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ERROR BOUNDS FOR GAUSSIAN QUADRATURE FORMULAE WITH LEGENDRE WEIGHT FUNCTION FOR ANALYTIC INTEGRANDS*

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Abstract. In this paper we are concerned with a method for the numerical evaluation of the error terms in Gaussian quadrature formulae with the Legendre weight function. Inspired by the work of H. Wang and L. Zhang [J. Sci. Comput., 75 (2018), pp. 457–477] and applying the results of S. Notaris [Math. Comp., 75 (2006), pp. 1217–1231], we determine an explicit formula for the kernel. This explicit expression is used for finding the points on ellipses where the maximum of the modulus of the kernel is attained. Effective error bounds for this quadrature formula for analytic integrands are derived.

Key words. Gauss quadrature formulae, Legendre polynomials, remainder term for analytic function, error bound

AMS subject classifications. 65D32, 65D30, 41A55

1. Introduction. Numerical integration is the process of approximating the definite integral of a given function. An n-point quadrature formula (QF) with respect to some positive weight function ω on a finite interval, which we normalize to be $[-1, 1]$, has the form

$$\int_{-1}^{1} \omega(t) f(t)\, dt = \sum_{i=1}^{n} \omega_i f(\xi_i) + R_n(f) \tag{1.1}$$

for some set of nodes ξ_i and weights ω_i. There are many choices for these nodes and weights. The QF (1.1) is said to have (algebraic) degree of precision d if $R_n(f) = 0$ for all $f \in \mathcal{P}_d$, where $\mathcal{P}_d$ denotes the set of all (algebraic) polynomials of degree at most d. The unique optimal interpolatory QF with n nodes that has maximal degree of precision $2n - 1$ is the Gauss quadrature formula. It is named after Gauss who discovered it in [3]. We are concerned with the Gauss-Legendre QF associated with the Legendre weight function. In the work [11], which inspired us, the authors considered Jacobi polynomials $P_n^{(\alpha,\beta)}$, which are orthogonal over $[-1, 1]$ with respect to the Jacobi weight function

$$\omega(t) = (1 - t)^{\alpha} (1 + t)^{\beta}, \qquad \alpha, \beta > -1.$$

Here, we consider the particular case where $\alpha = \beta = 0$, which leads to the Gauss-Legendre quadrature (1.1) with weight function $\omega(t) = 1$, and we will estimate the remainder term of this QF, R_n. When f is an analytic function, the remainder term can be represented as a contour integral with a complex kernel. We study the kernel on elliptic contours with foci at the points ∓ 1 and the sum of semi-axes $\rho > 1$ for the given QF. We determine an explicit expression for the kernel, determine the location on the ellipses where the maximum modulus of the kernel is attained, and we derive effective error bounds for this QF.

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1.1. Error bounds of QFs for analytic functions. Let Γ be a simple closed curve in the complex plane encompassing the interval $[-1,1]$, and let $\mathcal{D}$ be its interior. Suppose that f is a function that is analytic in $\mathcal{D}$ and continuous on $\overline{\mathcal{D}}$. It follows from the Lagrange interpolation formula (see, e. g., [9, Chapter 2]) that

$$r_n(f;t) = f(t) - \sum_{i=1}^{n} l_i(t) f(\xi_i) = \frac{1}{2\pi\, i} \oint_\Gamma \frac{f(z)\Omega_n(t)}{(z-t)\Omega_n(z)}\, dz, \tag{1.2}$$

with

$$\Omega_n(z) = c_n \prod_{i=1}^{n} (z-\xi_i) \qquad (c_n \neq 0),$$

where ξ_i are the zeros of the corresponding orthogonal polynomial $\Omega_n(t)$ (which is monic when $c_n = 1$) and l_i are the so-called fundamental functions of Lagrange interpolation. By multiplying (1.2) by the weight function $\omega(t)$ and integrating in t over $(-1,1)$, we get a contour integral representation for the remainder term $R_n(f)$ in the Gauss QF (1.1),

$$R_n(f) = I(f;\omega) - \sum_{i=1}^{n} \omega_i f(\xi_i) = \frac{1}{2\pi\, i} \oint_\Gamma K_n(z;\omega) f(z)\, dz, \tag{1.3}$$

where

$$I(f;\omega) = \int_{-1}^{1} \omega(t)\, f(t)\, dt, \qquad \omega_i = \int_{-1}^{1} \omega(t)\, l_i(t)\, dt,$$

and the *kernel* $K_n(z) = K_n(z;\omega)$ can be expressed in the form

$$K_n(z;\omega) = \frac{\varrho_n(z;\omega)}{\Omega_n(z)}, \qquad \varrho_n(z;\omega) = \int_{-1}^{1} \omega(t)\, \frac{\Omega_n(t)}{z-t}\, dt, \qquad z \in \mathbb{C} \setminus [-1,1]. \tag{1.4}$$

The integral representation (1.3) directly leads to the error bound

$$|R_n(f)| \le \frac{l(\Gamma)}{2\pi} \left(\max_{z\in\Gamma} |K_n(z)| \right) \left(\max_{z\in\Gamma} |f(z)| \right), \tag{1.5}$$

where $l(\Gamma)$ is the length of the contour Γ (see [2]).

A common choice for the contour Γ is one of the confocal ellipses with foci at the points ∓ 1, also known as the Bernstein ellipses, and the sum of semi-axes $\rho > 1$,

$$\mathcal{E}_\rho = \left\{ z \in \mathbb{C} :\ z = \frac{1}{2}\left(u + u^{-1}\right), u = \rho e^{i\theta},\ 0 \le \theta < 2\pi \right\}. \tag{1.6}$$

The Bernstein ellipse has major and minor semi-axes given by $\frac{1}{2}(\rho + \rho^{-1})$ and $\frac{1}{2}(\rho - \rho^{-1})$, respectively. A recent survey on error bounds (1.5) and others topics, when $\Gamma = \mathcal{E}_\rho$, for Gaussian-type QFs can be found in [2].

In this paper, we consider Legendre polynomials $\pi_n(t) = P_n^{(0,0)}(t)$ as the set of $\Omega_n(t)$, which are a particular instance of the well-known Jacobi polynomials $P_n^{(\alpha,\beta)}(t)$ for the parameters $\alpha = \beta = 0$. The behavior of these polynomials is studied and established for problems involving convergence rates of spectral interpolation and for spectral collocation method for solving integral and differential equations. By studying these problems, in [11] an explicit representation of $P_n^{(\alpha,\beta)}(t)$ in the parametrization variable was derived, the extrema of

$|P_n^{(\alpha,\beta)}(z)|$ on the Bernstein ellipse were identified for some parameters, and refined asymptotic estimates were provided. We use the following explicit formula for Jacobi polynomials obtained in [11, Lemma 3.2 and formula (3.11)],

$$P_n^{(\alpha,\beta)}(z) = \sum_{k=0}^{n} d_{|n-2k|,n} u^{n-2k}, \qquad z = \frac{1}{2}\left(u+u^{-1}\right), \tag{1.7}$$

where, in the case $\alpha=\beta>-1$,

$$d_{k,n} = \begin{cases} \frac{2^{2\alpha}\Gamma(n+\alpha+1)\Gamma\left(\frac{k+n+1}{2}+\alpha\right)\Gamma\left(\frac{n-k+1}{2}+\alpha\right)}{\sqrt{\pi}\Gamma(n+2\alpha+1)\Gamma\left(\frac{k+n}{2}+1\right)\Gamma\left(\frac{n-k}{2}+1\right)\Gamma(\alpha+1/2)}, & n-k \text{ even},\\ 0, & n-k \text{ odd}. \end{cases} \tag{1.8}$$

This general case will be used and adopted to the particular case of Legendre polynomials. Using properties of the Chebyshev polynomials of the first and second kind

$$T_n(\cos\theta) = \cos(n\theta), \qquad U_n(\cos\theta) = \frac{\sin((n+1)\theta)}{\sin\theta}, \qquad n \geq 0,$$

and the representations of them when $z \in \mathcal{E}_\rho$ in (cf. (1.6)), $z = \frac{1}{2}(u+u^{-1})$, $u = \rho e^{i\theta}$, $0 \leq \theta < 2\pi$ (see [6, pp. 1176–1177]),

$$T_n(z) = \frac{1}{2}(u^n + u^{-n}), \qquad U_n(z) = \frac{u^{n+1}-u^{-n-1}}{u-u^{-1}},$$

the authors in [11] obtained trigonometric representations of (1.7):

$$P_n^{(\alpha,\beta)}(\cos\theta) = d_{0,n} + 2\sum_{k=1}^{n} d_{k,n}\cos(k\theta). \tag{1.9}$$

There, some connection with Chebyshev polynomials were established. Some of the properties of Chebyshev polynomials are described by Notaris [8]. It is shown that the integrals

$$\int_{-1}^{1} \frac{p_n(t)}{z \mp t}\, dt, \qquad |z| \neq 1,$$

can be computed explicitly (see [8, Proposition 2.2.]) with p_n being one of the Chebysev polynomials of degree n. This particular property finds direct application in the computation of an explicit kernel formula in our case and further in the estimation of the error, which is described in the next sections.

2. The modulus of the kernel. The *kernel* is given by $K_n(z) = \frac{\varrho_n(z)}{\pi_n(z)}$, $z \notin [-1,1]$ (see (1.4)), where $\pi_n(z) = \Omega_n(z)$ is the Legendre polynomial of degree n and

$$\begin{aligned} \varrho_n(z) &= \int_{-1}^{1} \frac{\pi_n(t)}{z-t}\, dt = \int_0^\pi \frac{1}{z-\cos\theta}\left(2{\sum_{k=0}^{n}}'' d_{k,n}\cos k\theta\right)\sin\theta\, d\theta \\ &= 2{\sum_{k=0}^{n}}'' d_{k,n} \int_0^\pi \frac{\cos k\theta\, \sin\theta}{z-\cos\theta}\, d\theta. \end{aligned} \tag{2.1}$$

The notation $\sum''$ means that the first term $d_{0,n}$ in the sum must be halved. We consider (1.9) with $\alpha=\beta=0$, where $d_{k,n}$ is given by (1.8) with $\alpha=0$, i.e.,

$$d_{k,n} = \begin{cases} \frac{(n+k-1)!!(n-k-1)!!}{(n+k)!!(n-k)!!}, & n-k \text{ even},\\ 0, & n-k \text{ odd}, \end{cases}$$

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where

$$k!! = \begin{cases} \prod_{i=0}^{k/2-1}(k-2i), & k \text{ even}, \\ \prod_{i=0}^{(k-1)/2}(k-2i), & k \text{ odd}. \end{cases}$$

Further, using [8, Proposition 2.2, equation (2.8)] and its proof, for the expressions

$$I_k = \int_{-1}^{1} \frac{T_k(t)}{z-t}\,dt, \tag{2.2}$$

i.e., $I_k = \int_0^\pi \frac{\cos k\theta\, \sin\theta}{z-\cos\theta}\,d\theta$, it holds that

$$I_k = T_k(z)\log\frac{z+1}{z-1} - 4\sum_{j=1}^{\left[\frac{k+1}{2}\right]}{}' \frac{T_{k-2j+1}(z)}{2j-1} \qquad (|z|>1), \tag{2.3}$$

with the principal value of the logarithmic function $\log z = \log|z| + i\arg z$ $(-\pi < \arg z \leq \pi)$ and where the symbol $\sum'$ means that the last term in the sum must be halved if k is odd.

2.1. Expressions for the modulus of the kernel. Inserting the relation $z = (u+u)^{-1}/2$ $(|u|>1)$ in (2.3), it follows that

$$I_k = \frac{u^k + u^{-k}}{2}\log\frac{z+1}{z-1} - 2\sum_{j=1}^{\left[\frac{k+1}{2}\right]}{}' \frac{u^{k-2j+1} + u^{-(k-2j+1)}}{2j-1}. \tag{2.4}$$

Next, we note that

$$\log\frac{z+1}{z-1} = \log\frac{\frac{1}{2}(u+u^{-1})+1}{\frac{1}{2}(u+u^{-1})-1} = \log\frac{(1+u^{-1})^2}{(1-u^{-1})^2} = 2\log\frac{1+u^{-1}}{1-u^{-1}}. \tag{2.5}$$

Since

$$\log(1+u^{-1}) = \sum_{j=0}^{\infty}\frac{(-1)^j u^{-j-1}}{j+1}, \qquad \log(1-u^{-1}) = -\sum_{j=0}^{\infty}\frac{u^{-j-1}}{j+1} \qquad (|u^{-1}|<1),$$

in view of (2.5), it follows that

$$\log\frac{z+1}{z-1} = 4\sum_{j=0}^{\infty}\frac{u^{-2j-1}}{2j+1}. \tag{2.6}$$

Inserting (2.6) into (2.4) gives the relation

$$I_k = 2\left[\left(u^k + \frac{1}{u^k}\right)\sum_{j=0}^{\infty}\frac{1}{(2j+1)u^{2j+1}} - \sum_{j=1}^{\left[\frac{k+1}{2}\right]}{}' \frac{u^{k-2j+1} + \frac{1}{u^{k-2j+1}}}{2j-1}\right]. \tag{2.7}$$

Now, we can declare the following proposition.

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PROPOSITION 2.1. *It holds that*

$$I_k = \begin{cases} -4\sum_{j=0}^{\infty} \frac{(2j+1)u^{-2j-1}}{k^2-(2j+1)^2} = -4\left[\frac{u^{-1}}{k^2-1} + \frac{3u^{-3}}{k^2-9}\right] + o\left(u^{-4}\right), & k \text{ even},\\ -4\sum_{j=1}^{\infty} \frac{2ju^{-2j}}{k^2-(2j)^2} = -4\left[\frac{2u^{-2}}{k^2-4} + \frac{4u^{-4}}{k^2-16}\right] + o\left(u^{-5}\right), & k \text{ odd}. \end{cases}$$

Proof. In the case $k = 2m$, from (2.7), we see that

$$\begin{aligned} \frac{I_k}{2} &= \sum_{j=0}^{\infty} \frac{u^{k-2j-1}}{2j+1} + \sum_{j=0}^{\infty} \frac{u^{-k-2j-1}}{2j+1} - \sum_{j=1}^{m} \frac{u^{k-2j+1}}{2j-1} - \sum_{j=1}^{m} \frac{u^{-k+2j-1}}{2j-1} \\ &= \sum_{j=-m}^{\infty} \frac{u^{-2j-1}}{k+2j+1} + \sum_{j=m}^{\infty} \frac{u^{-2j-1}}{-k+2j+1} - \sum_{j=-m}^{-1} \frac{u^{-2j-1}}{k+2j+1} - \sum_{j=0}^{m-1} \frac{u^{-2j-1}}{k-2j-1}. \end{aligned}$$

Combining the first and the third terms of the last expression above and the second and fourth terms gives

$$\frac{I_k}{2} = \sum_{j=0}^{\infty} \frac{u^{-2j-1}}{k+2j+1} - \sum_{j=0}^{\infty} \frac{u^{-2j-1}}{k-2j-1} = -2\sum_{j=0}^{\infty} \frac{(2j+1)u^{-2j-1}}{k^2-(2j+1)^2}.$$

In the case $k = 2m+1$, we see that

$$\begin{aligned} \frac{I_k}{2} &= \sum_{j=0}^{\infty} \frac{u^{k-2j-1}}{2j+1} + \sum_{j=0}^{\infty} \frac{u^{-k-2j-1}}{2j+1} - \sum_{j=1}^{m} \frac{u^{k-2j+1}}{2j-1} - \sum_{j=1}^{m} \frac{u^{-k+2j-1}}{2j-1} - \frac{1}{k} \\ &= \sum_{j=-m}^{\infty} \frac{u^{-2j}}{k+2j} + \sum_{j=m+1}^{\infty} \frac{u^{-2j}}{-k+2j} - \sum_{j=-m}^{-1} \frac{u^{-2j}}{k+2j} - \sum_{j=1}^{m} \frac{u^{-2j}}{k-2j} - \frac{1}{k}. \end{aligned}$$

Combining the first, third, and fifth terms of the last expression above and the second and fourth terms gives

$$\frac{I_k}{2} = \sum_{j=1}^{\infty} \frac{u^{-2j}}{k+2j} - \sum_{j=1}^{\infty} \frac{u^{-2j}}{k-2j} = -2\sum_{j=1}^{\infty} \frac{(2j)u^{-2j}}{k^2-(2j)^2}. \qquad \square$$

Finally, on basis of (2.1), we have

$$\rho_n(z) = 2\sum_{k=0}^{n}{}'' d_{k,n} I_k, \tag{2.8}$$

where I_k are given by (2.7). Further,

$$\begin{aligned} \rho_{2m}(z) &= -16\left(\sum_{l=0}^{m}{}'' \frac{d_{2l,2m}}{4l^2-1}\cdot\frac{1}{u} + 3\sum_{l=0}^{m}{}'' \frac{d_{2l,2m}}{4l^2-9}\cdot\frac{1}{u^3}\right) + o\left(\frac{1}{u^4}\right),\\ \rho_{2m+1}(z) &= -32\left(\sum_{l=0}^{m} \frac{d_{2l+1,2m+1}}{(2l+1)^2-4}\cdot\frac{1}{u^2} + 2\sum_{l=0}^{m} \frac{d_{2l+1,2m+1}}{(2l+1)^2-16}\cdot\frac{1}{u^4}\right) + o\left(\frac{1}{u^5}\right), \end{aligned}$$

for $\rho \to \infty$ and $m \in \mathbb{N}$, which together with

$$\pi_n(z) = \sum_{k=0}^{n} d_{|n-2k|,n} u^{n-2k} = d_{n,n}u^n + d_{n-2,n}u^{n-2} + o\left(u^{n-3}\right) \quad (\rho \to \infty)$$

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from [11] yields, for $\rho \to \infty$,

$$K_{2m}(z) = \frac{-16\left(\sum\nolimits_{l=0}^{\prime\prime m} \frac{d_{2l,2m}}{4l^2-1} \cdot \frac{1}{u} + 3\sum\nolimits_{l=0}^{\prime\prime m} \frac{d_{2l,2m}}{4l^2-9} \cdot \frac{1}{u^3}\right) + o\left(\frac{1}{u^4}\right)}{d_{2m,2m}u^{2m} + d_{2m-2,2m}u^{2m-2} + o\left(u^{2m-3}\right)}$$

$$(2.9) \qquad = \frac{-16\sum\nolimits_{l=0}^{\prime\prime m} \frac{d_{2l,2m}}{4l^2-1}}{d_{2m,2m}u^{2m+1}} \cdot \frac{u^2 + 3\frac{\sum\nolimits_{l=0}^{\prime\prime m} \frac{d_{2l,2m}}{4l^2-9}}{\sum\nolimits_{l=0}^{\prime\prime m} \frac{d_{2l,2m}}{4l^2-1}} + o\left(\frac{1}{\rho}\right)}{u^2 + \frac{d_{2m-2,2m}}{d_{2m,2m}} + o\left(\frac{1}{\rho}\right)},$$

$$K_{2m+1}(z) = \frac{-32\left(\sum_{l=0}^{m} \frac{d_{2l+1,2m+1}}{(2l+1)^2-4} \cdot \frac{1}{u^2} + 2\sum_{l=0}^{m} \frac{d_{2l+1,2m+1}}{(2l+1)^2-16} \cdot \frac{1}{u^4}\right) + o\left(\frac{1}{u^5}\right)}{d_{2m+1,2m+1}u^{2m+1} + d_{2m-1,2m+1}u^{2m-1} + o\left(u^{2m-2}\right)}$$

$$(2.10) \qquad = \frac{-32\sum_{l=0}^{m} \frac{d_{2l+1,2m+1}}{(2l+1)^2-4}}{d_{2m+1,2m+1}u^{2m+3}} \cdot \frac{u^2 + 2\frac{\sum_{l=0}^{m} \frac{d_{2l+1,2m+1}}{(2l+1)^2-16}}{\sum_{l=0}^{m} \frac{d_{2l+1,2m+1}}{(2l+1)^2-4}} + o\left(\frac{1}{\rho}\right)}{u^2 + \frac{d_{2m-1,2m+1}}{d_{2m+1,2m+1}} + o\left(\frac{1}{\rho}\right)}.$$

The following observations are initiated on basis of many numerical experiments that we performed. The second factor in the kernels in (2.9), (2.10) is of the form

$$I(\rho,\theta) = \frac{u^2 + A + o\left(\frac{1}{\rho}\right)}{u^2 + B + o\left(\frac{1}{\rho}\right)} \qquad (\rho \to \infty),$$

where A and B are different real numbers and $u = \rho e^{i\theta}$ and $I(\rho,\theta) = I(\rho,\theta+\pi)$. For each $X \in \mathbb{R}$ we have

$$\left|u^2 + X + o\left(\frac{1}{\rho}\right)\right|^2 = \left(\rho^2\cos 2\theta + X + o\left(\frac{1}{\rho}\right)\right)^2 + \left(\rho^2 \sin 2\theta + o\left(\frac{1}{\rho}\right)\right)^2$$
$$= \rho^4 + 2X\rho^2\cos 2\theta + o(\rho) = \rho^2\left(\rho^2 + 2X\cos 2\theta + o\left(\rho^{-1}\right)\right) \quad (\rho \to \infty).$$

For ρ large enough, we are interesting in estimating $I(\rho,\theta)$, i.e., whether it holds that

$$I(\rho,\theta) = \frac{\rho^2 + 2A\cos 2\theta + o\left(\rho^{-1}\right)_{(\rho\to\infty)}}{\rho^2 + 2B\cos 2\theta + o\left(\rho^{-1}\right)_{(\rho\to\infty)}}$$
$$\le \frac{\rho^2 - 2A + o\left(\rho^{-1}\right)_{(\rho\to\infty)}}{\rho^2 - 2B + o\left(\rho^{-1}\right)_{(\rho\to\infty)}} = \left|I\left(\rho, \frac{\pi}{2}\right)\right| = \left|I\left(\rho, \frac{3\pi}{2}\right)\right|,$$

for each $\theta \in [0, 2\pi)$ if $A < B$, and similarly, if $A > B$, whether it holds that

$$I(\rho,\theta) = \frac{\rho^2 + 2A\cos 2\theta + o\left(\rho^{-1}\right)_{(\rho\to\infty)}}{\rho^2 + 2B\cos 2\theta + o\left(\rho^{-1}\right)_{(\rho\to\infty)}}$$
$$\le \frac{\rho^2 + 2A + o\left(\rho^{-1}\right)_{(\rho\to\infty)}}{\rho^2 + 2B + o\left(\rho^{-1}\right)_{(\rho\to\infty)}} = |I(\rho,0)| = |I(\rho,\pi)|$$

for each $\theta \in [0, 2\pi)$. That means that

$$\left(\rho^2 + 2A\cos 2\theta + o\left(\rho^{-1}\right)_{(\rho\to\infty)}\right)\left(\rho^2 - 2B + o\left(\rho^{-1}\right)_{(\rho\to\infty)}\right)$$
$$- \left(\rho^2 - 2A + o\left(\rho^{-1}\right)_{(\rho\to\infty)}\right)\left(\rho^2 + 2B\cos 2\theta + o\left(\rho^{-1}\right)_{(\rho\to\infty)}\right) \le 0$$

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for each $\theta \in [0, 2\pi)$ if $A < B$. Analogously, when $A > B$, we obtain the corresponding inequality

$$\left(\rho^2 + 2A\cos 2\theta + o\left(\rho^{-1}\right)_{(\rho\to\infty)}\right)\left(\rho^2 + 2B + o\left(\rho^{-1}\right)_{(\rho\to\infty)}\right) - \left(\rho^2 + 2A + o\left(\rho^{-1}\right)_{(\rho\to\infty)}\right)\left(\rho^2 + 2B\cos 2\theta + o\left(\rho^{-1}\right)_{(\rho\to\infty)}\right) \le 0$$

for each $\theta \in [0, 2\pi)$. The expressions on the left-hand sides in the previous two inequalities are of the form, for $\rho \to \infty$,

$$2(A-B)(1+\cos 2\theta)\rho^2 + o(\rho) \qquad \text{and} \qquad 2(B-A)(1-\cos 2\theta)\rho^2 + o(\rho),$$

for the cases $A < B$ and $A > B$, respectively. The last two inequalities always hold, expect when in the left-hand sides $\theta = \pi/2$ and $\theta = 3\pi/2$ ($A < B$) or $\theta = 0$ and $\theta = \pi$ ($A > B$), respectively.

The result of these considerations is that the value θ where the modulus of the kernel attains its maximum value depends only on the sign of the difference

$$D_n = 3\,\frac{\sum\nolimits''^{m}_{l=0} \frac{d_{2l,n}}{4l^2-9}}{\sum\nolimits''^{m}_{l=0} \frac{d_{2l,n}}{4l^2-1}} - \frac{d_{n-2,n}}{d_{n,n}} = 3\,\frac{\sum\nolimits''^{m}_{l=0} \frac{d_{2l,n}}{4l^2-9}}{\sum\nolimits''^{m}_{l=0} \frac{d_{2l,n}}{4l^2-1}} - \frac{n}{2n-1},$$

if n is even, and

$$D_n = 2\,\frac{\sum_{l=0}^{m} \frac{d_{2l+1,n}}{(2l+1)^2-16}}{\sum_{l=0}^{m} \frac{d_{2l+1,n}}{(2l+1)^2-4}} - \frac{d_{n-2,n}}{d_{n,n}} = 2\,\frac{\sum_{l=0}^{m} \frac{d_{2l+1,n}}{(2l+1)^2-16}}{\sum_{l=0}^{m} \frac{d_{2l+1,n}}{(2l+1)^2-4}} - \frac{n}{2n-1},$$

if n is odd (if $D_n \neq 0$), i.e.,

1. if $D_n < 0$, then the modulus of the kernel should attain its maximum at $\theta = \pi/2$ (and $\theta = 3\pi/2$);
2. if $D_n > 0$, then the modulus of the kernel should attain its maximum at $\theta = 0$ (and $\theta = \pi$).

We performed a substantial amount of numerical calculations that confirmed that the modulus of the kernel attains its maximum at $\theta = \pi/2$ (and at $\theta = 3\pi/2$) for ρ large enough (i.e., in our case $D_n < 0$). In that sense we suggest the following conjecture based on our observations.

CONJECTURE 2.1. *It is conjectured that the maximum modulus of the kernel $K_n(z)$ is attained at $\theta = \pi/2$ (and $\theta = 3\pi/2$), i.e.,*

$$\max_{z\in\mathcal{E}_\rho} |K_n(z)| = \max_{\theta\in[0,2\pi)} |K_n(z)| = \left|K_n\left(\pm\frac{i}{2}(\rho - \rho^{-1})\right)\right|,$$

for $\rho \ge \rho^*$, i.e., for ρ large enough.

In Figures 2.1 and 2.2, some graphs of the modulus of the kernels are presented, for $n = 3$ and $n = 4$, respectively, and for different choices of ρ.

2.2. Explicit expressions for the modulus of the kernel. In this section we present an analytical representation of the modulus of the *kernel* $K_n(z)$. Since the *kernel* is given by

$$K_n(z) = \frac{\varrho_n(z)}{\pi_n(z)} = \frac{A + iB}{C + iD},$$

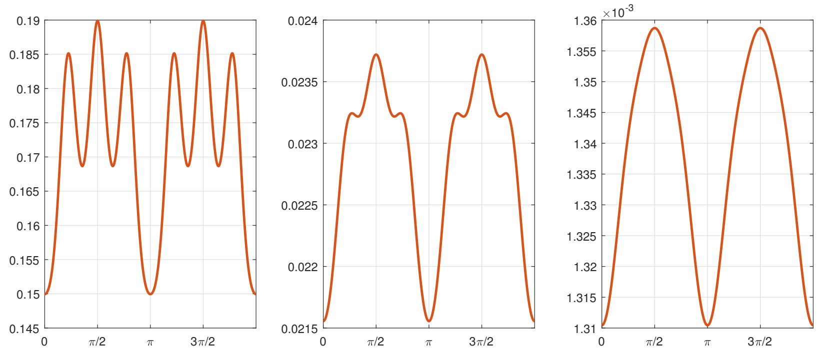

FIG. 2.1. $|K_3(z)|$ *for the cases* $\rho = 1.5, 2, 3$*, respectively.*

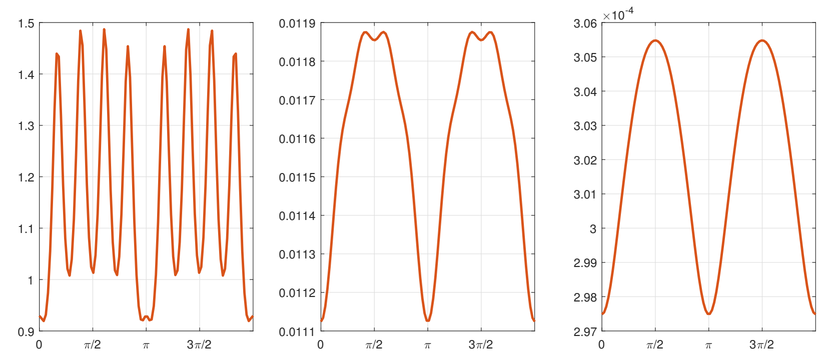

FIG. 2.2. $|K_4(z)|$ *for the cases* $\rho = 1.5, 2, 3$*, respectively.*

an explicit representation of its modulus is given by

$$|K_n(z)| = \frac{\sqrt{A^2 + B^2}}{\sqrt{C^2 + D^2}},$$

with some appropriate replacements stated below. In order to express $\varrho_n(z)$, we need some auxiliary considerations based on a separation of the real and imaginary parts of the terms I_0, $T_k(z)$ and the term involving linear combinations of $T_k(z)$ (see (2.2), (2.3)).

- $I_0 = Re(I_0) + i \cdot Im(I_0)$, i.e.,

$$\begin{aligned} I_0 &= \int_{-1}^{1} \frac{1}{\frac{1}{2}(u + \frac{1}{u}) - t}\, dt = \int_{-1}^{1} \frac{1}{\frac{\rho+\rho^{-1}}{2}\cos\theta + i \cdot \frac{\rho-\rho^{-1}}{2}\sin\theta\; - t}\, dt \\ &= \int_{-1}^{1} \frac{\gamma - t - i\cdot\delta}{(\gamma - t)^2 + \delta^2} dt = \underbrace{\int_{-1}^{1} \frac{\gamma - t}{(\gamma - t)^2 + \delta^2} dt}_{Re(I_0)} + i \cdot \underbrace{\int_{-1}^{1} \frac{-\delta}{(\gamma - t)^2 + \delta^2} dt}_{Im(I_0)}, \end{aligned}$$

by means of the substitutions $\gamma = \frac{\rho+\rho^{-1}}{2}\cos\theta$ and $\delta = \frac{\rho-\rho^{-1}}{2}\sin\theta$. Finally,

$$\begin{aligned} Re(I_0) &= -\frac{1}{2}\ln\frac{(\gamma - 1)^2 + \delta^2}{(\gamma + 1)^2 + \delta^2}, \\ Im(I_0) &= \arctan\left(\frac{\gamma - 1}{\delta}\right) - \arctan\left(\frac{\gamma + 1}{\delta}\right). \end{aligned}$$

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- $T_k = Re(T_k(z)) + i \cdot Im(T_k(z))$, i.e.,

$$T_k = \frac{1}{2}\left(u^k + \frac{1}{u^k}\right) = \frac{1}{2}\left(\rho^k(\cos k\theta + i\sin k\theta) + \rho^{-k}(\cos k\theta - i\sin k\theta)\right)$$
$$= \underbrace{\frac{\rho^k + \rho^{-k}}{2}\cos k\theta}_{Re(T_k)} + i\cdot \underbrace{\frac{\rho^k - \rho^{-k}}{2}\sin k\theta}_{Im(T_k)}.$$

- $S = -4\sum_{j=1}^{\prime\left[\frac{k+1}{2}\right]} \frac{T_{k-2j+1}(z)}{2j-1} = Re(S) + i \cdot Im(S)$.

Since

$$T_s(z) = \frac{\rho^s + \rho^{-s}}{2}\cos s\theta + i\cdot\frac{\rho^s - \rho^{-s}}{2}\sin s\theta,$$

with $s = k - 2j + 1$, we get

$$Re(S) = -4\sum_{j=1}^{\left[\frac{k+1}{2}\right]}{}' \frac{1}{2j-1}\left(\frac{\rho^{k-2j+1} + \rho^{-(k-2j+1)}}{2}\cos(k-2j+1)\theta\right),$$
$$Im(S) = -4\sum_{j=1}^{\left[\frac{k+1}{2}\right]}{}' \frac{1}{2j-1}\left(\frac{\rho^{k-2j+1} - \rho^{-(k-2j+1)}}{2}\sin(k-2j+1)\theta\right).$$

We have extracted the real and imaginary parts of the terms in $\varrho_n(z)$ (see (2.1)). Hence,

$$\varrho_n(z) = 2\sum_{k=0}^{n}{}'' d_{k,n}I_k = 2\sum_{k=0}^{n}{}'' d_{k,n}\left(T_k(z)I_0 - 4\sum_{j=1}^{\left[\frac{k+1}{2}\right]}{}' \frac{T_{k-2j+1}(z)}{2j-1}\right)$$
$$= 2\sum_{k=0}^{n}{}'' d_{k,n}\Big(\big(Re(T_k) + iIm(T_k)\big)\big(Re(I_0) + iIm(I_0)\big) + Re(S) + iIm(S)\Big)$$
$$= \underbrace{\sum_{k=0}^{n}{}'' 2d_{k,n}\big(Re(T_k)Re(I_0) - Im(T_k)Im(I_0) + Re(S)\big)}_{A}$$
$$+ i\cdot\underbrace{\sum_{k=0}^{n}{}'' 2d_{k,n}\big(Re(T_k)Im(I_0) + Im(T_k)Re(I_0) + Im(S)\big)}_{B}.$$

Thus, it is now easy to compute the modulus $|\varrho_n(z)| = \sqrt{A^2+B^2}$.

Similarly, in order to calculate $|\pi_n(z)| = \left|\sum_{k=0}^{n} d_{|n-2k|,n}u^{n-2k}\right| = \sqrt{C^2+D^2}$ (see (1.7) with $\alpha = \beta = 0$), we need to express its real and imaginary parts:

$$C = \begin{cases} \sum_{k=0}^{\frac{n}{2}-1} d_{n-2k,n}\left(\rho^{n-2k} + \rho^{-(n-2k)}\right)\cos(n-2k)\theta + d_{0,n}, & n \text{ even},\\ \sum_{k=0}^{\frac{n-1}{2}} d_{n-2k,n}\left(\rho^{n-2k} + \rho^{-(n-2k)}\right)\cos(n-2k)\theta, & n \text{ odd}, \end{cases}$$

$$D = \sum_{k=0}^{\left[\frac{n-1}{2}\right]} d_{n-2k,n}\left(\rho^{n-2k} - \rho^{-(n-2k)}\right)\sin(n-2k)\theta.$$

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REMARK 2.2. The previous derivation can be done easier if we use the relation $I_0 = 2\log\frac{1+u^{-1}}{1-u^{-1}}$ $(|u|>1)$ from (2.5). In this case, on basis of (2.8), we have, say, for n odd (analogously when n is even),

$$\rho_n(z) = 2\sum_{k=0}^{n}{}'' d_{k,n} I_k = -8\sum_{k=0}^{n}{}'' d_{k,n}\sum_{j=1}^{\infty}\frac{2j}{k^2-(2j)^2}\cdot\frac{1}{u^{2j}} = \sum_{j=1}^{\infty}\frac{c_j}{u^{2j}},$$

with

$$c_j = -16j\sum_{k=0}^{n}{}''\frac{d_{k,n}}{k^2-(2j)^2}.$$

Finally, we derive

$$|\varrho_n(z)| = \sqrt{\sum_{j=1}^{\infty} c_j^2\rho^{-4j} + 2\sum_{i=2}^{\infty}\sum_{j=1}^{i-1} c_i c_j \rho^{-2i-2j}\cos 2(i-j)\theta}.$$

In Figure 2.3 the graphs of the modulus of the kernels K_5 is displayed for $n=5$ and for different choices of ρ.

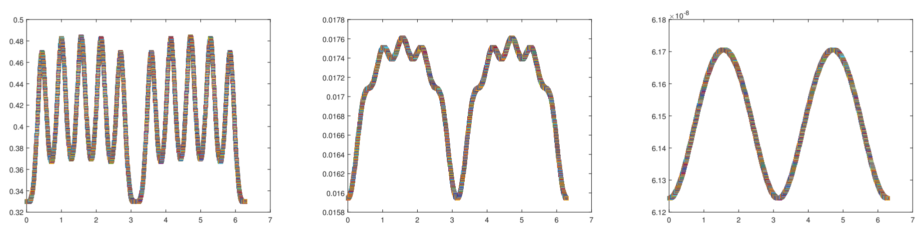

FIG. 2.3. $|K_5|$ *for the cases* $\rho = 1.2, 1.6, 5$, *respectively.*

3. Numerical results. According to the previous notation, under the assumption that f is analytic inside $\mathcal{E}_{\rho_{\max}}$, the error bound for the corresponding quadrature formula can be optimized by

$$|R_n(f)| \le r_n(f),$$

where, according to (1.5) with $\Gamma = \mathcal{E}_\rho$,

$$r_n(f) = \inf_{\rho^*<\rho<\rho_{\max}}\left[\frac{\ell(\mathcal{E}_\rho)}{2\pi}\left(\max_{z\in\mathcal{E}_\rho}|K_n(z)|\right)\left(\max_{z\in\mathcal{E}_\rho}|f(z)|\right)\right].$$

Here, ρ^* is the smallest possible value of ρ^* from Conjecture 2.1, which is obtained empirically by starting from the value 1.0001; $\rho_{\max}$ depends on the integrand (it is specified in the examples below), and $\ell(\mathcal{E}_\rho)$ represents the length of the ellipse $\mathcal{E}_\rho$ (1.6), which can be estimated by (see [1])

$$\ell(\mathcal{E}_\rho) \le 2\pi a_1\left(1-\frac{1}{4}a_1^{-2}-\frac{3}{64}a_1^{-4}-\frac{5}{256}a_1^{-6}\right),$$

where $a_1 = (\rho + \rho^{-1})/2$.

The error bound $r_n(f)$ reduces to

$$r_n(f,\omega) = \inf_{\rho^* < \rho < \rho_{\max}} \left[a_1 \left(1 - \frac{1}{4} a_1^{-2} - \frac{3}{64} a_1^{-4} - \frac{5}{256} a_1^{-6} \right) \left(\max_{z \in \mathcal{E}_\rho} |K_n(z)| \right) \left(\max_{z \in \mathcal{E}_\rho} |f(z)| \right) \right].$$

In order to verify the proposed error bounds, we made several tests and compared them with respect to the exact (actual) errors. Various examples are presented for some special functions appearing in the literature.

"*Error*" denotes the sharp (actual) error bound of the corresponding formula. All results in our experiments are calculated by using high precision arithmetic. Our program codes are based on the codes *sgauss.m, sr_jacobi.m* for symbolic calculation (cf. [5] and [4]). The results are summarized in Tables 3.1, 3.2, and 3.3 for the examples given below. The numbers in parentheses indicate decimal exponents. The value of ρ_{opt} where the infimum of the bound is attained is computed and given in the column named ρ_{opt}.

The actual error presents the absolute difference between the values of the integral

$$I(f_i) = \int_{-1}^{1} f_i(t)\, dt, \qquad i = 1, 2, 3,$$

and the values calculated by the corresponding Gauss quadrature with n nodes $I_n(f_i)$, i.e., $|I(f_i) - I_n(f_i)|$, which can be approximated by

$$\textit{Error} = \textit{Error}(n) = |I_{150}(f_i) - I_n(f_i)|.$$

EXAMPLE 3.1. Let $f_1(z) = e^{e^{\cos(\omega z)}}$, $\omega > 0$. The function f_1 is entire, and it is known that (see [10])

$$\max_{z \in \mathcal{E}_\rho} |f_1(z)| = e^{e^{\cosh(\omega b_1)}}, \qquad b_1 = (\rho - \rho^{-1})/2, \quad \rho_{\max} = +\infty.$$

EXAMPLE 3.2. Let $f_2(z) = e^{\omega z^2}$, $\omega > 0$. The function f_2 is entire, and it is known that (see [8])

$$\max_{z \in \mathcal{E}_\rho} |f_1(z)| = e^{\omega a_1^2}, \qquad a_1 = (\rho + \rho^{-1})/2, \quad \rho_{\max} = +\infty.$$

EXAMPLE 3.3. Let $f_3(z) = \dfrac{\cos(z)}{z^2 + \omega^2}$, $\omega > 0$. For the function $f_3(z)$ (see [7], [1, p. 25]), it holds that

$$\max_{z \in \mathcal{E}_\rho} |f_3(z)| = \frac{\cosh(b_1)}{-a_1^2 + \omega^2},$$

where $b_1 = (\rho - \rho^{-1})/2$. Here the infimum is calculated with respect to the interval $\rho \in (\rho^*, \rho_{\max})$, where $\rho_{\max} = \omega + \sqrt{1 + \omega^2}$. We made a couple of experiments with values of ρ in the intervals $(\rho^*, \rho_{\max})$ and obtained in each case an effective bound. The corresponding error bounds and the actual errors are displayed in Table 3.3.

In Examples 3.1 and 3.2, as n increases, the value of ρ_{opt} increases and that of r_n decreases. The bound r_n is also very effective for large enough ρ when the ellipse looks more and more like a circle. The corresponding error bounds and actual errors are displayed in Tables 3.1 and 3.2. The reported results in Tables 3.1, 3.2, 3.3 show the efficiency of the error bound r_n.

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TABLE 3.1
Error bounds $r_n(f_1)$, actual errors (Error), and the exact value of the integral (I_ω).

(n,ω)	$r_n(f_1)$	*Error*	ρ_{opt}	I_ω
(2,1)	7.328 (00)	1.592 (00)	2.071	21.7719...
(4,1)	2.839 (00)	4.175 (-02)	2.117	21.7719...
(5,1)	2.289 (-02)	5.849 (-03)	2.560	21.7719...
(6,1)	6.700 (-03)	7.669(-04)	2.661	21.7719...
(7,1)	4.622 (-04)	9.527(-05)	2.747	21.7719...
(8,1)	1.195(-04)	1.131(-05)	2.821	21.7719...
(9,1)	7.364 (-06)	1.291(-06)	2.884	21.7719...
(10,1)	1.738(-06)	1.423(-07)	2.941	21.7719...
(11,1)	9.894 (-08)	1.523(-08)	2.992	21.7719...
(13,1)	1.166 (-09)	1.611(-10)	3.078	21.7719...
(15,1)	1.237(-11)	1.558(-12)	3.150	21.7719...
(25,1)	5.573(-22)	5.046(-23)	3.410	21.7719...
(3,2)	4.812 (00)	2.477 (00)	1.145	14.0805...
(6,2)	1.086 (00)	1.251(-01)	1.621	14.0805...
(7,2)	2.028 (-01)	4.261(-02)	1.657	14.0805...
(8,2)	1.448(-01)	1.401(-02)	1.691	14.0805...
(9,2)	2.488 (-02)	4.474(-03)	1.722	14.0805...
(10,2)	1.650(-02)	1.391(-03)	1.751	14.0805...
(11,2)	2.666 (-03)	4.224(-04)	1.774	14.0805...
(13,2)	2.570 (-04)	3.661(-05)	1.816	14.0805...
(15,2)	2.273(-05)	2.955(-06)	1.859	14.0805...
(17,2)	1.872 (-06)	2.245(-07)	1.861	14.0805...
(18,2)	1.050(-06)	6.065(-08)	1.901	14.0805...
(19,2)	1.449 (-07)	1.618(-08)	1.909	14.0805...
(20,2)	7.905(-08)	4.269(-09)	1.921	14.0805...
(25,2)	5.008(-11)	4.680(-12)	1.955	14.0805...
(2,4)	4.940(+01)	5.267(00)	1.171	8.5977...
(4,4)	2.697(+01)	3.100(00)	1.175	8.5977...
(5,4)	1.250(+01)	2.443(00)	1.205	8.5977...
(6,4)	1.407(+01)	1.412(00)	1.221	8.5977...
(8,4)	7.541(00)	5.538(-01)	1.247	8.5977...
(10,4)	2.703(00)	1.987(-01)	1.272	8.5977...
(13,4)	2.990(-01)	3.822(-02)	1.300	8.5977...
(15,4)	1.316(-01)	1.201(-02)	1.321	8.5977...
(18,4)	3.740(-02)	1.973(-03)	1.341	8.5977...
(25,4)	2.600(-04)	2.254(-05)	1.374	8.5977...
(2,10)	9.321(+01)	3.221(+01)	1.010	10.7051...
(8,10)	4.057(+01)	3.402(00)	1.070	10.7051...
(15,10)	8.923(00)	4.246(-01)	1.083	10.7051...
(17,10)	6.289(00)	4.667(-01)	1.087	10.7051...
(19,10)	4.403 (00)	4.067(-01)	1.091	10.7051...
(25,10)	1.435(00)	5.389(-02)	1.101	10.7051...
(35,10)	1.803(-01)	7.770(-03)	1.101	10.7051...
(36,10)	8.811(-01)	7.681(-03)	1.103	10.7051...
(40,10)	1.176(-01)	2.590(-03)	1.119	10.7051...
(44,10)	4.710(-02)	9.681(-04)	1.121	10.7051...

TABLE 3.2
Error bounds $r_n(f_2)$, actual errors (Error), and the exact value of the integral (I_ω).

(n,ω)	$r_n(f_2)$	*Error*	ρ_{opt}	I_ω
(2,0.5)	1.068(-01)	2.719(-02)	4.015	2.3899...
(4,0.5)	2.060(-04)	3.785(-05)	6.176	2.3899...
(7,0.5)	1.243(-09)	3.637(-10)	7.481	2.3899...
(9, 0.5)	3.069(-13)	7.974(-14)	8.490	2.3899...
(10, 0.5)	8.098(-15)	1.000(-15)	8.719	2.3899...
(11, 0.5)	4.830(-17)	6.938(-18)	9.382	2.3899...
(15, 0.5)	4.261(-25)	8.566(-26)	10.930	2.3899...
(16, 0.5)	8.438(-27)	6.702(-28)	10.880	2.3899...
(7,1)	2.059(-07)	5.911(-08)	5.291	2.9253...
(9, 1)	2.072(-10)	5.196(-11)	5.961	2.9253...
(11, 1)	1.276(-13)	2.977(-14)	6.640	2.9253...
(13, 1)	1.112(-16)	2.081(-17)	7.211	2.9253...
(15, 1)	1.780(-20)	3.585(-21)	7.750	2.9253...
(16, 1)	5.755(-22)	5.612(-23)	7.699	2.9253...
(19, 1)	2.203(-27)	1.514(-28)	7.810	2.9253...
(2, 2)	4.312(00)	8.334(-01)	1.741	4.7289...
(4, 2)	1.165(-01)	1.966(-02)	2.181	4.7289...
(7, 2)	4.478(-05)	1.233(-05)	3.751	4.7289...
(8, 2)	6.264(-06)	7.774(-07)	3.791	4.7289...
(9, 2)	1.753(-07)	4.349(-08)	4.251	4.7289...
(10, 2)	1.844(-08)	2.186(-09)	4.481	4.7289...
(11, 2)	4.731(-10)	9.983(-11)	4.531	4.7289...
(13, 2)	5.409(-12)	1.611(-13)	3.941	4.7289...
(15, 2)	6.869(-15)	1.928(-16)	4.461	4.7289...

TABLE 3.3
Error bounds $r_n(f_3)$, actual errors (Error), and the exact value of the integral (I_ω).

(n,ω)	$r_n(f_3)$	*Error*	I_ω
(2,0.5)	1.281 (00)	1.031 (00)	4.3181...
(3,0.5)	5.793 (-01)	4.478 (-01)	4.3181...
(4,0.5)	1.913 (-01)	1.643 (-01)	4.3181...
(5,0.5)	7.059 (-02)	6.415 (-02)	4.3181...
(6,0.5)	2.560 (-02)	2.441 (-02)	4.3181...
(7,0.5)	1.139 (-02)	9.370 (-03)	4.3181...
(8,0.5)	5.068 (-03)	3.581 (-03)	4.3181...
(10,0.5)	1.004 (-03)	5.239 (-04)	4.3181...
(2,1)	2.330 (-01)	1.090 (-01)	1.3658...
(3,1)	2.749 (-01)	1.934 (-02)	1.3658...
(4,1)	3.741 (-02)	3.347 (-03)	1.3658...
(5,1)	2.501 (-02)	5.784 (-04)	1.3658...
(6,1)	7.203 (-03)	9.971 (-05)	1.3658...
(7,1)	1.717 (-04)	1.717 (-05)	1.3658...
(8,1)	1.316 (-05)	2.954 (-06)	1.3658...
(10,1)	7.928 (-07)	8.729 (-08)	1.3658...

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