



# Gaussian rule for integrals involving Bessel functions

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## Abstract

In this work we develop the Gaussian quadrature rule for weight functions involving powers, exponentials and Bessel functions of the first kind. Besides the computation based on the use of the standard and the modified Chebyshev algorithm, here we present a very stable algorithm based on the preconditioning of the moment matrix. Numerical experiments are provided and a geophysical application is considered.

**Keywords** Gaussian quadrature · Moment-based methods · Chebyshev algorithm · Bessel function of the first type

**Mathematics Subject Classification** 33C10 · 33C45 · 65D32 · 65F08

## 1 Introduction

This work deals with the construction of Gaussian quadrature rule for the computation of integrals of the type

$$I_{\nu, \alpha, c}(f) = \int_0^{\infty} f(x) x^{\alpha} e^{-cx} J_{\nu}(x) dx, \quad (1.1)$$

where  $J_{\nu}$  is the Bessel function of the first kind of order  $\nu \geq 0$ ,  $\alpha > -1$ ,  $c > 0$  and  $f$  is a smooth function. Since for the Bessel functions it holds  $|J_{\nu}(x)| \leq 1$ , for  $\nu \geq 0$ ,  $x \in \mathbb{R}$  (see [1, p. 362]), we consider weight functions of the type

$$w_{\nu, \alpha, c}(x) = x^{\alpha} e^{-cx} [J_{\nu}(x) + 1] \quad \text{on } [0, +\infty). \quad (1.2)$$

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Then, we rewrite (1.1) as

$$I_{v,\alpha,c}^J(f) - I_{\alpha,c}^L(f),$$

where

$$I_{v,\alpha,c}^J(f) = \int_0^\infty f(x)x^\alpha e^{-cx} [J_v(x) + 1] dx, \quad (1.3)$$

and

$$I_{\alpha,c}^L(f) = \int_0^\infty f(x)x^\alpha e^{-cx} dx. \quad (1.4)$$

We notice that the integral (1.4) can be accurately computed using a slight modification of the Gauss–Laguerre quadrature rule. In this setting, our aim is to construct a Gaussian rule with respect to the function  $w_{v,\alpha,c}$ . Since we do not know the explicit expression of the corresponding monic orthogonal polynomials, that we denote by  $\pi_k$ ,  $k \geq 0$ , we need to employ a numerical scheme to derive the coefficients of the three-term recursion

$$\begin{aligned} \pi_{k+1}(x) &= (x - \alpha_k)\pi_k(x) - \beta_k\pi_{k-1}(x), \quad k \geq 0, \\ \pi_{-1}(x) &= 0, \quad \pi_0(x) = 1, \end{aligned}$$

with  $\beta_k > 0$ . This can be done by computing the associated moments

$$\mu_k^{v,\alpha,c} = \int_0^\infty x^k w_{v,\alpha,c}(x) dx, \quad k \geq 0, \quad (1.5)$$

and then using the Chebyshev algorithm (see [9, Sect. 2.3]). These coefficients define the tridiagonal symmetric Jacobi matrix, whose eigenvalue decomposition provides abscissas and weights of the quadrature rule. This final step is efficiently implemented by the famous Golub and Welsh algorithm [14]. Some alternatives to this algorithm have been later developed and we refer to [17] for a general discussion and a rich bibliography. Nevertheless, it is well known (see e.g. [11]) that the computation of the recurrence coefficients can be inaccurate for growing  $k$  because the problem is severely ill conditioned when starting from the power moments (1.5). The ill conditioning can be partially overcome by using the modified moments, having at disposal a family of polynomials orthogonal with respect to a weight function similar to the one of the problem. This approach may be efficient in general but not always when working with unbounded intervals of integration (see [10, 11]). The idea of using modified moments was introduced by Sack and Donovan in [19], who developed an algorithm similar to the so called modified Chebyshev algorithm, advanced by Gautschi [9, Sect. 2.4]. The same algorithm was independently obtained by Wheeler [24].

In this work we present an alternative approach that is based on the preconditioning of the moment matrix. In particular, since the three-term recurrence coefficients can be

written in terms of ratios of determinants of the moment matrix or slight modifications of them (see [4, Sect. 2.7]), we exploit the Cramer rule to show that the coefficients can be computed by solving a linear system with the moment matrix. Since the weight function (1.2) can be interpreted as a perturbation of the weight function of the generalized Laguerre polynomials, we use the moment matrix of these polynomials as preconditioner. The numerical experiments show that this technique is always (independently of the parameters  $\nu, \alpha, c$ ) much more stable than the modified Chebyshev algorithm.

As an application we use the developed Gaussian quadrature to evaluate integrals of the type (1.1) arising in geophysical electromagnetic (EM) survey. In particular, we consider the electromagnetic fields over a layered earth due to magnetic dipoles above the surface (see [22]). In this framework,  $f$  is a smooth function,  $\nu = 0, 1, \alpha = 0$  and  $0 < c < 1$ .

We remark that other methods for the computation of the integral in (1.1), still of Gaussian type, have been developed over the years. Among the others we quote here [2, 25] and the references therein.

The paper is organized as follows. In Sect. 2 we derive a recursive relation for the practical evaluation of the power moments. In Sect. 3 we show the necessary details for the construction of the Gaussian rule for (1.1) by using the Chebyshev algorithm. In Sect. 4 we employ the modified Chebyshev algorithm working with the modified moments generated by the generalized Laguerre polynomials. In Sect. 5 we present the alternative approach based on the preconditioning of the moment matrix, using again the generalized Laguerre polynomials. Finally, in Sect. 6 we apply the method for the computation of EM fields.

## 2 Computation of the moments

In order to compute the moments

$$\mu_k = \mu_k^{\nu, \alpha, c} = \int_0^\infty x^{k+\alpha} e^{-cx} [J_\nu(x) + 1] dx, \quad k \geq 0, \tag{2.1}$$

we first derive a recursive relation for the so called core moments, defined as

$$\mu_{k,0} = \mu_{k,0}^{\nu, \alpha, c} = \int_0^\infty x^{k+\alpha} e^{-cx} J_\nu(x) dx, \quad k \geq 0. \tag{2.2}$$

We remark that the term core moment was introduced by Gautschi [12].

**Proposition 2.1** *For  $k \geq 0$  it holds*

$$\mu_{k,0} = \frac{1}{(\sqrt{c^2 + 1})^{k+\alpha+1}} \Gamma(k + \alpha + \nu + 1) P_{k+\alpha}^{-\nu} \left( \frac{c}{\sqrt{c^2 + 1}} \right), \tag{2.3}$$

where  $\Gamma$  is the Gamma function and  $P_{k+\alpha}^{-\nu}$  is the associated Legendre function (see e.g. [1, ch.8] or [18, ch.14]) of order  $-\nu$  and degree  $k + \alpha$ .

**Proof** We start from the general relation [7, p.713]

$$\int_0^\infty e^{-t \cos \theta} J_\nu(t \sin \theta) t^{k+\alpha} dt = \Gamma(k + \alpha + \nu + 1) P_{k+\alpha}^{-\nu}(\cos \theta),$$

which holds for each  $k \geq 0$  whenever  $\alpha > -1$ ,  $\nu \geq 0$ . By the change of variable  $s = t \sin \theta$ , we have that

$$\int_0^\infty e^{-s \frac{\cos \theta}{\sin \theta}} J_\nu(s) s^{k+\alpha} ds = \sin^{k+\alpha+1}(\theta) \Gamma(k + \alpha + \nu + 1) P_{k+\alpha}^{-\nu}(\cos \theta).$$

Setting  $\theta = \arctan\left(\frac{1}{c}\right)$ ,  $0 < \theta < \frac{\pi}{2}$ , so that  $c = \frac{\cos \theta}{\sin \theta}$ , and using the relations

$$\sin(\arctan x) = \frac{x}{\sqrt{1+x^2}}, \quad \cos(\arctan x) = \frac{1}{\sqrt{1+x^2}},$$

we obtain the result.  $\square$

**Proposition 2.2** *The following three-term recursion holds*

$$\mu_{k+1,0} = \frac{1}{c^2 + 1} \{c [2(k + \alpha) + 1] \mu_{k,0} - [(k + \alpha)^2 - \nu^2] \mu_{k-1,0}\}, \quad k \geq 1, \quad (2.4)$$

with

$$\begin{aligned} \mu_{0,0} &= \frac{\Gamma(\alpha + \nu + 1)}{(\sqrt{c^2 + 1})^{\alpha+1} \Gamma(\nu + 1)} \left( \sqrt{c^2 + 1} + c \right)^{-\nu} \\ &\quad \times {}_2F_1 \left( -\alpha, \alpha + 1; 1 + \nu; \frac{1}{2\sqrt{c^2 + 1} (\sqrt{c^2 + 1} + c)} \right), \end{aligned} \quad (2.5)$$

$$\begin{aligned} \mu_{1,0} &= \frac{\Gamma(\alpha + \nu + 2)}{(\sqrt{c^2 + 1})^{\alpha+2} \Gamma(\nu + 1)} \left( \sqrt{c^2 + 1} + c \right)^{-\nu} \\ &\quad \times {}_2F_1 \left( -\alpha - 1, \alpha + 2; 1 + \nu; \frac{1}{2\sqrt{c^2 + 1} (\sqrt{c^2 + 1} + c)} \right), \end{aligned} \quad (2.6)$$

where  ${}_2F_1$  is the hypergeometric function.

**Proof** From Eq. (2.3) and using the following three-term recursive relation for the associated Legendre functions [1, p. 334]

$$(k + \alpha + \nu + 1) P_{k+\alpha+1}^{-\nu}(z) = (2k + 2\alpha + 1) z P_{k+\alpha}^{-\nu}(z) - (k + \alpha - \nu) P_{k+\alpha-1}^{-\nu}(z),$$

we can write

$$\begin{aligned} \mu_{k+1,0} &= \frac{1}{(\sqrt{c^2 + 1})^{k+\alpha+2}} \Gamma(k + \alpha + \nu + 2) P_{k+\alpha+1}^{-\nu} \left( \frac{c}{\sqrt{c^2 + 1}} \right) \\ &= \frac{\Gamma(k + \alpha + \nu + 2)}{(\sqrt{c^2 + 1})^{k+\alpha+2}} \left[ \frac{2(k + \alpha) + 1}{k + \alpha + \nu + 1} \frac{c}{\sqrt{c^2 + 1}} P_{k+\alpha}^{-\nu} \left( \frac{c}{\sqrt{c^2 + 1}} \right) \right. \\ &\quad \left. - \frac{k + \alpha - \nu}{k + \alpha + \nu + 1} P_{k+\alpha-1}^{-\nu} \left( \frac{c}{\sqrt{c^2 + 1}} \right) \right]. \end{aligned} \tag{2.7}$$

Rearranging (2.7) and using again (2.3) for  $\mu_{k,0}$  and  $\mu_{k-1,0}$ , we obtain the relation (2.4). Equations (2.5) and (2.6) follow directly from (2.3) with  $k = 0$  and  $k = 1$ , respectively, and from the relation [7, p. 999]

$$P_{k+\alpha}^{-\nu}(x) = \frac{1}{\Gamma(\nu + 1)} \left( \frac{1+x}{1-x} \right)^{-\frac{\nu}{2}} {}_2F_1 \left( -k - \alpha, k + \alpha + 1; 1 + \nu; \frac{1-x}{2} \right),$$

for  $x \in (0, 1)$ .

□

Finally, we can derive a recursive relation for the moments.

**Proposition 2.3** *For  $k \geq 1$  it holds*

$$\begin{aligned} \mu_{k+1} &= \frac{1}{c^2 + 1} \left\{ c [2(k + \alpha) + 1] \mu_k - [(k + \alpha)^2 - \nu^2] \mu_{k-1} \right. \\ &\quad \left. + \frac{\Gamma(k + \alpha)[(k + \alpha)^2 + (k + \alpha) - c^2 \nu^2]}{c^{k+\alpha+2}} \right\}, \end{aligned} \tag{2.8}$$

with

$$\mu_0 = \mu_{0,0} + \frac{\Gamma(\alpha + 1)}{c^{\alpha+1}}, \quad \mu_1 = \mu_{1,0} + \frac{\Gamma(\alpha + 2)}{c^{\alpha+2}}.$$

**Proof** By definition (2.1), the moments  $\mu_k$  are given by

$$\begin{aligned} \mu_k &= \int_0^\infty x^{k+\alpha} e^{-cx} J_\nu(x) dx + \int_0^\infty x^{k+\alpha} e^{-cx} dx \\ &= \mu_{k,0} + \frac{\Gamma(k + \alpha + 1)}{c^{k+\alpha+1}}, \end{aligned}$$

where we have used [7, Sect. 3.381, n.4]. Therefore, from relation (2.4) for  $k \geq 1$ , we can write

$$\begin{aligned} \mu_{k+1} &= \mu_{k+1,0} + \frac{\Gamma(k + \alpha + 2)}{c^{k+\alpha+2}} \\ &= \frac{c[2(k + \alpha) + 1]}{c^2 + 1} \left( \mu_k - \frac{\Gamma(k + \alpha + 1)}{c^{k+\alpha+1}} \right) - \frac{(k + \alpha)^2 - v^2}{c^2 + 1} \left( \mu_{k-1} - \frac{\Gamma(k + \alpha)}{c^{k+\alpha}} \right) \\ &\quad + \frac{\Gamma(k + \alpha + 2)}{c^{k+\alpha+2}}. \end{aligned}$$

After some simple manipulations, we obtain the result. □

### 3 Computing the three-term recursion

One of the most used method for the computation of the coefficients  $\alpha_k$  and  $\beta_k$  of the recurrence relation

$$\pi_{k+1}(x) = (x - \alpha_k)\pi_k(x) - \beta_k\pi_{k-1}(x), \quad k \geq 0, \pi_{-1}(x) = 0, \quad \pi_0(x) = 1, \tag{3.1}$$

with  $\beta_k > 0$ , is the Chebyshev algorithm (see [9, sect.2.3] and [11]).

Given the first  $2n$  moments  $\mu_0, \dots, \mu_{2n-1}$ , the algorithm uniquely determines the first  $n$  recurrence coefficients  $\alpha_k$  and  $\beta_k, k = 0, \dots, n-1$ , by using the mixed moments

$$\sigma_{kl} = \int_0^\infty \pi_k(x)x^l w_{v,\alpha,c}(x)dx, \quad k, l \geq -1.$$

The Chebyshev algorithm is summarized in Algorithm 3.1.

#### Algorithm 3.1 Initialization

$$\begin{aligned} \alpha_0 &= \frac{\mu_1}{\mu_0}, \quad \beta_0 = \mu_0, \\ \sigma_{-1,l} &= 0, \quad l = 1, 2, \dots, 2n - 2, \\ \sigma_{0,l} &= \mu_l, \quad 0, 1, \dots, 2n - 1, \end{aligned}$$

for  $k = 1, 2, \dots, n - 1$   
 for  $l = k, k + 1, \dots, 2n - k - 1$

$$\begin{aligned} \sigma_{k,l} &= \sigma_{k-1,l+1} - \alpha_{k-1}\sigma_{k-1,l} - \beta_{k-1}\sigma_{k-2,l}, \\ \alpha_k &= \frac{\sigma_{k,k+1}}{\sigma_{k,k}} - \frac{\sigma_{k-1,k}}{\sigma_{k-1,k-1}}, \quad \beta_k = \frac{\sigma_{k,k}}{\sigma_{k-1,k-1}}. \end{aligned}$$

The corresponding Jacobi matrix

$$J = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & 0 \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & \\ & \sqrt{\beta_2} & \alpha_2 & \ddots & \\ & & \ddots & \ddots & \sqrt{\beta_{n-1}} \\ 0 & & & \sqrt{\beta_{n-1}} & \alpha_{n-1} \end{bmatrix} \in \mathbb{R}^{n \times n},$$

contains the coefficients of the three term recurrence relation for the orthonormal polynomials, that is,

$$\begin{aligned} \sqrt{\beta_{k+1}}\tilde{\pi}_{k+1}(x) &= (x - \alpha_k)\tilde{\pi}_k(x) - \sqrt{\beta_k}\tilde{\pi}_{k-1}(x), \quad k \geq 0, \\ \tilde{\pi}_{-1}(x) &= 0, \quad \tilde{\pi}_0(x) = \frac{1}{\sqrt{\beta_0}}. \end{aligned}$$

It is well known that the eigendecomposition of the matrix  $J$  provides the nodes  $x_i$  and the weights  $w_i, i = 1, \dots, n$  of the  $n$ -point Gauss rule (see e.g. [4, Sect. 2.7], and the reference therein).

Finally, for the computation of (1.1), we use the approximation

$$I_{\nu,\alpha,c}^J(f) \approx I_n^J(f) = \sum_{i=1}^n w_i f(x_i),$$

for the integral (1.3). Then, denoting by  $t_i^L, w_i^L$  respectively the nodes and the weights of the Gauss–Laguerre rule with respect to the weight function  $w_\alpha(t) = t^\alpha e^{-t}, \alpha > -1$ , the integral (1.4) is approximated by

$$\begin{aligned} I_{\alpha,c}^L(f) &= \frac{1}{c^{\alpha+1}} \int_0^\infty f\left(\frac{t}{c}\right) t^\alpha e^{-t} dt \\ &\approx I_n^L(f) = \frac{1}{c^{\alpha+1}} \sum_{i=1}^n w_i^L f\left(\frac{t_i^L}{c}\right). \end{aligned}$$

Finally, we thus have

$$I_{\nu,\alpha,c}(f) \approx I_n^J(f) - I_n^L(f). \tag{3.2}$$

Below we present the results of the numerical experiments carried out in Matlab. In particular, the Matlab routine that implements the Chebyshev algorithm is taken from [13]. Since for integrals involving Bessel functions, exponentials and powers the exact solution is known, in our simulations we choose  $f(x) = e^{-0.5x}$ . In Fig. 1 we consider two examples, for different values of the parameters  $\nu, \alpha$  and  $c$ , and plot the error between the approximation obtained with the developed Gaussian rule and the

exact solution (see [7, Sect. 6.624, n. 6] and [7, Sect. 8.704]) given by

$$I_{v,\alpha,d}(f) = \frac{\Gamma(d+v+1)}{(\sqrt{c^2+1})^{d+1}\Gamma(v+1)} \left( \frac{\sqrt{c^2+1}+c}{\sqrt{c^2+1}-c} \right)^{-\frac{v}{2}} \\ \times {}_2F_1 \left( -d, d+1; 1+v; \frac{1}{2} - \frac{c}{2\sqrt{c^2+1}} \right),$$

where  $d = c + 0.5$ .

Moreover, since for the truncation error it holds (see [4, Sect. 4.4])

$$E_n(f) = I_{v,\alpha,c}(f) - (I_n^J(f) - I_n^L(f)) \\ = (I_{v,\alpha,c}^J(f) - I_n^J(f)) - (I_{\alpha,c}^L(f) - I_n^L(f)) \\ = \frac{f^{(2n)}(\eta^J)}{(2n)!(k_n^J)^2} - \frac{f^{(2n)}(\eta^L)}{(2n)!(k_n^L)^2}, \quad \eta^J, \eta^L \in (0, \infty),$$

where  $k_n^J$  and  $k_n^L$  are the leading coefficients of the corresponding orthonormal polynomials of degree  $n$ , in Fig. 1 we also provide the plot of the upper bound of  $E_n(f)$  given by

$$|E_n(f)| \leq \frac{\|f^{(2n)}\|_\infty}{(2n)!} \left( \frac{1}{(k_n^J)^2} + \frac{1}{(k_n^L)^2} \right). \quad (3.3)$$

The coefficients  $k_n^J$  are numerically evaluated by using the relation (see [4, sect.2.7])

$$k_n^J = \frac{1}{\prod_{j=0}^n \sqrt{\beta_j}},$$

while for  $k_n^L$  we employ the known explicit formulation

$$k_n^L = \frac{1}{\sqrt{n! \Gamma(n + \alpha + 1)}}.$$

It is well known that, in general, the error bound (3.3) is not very sharp. More reliable a posteriori and a priori error estimates for the approximation (3.2) are studied in [5].

## 4 The modified Chebyshev algorithm

The picture on the right of Fig. 1 shows the stability problem when working with the power moments  $\mu_k$ . Indeed the Chebyshev algorithm typically starts to produce negative values of  $\beta_k$  for  $k$  around 20 or even before. This behavior is rather common and has been observed by many authors in the past [11, 14, 24]. As already mentioned,



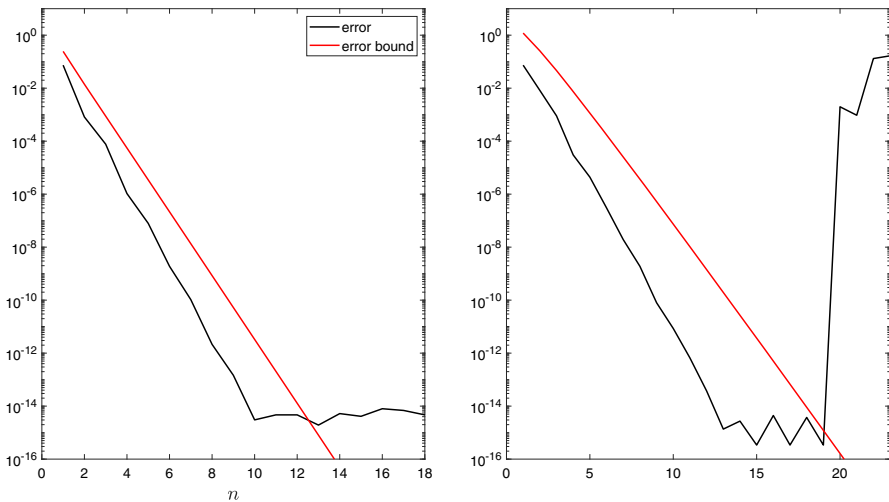


Fig. 1 Error behavior of (3.2) and error bound (3.3) with respect to  $n$  for  $\nu = 1, \alpha = -0.5, c = 1$  on the left and for  $\nu = 0.5, \alpha = 0.5, c = 0.2$  on the right. In both cases  $f(x) = e^{-0.5x}$

the problem is that the coefficients  $\alpha_k$  and  $\beta_k$  are extremely sensitive to small changes in the moments. In fact, the nonlinear map

$$K_n : \mathbb{R}^{2n} \rightarrow \mathbb{R}^{2n}$$

$$\mu \mapsto \rho$$

which maps the moment vector  $\mu = [\mu_0, \mu_1, \dots, \mu_{2n-1}]^T$  to the vector  $\rho = [\alpha_0, \dots, \alpha_{n-1}, \beta_0, \dots, \beta_{n-1}]^T$  of recursion coefficients becomes extremely ill conditioned as  $n$  increases (see [11] for the complete analysis).

In order to overcome this difficulty, the modified Chebyshev algorithm (see [9, Sect. 2.4]) can be employed. It is based on the use of the modified moments

$$m_k = m_k^{\nu, \alpha, c} = \int_0^\infty p_k(x) w_{\nu, \alpha, c}(x) dx, \quad k \geq 0, \tag{4.1}$$

and on the mixed moments

$$\tilde{\sigma}_{kl} = \int_0^\infty \pi_k(x) p_l(x) w_{\nu, \alpha, c}(x) dx, \quad k, l \geq -1,$$

where  $\{p_k\}_{k \geq 0}$  is a given system of orthogonal polynomials, chosen to be close to the desired polynomials  $\{\pi_k\}_{k \geq 0}$ , which satisfies the three-term recurrence relation

$$p_{k+1}(x) = (x - a_k)p_k(x) - b_k p_{k-1}(x), \quad k \geq 0$$

$$p_{-1}(x) = 0, \quad p_0(x) = 1,$$

with coefficients  $a_k \in \mathbb{R}, b_k \geq 0$  that are known.

In our case, since the weight function can be interpreted as a perturbation of the weight function relative to the generalized Laguerre polynomials  $\{L_k^\alpha\}_{k \geq 0}$ , we choose as  $\{p_k\}_{k \geq 0}$  the system  $\{L_k^{\alpha,c}\}_{k \geq 0}$  of the monic polynomials

$$L_k^{\alpha,c}(x) = \frac{1}{c^k} \tilde{L}_k^\alpha(cx), \tag{4.2}$$

where  $\tilde{L}_k^\alpha(t) = (-1)^k k! L_k^\alpha(t)$  is the monic generalized Laguerre polynomial of degree  $k$ . This system satisfies the relation

$$\tilde{L}_{k+1}^\alpha(t) = (t - A_k) \tilde{L}_k^\alpha(t) - B_k \tilde{L}_{k-1}^\alpha(t),$$

with

$$A_k = 2k + \alpha + 1, \quad B_k = k(k + \alpha) \quad k \geq 1. \tag{4.3}$$

As a general reference on orthogonal polynomials, here we quote [18, ch.18].

**Proposition 4.1** *The monic polynomials  $\{L_k^{\alpha,c}\}_{k \geq 0}$  defined by (4.2) are orthogonal with respect to the weight function  $x^\alpha e^{-cx}$  and satisfy the three-term recurrence relation*

$$L_{k+1}^{\alpha,c}(x) = \left(x - \frac{A_k}{c}\right) L_k^{\alpha,c}(x) - \frac{B_k}{c^2} L_{k-1}^{\alpha,c}(x), \tag{4.4}$$

in which  $A_k$  and  $B_k$  are defined in (4.3).

**Proof** The orthogonality follows from the change of variable  $cx = t$ , that leads to

$$\begin{aligned} \int_0^\infty L_k^{\alpha,c}(x) L_l^{\alpha,c}(x) x^\alpha e^{-cx} dx &= \frac{1}{c^{k+l}} (-1)^{k+l} k! l! \int_0^\infty L_k^\alpha(cx) L_l^\alpha(cx) x^\alpha e^{-cx} dx \\ &= \frac{(-1)^{k+l} k! l!}{c^{k+l+1-\alpha}} \int_0^\infty L_k^\alpha(t) L_l^\alpha(t) t^\alpha e^{-t} dt. \end{aligned}$$

Now, from the recursive relation for the monic generalized Laguerre polynomials  $\{\tilde{L}_k^\alpha\}_{k \geq 0}$

$$\tilde{L}_{k+1}^\alpha(cx) = (cx - A_k) \tilde{L}_k^\alpha(cx) - B_k \tilde{L}_{k-1}^\alpha(cx), \tag{4.5}$$

by (4.2) we obtain

$$c^{k+1} L_{k+1}^{\alpha,c}(x) = c \left(x - \frac{A_k}{c}\right) c^k L_k^{\alpha,c}(x) - B_k c^{k-1} L_{k-1}^{\alpha,c}(x),$$

and then (4.4). □

Using the polynomials  $\{L_k^{\alpha,c}\}_{k \geq 0}$ , the modified moments (see Eq. 4.1) can be written as

$$m_k = \int_0^\infty L_k^{\alpha,c}(x)x^\alpha e^{-cx} J_\nu(x)dx + \int_0^\infty L_k^{\alpha,c}(x)x^\alpha e^{-cx} dx.$$

Clearly, by orthogonality, the second integral is zero for  $k \geq 1$ . Hence, for  $k \geq 1$ , by (4.2) and the following explicit expression for the generalized Laguerre polynomials (see [1, p. 775])

$$L_k^\alpha(x) = \sum_{j=0}^k (-1)^j \binom{k+\alpha}{k-j} \frac{1}{j!} x^j,$$

we have that

$$\begin{aligned} m_k &= \int_0^\infty L_k^{\alpha,c}(x)x^\alpha e^{-cx} J_\nu(x)dx \\ &= \frac{(-1)^k k!}{c^k} \int_0^\infty L_k^\alpha(cx)x^\alpha e^{-cx} J_\nu(x)dx \\ &= \frac{(-1)^k k!}{c^k} \sum_{j=0}^k (-1)^j \binom{k+\alpha}{k-j} \frac{1}{j!} c^j \int_0^\infty x^{\alpha+j} e^{-cx} J_\nu(x)dx \\ &= \frac{(-1)^k k!}{c^k} \sum_{j=0}^k (-1)^j \binom{k+\alpha}{k-j} \frac{1}{j!} c^j \mu_{j,0}, \end{aligned} \tag{4.6}$$

where the last equality comes from (2.2). Finally, for  $k = 0$  we obtain

$$m_0 = \mu_{0,0} + \frac{\Gamma(\alpha + 1)}{c^{\alpha+1}},$$

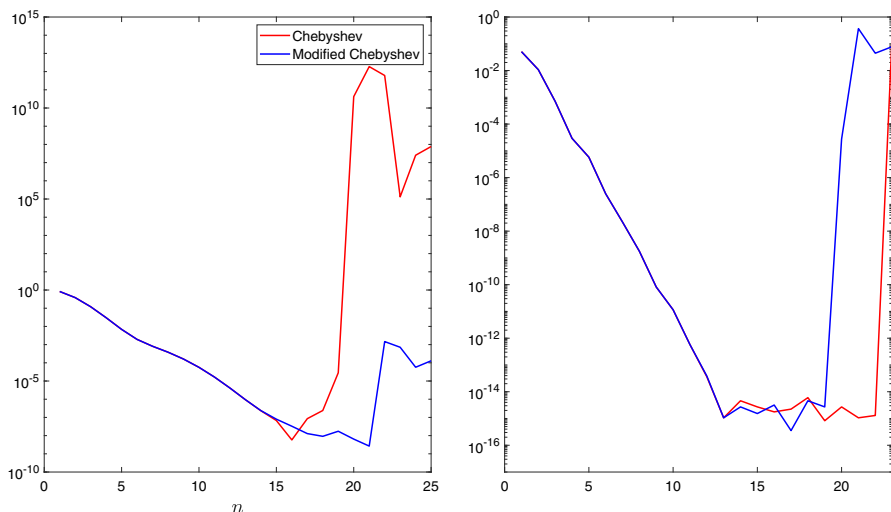
by [7, Sect. 3.381, n.4].

Using the modified moments, we can employ the Chebyshev algorithm, summarized in Algorithm 4.1. We remark that the case  $a_k = b_k = 0$  yields  $p_k(x) = x^k$ , and Algorithm 4.1 reduces to Algorithm 3.1.

**Algorithm 4.1** Initialization

$$\begin{aligned} \alpha_0 &= a_0 + \frac{m_1}{m_0}, \quad \beta_0 = m_0, \\ \sigma_{-1,l} &= 0, \quad l = 1, 2, \dots, 2n - 2, \\ \sigma_{0,l} &= m_l, \quad 0, 1, \dots, 2n - 1, \end{aligned}$$

for  $k = 1, 2, \dots, n - 1$



**Fig. 2** Relative error behavior with respect to  $n$  for  $\nu = 0.5, \alpha = 0.5, c = 0.2$  on the left and for  $\nu = 1, \alpha = 0.5, c = 0.7$  on the right. In both cases  $f(x) = e^{-0.5x}$

for  $l = k, k + 1, \dots, 2n - k - 1$

$$\sigma_{k,l} = \sigma_{k-1,l+1} - (\alpha_{k-1} - a_l)\sigma_{k-1,l} - \beta_{k-1}\sigma_{k-2,l} + b_l\sigma_{k-1,l-1},$$

$$\alpha_k = a_k + \frac{\sigma_{k,k+1}}{\sigma_{k,k}} - \frac{\sigma_{k-1,k}}{\sigma_{k-1,l-1}}, \quad \beta_k = \frac{\sigma_{k,k}}{\sigma_{k-1,k-1}}.$$

In Fig. 2 we compare the results of Algorithms 3.1 and 4.1. We provide only two representative examples that, nevertheless, are sufficient to say that Algorithm 4.1 in general allows to gain stability for further  $5 \div 10$  iterations, working in double precision arithmetic, but in many cases there is no effective improvement.

### 5 A preconditioned Cramer based approach

Let

$$M_k = \begin{bmatrix} \mu_0 & \mu_1 & \cdots & \mu_{k-1} \\ \mu_1 & \mu_2 & \cdots & \mu_k \\ \vdots & \vdots & & \vdots \\ \mu_{k-1} & \mu_k & \cdots & \mu_{2k-2} \end{bmatrix} \in \mathbb{R}^{k \times k},$$

be the moment matrix, and

$$N_k = \begin{bmatrix} \mu_0 & \mu_1 & \cdots & \mu_{k-2} & \mu_k \\ \mu_1 & \mu_2 & \cdots & \mu_{k-1} & \mu_{k+1} \\ \vdots & \vdots & & \vdots & \vdots \\ \mu_{k-1} & \mu_k & \cdots & \mu_{2k-3} & \mu_{2k-1} \end{bmatrix} \in \mathbb{R}^{k \times k}.$$

It is known (see [4, 21]) that the recurrence coefficients in (3.1) can also be written as

$$\alpha_k = \frac{F_{k+1}}{D_{k+1}} - \frac{F_k}{D_k}, \quad \beta_k = \frac{D_{k-1}D_{k+1}}{D_k^2} \quad k \geq 0, \tag{5.1}$$

where

$$\begin{aligned} D_k &= \det(M_k), \quad \text{for } k \geq 1, \\ F_k &= \det(N_k), \quad \text{for } k \geq 2, \end{aligned}$$

and

$$\begin{aligned} D_0 &= D_{-1} = 1, \\ F_0 &= 0, \quad F_1 = \mu_1. \end{aligned}$$

Consider the linear system

$$M_{k+1}x^{(k+1)} = e_{k+1}, \tag{5.2}$$

where  $e_{k+1} = (0, \dots, 0, 1)^T \in \mathbb{R}^{k+1}$ . In the following, we denote by  $x_i^{(k+1)}$  the  $i$ -th component of the solution of (5.2). First of all, we observe that, by Cramer’s rule,

$$\frac{D_k}{D_{k+1}} = x_{k+1}^{(k+1)}.$$

Moreover, since

$$\det(N_k) = -\det M_{k+1,(k)},$$

in which  $M_{k+1,(k)}$  is the matrix  $M_{k+1}$  with the  $k$ -th column substituted by the vector  $e_{k+1}$ , we have that

$$\frac{F_k}{D_{k+1}} = -\frac{\det M_{k+1,(k)}}{\det M_{k+1}} = -x_k^{(k+1)}.$$

Hence, we obtain

$$\frac{F_k}{D_k} = \frac{F_k}{D_{k+1}} \frac{D_{k+1}}{D_k} = -\frac{x_k^{(k+1)}}{x_{k+1}^{(k+1)}}.$$

In this setting, the coefficients  $\alpha_k$  and  $\beta_k$  can be expressed in terms of the components of the solutions of appropriate linear systems as follows:

$$\alpha_k = -\frac{x_{k+1}^{(k+2)}}{x_{k+2}^{(k+2)}} + \frac{x_k^{(k+1)}}{x_{k+1}^{(k+1)}}, \quad \beta_k = \frac{x_k^{(k)}}{x_{k+1}^{(k+1)}}, \quad k \geq 1, \quad (5.3)$$

with

$$\alpha_0 = \frac{\mu_1}{\mu_0}, \quad \beta_0 = \mu_0.$$

The system (5.2) rapidly becomes severely ill conditioned, so that the procedure does not offer any improvement with respect to the Chebyshev algorithm. Nevertheless, since  $M_{k+1}$  is a symmetric positive definite matrix, the idea is to use a bilateral preconditioner in order to solve efficiently (5.2). Analogously to the choice made for the modified Chebyshev approach, here we want to use as preconditioner the moment matrix corresponding to the generalized Laguerre polynomials.

Let  $\eta_k, k \geq 0$ , be the moments relative to the weight function  $x^\alpha e^{-cx}$ , given by

$$\eta_k = \eta_k^{\alpha,c} = \int_0^\infty x^{k+\alpha} e^{-cx} dx = \frac{\Gamma(k+\alpha+1)}{c^{k+\alpha+1}},$$

where we have used again [7, Sect. 3.381, n.4]. We can write

$$\eta_k = \frac{1}{c^{\alpha+1}} \frac{\gamma_k}{c^k},$$

where

$$\gamma_k = \gamma_k^\alpha = \int_0^\infty x^{k+\alpha} e^{-x} dx = \Gamma(k+\alpha+1) \quad (5.4)$$

are the moments relative to the generalized Gauss–Laguerre rule. Hence, we can write the corresponding moment matrix

$$M_k^{\alpha,c} = \begin{bmatrix} \eta_0 & \eta_1 & \cdots & \eta_{k-1} \\ \vdots & \vdots & & \vdots \\ \eta_{k-1} & \eta_k & \cdots & \eta_{2k-2} \end{bmatrix} \in \mathbb{R}^{k \times k},$$

as

$$M_k^{\alpha,c} = \frac{1}{c^{\alpha+1}} E_k M_k^\alpha E_k,$$

where

$$M_k^\alpha = \begin{bmatrix} \gamma_0 & \gamma_1 & \cdots & \gamma_{k-1} \\ \vdots & \vdots & & \vdots \\ \gamma_{k-1} & \gamma_k & \cdots & \gamma_{2k-2} \end{bmatrix} \in \mathbb{R}^{k \times k},$$

and  $E_k = \text{diag}(c^0, c^{-1}, \dots, c^{1-k})$ .

At this point, if we consider the Cholesky decomposition of  $M_k^\alpha$

$$M_k^\alpha = (R_k^\alpha)^T R_k^\alpha,$$

we have

$$M_k^{\alpha,c} = \frac{1}{c^{\alpha+1}} E_k (R_k^\alpha)^T R_k^\alpha E_k = (R_k^{\alpha,c})^T R_k^{\alpha,c},$$

where

$$R_k^{\alpha,c} = \frac{1}{(\sqrt{c})^{\alpha+1}} R_k^\alpha E_k.$$

The following proposition provides the explicit expression for  $R_k^\alpha$ , and therefore for  $R_k^{\alpha,c}$ .

**Proposition 5.1** *The Cholesky decomposition of the matrix  $M_k^\alpha$  is*

$$M_k^\alpha = (R_k^\alpha)^T R_k^\alpha,$$

with

$$R_{ij}^\alpha = \frac{(j-1)!}{(j-i)!} \frac{\Gamma(\alpha+j)}{\sqrt{\Gamma(i)\Gamma(\alpha+i)}}, \quad \text{for } i \leq j \leq k.$$

**Proof** Since the matrix  $M_k^\alpha$  is symmetric, we can restrict the analysis to the case  $i \leq j$ . By (5.4) we know that

$$(M_k^\alpha)_{ij} = \Gamma(i + \alpha + j - 1).$$

Now,

$$\begin{aligned} ((R_k^\alpha)^T R_k^\alpha)_{ij} &= \sum_{l=1}^i R_{lj}^\alpha R_{li}^\alpha \\ &= \Gamma(j)\Gamma(\alpha+j)\Gamma(i)\Gamma(\alpha+i) \sum_{l=1}^i \frac{1}{(j-l)!(i-l)!\Gamma(l)\Gamma(\alpha+l)}. \end{aligned}$$

Writing

$$\binom{x}{y} = \frac{\Gamma(x+1)}{\Gamma(y+1)\Gamma(x-y+1)}, \tag{5.5}$$

with  $x = \alpha + i - 1$  and  $y = l - i$ , we have

$$\frac{1}{\Gamma(\alpha+l)(i-l)!} = \binom{\alpha+i-1}{i-l} \frac{1}{\Gamma(\alpha+i)}.$$

Moreover,

$$\frac{1}{(j-l)!(l-1)!} = \binom{j-1}{l-1} \frac{1}{(j-1)!}.$$

Using the above relations, we obtain

$$((R_k^\alpha)^T R_k^\alpha)_{ij} = \Gamma(\alpha + j)\Gamma(i) \sum_{l=1}^i \binom{\alpha + i - 1}{i - l} \binom{j - 1}{l - 1}.$$

At this point, by the following slight modification of the Chu–Vandermonde identity (see [3]),

$$\sum_{u=1}^q \binom{t}{u-1} \binom{s-t}{q-u} = \binom{s}{q-1},$$

we obtain

$$((R_k^\alpha)^T R_k^\alpha)_{ij} = \Gamma(\alpha + j)\Gamma(i) \binom{\alpha + j + i - 2}{i - 1}.$$

Using again (5.5), with  $x = \alpha + j + i - 2$  and  $y = i + 1$ , it holds

$$\binom{\alpha + j + i - 2}{i - 1} = \frac{\Gamma(i + j + \alpha - 1)}{\Gamma(\alpha + j)\Gamma(i)},$$

and finally

$$((R_k^\alpha)^T R_k^\alpha)_{ij} = \Gamma(i + \alpha + j - 1).$$

□

We observe that the matrix  $R_k^\alpha$  can be written as

$$R_k^\alpha = D_k \tilde{R}_k^\alpha,$$

with

$$(\tilde{R}_k^\alpha)_{ij} = \frac{(j-1)!\Gamma(\alpha + j)}{(j-i)!\Gamma(i)\Gamma(\alpha + i)}, \quad \text{for } i \leq j,$$

and  $D_k$  diagonal matrix such that

$$(D_k)_{ii} = \sqrt{\Gamma(i)\Gamma(\alpha + i)}.$$



Since

$$(R_k^\alpha)^{-1} = (\tilde{R}_k^\alpha)^{-1}(D_k^\alpha)^{-1}.$$

and

$$(\tilde{R}_k^\alpha)^{-1}_{ij} = (-1)^{i+j}(\tilde{R}_k^\alpha)_{ij},$$

we have that the explicit expression for  $(R_k^\alpha)^{-1}$  is given by

$$(R_k^\alpha)^{-1}_{ij} = (-1)^{i+j} \frac{\sqrt{(j-1)! \Gamma(\alpha+j)}}{(j-i)! \Gamma(i) \Gamma(\alpha+i)}, \quad \text{for } i \leq j.$$

Therefore, the matrix  $(R_k^{\alpha,c})^{-1}$  can be written as

$$(R_k^{\alpha,c})^{-1} = (\sqrt{c})^{\alpha+1} E_k^{-1} (\tilde{R}_k^\alpha)^{-1} (D_k^\alpha)^{-1},$$

with

$$(R_k^{\alpha,c})^{-1}_{ij} = \frac{\sqrt{c^{\alpha+1}} c^{i-1} (-1)^{i+j} \sqrt{(j-1)! \Gamma(\alpha+j)}}{(j-i)! \Gamma(i) \Gamma(\alpha+i)}. \tag{5.6}$$

Finally, the linear system (5.2) can be preconditioned as

$$(R_{k+1}^{\alpha,c})^{-T} M_{k+1} (R_{k+1}^{\alpha,c})^{-1} y^{(k+1)} = (R_{k+1}^{\alpha,c})^{-T} e_{k+1}, \tag{5.7}$$

with

$$x^{(k+1)} = (R_{k+1}^{\alpha,c})^{-1} y^{(k+1)}. \tag{5.8}$$

Since the matrix  $M_{k+1}$  can be written as  $M_{k+1} = M_{k+1}^{\alpha,c} + M_{k+1,0}^{\alpha,c}$ , where  $M_{k+1,0}^{\alpha,c}$  is the matrix of the core moments defined by Eq. (2.2), we have that

$$\begin{aligned} (R_{k+1}^{\alpha,c})^{-T} M_{k+1} (R_{k+1}^{\alpha,c})^{-1} &= (R_{k+1}^{\alpha,c})^{-T} (M_{k+1}^{\alpha,c} + M_{k+1,0}^{\alpha,c}) (R_{k+1}^{\alpha,c})^{-1} \\ &= (R_{k+1}^{\alpha,c})^{-T} M_{k+1}^{\alpha,c} (R_{k+1}^{\alpha,c})^{-1} + (R_{k+1}^{\alpha,c})^{-T} M_{k+1,0}^{\alpha,c} (R_{k+1}^{\alpha,c})^{-1} \\ &= I_{k+1} + (R_{k+1}^{\alpha,c})^{-T} M_{k+1,0}^{\alpha,c} (R_{k+1}^{\alpha,c})^{-1} := Q_{k+1}, \end{aligned} \tag{5.9}$$

where  $I_{k+1}$  is the identity matrix. The system (5.7) becomes

$$(I_{k+1} + (R_{k+1}^{\alpha,c})^{-T} M_{k+1,0}^{\alpha,c} (R_{k+1}^{\alpha,c})^{-1}) y^{(k+1)} = (R_{k+1}^{\alpha,c})^{-T} e_{k+1}. \tag{5.10}$$

In Table 1 we show the remarkable effect of the preconditioning.

**Table 1** The Euclidean condition number of the matrix  $M_k$  and of the preconditioned matrix  $Q_k$ , defined in (5.9), for different values of  $k$

$k$	5	10	15	20	25	30
$\kappa_2(M_k)$	$2.4e + 13$	$7.8e + 32$	$1.0e + 51$	$2.2e + 69$	$4.6e + 88$	$1.1e + 107$
$\kappa_2(Q_k)$	$1.0e + 00$	$1.3e + 00$	$1.4e + 00$	$1.4e + 00$	$1.5e + 00$	$1.6e + 00$

In this example  $\nu = 0.9, \alpha = 0.1$  and  $c = 0.1$

We observe that, since  $(R_{k+1}^{\alpha,c})^{-1}$  is an upper triangular matrix, the components of the solution used in (5.1) can be written as

$$x_k^{(k+1)} = (R_{k+1}^{\alpha,c})_{kk}^{-1} y_k^{(k+1)} + (R_{k+1}^{\alpha,c})_{k,k+1}^{-1} y_{k+1}^{(k+1)}, \tag{5.11}$$

$$x_{k+1}^{(k+1)} = (R_{k+1}^{\alpha,c})_{k+1,k+1}^{-1} y_{k+1}^{(k+1)}. \tag{5.12}$$

We notice that the numerical implementation of the procedure to calculate  $\alpha_k$  and  $\beta_k$  as in (5.3), by using expressions (5.11) and (5.12), starts to show instability around  $k = 60 \div 70$ , depending on the parameters, when  $x_k^{(k+1)}$  and  $x_{k+1}^{(k+1)}$  are close to the underflow. In order to gain more stability the idea is to rewrite the coefficients  $\alpha_k$  and  $\beta_k$ , for  $k \geq 1$ , in terms of the components of the vectors  $y^{(k)}, y^{(k+1)}, y^{(k+2)}$ , defined in (5.8), and exploit the relation (5.6). Indeed, we observe that for  $i \sim j \sim k$ ,

$$(R_k^{\alpha,c})_{ij}^{-1} \sim \frac{c^k}{k!},$$

and therefore  $y_i^{(k+1)} \gg x_i^{(k+1)}$  for  $i = k, k + 1$ . By (5.1) and (5.6), we obtain

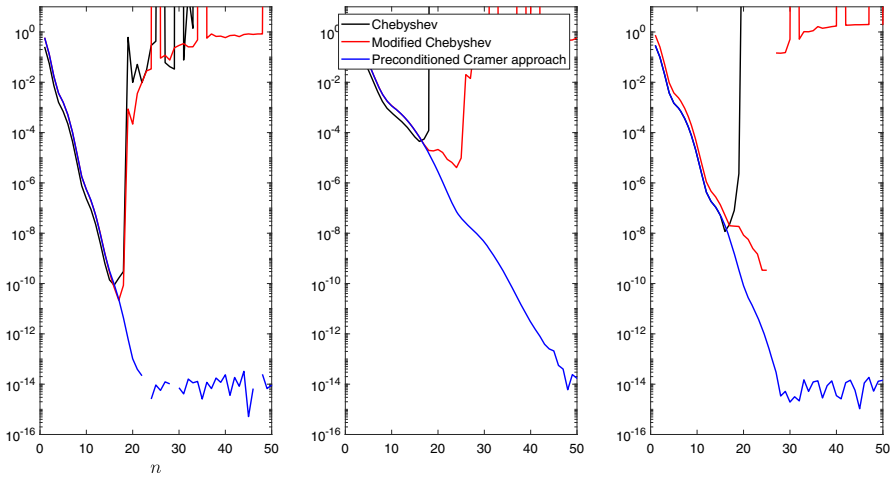
$$\alpha_k = -\frac{\sqrt{(k+1)(\alpha+k+1)}}{c} \left( \frac{y_{k+1}^{(k+2)}}{y_{k+2}^{(k+2)}} - \sqrt{(k+1)(\alpha+k+1)} \right) + \frac{\sqrt{k(\alpha+k)}}{c} \left( \frac{y_k^{(k+1)}}{y_{k+1}^{(k+1)}} - \sqrt{k(\alpha+k)} \right), \tag{5.13}$$

$$\beta_k = \frac{\sqrt{k(\alpha+k)}}{c} \left( \frac{y_k^{(k)}}{y_{k+1}^{(k+1)}} \right). \tag{5.14}$$

The final procedure, explained in Algorithm 5.1, allows to work with  $80 \div 90$  points, dependently on the parameters.

**Algorithm 5.1** Define  $\alpha_0, \beta_0, \beta_1, y^{(1)}, y^{(2)}$ .

- for  $k = 2, \dots, n - 1$
- calculate  $y^{(k+1)}$  by solving (5.10)
- $\beta_k \leftarrow y^{(k+1)}, y^{(k)}$  by (5.14)
- $\alpha_{k-1} \leftarrow y^{(k+1)}, y^{(k)}$  by (5.13)
- end

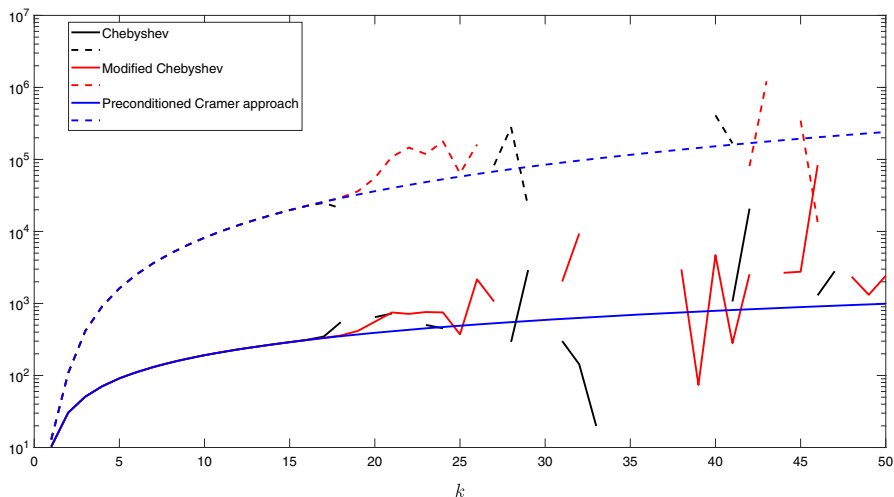


**Fig. 3** Relative error histories for  $\nu = 1, \alpha = 0.7, c = 0.3$  on the left, for  $\nu = 0.9, \alpha = 0.1, c = 0.1$  in the middle and for  $\nu = 1.5, \alpha = 0.5, c = 0.2$  on the right. In all cases  $f(x) = e^{-0.5x}$

We remark that the computational cost of Algorithm 5.1 is, in general, higher than the one of the Chebyshev algorithm, which requires  $\mathcal{O}(n^2)$  operations. This is due to the solution of system (5.10) in which the coefficient matrix  $Q_{k+1}$  (5.9) is symmetric and positive definite, but full. Anyway, the point in favour is that  $Q_{k+1}$  is actually a perturbation of the identity (thanks to the preconditioner), so that using for instance the Conjugate Gradient it is possible to achieve a good approximate solution in just few iterations. This allows to keep the cost in the order of  $\mathcal{O}(n^2)$  operations.

In Fig. 3 we compare the results of Algorithms 3.1, 4.1 and 5.1. For all the examples we can say that only the preconditioned Cramer based approach allows to achieve a relative error around the machine precision, while the Chebyshev and modified Chebyshev algorithms lose stability much earlier. In fact, as shown in Fig. 4, Algorithms 3.1 and 4.1 start to provide inaccurate values of the coefficients  $\alpha_k$  and  $\beta_k$  for  $k$  around  $15 \div 25$ , while Algorithm 5.1 is definitely more stable. Since the plot is in logarithmic scale, the missing parts of the curves are relative to negative entries.

Further examples are reported in Table 2, where we consider different values of the parameters  $\nu, \alpha, c$  and test the performance of the Gaussian rule (3.2) for the integral in (1.1). In particular, working with  $f(x) = e^{-0.5x}$  and  $f(x) = (1 + e^{-x})^{-1}$ , we report the total number of points used in formula (3.2), that is,  $2n$ , necessary to achieve a relative error  $\sim 10^{-8}$ . In general, at least in the interval  $[0, 1]$ , we can observe that the value of  $\alpha$  does not significantly affect the results. In the case of the entire function  $f(x) = e^{-0.5x}$ , we have that the complexity of the problem increases with increasing  $\nu$  and decreasing  $c$ . As for the meromorphic function  $f(x) = (1 + e^{-x})^{-1}$ , we observe different behaviors depending on the parameters  $\nu$  and  $c$ . For small values of  $c$  (that is,  $c \leq 0.3$ ) the method is more accurate for increasing  $\nu$ , while for  $c > 0.3$  the behavior is opposite. On the other side, for  $\alpha$  and  $\nu$  fixed, by increasing the value of  $c$  the complexity of the problem reduces.



**Fig. 4** Plot of the coefficients  $\alpha_k$  (solid lines) and  $\beta_k$  (dashed lines) for  $\nu = 0.9$ ,  $\alpha = 0.1$  and  $c = 0.1$

**Table 2** Number of function evaluations necessary to achieve a relative error  $\sim 10^{-8}$  by changing the parameters of the weight function

$\alpha$	$c$	$f(x) = e^{-0.5x}$			$f(x) = (1 + e^{-x})^{-1}$		
		$\nu = 1$	$\nu = 10$	$\nu = 20$	$\nu = 1$	$\nu = 10$	$\nu = 20$
0.1	0.15	36	46	60	160	118	64
	0.3	22	28	40	80	80	50
	0.5	16	22	30	50	56	52
	1	12	18	26	28	40	80
0.3	0.15	36	46	58	162	126	96
	0.3	24	28	38	82	66	50
	0.5	16	22	30	52	56	60
	1	12	18	30	28	42	56
0.5	0.15	48	44	52	156	130	100
	0.3	24	28	32	84	66	56
	0.5	16	22	30	54	64	62
	1	12	18	30	28	36	72
0.7	0.15	38	42	52	158	134	98
	0.3	24	30	34	88	64	60
	0.5	18	22	28	56	58	50
	1	12	18	28	28	36	46
1	0.15	40	44	54	128	118	102
	0.3	24	30	39	88	70	54
	0.5	18	22	28	52	46	40
	1	12	18	30	24	40	54

### 6 Electromagnetic fields

In this section we deal with an interesting application arising in geophysical electromagnetic (EM) survey. We consider the theoretical EM response, i.e. the electromagnetic fields components, over a  $N$ -layered earth due to vertical magnetic dipoles above the surface, composed of a transmitter coil and couples of receiver coils. The receiver couples are placed at different distances (offsets) from the transmitter coil. In this case, the electromagnetic induction effect, encoded in the first-order linear differential equations, produces eddy alternating currents in the soil which on their turn, induce response EM fields. Under the assumption that each layer is characterized by a certain conductivity  $\sigma_i$  and thickness  $h_i$  (the deeper layer is assumed to have infinite thickness), the general integral solutions of Maxwell equations are given by (see [16, 22])

$$H_z^{(N)} = \frac{m}{4\pi} \int_0^\infty (1 + R_0(\lambda)e^{-2H\lambda})\lambda^2 J_0(\lambda r)d\lambda,$$

$$H_\rho^{(N)} = \frac{m}{4\pi} \int_0^\infty (1 - R_0(\lambda)e^{-2H\lambda})\lambda^2 J_1(\lambda r)d\lambda,$$

where  $m$  is the magnetic moment,  $H$  is the height of the dipole with respect to the surface and  $r$  is the offset. In the above formulas  $R_0(\lambda)$  is the reflection term, recursively defined by

$$R_0(\lambda) = \frac{R_1(\lambda) + \Psi_1(\lambda)}{R_1(\lambda)\Psi_1(\lambda) + 1},$$

$$R_j(\lambda) = \frac{R_{j+1}(\lambda) + \Psi_{j+1}(\lambda)}{R_{j+1}(\lambda)\Psi_{j+1}(\lambda) + 1} e^{-2u_j(\lambda)h_j}, \quad j = 1, \dots, N - 1,$$

$$R_N(\lambda) = 0,$$

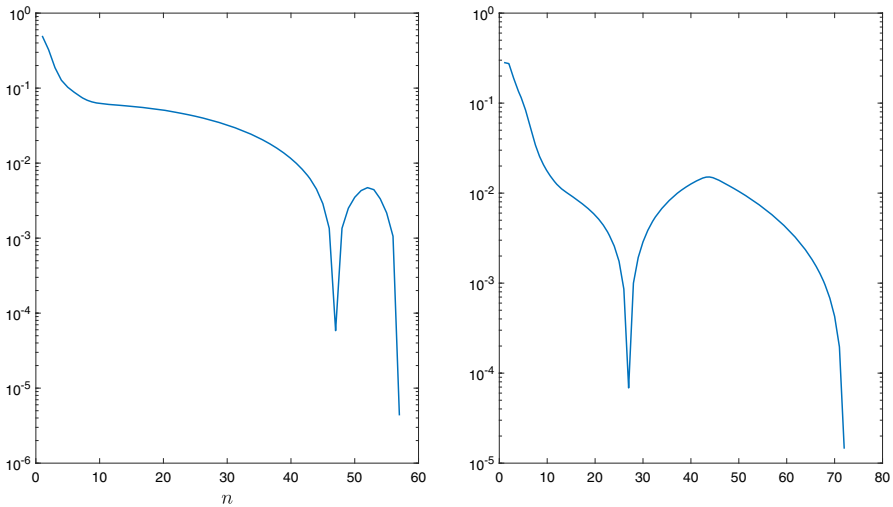
with

$$\Psi_j(\lambda) = \frac{u_{j-1}(\lambda) - u_j(\lambda)}{u_{j-1}(\lambda) + u_j(\lambda)}, \quad j = 1, \dots, N,$$

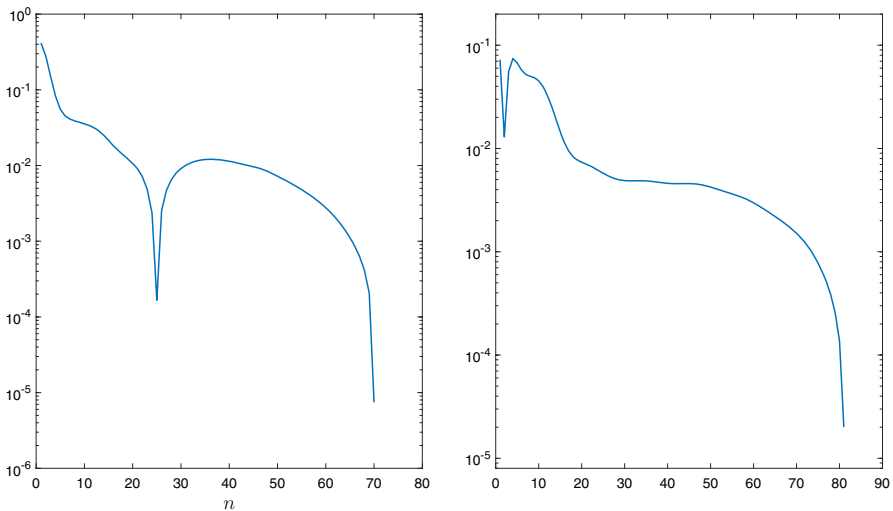
in which  $u_0(\lambda) = \lambda$  and  $u_j(\lambda) = \sqrt{\lambda^2 - k_j^2}$ ,  $k_j = \sqrt{-i\omega\mu\sigma_j}$ , for  $j = 1, \dots, N$ , where  $\omega$  is the angular frequency and  $\mu$  is the magnetic permeability of vacuum. We refer to [22, Section 4] and the reference therein for an exhaustive background. Since in the case of conductivity of geological materials only the imaginary part of the fields are considered, using the change of variable  $\lambda r = x$ , we obtain

$$\Im(H_z^{(N)}) = \frac{m}{4\pi r^3} \int_0^\infty \Im\left(R_0\left(\frac{x}{r}\right)\right) e^{-\frac{2H}{r}x} x^2 J_0(x) dx, \tag{6.1}$$

$$\Im(H_\rho^{(N)}) = -\frac{m}{4\pi r^3} \int_0^\infty \Im\left(R_0\left(\frac{x}{r}\right)\right) e^{-\frac{2H}{r}x} x^2 J_1(x) dx. \tag{6.2}$$



**Fig. 5** Relative error history for the computation of  $\mathfrak{N}(H_z^{(3)})$  with respect to  $n$  for parameters  $H = 0.4$  m,  $r = 3$  m,  $h_1 = 2.5$  m,  $h_2 = 0.5$  m,  $\sigma_1 = 0.05$  S/m,  $\sigma_2 = 0.0055$  S/m,  $\sigma_3 = 0.02$  S/m on the left and for parameters  $H = 0.5$  m,  $r = 3$  m,  $h_1 = 2.5$  m,  $h_2 = 0.5$  m,  $\sigma_1 = 0.033$  S/m,  $\sigma_2 = 0.1$  S/m,  $\sigma_3 = 0.01$  S/m on the right



**Fig. 6** Relative error history for the computation of  $\mathfrak{N}(H_\rho^{(3)})$  with respect to  $n$  for parameters  $H = 0.4$  m,  $r = 6$  m,  $h_1 = 2.5$  m,  $h_2 = 0.5$  m,  $\sigma_1 = 0.333$  S/m,  $\sigma_2 = 0.02$  S/m,  $\sigma_3 = 0.1$  S/m on the left and for parameters  $H = 0.4$  m,  $r = 6$  m,  $h_1 = 3.5$  m,  $h_2 = 1.5$  m,  $\sigma_1 = 0.033$  S/m,  $\sigma_2 = 0.1$  S/m,  $\sigma_3 = 0.01$  S/m on the right

In the numerical experiments we use Algorithm 5.1 to evaluate the fields (6.1) and (6.2) in the case of a 3-layered underground model. Referring to (1.1), in our examples we set  $\nu = 0, 1, \alpha = 0, c = \frac{2H}{r}$  and  $f(x) = \mathfrak{N}\left(R_0\left(\frac{x}{r}\right)\right)x^2$ . Regarding the choice of the parameters  $\sigma_i$  and  $h_i$ , i.e. of the underground models, we consider real life values of river levees (see e.g. [6]).

In Figs. 5 and 6 we provide the relative error between the approximated fields  $\mathfrak{S}(H_z^{(3)})$  and  $\mathfrak{S}(H_\rho^{(3)})$ , and a corresponding reference solution (see e.g. [15, 20]). In all examples we stop the procedure when the relative error is less than  $10^{-5}$ . The main reason of this choice is that for these parameters the method works with  $k_{\max} \sim 85$ , but in order to reach higher accuracy more points are necessary. To overcome this issue, extended precision arithmetic is necessary (see e.g. [12]), but this is beyond the purpose of the present paper.

## 7 Conclusions

In this work a Gaussian type quadrature rule for the computation of integrals involving fractional powers, exponentials and Bessel functions of the first kind, is presented. In this framework, the techniques commonly used in the computation of the coefficients of the three-term recurrence relation, for the corresponding orthogonal polynomials, are the standard and the modified Chebyshev algorithm. Since it is well known that the results of these methods can be inaccurate for growing number of quadrature points and especially for unbounded intervals of integration, an alternative and very stable approach, based on the preconditioning of the moment matrix, is developed. In particular, an algorithm, which exploits the Cramer rule to compute the coefficients by solving a linear system with the moment matrix, is presented. The numerical experiments confirm the reliability of this preconditioned Cramer based approach and shows that it is definitely more stable than the modified Chebyshev algorithm, since, in double precision arithmetic, it allows to work with further  $40 \div 60$  points, depending on the parameters.

We remark that, in principle, the approach can be applied to each weight function that is not so far to the standard ones, because it is necessary to be able to construct the preconditioner. Finally, we also point out that, similarly to the Gauss Laguerre rule, the weights decay exponentially and therefore a truncated approach can also be introduced as well.

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## Declarations

**Conflict of interest** The authors declare that there is not conflict of interest.

## References

1. Abramowitz, M., Stegun, I.A.: Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables, 7th edn. Dover Publications Inc, New York (1970)
2. Asheim, A., Huybrechs, D.: Complex Gaussian quadrature for oscillatory integral transforms. IMA J. Numer. Anal. **33**(4), 1322–1341 (2013). <https://doi.org/10.1093/imanum/drs060>

3. Askey, R.: Orthogonal polynomials and special functions. Reg. Conf. Ser. Appl. Math. **21**, 59–60 (1975)
4. Davis, P.J., Rabinowitz, P.: Methods of Numerical Integration. Academic Press Inc, New York (1975)
5. Denich, E.: Error estimates for a Gaussian rule involving Bessel functions. J. Comput. Appl. Math. **436**, 115448 (2024). <https://doi.org/10.1016/j.cam.2023.115448>
6. Francese, R., Morelli, G., Santos, F.M., Bondesan, A., Giorgi, M., Tesarollo, A.: An integrated geophysical approach to scan river embankments. Fast Times **23**(3), 86–96 (2018)
7. Gradshteyn, I.S., Ryzhik, I.M.: Tables of Integrals, Series, and Products. Academic Press, New York (1980)
8. Gautschi, W.: On the construction of Gaussian quadrature rules from modified moments. Math. Comput. **24**(110), 245–260 (1980). <https://doi.org/10.1090/S0025-5718-1970-0285117-6>
9. Gautschi, W.: On generating orthogonal polynomials. SIAM J. Sci. Stat. Comput. **3**(3), 289–317 (1982). <https://doi.org/10.1137/0903018>
10. Gautschi, W.: Algorithm 726: ORTHPOL—a package of routines for generating orthogonal polynomials and Gauss-type quadrature rules. ACM Trans. Math. Softw. **20**(1), 21–62 (1994). <https://doi.org/10.1145/174603.174605>
11. Gautschi, W.: Orthogonal polynomials: applications and computation. Acta Numer. (1996). <https://doi.org/10.1017/S0962492900002622>
12. Gautschi, W.: Computing polynomials orthogonal with respect to densely oscillating and exponentially decaying weight functions and related integrals. J. Comput. Appl. Math. **184**, 493–504 (2005). <https://doi.org/10.1016/j.cam.2005.01.023>
13. Gautschi, W.: Orthogonal polynomials, quadrature, and approximation: computational methods and software (in Matlab). In: Marcellán, F., Van Assche, W. (eds.) Orthogonal Polynomials and Special Functions. Lecture Notes in Mathematics, vol. 1883. Springer, Berlin (2006). [https://doi.org/10.1007/978-3-540-36716-1\\_1](https://doi.org/10.1007/978-3-540-36716-1_1)
14. Golub, G.H., Welsch, J.H.: Calculation of Gauss quadrature rules. Math. Comput. **23**(106), 221–230 (1969). <https://doi.org/10.1090/S0025-5718-69-99647-1>
15. Guptasarma, D., Singh, B.: New digital linear filters for Hankel  $J_0$  and  $J_1$  transform. Geophys. Prospect. **45**, 745–762 (1997). <https://doi.org/10.1046/j.1365-2478.1997.500292.x>
16. Ingeman-Nielsen, T., Baumgartner, F.: CR1Dmod: a Matlab program to model 1D complex resistivity effects in electrical and electromagnetic surveys. Comput. Geosci. **32**, 1411–1419 (2006). <https://doi.org/10.1016/j.cageo.2006.01.001>
17. Laurie, D.P.: Computation of Gauss-type quadrature formulas. J. Comput. Appl. Math. **127**, 201–217 (2001). [https://doi.org/10.1016/S0377-0427\(00\)00506-9](https://doi.org/10.1016/S0377-0427(00)00506-9)
18. Olver, F., Lozier, D., Boisvert, R., Clark, C.: The NIST Handbook of Mathematical Functions. Cambridge University Press, New York (2010)
19. Sack, R.A., Donovan, A.F.: An algorithm for Gaussian quadrature given modified moments. Numer. Math. **18**, 465–478 (1972). <https://doi.org/10.1007/BF01406683>
20. Singh, N.P., Mogi, T.: EMDPLER: a F77 program for modelling the EM response of dipolar sources over the non-magnetic layer earth models. Comput. Geosci. **36**, 430–440 (2010). <https://doi.org/10.1016/j.cageo.2009.08.009>
21. Szegő, G.: Orthogonal Polynomials, 4th edn. American Mathematical Society, Providence (1975). <https://doi.org/10.1090/S0002-9939-2010-10592-0>
22. Ward, S.H., Hohmann, G.W.: Electromagnetic theory for geophysical applications. In: Nabighian, M.N. (ed.) Electromagnetic Methods in Applied Geophysics, pp. 131–311. Tulsa, Oklahoma (1988). <https://doi.org/10.4236/wjnst.2016.64021>
23. Watson, G.N.: A Treatise on the Theory of Bessel Functions, 2nd edn. Cambridge University Press, Cambridge (1966)
24. Wheeler, J.C.: Modified moments and Gaussian quadratures. Rocky Mt. J. Math. **4**(2), 287–296 (1974). <https://doi.org/10.1216/RMJ-1974-4-2-287>
25. Wong, R.S.C.: Quadrature formulas for oscillatory integral transforms. Numer. Math. **39**, 351–360 (1982)



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