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ASYMPTOTIC ESTIMATES OF THE ERROR BOUND FOR GAUSS–RADAU QUADRATURES*

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Abstract. This paper deals with the derivation of asymptotic expressions for the quadrature error of Gauss–Radau–Jacobi and Gauss–Radau–Laguerre formulas. Starting from the contour integral representation of the remainder term, the analysis is derivative-free and based on the theory of analytic functions. The final error estimates allow to select a-priori the number of quadrature points necessary to achieve a prescribed accuracy. Several numerical examples are reported.

Key words. Gauss–Radau rule, contour integral representation, error estimate

AMS subject classifications. 65D32, 33C45

1. Introduction.

Let w be a positive weight function on $[a, b]$, with a a finite real number, such that all the moments exist and are finite. The $(n+1)$-point Gauss–Radau rule with preassigned node a and relative to the weight w is given by (see, e.g., [5, 9])

$$\int_a^b f(t)w(t)dt = \lambda_0 f(a) + \sum_{k=1}^{n} \lambda_k f(t_k) + R_n(f), \tag{1.1}$$

in which the interior nodes t_k, $k = 1, \dots, n$, are the zeros of the polynomial π_n^R of degree n that is orthogonal with respect to the modified weight $w^R(t) = (t-a)w(t)$. The weights λ_0 and λ_k, for $k = 1, \dots, n$, are obtainable by interpolating at the nodes a and t_k, for $k = 1, \dots, n$. The remainder term in the above formula is such that

$$R_n(f) = 0, \quad \forall f \in \mathbb{P}_{2n},$$

where $\mathbb{P}_{2n}$ is the space of polynomials of degree at most $2n$. Denoting by J_n the Jacobi matrix associated to the weight function w, that is,

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

in which $\alpha_k \in \mathbb{R}$, $\beta_k > 0$ are the recursion coefficients of the monic orthogonal polynomials $\{\pi_k\}_{k\geq 0}$ relative to w, the Gauss–Radau rule can be associated to the symmetric tridiagonal matrix (see again [9])

$$J_{n+1}^R = \begin{bmatrix} J_n & \sqrt{\beta_n} e_n \\ \sqrt{\beta_n} e_n^T & \alpha_n^R \end{bmatrix} \in \mathbb{R}^{(n+1)\times(n+1)}, \quad \alpha_n^R = a - \beta_n \frac{\pi_{n-1}(a)}{\pi_n(a)}, \tag{1.2}$$

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where $e_n = (0, \ldots, 0, 1)^T \in \mathbb{R}^n$. The nodes of formula (1.1), including a, are the eigenvalues of J_{n+1}^R, and the weights can be written as

$$\lambda_j = \beta_0 v_{j,1}^2, \quad j = 0, 1, \ldots, n,$$

in which $\beta_0 = \int_a^b w(t)dt$ and $v_{j,1}$ is the first component of the associated normalized vector v_j [11]. In particular, for the Gauss–Radau–Jacobi and Gauss–Radau–Laguerre rules, explicit expressions for α_n^R in (1.2) and all the weights in equation (1.1) are given in terms of n and the parameters of the quadrature formulas in [8].

As for the error analysis, in general, it is known that, by means of the Cauchy formula, the remainder term R_n in (1.1) can be written as the contour integral

$$R_n(f) = \frac{1}{2\pi i} \int_{\mathcal{C}} K_n(z) f(z) dz, \tag{1.3}$$

where the kernel $K_n(z)$ is defined as

$$K_n(z) = \frac{\psi(z)}{\phi(z)},$$

with

$$\phi(z) = (z - a)\pi_n^R(z), \tag{1.4}$$

$$\psi(z) = \int_a^b \frac{w(t)\phi(t)}{z - t} dt \tag{1.5}$$

(see [3]). In formula (1.3), the contour $\mathcal{C}$ contains the interval $[a, b]$ in its interior, but no singularity of the function $f(z)$ lies on or within the contour.

In this work, assuming that the function f in (1.1) is analytic in the interior of $\mathcal{C}$, we develop a-priori and derivative-free error estimates for the Gauss–Radau–Jacobi and Gauss–Radau–Laguerre rules. In particular, the idea is to first consider asymptotic estimates of the kernels for growing number of quadrature points n; see, e.g., [3]. Then, we suitably choose the contour $\mathcal{C}$ in order to exploit these asymptotics and also, in the case of meromorphic functions, the position of the poles (cf. [1]). We remark that derivative-free error estimates for Gauss–Radau rules have been developed, amongst others, in [6, 7, 10, 13].

In this work, by characterizing the type of singularity of the function f that defines the problem, we present explicit approximations of the remainder in terms of the number of interior nodes n (cf. (1.1)). In this setting, it is possible to have a quite reliable estimate of the number of quadrature points necessary to achieve a prescribed accuracy. The analysis reveals the typical observed rate of convergence, that is, linear for the Jacobi case and sublinear for the Laguerre one.

Throughout this work we use the symbols $\sim$ and $\approx$ to denote an asymptotic equivalence and a generic approximation, respectively. The symbol $\lesssim$ stands for less than or asymptotically equal to.

The paper is organized as follows. In Sections 2 and 3 we introduce the Gauss–Radau–Jacobi and Gauss–Radau–Laguerre formulas, respectively, and develop the derivative-free error analysis. In Section 4 we present several numerical experiments to test the reliability of the previously obtained error estimates. In Section 5 we conclude by giving some additional remarks.

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2. Gauss–Radau–Jacobi formula. In the case of the Gauss–Jacobi weight function $w^{(\alpha,\beta)}(t) = (1-t)^\alpha(1+t)^\beta$, $\alpha > -1$, $\beta > -1$, formula (1.1) becomes

$$\int_{-1}^{1} f(t)w^{(\alpha,\beta)}(t)dt = \lambda_0^{(\alpha,\beta)} f(-1) + \sum_{k=1}^{n} \lambda_k^{(\alpha,\beta)} f\left(t_k^{(\alpha,\beta)}\right) + R_n^{(\alpha,\beta)}(f), \tag{2.1}$$

and the modified weight is given by

$$w_R^{(\alpha,\beta)}(t) = (1+t)w^{(\alpha,\beta)}(t) = (1-t)^\alpha(1+t)^{\beta+1} = w^{(\alpha,\beta+1)}(t)$$

(see [8]). Hence, denoting by $P_k^{(\alpha,\beta)}$ the Jacobi polynomial of degree k orthogonal with respect to $w^{(\alpha,\beta)}$, the interior nodes $t_k^{(\alpha,\beta)}$ are the zeros of $P_n^{(\alpha,\beta+1)}$. As said in the introduction, explicit expressions for the weights in terms of α, β and n can be found in [8]. By (1.4)–(1.5), we have that

$$\phi^{(\alpha,\beta)}(z) = (z+1)P_n^{(\alpha,\beta+1)}(z),$$

and

$$\begin{aligned}\psi^{(\alpha,\beta)}(z) &= \int_{-1}^{1} \frac{(1-t)^\alpha(1+t)^{\beta+1}P_n^{(\alpha,\beta+1)}(t)}{z-t}dt \\ &= \int_{-1}^{1} \frac{w^{(\alpha,\beta+1)}P_n^{(\alpha,\beta+1)}(t)}{z-t}dt \\ &= \Pi_n^{(\alpha,\beta+1)}(z),\end{aligned}$$

where $\Pi_n^{(\alpha,\beta+1)}$ is known as the associated Jacobi function (see [2, Sect. 1.12]). In this setting, the kernel is given by

$$K_n^{(\alpha,\beta)}(z) = \frac{\Pi_n^{(\alpha,\beta+1)}(z)}{(z+1)P_n^{(\alpha,\beta+1)}(z)}. \tag{2.2}$$

As for the choice of the contour in the integral representation of the remainder

$$R_n^{(\alpha,\beta)}(f) = \frac{1}{2\pi i}\int_{\mathcal{C}} K_n^{(\alpha,\beta)}(z)f(z)dz, \tag{2.3}$$

we consider the family of confocal ellipses

$$\varepsilon_\rho = \left\{ z \in \mathbb{C} \mid z = \frac{1}{2}\left(\rho e^{i\theta} + \frac{1}{\rho e^{i\theta}}\right),\ 0 \le \theta < 2\pi \right\}, \quad \rho > 1, \tag{2.4}$$

having foci at ± 1 and the sum of the semiaxes equal to ρ. Before going on, we first need an asymptotic estimate of the kernel $K_n^{(\alpha,\beta)}$.

PROPOSITION 2.1. *For $n \to +\infty$ and z not in the neighborhood of $[-1,1]$, it holds*

$$K_n^{(\alpha,\beta)}(z) \sim 2^{2\alpha+2\beta+1}\pi(z-1)^\alpha(z+1)^\beta\left[z + (z^2-1)^{1/2}\right]^{-2n-\alpha-\beta-2}. \tag{2.5}$$

Proof. From [4], when z is not in the neighborhood of $[-1,1]$ and for large n, we have the following asymptotic expansions:

$$\begin{aligned}\Pi_n^{(\alpha,\beta+1)}(z) &\sim 2^{2n+\frac{3}{2}(\alpha+\beta+2)}\frac{\Gamma(n+\alpha+1)\Gamma(n+\beta+2)}{\Gamma(2n+\alpha+\beta+3)}\\ &\quad\times\frac{(z-1)^{\frac{2\alpha-1}{4}}(z+1)^{\frac{2\beta+1}{4}}}{\left[z+(z^2-1)^{1/2}\right]^{n+\frac{\alpha+\beta+2}{2}}},\\ P_n^{(\alpha,\beta+1)}(z) &\sim 2^{-2n-(\alpha+\beta+1)/2}\frac{\Gamma(2n+\alpha+\beta+2)}{\Gamma(n+1)\Gamma(n+\alpha+\beta+2)}\\ &\quad\times\frac{\left[z+(z^2-1)^{1/2}\right]^{n+\frac{\alpha+\beta+2}{2}}}{(z-1)^{\frac{2\alpha+1}{4}}(z+1)^{\frac{2\beta+3}{4}}},\end{aligned}$$

where $\Gamma(\cdot)$ denotes the Gamma function. Now, by using the above formulas and the identity $\Gamma(x+1)=x\Gamma(x)$, for $n\to+\infty$, we obtain

$$\begin{aligned}\frac{\Pi_n^{(\alpha,\beta+1)}(z)}{(z+1)P_n^{(\alpha,\beta+1)}(z)} &\sim 2^{4n+2\alpha+2\beta+4}\frac{n^2\left(\Gamma(n+1)\right)^4}{(2n)^3\left(\Gamma(2n+1)\right)^2}\\ &\qquad\times(z-1)^{\alpha}(z+1)^{\beta}\left[z+(z^2-1)^{1/2}\right]^{-2n-\alpha-\beta-2}.\end{aligned}$$

By employing Stirling's formula for the Gamma function

$$\Gamma(x+1)\sim\sqrt{2\pi x}\left(\frac{x}{e}\right)^{x},\quad x\to+\infty,$$

and after some computations, we obtain the result. □

REMARK 2.2. The choice made in (2.4) for the contour in formula (2.3) is justified by the following observation: The quantity $\left|z+(z^2-1)^{1/2}\right|$ (cf. (2.5)) is constant and equal to ρ on any particular ellipse of type (2.4).

At this point, having at disposal the asymptotic (2.5), we can proceed by assuming f to be analytic inside a generic ellipse ε_r, $r>1$, of type (2.4) and continuous on the boundary. Moreover, let $R>1$ be the smallest real number such that, on the corresponding ellipse ε_R of type (2.4), the function f has a singularity. It follows that r must be such that $1<r<R$ (we will see that in some cases one can take $r=R$). Then, for the remainder term $R_n^{(\alpha,\beta)}$ we can write (cf. (2.3))

$$\begin{aligned}\left|R_n^{(\alpha,\beta)}(f)\right| &\le \frac{1}{2\pi}\max_{z\in\varepsilon_r}|f(z)|\int_{\varepsilon_r}|K_n^{(\alpha,\beta)}||dz|\\ &\lesssim 2^{2\alpha+2\beta}r^{-2n-\alpha-\beta-2}\max_{z\in\varepsilon_r}|f(z)|\int_{\varepsilon_r}|z-1|^{\alpha}|z+1|^{\beta}|dz|,\quad 1<r<R,\end{aligned}\tag{2.6}$$

where we have used the asymptotic (2.5) and Remark 2.2. At this point, setting

$$r_+=r+\frac{1}{r}\tag{2.7}$$

and since $z\in\varepsilon_r$ iff $z=\frac{1}{2}\left(re^{i\theta}+\frac{1}{re^{i\theta}}\right)$, with $0\le\theta<2\pi$ (cf. (2.4)), the above integral becomes

$$\begin{aligned}I_r &= \int_0^{2\pi}\left(\frac{r_+}{2}-\cos\theta\right)^{\alpha+\frac{1}{2}}\left(\frac{r_+}{2}+\cos\theta\right)^{\beta+\frac{1}{2}}d\theta\\ &= 2\int_0^{\pi}\left(\frac{r_+}{2}-\cos\theta\right)^{\alpha+\frac{1}{2}}\left(\frac{r_+}{2}+\cos\theta\right)^{\beta+\frac{1}{2}}d\theta.\end{aligned}$$

By means of the midpoint rule, we can write

$$2\int_0^{\pi}\left(\frac{r_+}{2}-\cos\theta\right)^{\alpha+\frac{1}{2}}\left(\frac{r_+}{2}+\cos\theta\right)^{\beta+\frac{1}{2}}d\theta = 2\pi\left(\frac{r_+}{2}\right)^{\alpha+\frac{1}{2}}\left(\frac{r_+}{2}\right)^{\beta+\frac{1}{2}}+\mathcal{R}_M$$
$$= 2^{-\alpha-\beta}\pi(r^2+1)^{\alpha+\beta+1}r^{-\alpha-\beta-1}+\mathcal{R}_M$$

(see (2.7)), where $\mathcal{R}_M$ denotes the error of the midpoint rule. Therefore, by inserting the above formula in (2.6), we obtain

$$\left|R_n^{(\alpha,\beta)}(f)\right| \lesssim 2^{2\alpha+2\beta}\left(2^{-\alpha-\beta}\pi(r^2+1)^{\alpha+\beta+1}r^{-\alpha-\beta-1}+\mathcal{R}_M\right) \times r^{-2n-\alpha-\beta-2}\max_{z\in\varepsilon_r}|f(z)|. \tag{2.8}$$

At this point, in order to employ formula (2.8) one need to be able to compute or approximate the value of $f(z)$ on the ellipse ε_r. Even if this obviously depends on the particular function f involved in the problem, it is possible to give some general hints on how to proceed by characterizing the type of singularity of f along ε_R. Suppose, for example, that $f(t) \sim (t-c)^\gamma$, with $c < -1$ and $\gamma \notin \mathbb{Z}$, in a neighborhood of c. In this case c is a branch point, and ε_R, with $R = -c + \sqrt{c^2-1}$, is the ellipse passing through c. As for the choice of r in formula (2.6), we have to distinguish two cases, depending on the sign of γ.

• Case $\gamma < 0$.

In this situation, since f is unbounded on ε_R, we want to optimize the choice of $r < R$ in (2.6). We first observe that, by definition of ε_R, it holds

$$c = -\frac{1}{2}\left(R+\frac{1}{R}\right).$$

Then, we have (cf. formula (2.6))

$$\begin{aligned}\max_{z\in\varepsilon_r}|f(z)| &= \left|f\left(-\frac{1}{2}\left(r+\frac{1}{r}\right)\right)\right| = \left|-\frac{1}{2}\left(r+\frac{1}{r}\right)-c\right|^\gamma \\ &= \left|\frac{1}{2}\left(R+\frac{1}{R}-r-\frac{1}{r}\right)\right|^\gamma = \left[\frac{1}{2}(R-r)\left(1-\frac{1}{Rr}\right)\right]^\gamma \\ &\leq 2^{-\gamma}r^{-\gamma}R^{-\gamma}(r^2-1)^\gamma(R-r)^\gamma.\end{aligned} \tag{2.9}$$

By inserting (2.9) in (2.8) we obtain

$$\left|R_n^{(\alpha,\beta)}(f)\right| \lesssim 2^{2\alpha+2\beta-\gamma}R^{-\gamma}\left(2^{-\alpha-\beta}\pi(r^2+1)^{\alpha+\beta+1}r^{-\alpha-\beta-1}+\mathcal{R}_M\right) \times (r^2-1)^\gamma r^{-(2n+\alpha+\beta+\gamma+2)}(R-r)^\gamma. \tag{2.10}$$

At this point, we look for the minimum with respect to r. In order to simplify the computations, we first consider the following further approximations:

$$(r^2+1)\approx r^2 \quad \text{and} \quad (r^2-1)\approx r^2,$$

and neglect the term $\mathcal{R}_M$. This leads to

$$\left|R_n^{(\alpha,\beta)}(f)\right| \approx 2^{\alpha+\beta-\gamma}\pi R^{-\gamma}(R-r)^\gamma r^{-(2n+1-\gamma)} =: \mathcal{E}_n^J(r).$$

Defining, for n large enough,

$$r^\star = \arg\min_{1<r<R}\mathcal{E}_n^J(r),$$

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we find

$$r^\star = \frac{(m-\gamma)R}{m-2\gamma}, \quad \text{with} \quad m = 2n+1.$$

By inserting the above value in (2.10), for $m \to +\infty$, we obtain

$$\left|R_n^{(\alpha,\beta)}(f)\right| \lesssim 2^{2\alpha+2\beta-\gamma} R^{-\gamma} \left(2^{-\alpha-\beta}\pi(R^2+1)^{\alpha+\beta+1}R^{-\alpha-\beta-1} + \mathcal{R}_M\right) \times (-\gamma)^\gamma (R^2-1)^\gamma R^{-(m+\alpha+\beta+\gamma+1)} m^{-\gamma}. \tag{2.11}$$

• Case $\gamma > 0$.
In this situation the function is continuous on ε_R, and hence, we can take $r = R$. From (2.8), we have

$$\left|R_n^{(\alpha,\beta)}(f)\right| \lesssim 2^{2\alpha+2\beta} \left(2^{-\alpha-\beta}\pi(R^2+1)^{\alpha+\beta+1}R^{-\alpha-\beta-1} + \mathcal{R}_M\right) \times R^{-(m+\alpha+\beta+1)} \max_{z\in\varepsilon_R} |f(z)|. \tag{2.12}$$

REMARK 2.3. In the numerical experiments of Section 4 we will consider the case $f(t) = (t-c)^\gamma$. In this situation, the maximum of $f(z)$ with $z \in \varepsilon_R$ is reached at the point $z = \frac{1}{2}\left(R + \frac{1}{R}\right)$, hence,

$$\max_{z\in\varepsilon_R} |f(z)| = R^{-\gamma}(R^2+1)^\gamma,$$

and the estimate (2.12) becomes

$$\left|R_n^{(\alpha,\beta)}(f)\right| \lesssim 2^{2\alpha+2\beta} \left(2^{-\alpha-\beta}\pi(R^2+1)^{\alpha+\beta+1}R^{-\alpha-\beta-1} + \mathcal{R}_M\right) \times R^{-(m+\alpha+\beta+\gamma+1)}(R^2+1)^\gamma. \tag{2.13}$$

REMARK 2.4. We point out that the above analysis can be exploited also for functions having other types of singularities. Denoting by $w \in \mathbb{C}$ a generic singularity of f on the boundary ε_R, the procedure described for the case $\gamma < 0$ can be followed also if w represents a cluster singularity or if w belongs to the natural boundary of f and is such that $f(w) = \infty$. On the other hand, the case $\gamma > 0$ applies also if w belongs to a cut of the function or the natural boundary of f with $|f(w)| < \infty$. Clearly, γ needs to be explicitly known.

In the following section we show that, if f is meromorphic, the position of the poles can be exploited in the error analysis by using the residue theorem (see [1]).

2.1. Meromorphic functions. Suppose that f has no singularities within or on a particular ellipse $\varepsilon_{\tilde r}$ of type (2.4), except for a pair of simple poles z_0 and $\bar z_0$. Denoting by $\mathcal{C}_1$ and $\mathcal{C}_2$ two arbitrary small circles surrounding the two poles, we take as contour in (2.3) $\mathcal{C} = \varepsilon_{\tilde r} \cup \mathcal{C}_1 \cup \mathcal{C}_2$. By running through $\mathcal{C}$ in the counterclockwise direction, we obtain

$$R_n^{(\alpha,\beta)}(f) = \frac{1}{2\pi i}\left(\int_{\varepsilon_{\tilde r}} K_n^{(\alpha,\beta)}(z) f(z) dz - \int_{\mathcal{C}_1\cup\mathcal{C}_2} K_n^{(\alpha,\beta)}(z) f(z) dz\right).$$

By using, for $n \to +\infty$, the asymptotic (2.5), and Remark 2.2, the contribution on the ellipse $\varepsilon_{\tilde r}$ is given by

$$\left|\frac{1}{2\pi i}\int_{\varepsilon_{\tilde r}} K_n^{(\alpha,\beta)}(z) f(z) dz\right| \sim 2^{2(\alpha+\beta)}(\tilde r)^{-2n-\alpha-\beta-2}\left|\int_{\varepsilon_{\tilde r}} (z-1)^\alpha (z+1)^\beta f(z) dz\right|$$
$$\leq 2^{2(\alpha+\beta)}(\tilde r)^{-2n-\alpha-\beta-2}\int_{\varepsilon_{\tilde r}} \left|w^{(\alpha,\beta)}(z) f(z)\right| |dz|.$$

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Then, by means of the residue theorem, we have

$$\begin{aligned}
&\frac{1}{2\pi i}\int_{\mathcal{C}_1\cup\mathcal{C}_2} K_n^{(\alpha,\beta)}(z)f(z)dz\\
&= \mathrm{Res}(f,z_0)K_n^{(\alpha,\beta)}(z_0) + \mathrm{Res}(f,\bar z_0)K_n^{(\alpha,\beta)}(\bar z_0)\\
&= 2\Re\left\{\mathrm{Res}(f,z_0)K_n^{(\alpha,\beta)}(z_0)\right\}\\
&= 4^{\alpha+\beta+1}\pi\Re\left\{\mathrm{Res}(f,z_0)w^{(\alpha,\beta)}(z_0)(z_0+(z_0^2-1)^{\frac{1}{2}})^{-(2n+\alpha+\beta+2)}\right\},
\end{aligned}$$

where the symbol $\Re(\cdot)$ denotes the real part and $\mathrm{Res}(f, z_0)$ is the residue of f at z_0. Denoting by ε_R the ellipse of the type given in (2.4) passing through z_0 and $\bar z_0$ and noting that $|z_0 + (z_0^2-1)^{\frac{1}{2}}| = R < \tilde r$, we neglect the contribution on the ellipse $\varepsilon_{\tilde r}$. Therefore, we consider the estimate ($n \to +\infty$)

$$R_n^{(\alpha,\beta)}(f) \sim -4^{\alpha+\beta+1}\pi\Re\left\{\mathrm{Res}(f,z_0)w^{(\alpha,\beta)}(z_0)(z_0+(z_0^2-1)^{\frac{1}{2}})^{-(2n+\alpha+\beta+2)}\right\},$$

which leads to

$$\left|R_n^{(\alpha,\beta)}(f)\right| \lesssim 4^{\alpha+\beta+1}\pi\left|\mathrm{Res}(f,z_0)w^{(\alpha,\beta)}(z_0)\right| R^{-m-1-\alpha-\beta}, \tag{2.14}$$

with $m = 2n + 1$ (see also [1]).

3. Gauss–Laguerre–Radau formula. In the case of the Gauss–Laguerre weight function $w^{(\alpha)}(t) = t^\alpha e^{-t}$, $\alpha > -1$, formula (1.1) becomes

$$\int_0^{+\infty} f(t)w^{(\alpha)}(t)dt = \lambda_0^{(\alpha)}f(0) + \sum_{k=1}^{n}\lambda_k^{(\alpha)}f\left(t_k^{(\alpha)}\right) + R_n^{(\alpha)}(f). \tag{3.1}$$

As before, explicit expressions for the weights in terms of n and α can be found in [8]. For this rule, the modified weight function is given by

$$w_R^{(\alpha)}(t) = t^{\alpha+1}e^{-t} = w^{(\alpha+1)}(t),$$

so that, denoting by $L_n^{(\alpha)}$ the generalized Laguerre polynomial of degree n orthogonal with respect to $w^{(\alpha)}$, the interior nodes $t_k^{(\alpha)}$ are the zeros of $L_n^{(\alpha+1)}$. As for the kernel

$$K_n^{(\alpha)}(z) = \frac{\psi^{(\alpha)}(z)}{\phi^{(\alpha)}(z)},$$

by (1.4)–(1.5) we have that

$$\phi^{(\alpha)}(z) = zL_n^{(\alpha+1)}(z)$$

and

$$\psi^{(\alpha)}(z) = \int_0^{+\infty}\frac{t^{\alpha+1}e^{-t}L_n^{(\alpha+1)}(t)}{z-t}dt = \int_0^{+\infty}\frac{w^{(\alpha+1)}L_n^{(\alpha+1)}(t)}{z-t}dt = q_n^{(\alpha+1)}(z),$$

where $q_n^{(\alpha+1)}$ is the associated Laguerre function (see [2, Sect. 1.12]). Regarding the choice of the contour in the integral representation of the remainder (cf. (1.3))

$$R_n^{(\alpha)}(f) = \frac{1}{2\pi i}\int_{\mathcal{C}} K_n^{(\alpha)}(z)f(z)dz, \tag{3.2}$$

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we consider the family of parabolas of the complex plane

$$\Gamma_\rho = \left\{ z \in \mathbb{C} \mid \Re(\sqrt{-z}) = \ln \rho \right\}, \quad \rho > 1, \tag{3.3}$$

symmetric with respect to the real axis having their vertices in $-(\ln \rho)^2$ and their convexity oriented towards the positive real axis. The following proposition describes the asymptotic behavior of $K_n^{(\alpha)}$ for $n \to +\infty$:

PROPOSITION 3.1. *For z bounded and $n \to +\infty$, it holds*

$$K_n^{(\alpha)}(z) \sim -2\pi e^{-i\pi(\alpha+1)} z^\alpha e^{-z} \left(e^{\sqrt{-z}} \right)^{-2\sqrt{\bar{n}}}, \tag{3.4}$$

with

$$\bar{n} = 4n + 4 + 2\alpha. \tag{3.5}$$

Proof. By using the asymptotic [3, formula (A.6)] for $n \to +\infty$, it follows immediately that

$$K_n^{(\alpha)}(z) \sim -2e^{-i\pi(\alpha+1)} z^\alpha e^{-z} \frac{K_{\alpha+1}\left[2\left(\left(n+1+\frac{\alpha}{2}\right) z e^{-i\pi}\right)^{1/2}\right]}{I_{\alpha+1}\left[2\left(\left(n+1+\frac{\alpha}{2}\right) z e^{-i\pi}\right)^{1/2}\right]}, \tag{3.6}$$

where $I_{\alpha+1}$ and $K_{\alpha+1}$ are the modified Bessel functions of order $(\alpha+1)$ of the first and second kind, respectively. Then, from [14, Sect.10.40], for $|w| \to +\infty$, it holds that

$$K_{\alpha+1}(w) \sim \sqrt{\frac{\pi}{2w}} e^{-w} \quad \text{and} \quad I_{\alpha+1}(w) \sim \frac{e^w}{\sqrt{2\pi w}}.$$

By substituting the above expressions in (3.6) and after some computations one obtains the result. □

REMARK 3.2. For any $z \in \Gamma_\rho$ (cf. (3.3)), it holds

$$\exp(\Re(\sqrt{-z})) = \rho.$$

Similarly to the previous section, we assume f to be analytic inside a generic parabola Γ_r, $r > 1$, of type (3.3) and continuous on the boundary. Then, let $R > 1$ be the smallest real number such that, on the corresponding parabola Γ_R of type (3.3), the function f has a singularity. Hence, r must be such that $1 < r < R$. In order to derive an estimate for the remainder term $R_n^{(\alpha)}$, we define

$$I(r, \alpha) = \int_0^{+\infty} \left(\frac{b^2}{4(\ln r)^2} + (\ln r)^2 \right)^{\alpha + \frac{1}{2}} e^{-\frac{b^2}{4(\ln r)^2}} db \tag{3.7}$$

and state the following preliminary result:

LEMMA 3.3. *For $r > 1$ it holds*

$$I(r, \alpha) \le \begin{cases} \ln r \, \Gamma(\alpha+1) & \text{for } -1 < \alpha < -\frac{1}{2}, \\ 2^{\alpha+\frac{1}{2}} \ln r \left((\ln r)^{2\alpha+1} \sqrt{\pi} + \Gamma(\alpha+1) \right) & \text{for } \alpha \ge -\frac{1}{2}. \end{cases}$$

Proof. If $-1 < \alpha < -\frac{1}{2}$, then (cf. (3.7))

$$\left(\frac{b^2}{4(\ln r)^2} + (\ln r)^2 \right)^{\alpha+\frac{1}{2}} \le \left(\frac{b^2}{4(\ln r)^2} \right)^{\alpha+\frac{1}{2}},$$

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hence,

$$I(r,\alpha) \leq \int_0^{+\infty} \left(\frac{b^2}{4(\ln r)^2}\right)^{\alpha+\frac{1}{2}} e^{-\frac{b^2}{4(\ln r)^2}} db.$$

By means of the change of variable $y = \frac{b^2}{4(\ln r)^2}$ and by definition of the Gamma function [12, 8.310],

$$I(r,\alpha) \leq \ln r \int_0^{+\infty} y^{\alpha} e^{-y} dy = \ln r \Gamma(\alpha+1).$$

For $\alpha \geq -\frac{1}{2}$, we can write

$$\begin{aligned} I(r,\alpha) &\leq \int_0^{2(\ln r)^2} \left(2(\ln r)^2\right)^{\alpha+\frac{1}{2}} e^{-\frac{b^2}{4(\ln r)^2}} db + \int_{2(\ln r)^2}^{+\infty} \left(\frac{b^2}{2(\ln r)^2}\right)^{\alpha+\frac{1}{2}} e^{-\frac{b^2}{4(\ln r)^2}} db \\ &\leq 2^{\alpha+\frac{1}{2}} (\ln r)^{2\alpha+1} \int_0^{2(\ln r)^2} e^{-\frac{b^2}{4(\ln r)^2}} db + 2^{\alpha+\frac{1}{2}} \int_0^{+\infty} \left(\frac{b^2}{4(\ln r)^2}\right)^{\alpha+\frac{1}{2}} e^{-\frac{b^2}{4(\ln r)^2}} db. \end{aligned}$$

For the first integral in the above formula, we consider the change of variable $x^2 = \frac{b^2}{4(\ln r)^2}$, while the second one is the same as for the case $-1 < \alpha < -\frac{1}{2}$. Therefore, we obtain

$$\begin{aligned} I(r,\alpha) &\leq 2^{\alpha+\frac{3}{2}} (\ln r)^{2\alpha+2} \int_0^{\ln r} e^{-x^2} dx + 2^{\alpha+\frac{1}{2}} \ln r \Gamma(\alpha+1) \\ &= 2^{\alpha+\frac{3}{2}} (\ln r)^{2\alpha+2} \frac{\sqrt{\pi}}{2} \operatorname{erf}(\ln r) + 2^{\alpha+\frac{1}{2}} \ln r \Gamma(\alpha+1), \end{aligned}$$

where $\operatorname{erf}(\cdot)$ is the error function (see [12, 8.250(1)]). By using the simple inequality $\operatorname{erf}(\ln r) < 1$, we obtain the result. ∎

At this point we have the following result for the remainder term:

PROPOSITION 3.4. *For f bounded on Γ_r it holds*

$$(3.8) \quad \begin{aligned} |R_n^{(\alpha)}(f)| &\lesssim \max_{z\in\Gamma_r} |f(z)| r^{-2\sqrt{\bar{n}}+\ln r} \\ &\times \begin{cases} 2\Gamma(\alpha+1) & \textit{for } -1 < \alpha < -\frac{1}{2}, \\ 2^{\alpha+\frac{3}{2}} \left((\ln r)^{2\alpha+1}\sqrt{\pi} + \Gamma(\alpha+1)\right) & \textit{for } \alpha \geq -\frac{1}{2}, \end{cases} \end{aligned}$$

with $\bar{n}$ as in (3.5).

Proof. By Remark 3.2 and since

$$\exp(\sqrt{-z}) = \exp(\Re(\sqrt{-z}))\exp(i\Im(\sqrt{-z})),$$

where the symbol $\Im(\cdot)$ denotes the imaginary part, we have

$$\begin{aligned} \left|R_n^{(\alpha)}(f)\right| &\lesssim r^{-2\sqrt{\bar{n}}} \int_{\Gamma_r} |z^{\alpha} e^{-z}||f(z)||dz| \\ &\leq \max_{z\in\Gamma_r} |f(z)| r^{-2\sqrt{\bar{n}}} \int_{\Gamma_r} |z^{\alpha}||e^{-z}||dz|. \end{aligned}$$

By writing $z = a + ib$ $(a, b \in \mathbb{R})$ and using (3.3), we have that $z \in \Gamma_r$ iff

$$a = \frac{b^2 - 4(\ln r)^4}{4(\ln r)^2}.$$

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With this parametrization of the parabola, we obtain

$$\left|R_n^{(\alpha)}(f)\right| \lesssim \max_{z\in\Gamma_r}|f(z)|r^{-2\sqrt{n}} \int_{-\infty}^{+\infty} \left|\frac{b^2-4(\ln r)^4+4b(\ln r)^2 i}{4(\ln r)^2}\right|^{\alpha} \times e^{-\frac{b^2}{4(\ln r)^2}} e^{(lnr)^2} \left|\frac{2b+4(\ln r)^2 i}{4(\ln r)^2}\right| db,$$

and, after some computations,

$$\begin{aligned}\left|R_n^{(\alpha)}(f)\right| &\lesssim \max_{z\in\Gamma_r}|f(z)|\frac{r^{-2\sqrt{n}+\ln r}}{2^{2\alpha+1}(\ln r)^{2\alpha+2}} \int_{-\infty}^{+\infty} \left((b^2+4(\ln r)^4\right)^{\alpha+\frac{1}{2}} e^{-\frac{b^2}{4(\ln r)^2}} db \\ &= \max_{z\in\Gamma_r}|f(z)|\frac{r^{-2\sqrt{n}+\ln r}}{\ln r} \int_{-\infty}^{+\infty} \left(\frac{b^2}{4(\ln r)^2}+(\ln r)^2\right)^{\alpha+\frac{1}{2}} e^{-\frac{b^2}{4(\ln r)^2}} db \\ &= \max_{z\in\Gamma_r}|f(z)|\frac{r^{-2\sqrt{n}+\ln r}}{\ln r} 2\int_{0}^{+\infty} \left(\frac{b^2}{4(\ln r)^2}+(\ln r)^2\right)^{\alpha+\frac{1}{2}} e^{-\frac{b^2}{4(\ln r)^2}} db \\ &= \max_{z\in\Gamma_r}|f(z)|\frac{r^{-2\sqrt{n}+\ln r}}{\ln r} 2I(r,\alpha)\end{aligned}$$

(cf. (3.7)). By using Lemma 3.3 we obtain the result. ☐

As in the previous section, the analysis depends on the particular function f (cf. (3.8)). In order to characterize the singularity of f on the boundary Γ_R, suppose for example that $f(t) \sim (t+B)^\nu$, with $B > 0$ and $\nu \notin \mathbb{Z}$, in a neighborhood of $-B$. In this case $-B$ is a branch point, and Γ_R, $R = e^{\sqrt{B}}$, is a parabola of type (3.3) with vertex in $-B$. Moreover, in order to employ formula (3.8), we need to assume $\nu < 0$. As for the choice of r, first, by using (3.3), we observe that $z = |z|e^{i\theta} \in \Gamma_r$ iff

$$\Re\left(\sqrt{-|z|e^{i\theta}}\right) = \ln r,$$

from which it follows that

$$|z| = \frac{(\ln r)^2}{\sin^2\left(\frac{\theta}{2}\right)}, \quad \text{and therefore,} \quad z = \frac{(\ln r)^2}{\sin^2\left(\frac{\theta}{2}\right)} e^{i\theta}.$$

Then, we have

$$\max_{z\in\Gamma_r}|f(z)| = \max_{\theta\in[0,2\pi]}\left|\frac{(\ln r)^2 e^{i\theta}}{\sin^2(\theta/2)}+B\right|^{\nu},$$

in which the maximum is reached at $\theta = \pi$. Hence, since by definition of Γ_R it holds that $B = (\ln R)^2$, we obtain

$$\begin{aligned}\max_{z\in\Gamma_r}|f(z)| &= [(\ln R)^2-(\ln r)^2]^\nu = (\ln R+\ln r)^\nu(\ln R-\ln r)^\nu \\ &= (\ln R+\ln r)^\nu\left[\ln\left(1+\frac{R-r}{r}\right)\right]^\nu \\ &\sim (\ln R+\ln r)^\nu\left(\frac{R-r}{r}\right)^\nu, \quad r\to R \\ &\le (2\ln r)^\nu\left(\frac{R-r}{r}\right)^\nu.\end{aligned}$$

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By inserting the above result in (3.8), we have that

$$|R_n^{(\alpha)}(f)| \lesssim \mathcal{E}_n^L(r)$$

with

$$\mathcal{E}_n^L(r) := (\ln r)^\nu (R-r)^\nu r^{-2\sqrt{n}-\nu+\ln r} \times \begin{cases} 2^{\nu+1}\Gamma(\alpha+1) & \text{for } -1<\alpha<-\frac{1}{2}, \\ 2^{\alpha+\nu+\frac{3}{2}}\left((\ln r)^{2\alpha+1}\sqrt{\pi}+\Gamma(\alpha+1)\right) & \text{for } \alpha \geq -\frac{1}{2}. \end{cases} \tag{3.9}$$

In order to optimize the above quantity with respect to r, we search for $\bar{r}$ such that

$$\bar{r} = \arg\min_{1<r<R} (R-r)^\nu r^{-2\sqrt{n}-\nu}.$$

This leads to

$$\bar{r} = \frac{(\overline{m}+\nu)R}{\overline{m}}, \quad \text{with} \quad \overline{m} = 2\sqrt{n}.$$

We decided to neglect the terms involving $\ln r$ in the minimization (cf (3.9)) in order to simplify the computations and to obtain an explicit expression for $\bar{r}$. Substituting the value of $\bar{r}$ in (3.9) leads to

$$\mathcal{E}_n^L(\bar{r}) \sim (\ln R)^\nu (-\nu)^\nu R^{-\overline{m}} (\overline{m})^{\overline{m}} (\overline{m}+\nu)^{-\overline{m}-\nu} \times \begin{cases} 2^{\nu+1}\Gamma(\alpha+1) & \text{for } -1<\alpha<-\frac{1}{2}, \\ 2^{\alpha+\nu+\frac{3}{2}}\left((\ln R)^{2\alpha+1}\sqrt{\pi}+\Gamma(\alpha+1)\right) & \text{for } \alpha \geq -\frac{1}{2}, \end{cases} \tag{3.10}$$

for $\overline{m} \to +\infty$.

Similar observations made in Remark 2.4 for the Gauss–Radau–Jacobi rule are valid also in this case. Moreover, if f is meromorphic, as considered in Section 2.1, we show in the next section how to exploit the position of the poles (see again [1]).

3.1. Meromorphic functions. Similarly to the Jacobi case, suppose that f has no singularities within or on a particular parabola $\Gamma_{\tilde{r}}$ of type (3.3), except for a pair of simple poles z_0 and $\bar{z}_0$. Denoting by $\mathcal{C}_1$ and $\mathcal{C}_2$ two arbitrary small circles surrounding the two poles, the idea is to define $\mathcal{C} = \Gamma_{\tilde{r}} \cup \mathcal{C}_1 \cup \mathcal{C}_2$ as for the contour in (3.2). By running through $\mathcal{C}$ in the counterclockwise direction, we obtain

$$R_n^{(\alpha)}(f) = \frac{1}{2\pi i}\left(\int_{\Gamma_{\tilde{r}}} \frac{\psi^{(\alpha)}(z)}{\phi^{(\alpha)}(z)} f(z)dz - \int_{\mathcal{C}_1\cup\mathcal{C}_2} \frac{\psi^{(\alpha)}(z)}{\phi^{(\alpha)}(z)} f(z)dz\right).$$

By using, for $n \to +\infty$, the asymptotic (3.4) and Remark 3.2, the contribution on the parabola is given by

$$\begin{aligned} \left|\frac{1}{2\pi i}\int_{\Gamma_{\tilde{r}}} \frac{\psi^{(\alpha)}(z)}{\phi^{(\alpha)}(z)} f(z)dz\right| &\sim (\tilde{r})^{-2\sqrt{n}} \left|\int_{\Gamma_{\tilde{r}}} z^\alpha e^{-z} f(z)dz\right| \\ &\leq (\tilde{r})^{-2\sqrt{n}} \int_{\Gamma_{\tilde{r}}} \left|w^{(\alpha)}(z)f(z)\right| |dz|. \end{aligned}$$

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Moreover, by the residue theorem and again formula (3.4), we can write

$$\begin{aligned}\frac{1}{2\pi i}\int_{\mathcal{C}_1\cup\mathcal{C}_2}\frac{\psi^{(\alpha)}(z)}{\phi^{(\alpha)}(z)}f(z)dz &= \mathrm{Res}(f,z_0)\frac{\psi^{(\alpha)}(z_0)}{\phi^{(\alpha)}(z_0)}+\mathrm{Res}(f,\bar z_0)\frac{\psi^{(\alpha)}(\bar z_0)}{\phi^{(\alpha)}(\bar z_0)}\\ &= 2\Re\left\{\mathrm{Res}(f,z_0)\frac{\psi^{(\alpha)}(z_0)}{\phi^{(\alpha)}(z_0)}\right\}\\ &\sim -4\pi\Re\left\{\mathrm{Res}(f,z_0)e^{-i\pi(\alpha+1)}w^{(\alpha)}(z_0)\left(e^{\sqrt{-z_0}}\right)^{-2\sqrt{\bar n}}\right\}.\end{aligned}$$

Denoting by Γ_R the parabola of type (3.3) passing through z_0 and $\bar z_0$, we have that $\exp(\Re(\sqrt{-z_0}))=R$. Since $\tilde r > R$, we can neglect the contribution on the parabola and consider the estimate

$$R_n^{(\alpha)}(f)\sim 4\pi\Re\left\{\mathrm{Res}(f,z_0)e^{-i\pi(\alpha+1)}w^{(\alpha)}(z_0)\left(e^{\sqrt{-z_0}}\right)^{-2\sqrt{\bar n}}\right\}.$$

This leads to

$$\left|R_n^{(\alpha)}(f)\right|\lesssim 4\pi\left|\mathrm{Res}(f,z_0)w^{(\alpha)}(z_0)\right|R^{-\overline{m}}, \tag{3.11}$$

with $\overline{m}=2\sqrt{\bar n}$.

4. Numerical experiments. In this section we test the previously derived error approximations on some examples. As for the Gauss–Radau–Jacobi rule (cf. (2.1)), we consider the integrals

$$\int_{-1}^{1}(t-c)^{\gamma}w^{(\alpha,\beta)}(t)dt,\quad c<-1,\ \gamma\notin\mathbb{Z}, \tag{4.1}$$

$$\int_{-1}^{1}\frac{1}{1+t^2}w^{(\alpha,\beta)}(t)dt, \tag{4.2}$$

for different values of the parameters. In Figure 4.1 and Figure 4.2 we display the relative error together with the estimates (2.11) and (2.13), where we neglect the term $\mathcal{R}_M$ for the computation of the integral (4.1) with $\gamma<0$ and $\gamma>0$, respectively. Here and in all remaining figures, the errors and the estimates are plotted in a logarithmic scale. We can observe that the error estimates lose accuracy as $c\to -1$, as a consequence of Proposition 2.1. In Figure 4.3 we display the error and the estimate (2.14) for the evaluation of integral (4.2), in which the meromorphic function $F(z)=\frac{1}{1+z^2}$ has poles $\pm i$.

As for the Gauss–Radau–Laguerre rule (3.1), we consider the integrals

$$\int_{0}^{+\infty}(t+B)^{\nu}w^{(\alpha)}(t)dt,\quad B>0,\nu<0,\nu\notin\mathbb{Z}, \tag{4.3}$$

$$\int_{0}^{+\infty}\frac{1}{1+e^t}w^{(\alpha)}(t)dt, \tag{4.4}$$

$$\int_{0}^{+\infty}\frac{1}{1+t^2}w^{(\alpha)}(t)dt. \tag{4.5}$$

In Figure 4.4 we display the relative error and the approximation (3.10) for different values of the parameters B, ν, and α for the computation of the integral (4.3). Finally, in Figure 4.5 we test the estimate (3.11) for the evaluation of the integrals (4.4) and (4.5). As for the meromorphic function $G(z)=\frac{1}{1+e^z}$, we have considered the poles closest to the real axis, that is, $\pm i\pi$.

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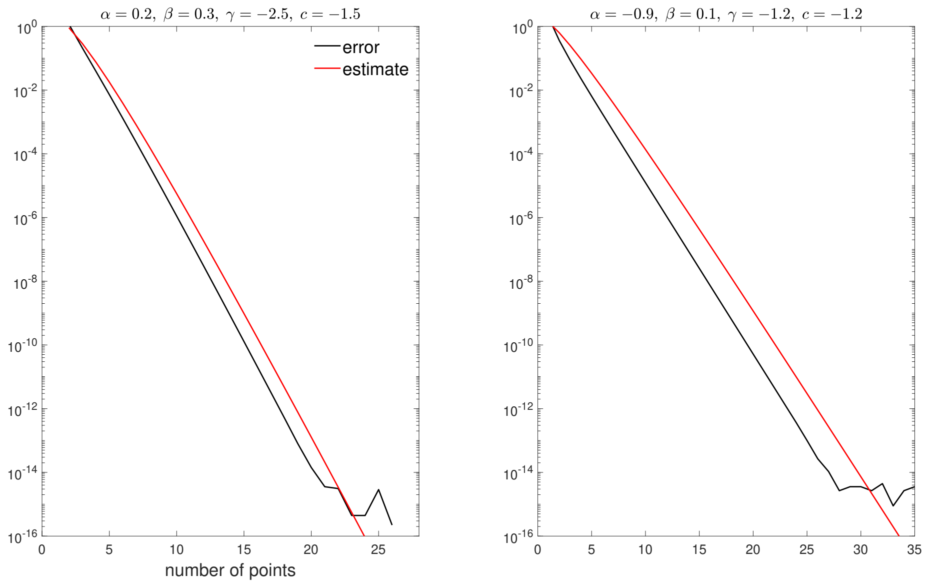

FIG. 4.1. *The relative error of the Gauss–Radau–Jacobi rule and the estimate* (2.11) *for the computation of the integral* (4.1)*, with* $\gamma < 0$*.*

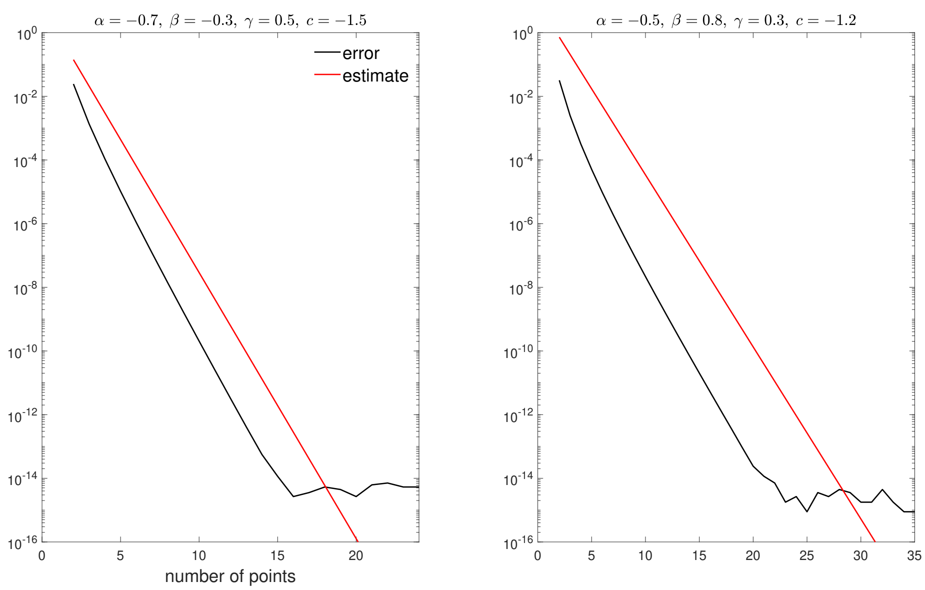

FIG. 4.2. *The relative error of the Gauss–Radau–Jacobi rule and the estimate* (2.13) *for the computation of the integral* (4.1)*, with* $\gamma > 0$*.*

5. Conclusions. In this work we have developed an a-priori and derivative-free error analysis for the Gauss–Radau–Jacobi and Gauss–Radau–Laguerre rules for analytic functions. By considering different types of singularities of the integrand functions, we have presented some strategies that allow to obtain quite accurate approximations of the error, in which the dependence on the number of interior points of the quadrature formula is made explicit.

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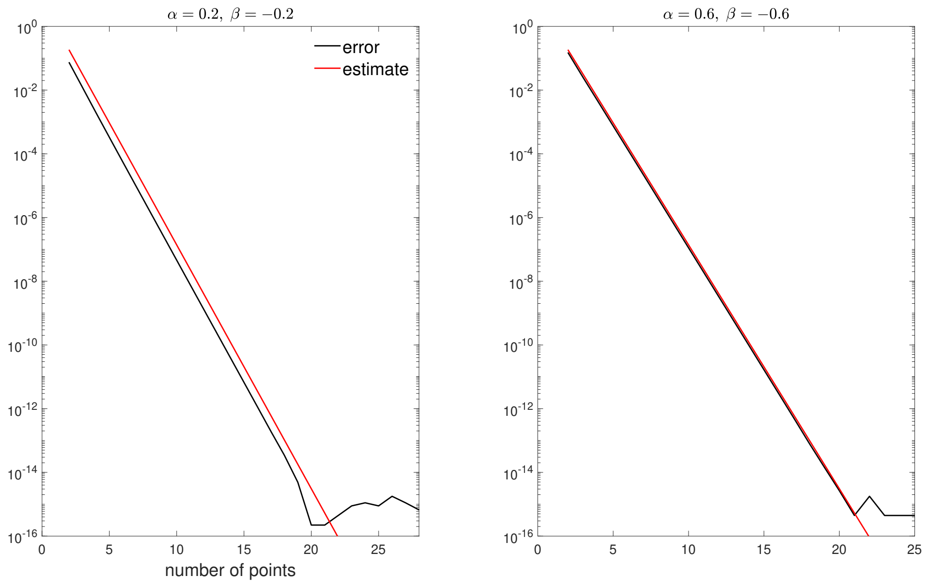

FIG. 4.3. *The relative error of the Gauss–Radau–Jacobi rule and the estimate* (2.14) *for the computation of the integral* (4.2).

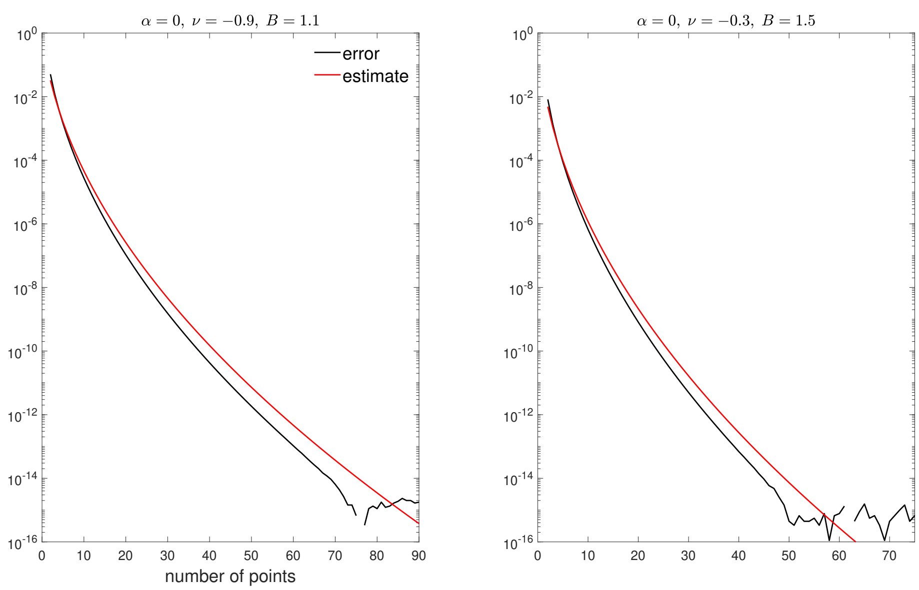

FIG. 4.4. *The relative error of the Gauss–Radau–Laguerre rule and the estimate* (3.10) *for the computation of the integral* (4.3).

We want to point out that, in the case of the Jacobi weight function, a similar analysis can be developed also for the $(n+2)$-point Gauss–Lobatto–Jacobi quadrature rule (see [9])

$$\int_{-1}^{1} f(t)w^{(\alpha,\beta)}(t)dt = \lambda_0^L f(-1) + \sum_{k=1}^{n} \lambda_k^L f\left(t_k^L\right) + \lambda_{n+1}^L f(1) + R_n^L(f).$$

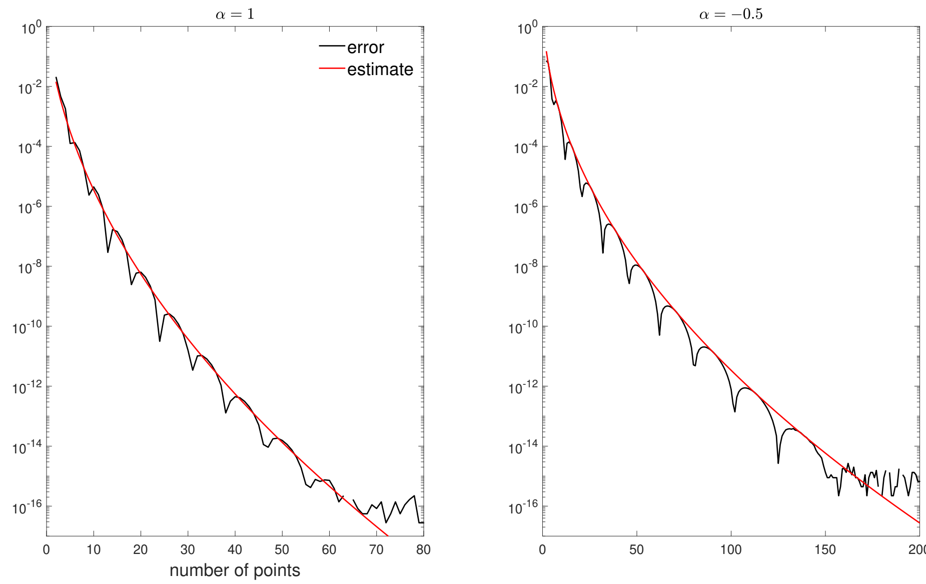

FIG. 4.5. *The relative error of the Gauss–Radau–Laguerre rule and the estimate* (3.11) *for the computation of the integral* (4.4) *(left) and the integral* (4.5) *(right).*

Indeed, the whole analysis presented in Section 2 can be adapted by observing that in the contour integral representation of the remainder

$$R_n(f) = \frac{1}{2\pi i}\int_{\mathcal{C}} K_n^L(z)f(z)dz,$$

the kernel is given by (see [3])

$$K_n^L(z) = \frac{\Pi_n^{(\alpha+1,\beta+1)}(z)}{(1-z)(1+z)P_n^{(\alpha+1,\beta+1)}(z)}$$

(cf. formula (2.2)). Recently, error bounds for Gauss–Lobatto quadrature of analytic functions have been derived in [15]. In this work, the authors examine the maximum of the kernel on an ellipse of type (2.4) and numerically provide the optimal value of r, i.e., the sum of the semiaxes of the ellipse. The main difference is that in the present work the asymptotic estimate of the kernel has been exploited to obtain explicit approximations of the error.

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