Error estimates for a Gaussian rule involving Bessel functions

Eleonora Denich

Department of Mathematics and Geosciences, via Valerio 12/1, Trieste, 34127, Italy

A B S T R A C T

This paper deals with the estimation of the quadrature error of a Gaussian formula for weight functions involving powers, exponentials and Bessel functions of the first kind. For this purpose, in this work the averaged and generalized averaged Gaussian rules are employed, together with a tentative a priori approximation of the error. The numerical examples confirm the reliability of these approaches.

1. Introduction

In this work we consider the approximation of integrals of the type

$$I_{\nu,\alpha,c}(f) = \int_0^\infty f(x) x^\alpha e^{-cx} J_\nu(x) dx, \tag{1}$$

where

$$J_\nu(x) = \sum_{m=0}^\infty \frac{(-1)^m}{m!\,\Gamma(m+\nu+1)} \left(\frac{x}{2}\right)^{2m+\nu}$$

is the Bessel function of the first kind of order $\nu \geq 0$ (see [1] for a background), $\alpha > -1$, $c > 0$ and f is a smooth function. We point out that integrals of type (1) are strongly related to Hankel transforms, which commonly appear in problems of mathematical physics and applied mathematics having axial symmetry. An example of application arises in geophysical electromagnetic survey. In particular, electromagnetic fields over a layered earth due to magnetic dipoles above the surface can be expressed in integral form as in (1) (see [2]).

Since $|J_\nu(x)| \leq 1$, for $\nu \geq 0$, $x \in \mathbb{R}$ (see [3, p. 362]), a Gaussian quadrature rule for the computation of integrals of type (1) was constructed in [4] by rewriting (1) as

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

with

$$I_{\nu,\alpha,c}^J(f) := \int_0^\infty f(x) x^\alpha e^{-cx} [J_\nu(x) + 1] dx, \tag{2}$$

E-mail address: eleonora.denich@phd.units.it.

and

$$I_{\alpha,c}^L(f) := \int_0^\infty f(x)x^\alpha e^{-cx}dx. \tag{3}$$

In this setting, the authors considered the approximations

$$I_{\nu,\alpha,c}^J(f) \approx I_n^J(f) \quad \text{and} \quad I_{\alpha,c}^L(f) \approx I_n^L(f),$$

where

$$I_n^J(f) = \sum_{i=1}^n w_i^{(n)} f\left(x_i^{(n)}\right) \tag{4}$$

is the Gaussian rule relative to the weight function

$$w_{\nu,\alpha,c}(x) := x^\alpha e^{-cx}[J_\nu(x) + 1] \quad \text{on} \quad [0, +\infty), \tag{5}$$

and

$$I_n^L(f) = \sum_{i=1}^n \lambda_i^{(n)} f\left(\xi_i^{(n)}\right) \tag{6}$$

is a slight modification of the Gauss–Laguerre quadrature rule, i.e., relative to the weight function

$$w_{\alpha,c}(x) = x^\alpha e^{-cx} \quad \text{on} \quad [0, +\infty). \tag{7}$$

Clearly, it is possible to consider a change of variable in (3) in order to work with the standard Laguerre rule, but our choice allows to treat in the same way integrals (2) and (3).

Denoting by $I_n(f)$ the n-point Gaussian rule for the integral

$$I(f) = \int_0^{+\infty} f(x)w(x)dx,$$

in which w is a generic weight function, it is not easy, in general, to derive an accurate estimate of the error

$$E_n(f) = I(f) - I_n(f). \tag{8}$$

A classical approach is to consider the $(2n+1)$-point Gauss–Kronrod quadrature rule associated with the n-point Gaussian formula $I_n(f)$ (see [5–7]). However, in [8] the nonexistence of Gauss–Kronrod rules, for $n > 2$, with real nodes and positive weights for the Gauss–Laguerre formula was proved. As consequence, this approach is not suitable for our case.

An alternative approach was proposed by Laurie [9], who introduced the so-called anti-Gaussian quadrature rule A_{n+1}, corresponding to I_n. It is a $(n + 1)$-point formula of degree $2n - 1$ which integrates polynomial of degree up to $2n + 1$ with an error equal in magnitude but of opposite sign to one of the n-point Gaussian formula. Then the idea is to estimate error (8) as

$$E_n(f) \approx \tilde{A}_{2n+1}(f) - I_n(f),$$

where the $(2n + 1)$-point formula

$$\tilde{A}_{2n+1}(f) = \frac{1}{2}\left(A_{n+1}(f) + I_n(f)\right)$$

is commonly named averaged Gaussian formula. The anti-Gaussian rule always exists, it is guaranteed to have real nodes and positive weights, and at most one of the nodes may be outside the integration interval (see [9]).

A more general formula, given by

$$H_{2n+1}(f) = \frac{1}{2+\gamma}\left((1+\gamma)I_n(f) + A_{n+1}(f)\right), \quad \gamma > 0, \tag{9}$$

was considered by Enrich in [10]. In particular, he constructed (9), for the Laguerre and Hermite weight functions, with the parameter γ chosen to reach the highest degree of exactness, that is, $2n + 1$. We refer to this formula as the generalized averaged Gaussian rule.

More recently, Spalević [11] derived a parameter free method for constructing generalized averaged Gauss rules for any weight function for which all moments exist. We denote these quadrature formulas by $\hat{A}_{2n+1}$. They have degree of exactness at least $2n + 1$ and are guaranteed to have real nodes and positive weights. Then the error is estimated as

$$E_n(f) \approx \hat{A}_{2n+1}(f) - I_n(f). \tag{10}$$

In this paper the averaged Gauss rules $\tilde{A}_{2n+1}^J$, $\tilde{A}_{2n+1}^L$ and generalized averaged Gauss rules $\hat{A}_{2n+1}^J$, $\hat{A}_{2n+1}^L$, corresponding to I_n^J and I_n^L, respectively, are constructed and used to estimate the error

$$E_{n,\nu,\alpha,c}(f) = E_{n,\nu,\alpha,c}^J(f) - E_{n,\alpha,c}^L(f), \tag{11}$$

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where

$$E^J_{n,v,\alpha,c}(f) = I^J_{v,\alpha,c}(f) - I^J_n(f) \quad \text{and} \quad E^L_{n,\alpha,c}(f) = I^L_{\alpha,c}(f) - I^L_n(f). \tag{12}$$

Unfortunately, the use of the heavy notation $E^{(\cdot)}_{n,v,\alpha,c}$ is necessary to avoid confusion with some general results reported in the paper.

The averaged and generalized averaged Gaussian rules are easy to construct and, moreover, typically lead to quite accurate estimates of (10) (see [12]). However, sometimes it can be useful to have at disposal an a priori estimate of the error to have an idea of the number of points necessary to reach a prescribed accuracy. In this view, here we also present a tentative a priori approximation of the quadrature error. In particular, by interpreting $w_{v,\alpha,c}$ as a perturbation of the weight function of the Gauss–Laguerre rule, the idea is to employ a result due to Barrett [13] and relative to the asymptotic behavior of the error of the Gauss–Laguerre formula, to estimate $E^L_{n,\alpha,c}$ and $E^J_{n,v,\alpha,c}$. Moreover, similarly to the Gauss–Laguerre rule, it can be verified that the weights of I^J_n decay exponentially. Hence, having at disposal a reliable error estimate, a truncated approach can also be introduced, but not considered in the present paper.

Throughout this work we use the symbol $\approx$ to indicate a generic approximation. The symbol $\sim$ is used to express the asymptotic equality.

This paper is organized as follows. Sections 2 and 3 deals with the representation of averaged and generalized averaged Gaussian rules. Moreover, some theoretical and experimental properties of the quadrature formulas are described. In Section 4 a tentative error approximation, which allows to have an a priori estimate of the error behavior, is presented. Section 5 deals with the discussion of some numerical examples, which show the performances of the error estimates. Concluding remarks can be found in Section 6.

2. Construction of averaged Gaussian rules

Let w be a generic weight function on $[0, +\infty)$ and consider the corresponding Gaussian quadrature formula

$$I_n(f) = \sum_{i=1}^{n} \sigma_i^{(n)} f\left(\tau_i^{(n)}\right), \tag{13}$$

of degree $2n - 1$, for the integral

$$I(f) = \int_0^{+\infty} f(x)w(x)dx.$$

Denoting by $\alpha_k \in \mathbb{R}$, $\beta_k > 0$ the recursion coefficients for the sequences of monic orthogonal polynomials $\{\pi_j\}_{j\geq 0}$ relative to the weight function w, the Gaussian rule (13) can be associated with the symmetric tridiagonal matrix

$$J_n = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & 0 \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & \\ & \sqrt{\beta_2} & \alpha_2 & \ddots & \\ & & \ddots & \ddots & \sqrt{\beta_{n-1}} \\ 0 & & & \sqrt{\beta_{n-1}} & \alpha_{n-1} \end{bmatrix} \in \mathbb{R}^{n\times n}. \tag{14}$$

It is well known that the eigendecomposition of the above matrix provides the nodes $\tau_i^{(n)}$ and the weights $\sigma_i^{(n)}$, $i = 1, \ldots, n$, of the Gaussian rule I_n (see e.g. [14] and the references therein). Now, the corresponding $(n + 1)$-point anti-Gaussian quadrature formula

$$A_{n+1}(f) := \sum_{i=1}^{n+1} \tilde{\sigma}_i^{(n+1)} f\left(\tilde{\tau}_i^{(n+1)}\right), \tag{15}$$

is such that

$$I(p) - A_{n+1}(p) = -\left(I(p) - I_n(p)\right), \quad \forall p \in \mathbb{P}_{2n+1}, \tag{16}$$

where $\mathbb{P}_{2n+1}$ denotes the space of polynomials of degree at most $2n+1$. Laurie [9] showed that formula (15) is associated with the symmetric tridiagonal matrix $\tilde{J}_{n+1} \in \mathbb{R}^{(n+1)\times(n+1)}$ defined by

$$\tilde{J}_{n+1} = \begin{bmatrix} J_n & e_n\sqrt{2\beta_n} \\ e_n^T\sqrt{2\beta_n} & \alpha_n \end{bmatrix}, \tag{17}$$

where $e_n = (0, \ldots, 0, 1)^T \in \mathbb{R}^n$. Therefore, having at disposal the recurrence coefficients α_k and β_k, it is trivial to compute the nodes $\tilde{\tau}_i^{(n+1)}$ and the weights $\tilde{\sigma}_i^{(n+1)}$, $i = 1, \ldots, n + 1$, of the anti-Gaussian rule. Moreover, quadrature formula (15) has the following properties (see [9, Theorem 1]):

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1. $\tilde{\sigma}_i^{(n+1)} > 0$, $i = 1, \ldots, n+1$;
2. the nodes $\tilde{\tau}_i^{(n+1)}$, $i = 1, \ldots, n+1$, are all real and are interlaced by those of the Gaussian formula I_n, that is,

$$\tilde{\tau}_1^{(n+1)} < \tau_1^{(n)} < \tilde{\tau}_2^{(n+1)} < \cdots < \tau_n^{(n)} < \tilde{\tau}_{n+1}^{(n+1)};$$

3. $\tilde{\tau}_i^{(n+1)} \in [0, +\infty)$, for $i \geq 2$;
4. $\tilde{\tau}_1^{(n+1)} \in [0, +\infty)$ if and only if

$$\frac{\pi_{n+1}(0)}{\pi_{n-1}(0)} \geq \beta_n, \quad n \geq 1. \tag{18}$$

At this point, the averaged quadrature formula $\tilde{A}_{2n+1}$ is defined as

$$\tilde{A}_{2n+1}(f) := \frac{1}{2} \left(I_n(f) + A_{n+1}(f) \right).$$

From property (16) it follows that the degree of exactness of $\tilde{A}_{2n+1}$ is $2n + 1$, and the quadrature error can be estimated by

$$E_n(f) \approx \tilde{A}_{2n+1}(f) - I_n(f) = \frac{1}{2} \left(A_{n+1}(f) - I_n(f) \right).$$

Going back to our case, we denote by α_k^J, β_k^J and α_k^L, β_k^L the recursion coefficients for the sequences of monic orthogonal polynomials relative to $w_{v,\alpha,c}$ and $w_{\alpha,c}$ (see (5)–(7)), respectively, and by $\tilde{J}_{n+1}^J$, $\tilde{J}_{n+1}^L$ the associated tridiagonal matrices of type (17). In particular, we have that α_k^L, β_k^L are strongly related to the recurrence coefficients a_k, b_k of the standard generalized Gauss–Laguerre rule. Indeed, it can be easily verified that

$$\alpha_k^L = \frac{a_k}{c} \quad \text{and} \quad \beta_k^L = \frac{b_k}{c^2}. \tag{19}$$

Moreover, the monic polynomials $\left\{ L_k^{(\alpha,c)} \right\}_{k \geq 0}$ defined by

$$L_k^{(\alpha,c)}(x) = \frac{1}{c^k} L_k^{(\alpha)}(cx), \tag{20}$$

where $L_k^{(\alpha)}(t)$ is the monic generalized Laguerre polynomial of degree k, are orthogonal with respect to the weight function $w_{\alpha,c}$. At this point, we denote by

$$A_{n+1}^J(f) = \sum_{i=1}^{n+1} \tilde{w}_i^{(n+1)} f \left(\tilde{x}_i^{(n+1)} \right) \tag{21}$$

and

$$A_{n+1}^L(f) = \sum_{i=1}^{n+1} \tilde{\lambda}_i^{(n+1)} f \left(\tilde{\xi}_i^{(n+1)} \right) \tag{22}$$

the anti-Gaussian quadrature rules (cf. (15)) relative to I_n^J and I_n^L (see (4) and (6)), respectively. Then, the corresponding averaged Gauss rules are

$$\tilde{A}_{2n+1}^J(f) = \frac{1}{2} \left(I_n^J(f) + A_{n+1}^J(f) \right)$$

and

$$\tilde{A}_{2n+1}^L(f) = \frac{1}{2} \left(I_n^L(f) + A_{n+1}^L(f) \right).$$

Finally, the error of the Gaussian quadrature formula (see (11)) is estimated as

$$E_{n,v,\alpha,c}(f) \approx \tilde{E}_{n,v,\alpha,c}(f) := \tilde{E}_{n,v,\alpha,c}^J(f) - \tilde{E}_{n,\alpha,c}^L(f), \tag{23}$$

where

$$\tilde{E}_{n,v,\alpha,c}^J(f) = \tilde{A}_{2n+1}^J(f) - I_n^J(f) \quad \text{and} \quad \tilde{E}_{n,\alpha,c}^L(f) = \tilde{A}_{2n+1}^L(f) - I_n^L(f).$$

For the generalized Gauss–Laguerre rule the recurrence coefficients and the values of the orthogonal polynomials are explicitly known, and condition (18) holds (see [9, Theorem 4]). Moreover, by using relations (19) and (20) it is not difficult to prove the same result also for the Gaussian rule I_n^L. Therefore, we have that the anti-Gaussian formula A_{n+1}^L is internal, i.e., $\tilde{\xi}_1^{(n+1)} \in [0, +\infty)$.

For what concerns the anti-Gaussian rule A_{n+1}^J, we do not have at disposal the recurrence coefficients and the expressions of the corresponding orthogonal polynomials (see [4]). Hence, condition (18) can only be verified numerically. In our numerical experiments, independently of v, c and working with $n = 100$, we have observed negative values of $\tilde{x}_1^{(n+1)}$ for $-1 < \alpha < \tilde{\alpha}$, where $\tilde{\alpha} \in (-0.8, -0.7)$.

3. Construction of generalized averaged Gauss rules

In this section we describe the generalized averaged Gauss rule $\hat{A}_{2n+1}$, introduced in [11], associated with a generic Gauss formula I_n. It is a $(2n + 1)$-point formula which can be represented by a single symmetric tridiagonal matrix $\hat{J}_{2n+1} \in \mathbb{R}^{(2n+1)\times(2n+1)}$, that is,

$$\hat{J}_{2n+1} = \begin{bmatrix} J_n & \sqrt{\beta_n}e_n & \mathbf{0} \\ \sqrt{\beta_n}e_n^T & \alpha_n & \sqrt{\beta_{n+1}}e_1^T \\ \mathbf{0} & \sqrt{\beta_{n+1}}e_1 & J_n' \end{bmatrix},$$

where $e_1 = (1, 0, \ldots, 0)^T \in \mathbb{R}^n$, J_n is as in (14) and J_n' is obtained by reversing the order of the rows and column of J_n, that is,

$$J_n' = \begin{bmatrix} \alpha_{n-1} & \sqrt{\beta_{n-1}} & & & 0 \\ \sqrt{\beta_{n-1}} & \alpha_{n-2} & \sqrt{\beta_{n-2}} & & \\ & \ddots & \ddots & \ddots & \\ & & \sqrt{\beta_2} & \alpha_1 & \sqrt{\beta_1} \\ 0 & & & \sqrt{\beta_1} & \alpha_0 \end{bmatrix} \in \mathbb{R}^{n\times n}.$$

The generalized averaged Gauss formula can also be described in a more compact form. Indeed, $\hat{A}_{2n+1}$ can be written as

$$\hat{A}_{2n+1}(f) = \frac{\beta_{n+1}}{\beta_n + \beta_{n+1}}I_n(f) + \frac{\beta_n}{\beta_n + \beta_{n+1}}\bar{A}_{n+1}(f), \tag{24}$$

where the quadrature formula

$$\bar{A}_{n+1}(f) = \sum_{i=1}^{n+1} \bar{\sigma}_i^{(n+1)} f\left(\bar{\tau}_i^{(n+1)}\right) \tag{25}$$

is determined by the symmetric tridiagonal matrix $\bar{J}_{n+1} \in \mathbb{R}^{(n+1)\times(n+1)}$, defined as

$$\bar{J}_{n+1} = \begin{bmatrix} J_n & e_n\sqrt{\beta_n + \beta_{n+1}} \\ e_n^T\sqrt{\beta_n + \beta_{n+1}} & \alpha_n \end{bmatrix}, \tag{26}$$

(see [15]). By construction, the $(n+1)$-point quadrature rule (25) has essentially the same properties of the anti-Gaussian rule A_{n+1}, but in this case the nodes are internal, i.e., $\bar{\tau}_1^{(n+1)} \in [0, +\infty)$, if and only if

$$\frac{\pi_{n+1}(0)}{\pi_{n-1}(0)} \geq \beta_{n+1}, \quad n \geq 1, \tag{27}$$

(see [11]).

At this point, we denote the generalized averaged Gaussian rules corresponding to I_n^J and I_n^L by

$$\hat{A}_{2n+1}^J(f) = \frac{\beta_{n+1}^J}{\beta_n^J + \beta_{n+1}^J}I_n^J(f) + \frac{\beta_n^J}{\beta_n^J + \beta_{n+1}^J}\bar{A}_{n+1}^J(f)$$

and

$$\hat{A}_{2n+1}^L(f) = \frac{\beta_{n+1}^L}{\beta_n^L + \beta_{n+1}^L}I_n^L(f) + \frac{\beta_n^L}{\beta_n^L + \beta_{n+1}^L}\bar{A}_{n+1}^L(f),$$

where the formulas

$$\bar{A}_{n+1}^J(f) = \sum_{i=1}^{n+1} \bar{w}_i^{(n+1)} f\left(\bar{x}_i^{(n+1)}\right) \quad \text{and} \quad \bar{A}_{n+1}^L(f) = \frac{1}{c^{\alpha+1}}\sum_{i=1}^{n+1} \bar{\lambda}_i^{(n+1)} f\left(\bar{\xi}_i^{(n+1)}\right)$$

are associated with the tridiagonal matrices $\bar{J}_{n+1}^J$ and $\bar{J}_{n+1}^L$, obtained by considering in (26) the recursion coefficients α_k^J, β_k^J and α_k^L, β_k^L, respectively. Finally, the error of the Gaussian quadrature (see (11)) is estimated as

$$E_{n,v,c}(f) \approx \hat{E}_{n,v,\alpha,c}(f) := \hat{E}_{n,v,\alpha,c}^J(f) - \hat{E}_{n,\alpha,c}^L(f), \tag{28}$$

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where

$$\hat{E}^J_{n,v,\alpha,c}(f) = \hat{A}^J_{2n+1}(f) - I^J_n(f) \quad \text{and} \quad \hat{E}^L_{n,\alpha,c}(f) = \hat{A}^L_{2n+1}(f) - I^L_n(f).$$

From (27) and by using again relations (19) and (20), it is trivial to prove that for the generalized averaged Gauss rule $\bar{A}^L_{n+1}$ the condition for the internality is $\alpha \geq 1$. This means that for $-1 < \alpha < 1$ the smallest node of $\bar{A}^L_{n+1}$ is negative. As before, the behavior of the rule $\bar{A}^J_{n+1}$ can only be verified numerically. In particular, independently of v, c and working with $n = 100$, we have found negative values of $\bar{x}^{(n+1)}_1$ for $-1 < \alpha < \bar{\alpha}$, with $\bar{\alpha} \in (1, 1.1)$.

4. A tentative a priori estimate

In the previous sections we have described how, having at disposal the recurrence coefficients of the corresponding orthogonal polynomials, the averaged and generalized averaged Gaussian rules can be easily constructed and employed to approximate the quadrature error $E_{n,v,\alpha,c}(f)$ (see (11)). In this section, by using the results of Barrett [13] regarding the derivation of an asymptotic expression for the error of the Gauss–Laguerre formula, we present a tentative a priori estimate of the error $E_{n,v,\alpha,c}(f)$. In particular, as remarked in the introduction, since $|J_v(x)| \leq 1$, for $v \geq 0$, $x \in \mathbb{R}$, we can interpret the weight function $w_{v,\alpha,c}$ as a perturbation of the weight of the Gauss–Laguerre rule. Therefore, the idea is to employ the error estimate for the Gauss–Laguerre formula to approximate not only $E^L_{n,\alpha,c}(f)$, but also $E^J_{n,v,\alpha,c}(f)$ (see (12)). First, let consider the error of the Laguerre rule for the classical case of $c = 1$, that is, $E^L_{n,\alpha,1}(f)$. For any given $R > 1$, the set $\Gamma_R = \{z \in \mathbb{C} \mid \Re\sqrt{-z} = \ln R\}$ represents a parabola of the complex plane positively oriented, symmetric with respect to the real axis and with vertex at $-\ln R$. Barrett [13] showed that, if $f(z)$ has no singularities on or within Γ_R, except for a pair of simple poles z_0 and its conjugate $\bar{z}_0$, then, for $n \to \infty$,

$$E^L_{n,\alpha,1}(f) \sim 4\pi \Re \left\{ \text{Res}(f(z), z_0) e^{-i\alpha\pi} \left[\exp \sqrt{-z_0} \right]^{-2\sqrt{\bar{n}}} \right\}, \tag{29}$$

where $\bar{n} = 4n + \alpha + 2$ and the symbol $\text{Res}(\cdot, \cdot)$ denotes the residue. Formula (29) follows from the fact that $E^L_{n,\alpha,1}(f)$ can be represented as the contour integral

$$E^L_{n,\alpha,1}(f) = \frac{1}{2\pi i} \int_\Gamma \frac{q^L_n(z)}{L^{(\alpha)}_n(z)} f(z) dz,$$

where $L^{(\alpha)}_n(z)$ is the generalized Laguerre polynomial, $q^L_n(z)$ is the associated function defined by

$$q^L_n(z) = \int_0^{+\infty} \frac{w_\alpha(x) L^{(\alpha)}_n(x)}{z - x} dx,$$

with $w_\alpha(x) = x^\alpha e^{-x}$ and Γ is a contour containing $[0, +\infty)$ and such that no singularity of $f(z)$ lies on or within the contour (see [16]). Then, by using the relation (see [17])

$$\frac{q^L_n(z)}{L^{(\alpha)}_n(z)} \sim -2e^{-i\pi\alpha} z^\alpha e^{-z} \frac{K_\alpha\left(\sqrt{\bar{n}z e^{-i\pi}}\right)}{I_\alpha\left(\sqrt{\bar{n}z e^{-i\pi}}\right)}, \tag{30}$$

where I_α, K_α are the modified Bessel functions of order α of the first and second kind, respectively, and the asymptotic formulas (see [3, p.377, 9.7.1–9.7.2])

$$I_\alpha(t) \sim \frac{e^t}{\sqrt{2\pi t}}, \quad K_\alpha(t) \sim e^{-t} \sqrt{\frac{\pi}{2t}},$$

valid for large $|t|$, $|\arg(t)| < \pi/2$, we obtain

$$\frac{q^L_n(z)}{L^{(\alpha)}_n(z)} \sim -2\pi e^{-i\alpha\pi} z^\alpha e^{-z} \left[\exp\left(\sqrt{-z}\right) \right]^{-2\sqrt{\bar{n}}} =: \Phi_n(z), \quad z \notin [0, +\infty). \tag{31}$$

Finally, formula (29) can be derived by choosing $\Gamma = \Gamma_R \cup C_1 \cup C_2$, where C_1, C_2 are two arbitrary small circles surrounding the two poles, and by using relation (31). After simple computations, it can be verified that, by replacing $w_\alpha(x)$ with $w_{\alpha,c}(x)$, one obtains

$$E^L_{n,\alpha,c}(f) \sim \frac{4\pi}{c^{\alpha-1}} \Re \left\{ \text{Res}(f(z), z_0) e^{-i\alpha\pi} \left[\exp \sqrt{-cz_0} \right]^{-2\sqrt{\bar{n}}} \right\}. \tag{32}$$

Now, let consider the error $E^J_{n,v,\alpha,c}(f)$. It can also be written as the contour integral

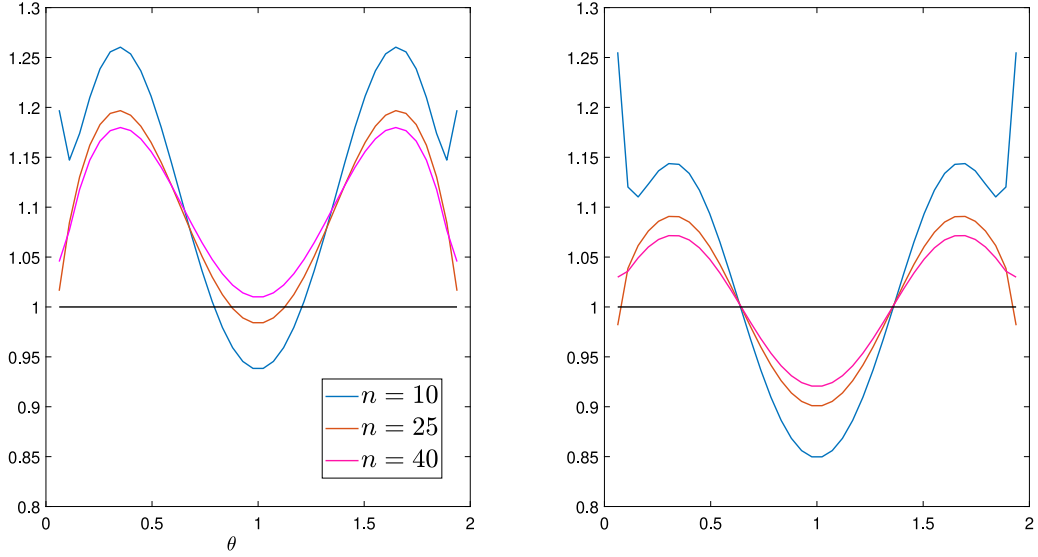$$E^J_{n,v,\alpha,c}(f) = \frac{1}{2\pi i} \int_\Gamma \frac{q^J_n(z)}{p_n(z)} f(z) dz,$$

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Fig. 1. The ratios $\frac{\Psi_n^J(z)}{\Phi_n(z)}$ (left) and $\frac{\Psi_n^L(z)}{\Phi_n(z)}$ (right) for $z = re^{i\theta\pi}$, with $r = 4$, $\theta \in (0, 2)$. In this case $\nu = 1, c = 0.5, \alpha = 0.3$.

where $p_n(z)$ is the orthogonal polynomial relative to the weight function $w_{\nu,\alpha,c}$ and

$$q_n^J(z) = \int_0^{+\infty} \frac{w_{\nu,\alpha,c}(x)p_n(x)}{z - x} dx.$$

However, as remarked before, we do not have at disposal the analytic expression of $p_n(z)$ and, therefore, an asymptotic formula analogous to (31) cannot be derived. In order to justify the use of estimate (32) also for $E_{n,\nu,\alpha,c}^J(f)$, we numerically evaluate the functions

$$\Psi_n^J(z) := \frac{q_n^J(z)}{p_n(z)} \quad \text{and} \quad \Psi_n^L(z) := \frac{q_n^L(z)}{L_n^{(\alpha)}(z)} \tag{33}$$

and check if the approximation $\Phi_n(z)$ (cf. (31)) can also be used for $\Psi_n^J(z)$. In Figs. 1–2, for different values of n, ν, α, c, we plot the ratios

$$\frac{\Psi_n^J(z)}{\Phi_n(z)} \quad \text{and} \quad \frac{\Psi_n^L(z)}{\Phi_n(z)},$$

in which $z = re^{i\theta\pi}$, with $r = 4$, $\theta \in (0, 2)$. We remark that $\frac{\Psi_n^L(z)}{\Phi_n(z)} \sim 1$, for $n \to \infty$, by (31). The results show that approximation (31) works rather good also for $\Psi_n^J(z)$, and the situation is analog for other values of the parameters. Hence, the idea is to use the approximation (32) also for $E_{n,\nu,\alpha,c}^J(f)$. Finally, since $E_{n,\nu,\alpha,c}(f) = E_{n,\nu,\alpha,c}^J(f) - E_{n,\alpha,c}^L(f)$, we consider the estimate

$$\left|E_{n,\nu,\alpha,c}(f)\right| \approx 2\mathcal{E}_{n,\alpha,c}(f), \tag{34}$$

with

$$\mathcal{E}_{n,\alpha,c}(f) := \frac{4\pi}{c^{\alpha-1}} \left| \text{Res}(f(z), z_0) \left[\exp\sqrt{-cz_0}\right]^{-2\sqrt{n}} \right|, \tag{35}$$

(cf. (32)).

5. Numerical examples

In this section we present some numerical experiments which confirm the reliability of the error estimates (23), (28) and (34). We remark that all the computations reported in this work are carried out in Matlab by using high-precision arithmetic, specifically with 120 significant decimal digits. The main reason for this choice is that we do not know explicitly the recurrence coefficients α_k^J, β_k^J and hence we are forced to employ a numerical scheme to derive them. However, it is well known (see e.g. [18]) that this computation can be inaccurate for growing k, because the problem is severely ill conditioned. Therefore, even if in [4] an alternative more stable approach is presented, the use of high-precision arithmetic
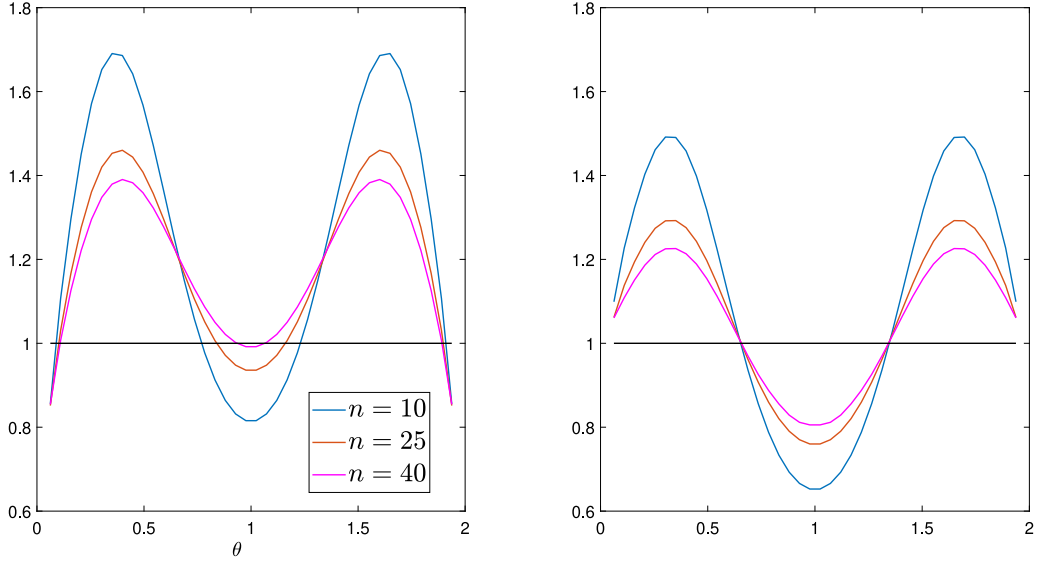
7

Fig. 2. The ratios $\frac{\psi_n^J(z)}{\Phi_n(z)}$ (left) and $\frac{\psi_n^L(z)}{\Phi_n(z)}$ (right) for $z = re^{i\theta\pi}$, with $r = 4$, $\theta \in (0, 2)$. In this case $\nu = 0, c = 1, \alpha = -0.5$.

allows to considerably increase the number of quadrature points and to obtain an absolute error in the approximations of the order of the machine precision. The Matlab routine for the computation of the recurrence coefficients α_k^J, β_k^J is taken from [19], while the code for the implementation of the Gauss–Laguerre quadrature rule from [20].

Before going on, we observe that, by using the change of variable $t = cx$ in (1), which leads to

$$I_{\nu,\alpha,c}(f) = \int_0^\infty F\left(\frac{t}{c}\right) t^\alpha e^{-t} dt, \quad F(t) = \frac{1}{c^{\alpha+1}} f\left(\frac{t}{c}\right) J_\nu\left(\frac{t}{c}\right),$$

and by considering as weight function

$$w_\alpha(t) = t^\alpha e^{-t}, \tag{36}$$

integral (1) can be computed by employing the n-point generalized Gauss–Laguerre formula, that is,

$$I_{\nu,\alpha,c}(f) \approx \sum_{i=1}^n F\left(t_i^{(n)}\right) \eta_i^{(n)}. \tag{37}$$

In Fig. 3, by considering a reference solution, we compare the results of the Gaussian rule constructed in [4] with the ones of the generalized Gauss–Laguerre formula (37). We remark that the former requires a double set of points, i.e., a double number of function evaluations, and the employment of a numerical scheme for the computation of the recurrence coefficients α_k^J, β_k^J. Nevertheless, since the oscillating term, i.e., the Bessel function, is not part of the weight function (36), the approach developed in [4] typically provides better results with respect to the generalized Gauss–Laguerre rule, especially for small values of the parameter c, which handles the frequency of the oscillations (see Fig. 3a). Anyway, for large c, the Laguerre formula appears to be reliable (see Fig. 3b). The same behavior has been observed in other experiments not reported.

Example 1. Consider the integral

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

with

$$f(x) = \frac{1}{1 + e^{-x}}.$$

In order to use error estimate (34), we start by studying the poles of f. A simple analysis shows that they are given by the set

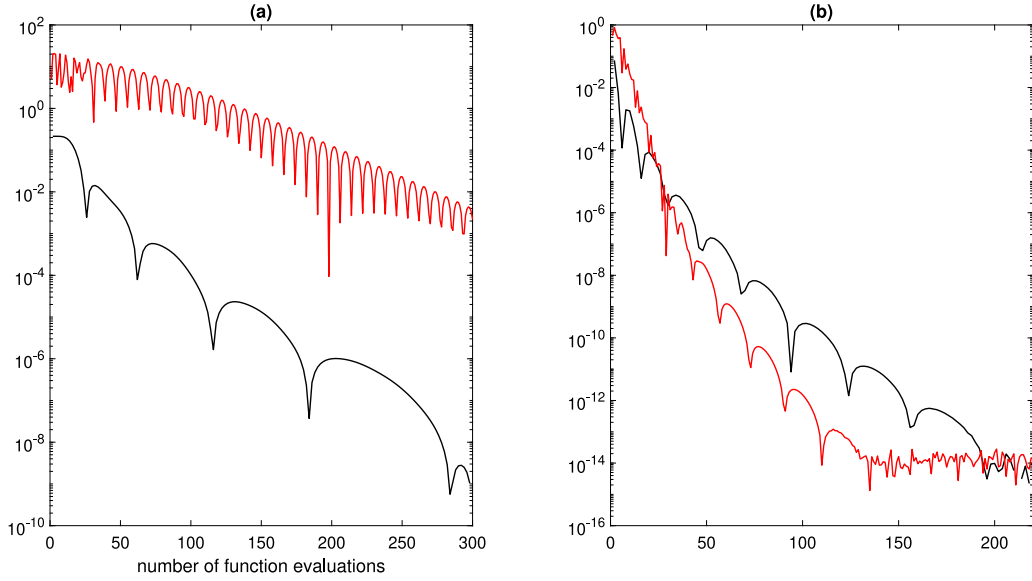$$z_k = -i(\pi + 2k\pi), \quad k \in \mathbb{Z},$$

8

Fig. 3. Comparison between the absolute error obtained by using the Gaussian approach developed in [4] (black) and the Gauss–Laguerre formula (37) (red) for $\alpha = 1.1, c = 0.1, \nu = 0$ (left) and $\alpha = 0.5, c = 0.4, \nu = 1$ (right). In both cases $f(t) = \frac{1}{1+e^{-t}}$.
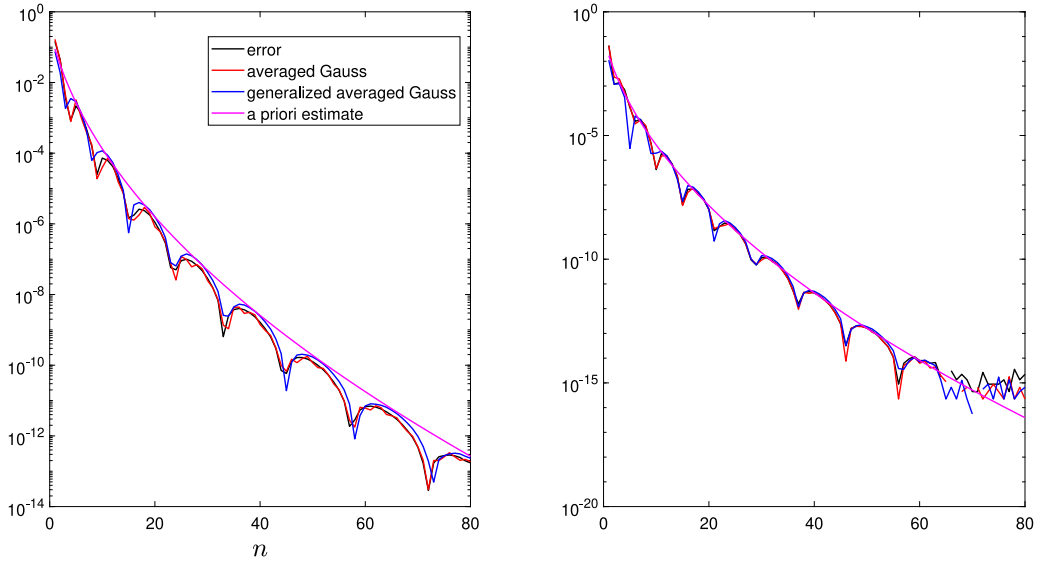

Fig. 4. The quadrature error and its approximations $|\tilde{E}_{n,\nu,\alpha,c}(f)|$, $|\hat{E}_{n,\nu,\alpha,c}(f)|$ and (38) for $\nu = 1, c = 0.5, \alpha = 1.7$ (left) and $\nu = 0.5, c = 0.8, \alpha = 1.5$ (right).

and the closest to the real axis are z_0 and its conjugate z_{-1}, that is, $\pm i\pi$. As for the residue (cf. (32)), we obtain

$$\text{Res}\,(f(z), z_0) = 1.$$

Therefore, by using (34) and (35), we have that

$$|E_{n,\nu,\alpha,c}(f)| \approx 8\pi c^{1-\alpha} e^{-\sqrt{2c\pi\bar{n}}}. \tag{38}$$

In Fig. 4 we compare, for different values of ν, α, c, the quadrature error $|E_{n,\nu,\alpha,c}(f)|$, obtained by considering a reference solution, with the approximations $|\tilde{E}_{n,\nu,\alpha,c}(f)|$, $|\hat{E}_{n,\nu,\alpha,c}(f)|$ (cf. (23)–(28)) and estimate (38). We can see the very good agreement between the error and the approximations given by the averaged and generalized averaged Gaussian rules. Moreover, the examples reveal that the a priori estimate (38) is rather accurate.
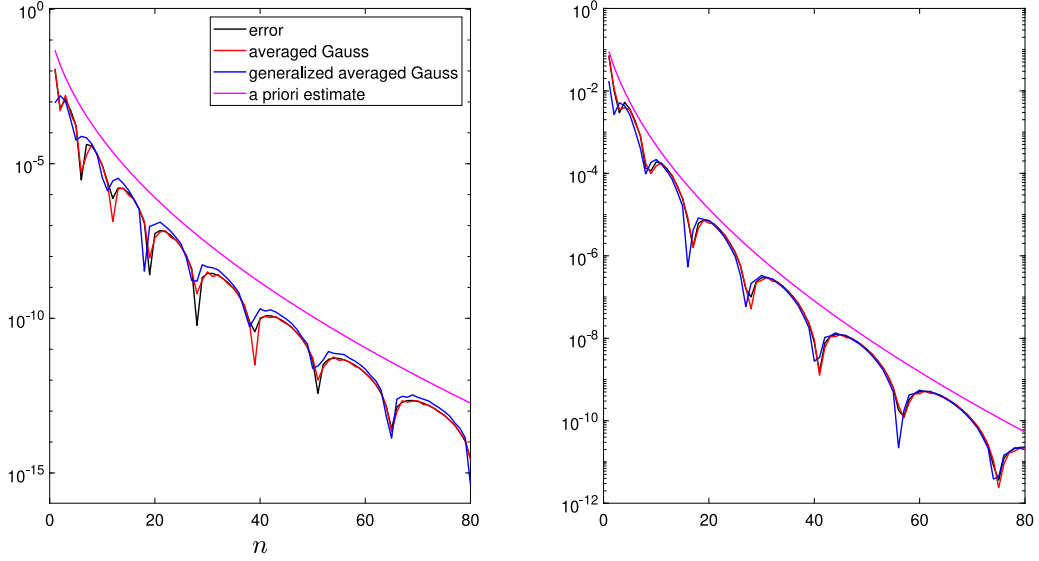
9

Fig. 5. The quadrature error and its approximations $|\tilde{E}_{n,\nu,\alpha,c}(f)|$, $|\hat{E}_{n,\nu,\alpha,c}(f)|$ and (39) for $\nu = 1, c = 1.5, \alpha = 1$ (left) and $\nu = 0, c = 1, \alpha = 1.5$ (right).

Example 2. Consider now the case of

$$f(x) = \frac{1}{1+x^2}.$$

This function has only two poles $\pm i$. As for the residue (cf. (32)), we obtain

$$\text{Res}\,(f(z), i) = -\frac{i}{2}.$$

Therefore, by using (34) and (35), we have that

$$|E_{n,\nu,\alpha,c}(f)| \approx 4\pi c^{1-\alpha} e^{-\sqrt{2c\pi\bar{n}}}. \tag{39}$$

In Fig. 5 we compare, for different values of ν, α, c, the quadrature error $|E_{n,\nu,\alpha,c}(f)|$, obtained by considering a reference solution, with the approximations $|\tilde{E}_{n,\nu,\alpha,c}(f)|$, $|\hat{E}_{n,\nu,\alpha,c}(f)|$ (cf. (23)–(28)) and estimate (39).

Example 3. Consider the integral

$$I_{\nu,0,c}(f) = \int_0^\infty f(x)e^{-cx}J_\nu(x)dx, \tag{40}$$

with

$$f(x) = \frac{\sin(\omega x)}{x}, \quad \omega > 0.$$

For $\nu = 0, 1$, we have that the exact solution of (40) is given by (see [21, p. 763, 6.752, n. 1-2])

$$I_{0,0,c}(f) = \arcsin\left(\frac{2\omega}{\sqrt{c^2 + (\omega+1)^2} + \sqrt{c^2 + (\omega-1)^2}}\right),$$

$$I_{1,0,c}(f) = \omega(1 - r),$$

where r is such that

$$\omega^2 = \frac{1}{1-r^2} - \frac{c^2}{r^2}.$$

In this case, since the function f has no poles, we can only consider the a posteriori approximations based on the averaged and generalized averaged Gaussian rules. In this setting, in Fig. 6 we compare, for different values of c and ω, the quadrature error $|E_{n,\nu,0,c}(f)|$ with the approximations $|\tilde{E}_{n,\nu,0,c}(f)|$, $|\hat{E}_{n,\nu,0,c}(f)|$ (cf. (23)–(28)). We observe that the error estimated by the averaged Gauss rule almost overlaps the quadrature error.
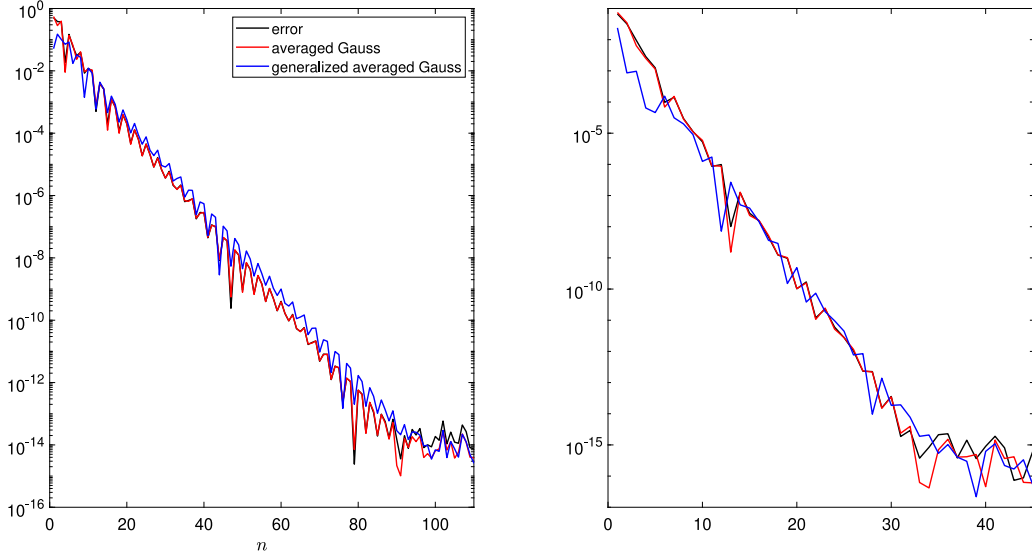
10

Fig. 6. The quadrature error and its approximations $|\tilde{E}_{n,\nu,\alpha,c}(f)|$, $|\hat{E}_{n,\nu,\alpha,c}(f)|$ for $\nu = 0, c = 1.5, \omega = 5$ (left), and $\nu = 1, c = 1.8, \omega = 3$ (right).
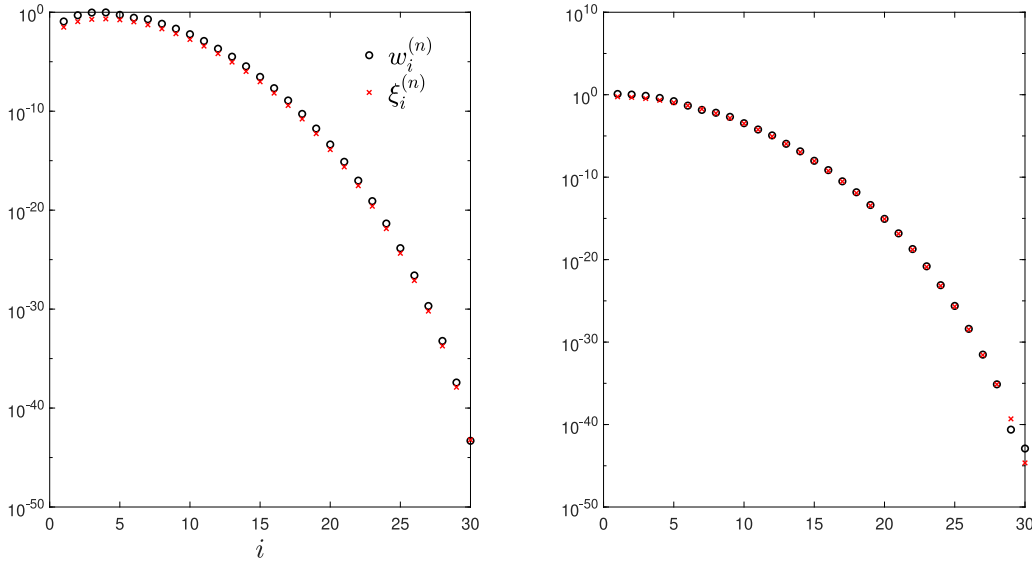

Fig. 7. The weights $w_i^{(n)}$, $\xi_i^{(n)}$, $i = 1, \ldots, n$ (cf. (4)–(6)) for $\nu = 1, \alpha = 0.7, c = 0.5$ (left) and $\nu = 0, \alpha = -0.5, c = 0.8$ (right). In both cases $n = 30$.

6. Conclusions

In this work the error estimates of the Gaussian quadrature formula introduced in [4] are considered. In particular, a posteriori error approximations given by the averaged and generalized averaged Gaussian rules have been constructed and showed to be very accurate. Moreover, starting from numerical experiments regarding the ratio q_n^J/p_n (see (33)), an heuristic but quite effective a priori error estimate has been introduced. We remark that, having at disposal an a-priori estimate of the error and by noting that, similar to the Gauss–Laguerre rule, the weights $w_i^{(n)}$, $i = 1, \ldots, n$, (cf. (4)) decay exponentially (see Fig. 7), a truncated approach can also be introduced, to reduce the number of function evaluations (see [22]).

Data availability

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

Acknowledgments

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