Finally, using (3) and (38), the multipliers $m_{i,j}$, $1 \le j < i \le n+1$, can be written as

$$m_{i,j} = \frac{p_{i,j}}{p_{i-1,j}} = \frac{\Gamma(a+i)}{(1-2\lambda)\Gamma(a+i-1)} = \frac{a+i-1}{1-2\lambda}.$$

Taking into account the symmetry of the Gramian $G_n^{(a,\lambda)}$, we conclude that $\widetilde{m}_{i,j} = m_{i,j}$, $1 \le j < i \le n+1$. ∎

As a consequence of Theorem 3, and taking into account formula (39) for the diagonal pivots of the Neville elimination, we can derive an explicit expression for the Hankel determinant $\det G_n^{(a,\lambda)}$.

Corollary 3. *Let $G_n^{(a,\lambda)}$ the Laguerre Gramian matrix in (33) for $a > -1$ and $\lambda < 1/2$. Then*

$$\det\ G_n^{(a,\lambda)} = \prod_{i=1}^{n+1}(i-1)!\frac{\Gamma(a+i)}{(1-2\lambda)^{a+2i-1}}.$$

Using Theorem 3, the decomposition (4) of $G_n^{(a,\lambda)}$ as well as the decomposition (7) of $(G_n^{(a,\lambda)})^{-1}$, can be represented through $BD(G_n^{(a,\lambda)}) = (BD(G_n^{(a,\lambda)})_{i,j})_{1\le i,j\le n+1}$ such that

$$BD(G_n^{(a,\lambda)})_{i,j} := \begin{cases} \frac{a+i-1}{1-2\lambda}, & \text{if } i > j, \\ (i-1)!\frac{\Gamma(a+i)}{(1-2\lambda)^{a+2i-1}}, & \text{if } i = j, \\ \frac{a+j-1}{1-2\lambda}, & \text{if } i < j. \end{cases} \tag{40}$$

Let us observe that the matrix $BD(G_n^{(0,\lambda)})$ provides the bidiagonal factorization of the Gramian matrices of the monomial basis $(1, t, \dots, t^n)$, with respect to the Laguerre inner product (32).

The total positivity of Laguerre Gramian matrices $G_n^{(a,\lambda)}$ can be derived by analysing the sign of the entries of $BD(G_n^{(a,\lambda)})$.

Corollary 4. *For any $a > -1$ and $\lambda < 1/2$, the Laguerre Gramian matrix $G_n^{(a,\lambda)}$ in (33) is STP. If, in addition, $\Gamma(a+1)$ can be evaluated to high relative accuracy, then $G_n^{(a,\lambda)}$ and its inverse matrix can also be computed to high relative accuracy.*

Finally, we are going to consider Hermite weights $w(t) = e^{-t^2}$. The polynomial space $\mathbf{P}^n(\mathbb{R})$ is a Hilbert space under the inner product

$$\langle u, v\rangle_H := \int_{-\infty}^{\infty} e^{-t^2} u(t)v(t)\, dt. \tag{41}$$

The Gramian matrix of $(1, t, \dots, t^n)$ with respect (41) is $G_H = (G_{i,j})_{1\le i,j\le n+1}$ with

$$G_{i,j} := \langle t^{i-1}, t^{j-1}\rangle_H = \int_{-\infty}^{\infty} t^{i+j-2} e^{-t^2}\, dt, \quad 1 \le i, j \le n+1. \tag{42}$$

We shall say that G in (42) is a Hermite Gramian matrix. The following result proves these matrices are not TP.

Theorem 4. *For $n \ge 2$, the Hermite Gramian matrix (42) is not TP.*

Proof. It can easily be checked that

$$G_{i,j} = \int_{-\infty}^{\infty} t^{i+j-2} e^{-t^2}\, dt = \begin{cases} 0, & \text{if } i+j \text{ is odd}, \\ > 0, & \text{if } i+j \text{ is even}. \end{cases} \tag{43}$$

Consequently, $\det G[2,3|1,2] = G_{2,1}G_{3,2} - G_{3,1}G_{2,2} = -G_{3,1}G_{2,2} = -G_{3,1}^2 < 0$. ∎

5 | GRAMIAN MATRICES OF MONOMIAL BASES OF EVEN DEGREE

In this section we shall consider the basis $(1, t^2, \dots, t^{2n})$ of the $(n+1)$-dimensional space $\widetilde{\mathbf{P}}^{2n}$ of even polynomials of degree not greater than $2n$ in the variable t. This space is a Hilbert space under the following Chebyshev-type inner product,

$$\langle u, v\rangle_{a,b} := \int_0^1 t^{2a}(1-t^2)^b u(t)v(t)\, dt, \quad a > -1/2,\ b > -1. \tag{44}$$

In order to deduce the expression of the entries of the Gramian matrix $G_n^{a,b}$ of the even power basis $(1, t^2, \dots, t^{2n})$ with respect (44), let us first observe that

$$2\int_0^1 t^{2a+2i+2j-4}(1-t^2)^b\, dt = \int_0^1 \tau^{a+i+j-5/2}(1-\tau)^b\, d\tau = \beta(a+i+j-3/2, b+1). \tag{45}$$

Consequently, we have:

$$G_n^{a,b} := \frac{1}{2}(\beta(a+i+j-3/2, b+1))_{1\le i,j\le n+1}. \tag{46}$$

Clearly, $G_n^{a,b}$ is a Hankel matrix. In the following result the pivots and multipliers of its Neville elimination are derived.

Theorem 5. *The diagonal pivots and multipliers of the Neville elimination of the Gramian matrix $G_n^{a,b}$ in (46) satisfy*

$$
\begin{aligned}
p_{1,1} &= \frac{1}{2}\beta\left(a+\frac{1}{2}, b+1\right),\\
p_{i+1,i+1} &= \frac{i(a+i-1/2)(a+b+i-1/2)(b+i)}{(a+b+2i-3/2)(a+b+2i-1/2)^2(a+b+2i+1/2)}p_{i,i}, \quad i=1,\ldots,n,
\end{aligned}
\tag{47}
$$

$$
m_{i,j} = \widetilde{m}_{i,j} = \frac{(2a+2i-3)(2a+2b+2i-3)}{(2a+2b+2i+2j-3)(2a+2b+2i+2j-5)}, \quad 1 \le j < i \le n+1. \tag{48}
$$

Proof. Let $G^{(k)} = (G_{i,j}^{(k)})_{1\le i,j\le n+1}$, $k = 1, \ldots, n+1$, be the matrices obtained after $k-1$ steps of the Neville elimination of G_n, with $G^{(1)} := G_n^{a,b}$. Considering the generalization of combinatorial numbers (12), let us prove by induction on k that

$$
G_{i,j}^{(k)} = \frac{1}{2}\binom{j-1}{k-1}\beta(a+i+j-k-1/2, b+k)\bigg/\binom{a+b+i+k-5/2}{k-1}, \tag{49}
$$

for $1 \le i,j \le n+1$. Since $G_n^{a,b}$ is defined by (46), equality (49) clearly holds for $k=1$. Suppose that (49) holds for $1 \le k \le n$. Using the well-known formulae (21) satisfied by the Γ and β functions, as well as (12), the following identity can be easily derived

$$
\frac{G_{i,k}^{(k)}}{G_{i-1,k}^{(k)}} = \frac{(2a+2i-3)(2a+2b+2i-3)}{(2a+2b+2i+2k-3)(2a+2b+2i+2k-5)}. \tag{50}
$$

The generalized combinatorial numbers in (12) satisfy

$$
\frac{\alpha+1}{\alpha-n+1}\binom{\alpha}{n} = \binom{\alpha+1}{n},
$$

then we have

$$
\frac{a+b+i+k-5/2}{a+b+i-3/2}\binom{a+b+i+k-7/2}{k-1} = \binom{a+b+i+k-5/2}{k-1}. \tag{51}
$$

Then, using (51), and taking into account identities (1), (49) and (50), we have

$$
G_{i,j}^{(k+1)} = G_{i,j}^{(k)} - \frac{G_{i,k}^{(k)}}{G_{i-1,k}^{(k)}}G_{i-1,j}^{(k)} = \frac{\binom{j-1}{k-1}}{2\binom{a+b+i+k-5/2}{k-1}}\frac{\Gamma(b+k)\Gamma(a+i+j-k-3/2)}{\Gamma(a+b+i+j-3/2)}F_{i,j}, \tag{52}
$$

where

$$
F_{i,j} := \frac{a+i+j-k-3/2}{a+b+i+j-3/2} - \frac{a+i-3/2}{a+b+i+k-3/2} = \frac{(b+k)(j-k)}{(a+b+i+j-3/2)(a+b+i+k-3/2)}.
$$

Finally, taking into account identities (13), we can write

$$
\begin{aligned}
G_{i,j}^{(k+1)} &= \frac{1}{2}\frac{(j-k)\binom{j-1}{k-1}}{(a+b+i+k-3/2)\binom{a+b+i+k-5/2}{k-1}}\frac{\Gamma(a+i+j-k-3/2)\,(b+k)\Gamma(b+k)}{(a+b+i+j-3/2)\Gamma(a+b+i+j-3/2)}\\
&= \frac{1}{2}\binom{j-1}{k}\bigg/\binom{a+b+i+k-3/2}{k}\frac{\Gamma(a+i+j-k-3/2)\,\Gamma(b+k+1)}{\Gamma(a+b+i+j-1/2)}\\
&= \frac{1}{2}\binom{j-1}{k}\beta(a+i+j-k-3/2, b+k+1)\bigg/\binom{a+b+i+k-3/2}{k},
\end{aligned}
$$

corresponding to identities (49) for $k+1$.

Taking into account (2) and (49), the pivots $p_{i,j}$ of the Neville elimination of G can be described as follows

$$p_{i,j} = G^{(j)}_{i,j} = \frac{1}{2}\beta(a+i-1/2, b+j) \Big/ \binom{a+b+i+j-5/2}{j-1}, \quad 1 \le i,j \le n+1, \tag{53}$$

and the diagonal pivots $p_{i,i}$ are

$$p_{i,i} = \frac{1}{2}\beta(a+i-1/2, b+i) \Big/ \binom{a+b+2i-5/2}{i-1}, \quad i = 1, \dots, n+1. \tag{54}$$

It can be checked that $p_{1,1} = \beta(a+1/2, b+1)/2$ and

$$\frac{p_{i+1,i+1}}{p_{i,i}} = \frac{i(a+i-1/2)(a+b+i-1/2)(b+i)}{(a+b+2i-3/2)(a+b+2i-1/2)^2(a+b+2i+1/2)},$$

so, (47) holds. Formula (48) for the multipliers $m_{i,j}$, $1 \le j < i \le n+1$ is obtained using (3) and (53). Finally, taking into account that the Gramian matrix $G_n^{a,b}$ is a symmetric matrix, we conclude that $\widetilde{m}_{i,j} = m_{i,j}$, $1 \le j < i \le n+1$. ■

As a consequence of Theorem 5, and taking into account formula (54) for the diagonal pivots of the NE, we can derive an explicit expression for the Hankel det $G_n^{a,b}$.

Corollary 5. *Let $G_n^{a,b}$ the Gramian matrix in (46) for $a > -1/2$ and $b > -1$. Then*

$$\det\ G_n^{a,b} = \frac{1}{2^{n+1}} \prod_{i=1}^{n+1} \frac{\beta(a+i-1/2, b+i)}{\binom{a+b+2i-5/2}{i-1}}.$$

Moreover, by Theorem 5, $BD(G_n^{a,b}) = (BD(G_n^{a,b})_{i,j})_{1\le i,j \le n+1}$ satisfies

$$BD(G_n^{a,b})_{i,j} := \begin{cases} \frac{(2a+2i-3)(2a+2b+2i-3)}{(2a+2b+2i+2j-3)(2a+2b+2i+2j-5)}, & \text{if } i > j, \\ \frac{1}{2}\beta(a+i-1/2, b+i)/\binom{a+b+2i-5/2}{i-1}, & \text{if } i = j, \\ \frac{(2a+2j-3)(2a+2b+2j-3)}{(2a+2b+2i+2j-3)(2a+2b+2i+2j-5)}, & \text{if } i < j. \end{cases} \tag{55}$$

Let us notice that the diagonal pivots and multipliers of the Neville elimination of the Gramian matrices $G_n^{a,b}$ in (46) are positive for any $a > -1/2$ and $b > -1$. Then, the strict total positivity of these matrices is deduced.

Corollary 6. *For any $a > -1/2$ and $b > -1$, the Gramian matrix $G_n^{a,b}$ in (46) is STP. If, in addition, $\Gamma(a+1/2)$ and $\Gamma(b+1)$ can be evaluated to high relative accuracy, then $G_n^{a,b}$ and its inverse matrix can also be computed to high relative accuracy.*

Now, we are going to consider Hermite weights of the form $w(t) = t^{2a}e^{-t^2}$. The polynomial space $\widetilde{\mathbf{P}}^{2n}(\mathbb{R})$ is a Hilbert space under the inner product

$$\langle u, v \rangle_a := \int_{-\infty}^{\infty} t^{2a} e^{-t^2} u(t)v(t)\, dt, \quad a > -1/2. \tag{56}$$

In order to deduce the expression of the entries of the Gramian matrix of $(1, t^2, \dots, t^{2n})$ with respect the inner product (56), let us first observe that, for $a > -1/2$,

$$\int_{-\infty}^{\infty} t^{2a} e^{-t^2}\, dt = 2\int_0^{\infty} t^{2a} e^{-t^2}\, dt = \int_0^{\infty} \tau^{a-1/2} e^{-\tau}\, d\tau = \Gamma(a+1/2). \tag{57}$$

Consequently, the Gramian matrix $G_n^{(a)} = (G_{i,j}^{(a)})_{1\le i,j\le n+1}$ with respect to (56) can be described as

$$G_{i,j}^{(a)} := \int_{-\infty}^{\infty} t^{2(i+j+a-2)} e^{-t^2}\, dt = \Gamma(i+j+a-3/2), \tag{58}$$

and can be considered as a Hankel matrix. The following result derives the pivots and multipliers of its Neville elimination.

Theorem 6. *The diagonal pivots and multipliers of the Neville elimination of the Gramian matrix $G_n^{(a)}$ in (58) satisfy*

$$p_{1,1} = \Gamma(a+1/2), \quad p_{i+1,i+1} = i(i+a-1/2)p_{i,i}, \quad 1 \le i \le n. \tag{59}$$

$$m_{i,j} = \widetilde{m}_{i,j} = a+i-3/2, \quad 1 \le j < i \le n+1. \tag{60}$$

Proof. Let $G^{(k)} = (G_{i,j}^{(k)})_{1\le i,j\le n+1}$, $k = 1, \ldots, n+1$, be the matrices obtained after $k-1$ steps of the Neville elimination of $G^{(a)}$, with $G^{(1)} := G_n^{(a)}$. By induction on k, we shall see that

$$G_{i,j}^{(k)} = (k-1)!\binom{j-1}{k-1}\Gamma(i+j+a-k-1/2), \quad 1 \le i,j \le n+1. \tag{61}$$

Taking into account (58), equality (61) clearly holds for $k = 1$. Suppose that (61) holds for $1 \le k \le n$. Using (21), it can be checked that

$$\frac{G_{i,k}^{(k)}}{G_{i-1,k}^{(k)}} = \frac{\Gamma(i+a-1/2)}{\Gamma(i+a-3/2)} = \frac{(i+a-3/2)\Gamma(i+a-3/2)}{\Gamma(i+a-3/2)} = i+a-3/2. \tag{62}$$

Defining

$$\widetilde{G}_{i,j}^{(k+1)} := \frac{1}{(k-1)!\binom{j-1}{k-1}} G_{i,j}^{(k+1)},$$

and using (1), formula (61) and (62), we can write

$$\widetilde{G}_{i,j}^{(k+1)} = \Gamma(i+j+a-k-1/2) - (i+a-3/2)\Gamma(i+j+a-k-3/2) = (j-k)\Gamma(i+j+a-k-3/2)$$

and, finally,

$$G_{i,j}^{(k+1)} = k!\binom{j-1}{k}\Gamma(i+j+a-k-3/2),$$

confirming identities (61) for $k+1$.

Now, using (2) and (61), we derive that the pivots $p_{i,j}$ can be described as follows

$$p_{i,j} = G_{i,j}^{(j)} = (j-1)!\Gamma(i+a-1/2), \quad 1 \le i,j \le n+1, \tag{63}$$

Then, the diagonal pivots $p_{i,i}$ are

$$p_{i,i} = (i-1)!\Gamma(i+a-1/2), \quad 1 \le i,j \le n+1, \tag{64}$$

and satisfy $p_{1,1} = \Gamma(a+1/2)$ and

$$\frac{p_{i+1,i+1}}{p_{i,i}} = i\frac{\Gamma(i+a+1/2)}{\Gamma(i+a-1/2)} = i\frac{(i+a-1/2)\Gamma(i+a-1/2)}{\Gamma(i+a-1/2)} = i(i+a-1/2),$$

and so, (59) holds. Now, for the multipliers of the NE, we have by (3) and (63) that

$$m_{i,j} = \frac{p_{i,j}}{p_{i-1,j}} = \frac{\Gamma(i+a-1/2)}{\Gamma(i+a-3/2)} = i+a-3/2,$$

and formula (60) holds. Finally, taking into account that the Gramian matrix $G_n^{(a)}$ is a symmetric matrix, we conclude that $\widetilde{m}_{i,j} = m_{i,j}$, $1 \le j < i \le n+1$. ■

As a consequence of Theorem 6, and taking into account formula (64) for the diagonal pivots of the NE, we can derive an explicit expression for the Hankel det $G_n^{(a)}$.

Corollary 7. *Let $G_n^{(a)}$ the Gramian matrix in (58) for $a > -1/2$. Then*

$$\det\ G_n^{(a)} = \prod_{i=1}^{n+1} (i-1)!\Gamma(i+a-1/2).$$

Taking into account Theorem 6, $BD(G_n^{(a)}) = (BD(G_n^{(a)})_{i,j})_{1\le i,j\le n+1}$ satisfies

$$BD(G_n^{(a)})_{i,j} := \begin{cases} a+i-3/2, & \text{if } i > j, \\ (i-1)!\Gamma(i+a-1/2), & \text{if } i = j, \\ a+j-3/2, & \text{if } i < j. \end{cases} \tag{65}$$

Let us notice that the diagonal pivots and multipliers of the Neville elimination of the Gramian matrices $G_n^{(a)}$ in (58) are positive for any $a > -1/2$. Then the strict total positivity of these matrices is deduced.

Corollary 8. *For any $a > -1/2$, the Gramian matrix $G_n^{(a)}$ in (58) is STP. If, in addition, $\Gamma(a+1/2)$ can be evaluated to high relative accuracy, then $G_n^{(a)}$ and its inverse matrix can also be computed to high relative accuracy.*

6 | NUMERICAL EXPERIMENTS

Some numerical tests are presented in this section supporting the obtained theoretical results. In this context, we have implemented different MATLAB functions in $O(n^2)$ time for computing the bidiagonal factorizations (4) proposed in the previous sections stored in the matrix form (9). For the Gramian matrix $\widetilde{G}_n^{(a,b)}$ of the basis $(1, t-t_0, \dots, (t-t_0)^n)$ with respect to the inner product (26), using Theorem 2, we have implemented a MATLAB function for computing $BD(\widetilde{G}_n^{(a,b)})$ (see (29)). Let us observe that, in the case that $t_0 = 0$ and $t_1 = 1$, the mentioned function can compute $BD(G_n^{(a,b)})$ for the Chebyshev Gramian matrix $G_n^{(a,b)}$ in (17). Moreover, for the Laguerre Gramian matrix $G_n^{(a,\lambda)}$ described by (33), considering Theorem 3, we have also implemented a MATLAB function for computing $BD(G_n^{(a,\lambda)})$ (see (40)). Furthermore, for the even monomial basis $(1, t^2, \dots, t^{2n})$ we have implemented two MATLAB functions. One of them, using Theorem 5, computes $BD(G_n^{a,b})$ (see (55)) for the Gramian matrix $G_n^{a,b}$ in (46), and the other, considering Theorem 6, computes $BD(G_n^{(a)})$ (see (65)), for the Gramian matrix $G_n^{(a)}$ in (58).

In the rest of the Section, for the sake of brevity, all the Gramian matrices will be denoted as G, and their corresponding bidiagonal decompositions will be denoted by $BD(G)$.

In order to check the accuracy of our algorithms, we have considered different STP Gramian matrices G with dimension $n+1 = 4, 5, \dots, 20$. Moreover, having in mind that for $\alpha \in \mathbb{N} \cup \{0\}$, $\Gamma(\alpha+1) = \alpha!$ and $\Gamma(n+1/2) = \frac{(2n)!}{4^n n!}\sqrt{\pi}$, $n \in \mathbb{N}$, we have chosen parameters a and b so that the conditions provided in Corollary 2 (for Chebyshev Gramian matrices), Corollary 4 (for Laguerre Gramian matrices), Corollary 6 (for Gramian matrices (46)) and Corollary 8 (for Gramian matrices (58)) are fulfilled and so, we can guarantee HRA in the computation of $BD(G)$. In particular, we have considered Chebyshev Gramian matrices (17) for $(a,b) = (1/2, 1/2)$, Laguerre Gramian matrices (33) for $(a,\lambda) = (1,0)$ and $(a,\lambda) = (1,1/3)$, Gramian matrices (46) for $(a,b) = (2,-1/2)$, and finally, Gramian matrices (58) for $a = 1$.

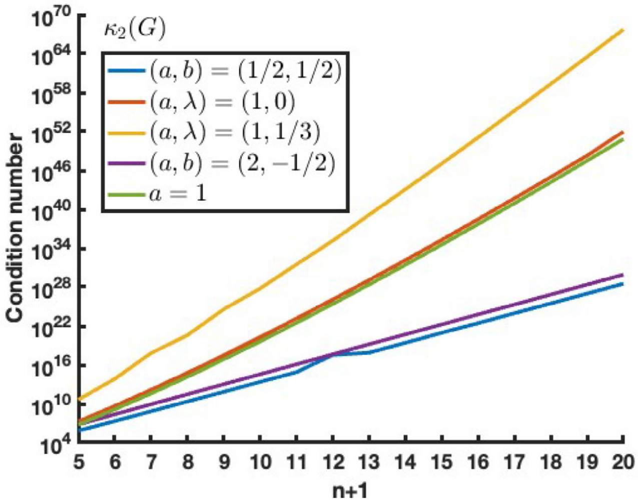

FIGURE 1 The 2-norm conditioning of Gramian matrices G.

In addition, we have performed with these matrices several matrix computations which include computing singular values (which coincide with the eigenvalues because the matrices are symmetric), inverses and linear equation solving. All the approximations computed by our algorithms have been compared with the respective approximations obtained by traditional methods provided in MATLAB *R2022b*. In this context, the values provided by Wolfram Mathematica 13.1 with 100-digit arithmetic have been taken as the exact solution of the considered linear algebra problem. Finally, the relative error of each approximation has also been computed in Mathematica with 100-digit arithmetic.

In addition, we have also computed the 2-norm condition number of all considered matrices. The conditioning obtained in Mathematica is depicted in Figure 1. It can easily be observed that the conditioning drastically increases with the size of the matrices. Due to the ill-conditioning of these matrices, standard routines do not obtain accurate solutions because they can suffer from inaccurate cancelations. In contrast, the algorithms using the factorizations obtained in this paper exploit the structure of the considered matrices achieving, as we will see, numerical results to high relative accuracy.

6.1 | Computation of singular values

Given $B = BD(A)$ to high relative accuracy, the MATLAB function `TNSingularValues(B)` available in Reference 33 computes the singular values of a matrix A to high relative accuracy. Its computational cost is $O(n^3)$ (see Reference 19).

In this context, we have compared the smallest singular value obtained using `TNSingularValues(BD(G))` and the MATLAB command `svd`. The values provided by Mathematica using 100-digit arithmetic have been considered as the exact solution of the linear algebra problem and the relative error e of each approximation has been computed as $e := |a - \tilde{a}|/|a|$, where a denotes the singular value computed in Mathematica and $\tilde{a}$ the singular value computed in Matlab.

The relative errors are shown in Figure 2. Note that our approach computes accurately the smallest singular value regardless of the 2-norm condition number of the considered matrices. In contrast, the MATLAB command `svd` returns results that are not accurate at all.

6.2 | Computation of inverses

Given $B = BD(A)$ to high relative accuracy, the MATLAB function `TNInverseExpand`(B) available in Reference 33 returns A^{-1} to high relative accuracy, requiring $O(n^2)$ arithmetic operations (see Reference 28).

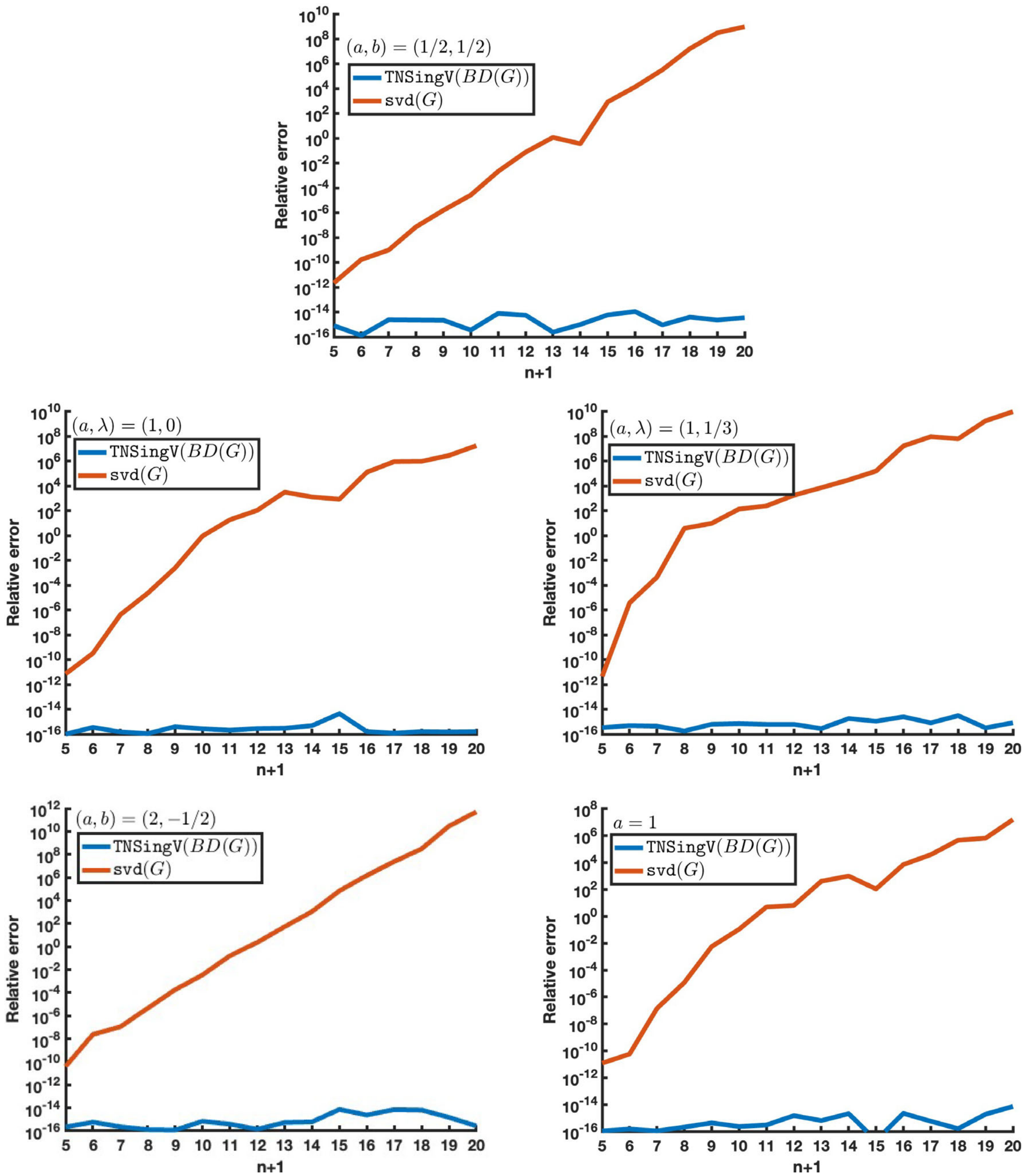

FIGURE 2 Relative error of the approximations to the smallest singular value of Gramian matrices G.

In addition, we have compared the inverses obtained using TNInverseExpand($BD(G)$) and the MATLAB command inv. To look over the accuracy of these two methods we have compared both approximations with the inverse matrix A^{-1} computed by Mathematica using 100-digit arithmetic, taking into account the formula $e = \|A^{-1} - \widetilde{A}^{-1}\|_2 / \|A^{-1}\|_2$ for the corresponding relative error, where $\widetilde{A}^{-1}$ denotes the inverse computed in Matlab.

As shown in Figure 3, our algorithm provides results to high relative accuracy. On the contrary, the results obtained with MATLAB reflect poor accuracy.

6.3 | Resolution of linear systems

Given $B = BD(A)$ to high relative accuracy and a vector d with alternating signs, the MATLAB function TNSolve(B, d) available in Reference 33 returns the solution c of $Ac = d$ to high relative accuracy. It requires $O(n^2)$ arithmetic operations (see Reference 33).

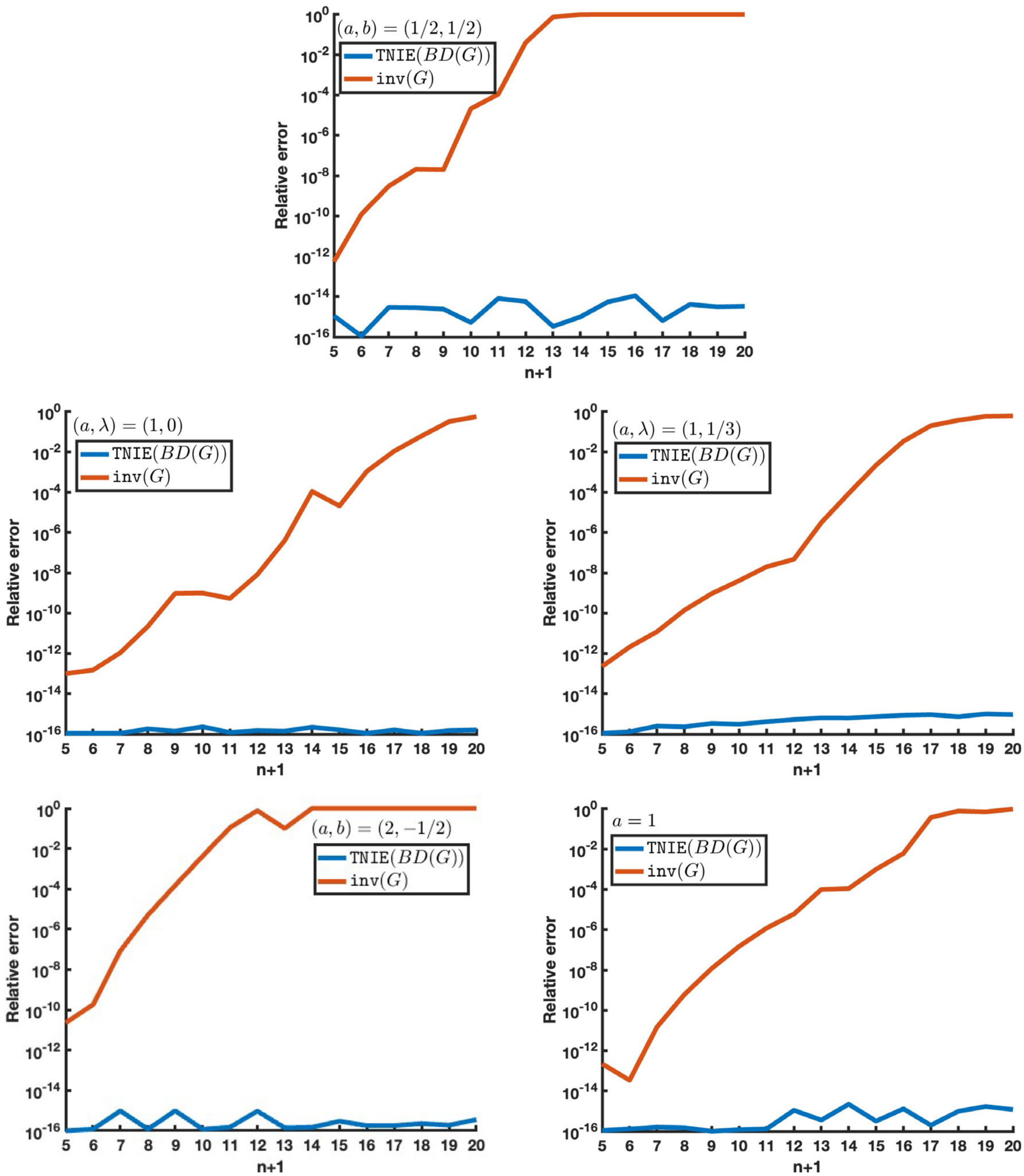

FIGURE 3 Relative error of the approximations to the inverse of Gramian matrices G.

For all considered Gramian matrices, we have compared the solution of the linear system $Gc = d$ obtained using TNSolve$(BD(G), d)$ and the MATLAB command \. The solution provided by Mathematica using 100-digit arithmetic has been considered as the exact solution c. Then, we have computed in Mathematica the relative error of the computed approximations $\tilde{c}$, taking into account the formula $e = \|c - \tilde{c}\|_2 / \|c\|_2$.

As opposed to the results obtained with the command \, the proposed algorithm preserves the accuracy for all the considered dimensions. Figure 4 illustrates the relative errors.

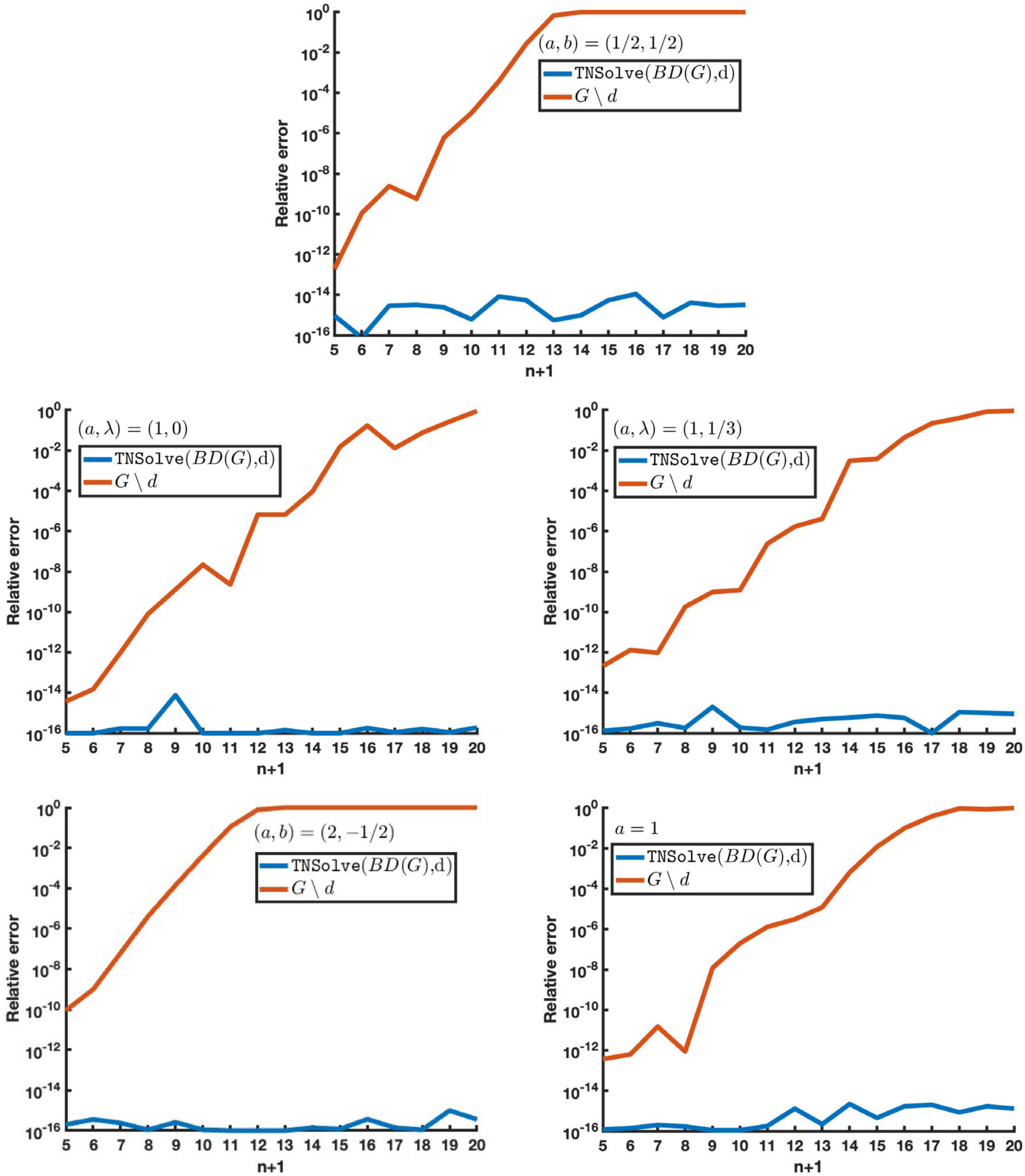

FIGURE 4 Relative error of the approximations to the solution of the linear systems $Gc = d$, where $d = ((-1)^{i+1} d_i)_{1 \le i \le n+1}$ and d_i, $i = 1, \ldots, n+1$ are random nonnegative integer values.

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CONFLICT OF INTEREST STATEMENT

This study does not have any conflicts to disclose.

DATA AVAILABILITY STATEMENT

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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