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THE REMAINDER TERM OF GAUSS–RADAU QUADRATURE RULE WITH SINGLE AND DOUBLE END POINT

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Abstract. The remainder term of quadrature formula can be represented as a contour integral with a complex kernel. We study the kernel on elliptic contours for Gauss–Radau quadrature formula with the Chebyshev weight function of the second kind with double and single end point. Starting from the explicit expression of the corresponding kernel, derived by Gautschi and Li, we determine the locations on the ellipses where the maximum modulus of the kernel is attained.

1. Gauss–Radau quadrature rule with double end point

In this section, we analyze the remainder term for the Gauss–Radau quadrature rule with the end point -1 of multiplicity r

$$\int_{-1}^{1} f(t)\,\omega(t)\,dt = \sum_{\rho=0}^{r-1} \kappa_\rho{}^R f^{(\rho)}(-1) + \sum_{\nu=1}^{n} \lambda_\nu{}^R f(\tau_\nu{}^R) + R_{n,r}^R(f), \tag{1.1}$$

where τ_ν^R are zeros of $\pi_n(\cdot;\omega^R)$, orthogonal polynomial on $[-1,1]$, with respect to the weight function

$$\omega^R(t) = (t+1)^r \omega(t).$$

Here, $R_{n,r}^R(f) = 0$ for all $f \in \mathbb{P}_{2n+2r-1}$ (polynomials of degree $\leqslant 2n+2r-1$). Let Γ be a simple closed curve in the complex plane surrounding the interval $[-1,1]$ and let $\mathcal{D} = \operatorname{int}\Gamma$ be its interior. If the integrand f is analytic in a domain $\mathcal{D}$ containing $[-1,1]$, then the remainder term $R_{n,r}^R(f)$ admits the contour integral representation

$$R_{n,r}^R(f) = \frac{1}{2\pi i} \oint_\Gamma K_{n,r}^R(z;\omega) f(z)\,dz. \tag{1.2}$$

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The *kernel* is given by

$$K^R_{n,r}(z;\omega) \equiv K_{n,r}(z,\omega) = \frac{\varrho^R_{n,r}(z;\omega)}{(z+1)^r \pi_n(z;\omega^R)}, \quad z \notin [-1,1],$$

where we denote $w_{n,r}(z;\omega) = (z+1)^r \pi_n(z;\omega^R)$. Also,

$$\varrho^R_{n,r}(z;\omega) \equiv \varrho_{n,r}(z,\omega) = \int_{-1}^{1} \frac{w_{n,r}(z;\omega)}{z-t}\,\omega(t)dt.$$

Integral representation (1.2) leads to the error bound

$$|R^R_{n,r}(f)| \leqslant \frac{\ell(\Gamma)}{2\pi}\Big(\max_{z\in\Gamma} |K_{n,r}(z;\omega)|\Big)\Big(\max_{z\in\Gamma} |f(z)|\Big),$$

where $\ell(\Gamma)$ is the length of the contour Γ. In this paper we take $\Gamma = \mathcal{E}_\rho$, where the ellipse $\mathcal{E}_\rho$ is given by

$$\mathcal{E}_\rho = \big\{z \in \mathbb{C} \mid z = \tfrac{1}{2}(u+u^{-1}),\ 0 \leqslant \theta \leqslant 2\pi\big\}, \quad u = \rho\, e^{i\theta}. \tag{1.3}$$

The upper bound on $|R^R_{n,r}(f)|$ reduces to

$$|R^R_{n,r}(f)| \leqslant \frac{\ell(\mathcal{E}_\rho)}{2\pi}\Big(\max_{z\in\mathcal{E}_\rho} |K_{n,r}(z;\omega)|\Big)\Big(\max_{z\in\mathcal{E}_\rho} |f(z)|\Big).$$

Furthermore, we take $r = 2$, meaning we are dealing with a double end point. The goal is to determine the points where the kernel attains its maximum modulus along the contour of integration. In [**2**] Gautschi and Li considered the Gauss–Radau and the Gauss–Lobatto quadrature rules with multiple end points with respect to four Chebyshev weight functions and derived explicit expressions of the corresponding kernels $K_{n,r}(z;\omega_j)$ in terms of the variable $u = \rho e^{i\theta}$.

1.1. Maximum modulus of the kernel. Gautschi and Li [**2**, Section 3.3] analyzed the maximum modulus of the kernel $K_{n,2}(z;\omega_2)$. Based on numerical calculations, they made the conjectures that the maximum is attained on the negative real axis if (i) $\rho > 1$ and $1 \leqslant n \leqslant 11$, and (ii) $\rho \geqslant \rho_n$ and $n \geqslant 12$.

Here, ρ_n are numbers determined for $12 \leqslant n \leqslant 20$. We can merge the cases from the previous conjectures. The maximum modulus of the kernel is attained on the negative real axis if $\rho > \rho^*$ and $n \geqslant 1$, where $\rho^* = 1$ if $1 \leqslant n \leqslant 11$, while $\rho^* = \rho_n$ if $n \geqslant 12$.

In this paper we prove the existence of the values ρ^* from the previous conjecture. We give the strong numerical evidence for the precise values of ρ^* for $n \geqslant 12$. Gautschi and Li [**2**, (2.7)] derived the explicit representation of the kernel

$$\begin{aligned} K_{n,2}(z;\omega_2) = {} & \frac{\pi(u^2-1)}{u^{n+4}} \\ & \times \frac{u^2+\alpha u+\beta}{\beta[u^{n+3}-u^{-(n+3)}]+\alpha[u^{n+2}-u^{-(n+2)}]+[u^{n+1}-u^{-(n+1)}]}, \end{aligned}$$

where $\alpha = \frac{4(n+1)}{2n+5}$, $\beta = \frac{(n+1)(2n+3)}{(n+3)(2n+5)}$, $z = (u+u^{-1})/2$ and $u = \rho e^{i\theta}$. We can determine the modulus of the kernel on $\mathcal{E}_\rho$. We are also interested in the modulus of the kernel at $\theta = \pi$. By introducing some substitutions, we can easily express the modulus of the kernel in the form

$$|K_{n,2}(z;\omega_2)| = \Big(\frac{\pi^2}{\rho^{2n+8}}\frac{ac}{\delta}\Big)^{1/2},$$

where

$$\begin{aligned}
a &= |u^2-1|^2 = \rho^4 - 2\rho^2\cos 2\theta + 1,\\
c &= |u^2+\alpha u+\beta|^2 = \rho^4 + 2\alpha\cos\theta\rho^3 + (\alpha^2+2\beta\cos 2\theta)\rho^2 + 2\alpha\beta\cos\theta\rho + \beta^2,\\
\delta &= \big|\beta[u^{n+3}-u^{-(n+3)}] + \alpha[u^{n+2}-u^{-(n+2)}] + [u^{n+1}-u^{-(n+1)}]\big|^2 = \frac{d}{\rho^{2n+6}},
\end{aligned}$$

i.e.,

$$\begin{aligned}
d &= \delta\cdot\rho^{2n+6}\\
&= |\beta[u^{n+3}-u^{-(n+3)}] + \alpha[u^{n+2}-u^{-(n+2)}] + [u^{n+1}-u^{-(n+1)}]|^2\cdot\rho^{2n+6}\\
&= \beta^2\cdot\rho^{4n+12} + 2\alpha\beta\cos\theta\cdot\rho^{4n+11} + [\alpha^2+2\beta\cos 2\theta]\cdot\rho^{4n+10}\\
&\quad + 2\alpha\cos\theta\cdot\rho^{4n+9} + \rho^{4n+8} - 2\beta\cos(2n+4)\theta\cdot\rho^{2n+8}\\
&\quad - [2\alpha\cos(2n+3)\theta + 2\alpha\beta\cos(2n+5)\theta]\cdot\rho^{2n+7}\\
&\quad - [2\cos(2n+2)\theta + 2\beta^2\cos(2n+6)\theta + 2\alpha^2\cos(2n+4)\theta]\cdot\rho^{2n+6}\\
&\quad - [2\alpha\beta\cos(2n+5)\theta + 2\alpha\cos(2n+3)\theta]\cdot\rho^{2n+5} - 2\beta\cos(2n+4)\theta\cdot\rho^{2n+4}\\
&\quad + \rho^4 + 2\alpha\cos\theta\cdot\rho^3 + [\alpha^2+2\beta\cos 2\theta]\cdot\rho^2 + 2\alpha\beta\cos\theta\cdot\rho + \beta^2.
\end{aligned}$$

In order to express $d(\rho)$ as a polynomial function in ρ, the term δ is multiplied by ρ^{2n+6}, which reduces the expression for the square of the modulus of the kernel to

$$|K_{n,2}(z;\omega_2)|^2 = \frac{\pi^2}{\rho^2}\frac{ac}{d}.$$

By letting A, C, D denote the values of a, c, d at the angle $\theta = \pi$, the square of the modulus of the kernel at $\theta = \pi$ can be expressed as

$$|K_{n,2}(z;\omega_3)|^2 = \frac{\pi^2}{\rho^2}\frac{AC}{D}.$$

The following substitutions are appropriate

$$\begin{aligned}
A &= \rho^4 - 2\rho^2 + 1,\\
C &= \rho^4 - 2\alpha\cdot\rho^3 + (\alpha^2+2\beta)\cdot\rho^2 - 2\alpha\beta\cdot\rho + \beta^2,\\
D &= \beta^2\cdot\rho^{4n+12} - 2\alpha\beta\cdot\rho^{4n+11} + (\alpha^2+2\beta)\cdot\rho^{4n+10}\\
&\quad - 2\alpha\cdot\rho^{4n+9} + \rho^{4n+8} - 2\beta\cdot\rho^{2n+8} + (2\alpha+2\alpha\beta)\cdot\rho^{2n+7}\\
&\quad - (2+2\beta^2+2\alpha^2)\cdot\rho^{2n+6} + (2\alpha\beta+2\alpha)\cdot\rho^{2n+5} - 2\beta\cdot\rho^{2n+4}\\
&\quad + \rho^4 - 2\alpha\cdot\rho^3 + (\alpha^2+2\beta)\cdot\rho^2 - 2\alpha\beta\cdot\rho + \beta^2.
\end{aligned}$$

According to Gautschi and Li's conjecture, there exist some value ρ^* such that the maximum modulus of the kernel is attained at $\theta = \pi$ for all $\rho > \rho^*$ and $n \geqslant 1$. In the case of conjecture (i) $\rho^* = 1$, while in the case of conjecture (ii) $\rho^* = \rho_n$.

We formulate the following theorem which states the existence of the value ρ^*. Whereas that conjectures hold for all ρ from the interval $[\rho^*, \infty)$, we separately derive a detailed numerical study.

THEOREM 1.1. *For the Gauss–Radau quadrature formula with a double end point* -1 $(r = 2)$ *with the Chebyshev weight function of the second kind, there exists a value* $\rho^* \in [1, \infty)$*, such that the modulus of the kernel* $|K_{n,2}(z; \omega_2)|$ *attains its maximum value on the negative real axis* $(\theta = \pi)$ *for* $\rho > \rho^*$ *and* $n \geqslant 1$*, i.e.,*

$$\max_{z \in \mathcal{E}_\rho} |K_{n,2}(z; \omega_2)| = \bigl|K_{n,2}\bigl(-\tfrac{1}{2}(\rho + \rho^{-1}), \omega_2\bigr)\bigr|;$$

for $\rho > \rho^*$, $n \geqslant 1$.

PROOF. i) Referring to the previously introduced notation, we have to show that $\frac{ac}{d} \leqslant \frac{AC}{D}$ for each $\rho > \rho^*$ and $n \geqslant 1$. The previous inequality can be written as $I(\rho) = [acD - ACd] \leqslant 0$. We can easily see that $I(\rho)$ is a polynomial in ρ, of degree equal to $4n + 19$, whose coefficients depend only on θ, i.e.,

$$I = I(\rho) = \sum_{i=0}^{4n+19} a_i(\theta)\rho^i. \tag{1.4}$$

In order to show the existence of numbers ρ^*, we use the well known fact that, starting from some value of ρ, the sign of the polynomial

$$I(\rho) = \rho^{4n+19}\Bigl(a_{4n+19} + \frac{a_{4n+18}}{\rho} + \frac{a_{4n+17}}{\rho^2} + \cdots + \frac{a_0}{\rho^{4n+19}}\Bigr)$$

coincides with the sign of the leading coefficient $a_{4n+19} = 2\alpha\beta(1 + \cos\theta)(\beta - 1)$, where $\alpha = 4\frac{n+1}{2n+5}$ and $\beta = \frac{(n+1)(2n+3)}{(n+3)(2n+5)}$. Therefore,

$$a_{4n+19} < 0 \quad \text{iff} \quad \beta < 1 \quad \text{iff} \quad (n+1)(2n+3) < (n+3)(2n+5).$$

The previous inequality reduces to $n > -2$. We conclude that the term a_{4n+19} is negative for all $n \geqslant 1$, i.e., for all $n \geqslant 1$ there exists a number ρ^* such that $I(\rho) \leqslant 0$ for all $\rho > \rho^*$. □

1.2. Gautschi and Li's conjecture. According to the conjecture, the maximum is attained at $\theta = \pi$ for all $\rho > \rho^*$ and $n \geqslant 1$. In order to ensure the nonpositivity of polynomial $I(\rho)$ given by (1.4) for each $\rho > \rho^*$, we can write the initial polynomial in the terms of positive differences $\rho - \rho^*$, and show the nonpositivity of its new coefficients. We have

$$J(\rho) = \sum_{i=0}^{4n+19} b_i(\theta, \rho^*)(\rho - \rho^*)^i \quad \text{for all } \rho > \rho^*.$$

Numerical calculations show that all functions $b_i(\theta, \rho^*)$, $i = 0, 1, \ldots, 4n + 19$ are strictly under the x-axis for all θ. In general, nonpositivity of the coefficients $b_i(\theta, \rho^*)$ is not a necessary condition for nonpositivity of a polynomial for each $\rho > \rho^*$, but in this case, it is obviously a sufficient condition.

Explicit formulae for $b_i(\theta, \rho^*)$ can be given in the terms of the coefficients $a_j(\theta)$ by using the binomial formula, but in MatLab implementation it is more practical to use a Horner scheme. The new coefficients $b_0(\theta,\rho^*), b_1(\theta,\rho^*), \dots, b_{4n+19}(\theta,\rho^*)$ are complicated trigonometric functions, inappropriate for further analytical consideration. The method has been tested for all values of n from 1 to 100 and it gives the optimal results. Some of the cases are displayed in Fig. 1.

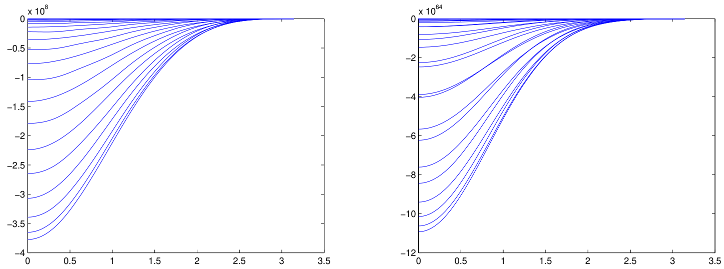

FIGURE 1. The functions $b_0(\theta,\rho^*),\dots,b_{31}(\theta,\rho^*)$, in the case $n=3$, $\rho^*=1$ (left) and the functions $b_0(\theta,\rho^*),\dots,b_{139}(\theta,\rho^*)$, in the case $n=30$, $\rho^*=16.8838$ (right).

1.3. The determination of ρ^* in the case $n \geqslant 12$. Our aim is to determine the minimal values of ρ^* for $n \geqslant 12$ by using MatLab. For fixed $n \geqslant 12$, we treated the terms $J(\rho)$ and tested the smallest possible values of ρ^* such that the terms $J(\rho)$ are nonpositive for each $\rho > \rho^*$ (Table 1).

TABLE 1. The values of ρ^* for $12 \leqslant n \leqslant 47$

n	ρ^*	n	ρ^*	n	ρ^*	n	ρ^*
12	2.3455	21	10.5861	30	16.8838	39	23.0093
13	3.4034	22	11.3053	31	17.5691	40	23.6857
14	4.7165	23	12.0172	32	18.2529	41	24.3615
15	5.8433	24	12.7232	33	18.9354	42	25.0367
16	6.7473	25	13.4245	34	19.6167	43	25.7115
17	7.5731	26	14.1219	35	20.2969	44	26.3859
18	8.3575	27	14.8161	36	20.9762	45	27.0599
19	9.1162	28	15.5076	37	21.6547	46	27.7334
20	9.8575	29	16.1967	38	22.3323	47	28.4066

1.4. The error bounds. Let us consider the numerical calculation of integral (1.1) with a Chebyshev weight function $\omega = \omega_2$

$$I(f) = \int_{-1}^{1} f(t)\sqrt{1-t^2}\,dt.$$

According to the previously introduced notation, the error bound of the corresponding quadrature formula is given by $|R_{n,2}(f)| \leqslant r_n(f)$, where

$$r_n(f) = \inf_{\rho_n<\rho<\rho_{\max}} \left[\frac{\ell(\mathcal{E}_\rho)}{2\pi}\Big(\max_{z\in\mathcal{E}_\rho}|K_{n,2}(z)|\Big)\Big(\max_{z\in\mathcal{E}_\rho}|f(z)|\Big)\right].$$

Here, $\ell(\mathcal{E}_\rho)$ represents the length of the ellipse $\mathcal{E}_\rho$, and can be estimated by

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

where $a_1 = (\rho+\rho^{-1})/2$ [**13**]. According to the conjecture, the kernel attains its maximum value at $\theta=\pi$, i.e., $\max_{z\in\mathcal{E}_\rho}|K_{n,2}(z)| = \frac{\pi}{\rho}\sqrt{AC/D}$, where A, C, D denote the values of the terms a, c, d for the fixed angle $\theta=\pi$. The error bound $r_n(f)$ reduces to

$$r_n(f) = \inf_{\rho_n<\rho<\rho_{\max}} \left[a_1\frac{\pi}{\rho}\Big(1-\frac{1}{4}a_1^{-2}-\frac{1}{64}a_1^{-4}-\frac{5}{256}a_1^{-6}\Big)\sqrt{\frac{AC}{D}}\Big(\max_{z\in\mathcal{E}_\rho}|f(z)|\Big)\right]. \tag{1.5}$$

In order to check the proposed error bounds we made several tests and compared them with respect to the exact errors (“Error”) calculated by using a modified Gautschi MatLab code `gradau.m` (cf. [**4, 5**]) to a high precision arithmetic.

EXAMPLE 1.1. Let $f_1(z) = \frac{\cos(z)}{z^2+\omega^2}$, $\omega>0$. For the function $f_1(z)$ (see [**15**]) it holds that

$$\max_{z\in\mathcal{E}_\rho}|f_1(z)| = \frac{\cos(b_1)}{-b_1^2+\omega^2},$$

where $b_1 = (\rho-\rho^{-1})/2$, and the infimum is calculated with respect to the interval $\rho\in(\rho_n,\rho_{\max})$, where $\rho_{\max} = \omega+\sqrt{1+\omega^2}$. The corresponding error bounds and actual errors are displayed in Table 2.

TABLE 2. Error bounds $r_n(f_1)$ and actual errors, where $f_1(z) = \frac{\cos(z)}{z^2+\omega^2}$

n	$r_n,\ \omega=2$	Error	$r_n,\ \omega=5$	Error	$r_n,\ \omega=20$	Error
1	1.082(−1)	2.544(−2)	2.800(−3)	1.549(−3)	8.426(−5)	6.903(−5)
2	5.601(−3)	1.051(−3)	4.087(−5)	1.671(−5)	6.819(−7)	4.226(−7)
3	3.224(−4)	4.858(−5)	5.367(−7)	1.572(−7)	3.089(−9)	1.665(−9)
4	1.909(−5)	2.395(−6)	6.547(−9)	1.417(−9)	9.374(−12)	4.491(−12)
5	1.142(−6)	1.225(−7)	7.637(−11)	1.285(−11)	2.045(−14)	8.808(−15)
10	8.600(−13)	5.335(−14)	1.215(−20)	9.504(−22)	4.433(−29)	1.046(−29)
13	1.761(−16)	2.714(−17)	1.432(−26)	8.481(−28)	2.155(−38)	3.104(−39)

The values $r_n(f_1)$, and $\rho_{\text{opt}}\in(\rho_n,\rho_{\max})$, for the same values n and ω from Table 2, in which the expression within the brackets under the sign of inf in (1.5) attains its minimum, are presented in Table 3.

EXAMPLE 1.2. Let $f_2(z) = e^{e^{\cos(\omega z)}}$, $\omega>0$. The function f_2 is entire and it is known (see [**14**]) that

$$\max_{z\in\mathcal{E}_\rho}|f_2(z)| = e^{e^{\cosh(\omega b_1)}}.$$

Table 4 displays some error bounds and actual errors.

TABLE 3. Error bounds $r_n(f_1)$ and values ρ_{opt}, where $f_1(z) = \frac{\cos(z)}{z^2+\omega^2}$

n	$r_n(f_1),\ \omega = 2$	ρ_{opt}	$r_n(f_1),\ \omega = 5$	ρ_{opt}	$r_n(f_1),\ \omega = 20$	ρ_{opt}
1	1.082(−1)	3.3511	2.800(−3)	6.2311	8.426(−5)	8.2831
2	5.601(−3)	3.5666	4.087(−5)	7.4816	6.819(−7)	11.8126
3	3.224(−4)	3.7104	5.367(−7)	8.2394	3.089(−9)	15.4024
4	1.909(−5)	3.8087	6.547(−9)	8.6927	9.374(−12)	18.9057
5	1.142(−6)	3.8765	7.637(−11)	8.9795	2.045(−14)	22.2445
10	8.600(−13)	4.0397	1.215(−20)	9.5587	4.433(−29)	33.8827
13	1.761(−16)	4.0814	1.432(−26)	9.6884	2.155(−38)	36.4644

TABLE 4. Error bounds $r_n(f_2)$ and actual errors, where $f_2(z) = e^{e^{\cos(wz)}}$

n	$r_n,\ \omega = 1$	Error	$r_n,\ \omega = 0.1$	Error	$r_n,\ \omega = 0.01$	Error
1	4.412(+1)	4.017(+0)	3.101(−3)	1.411(−3)	1.212(−5)	1.434(−7)
2	4.395(+0)	5.425(−1)	5.982(−6)	2.023(−6)	3.671(−9)	2.057(−12)
3	5.140(−1)	6.971(−2)	1.097(−8)	3.043(−9)	1.061(−16)	1.892(−15)
4	6.280(−2)	8.698(−2)	1.877(−11)	4.490(−12)	1.838(−21)	4.580(−22)
5	7.701(−3)	1.050(−3)	3.012(−14)	9.457(−15)	2.977(−26)	6.546(−27)
6	9.212(−4)	1.227(−4)	4.569(−17)	8.812(−18)	4.548(−31)	9.015(−32)
9	1.365(−6)	1.635(−7)	1.213(−25)	1.867(−26)	1.224(−45)	1.920(−46)
12	1.613(−9)	1.738(−10)	2.350(−34)	3.067(−35)	2.394(−60)	3.168(−61)

2. Gauss–Radau quadrature rule with single end point

In this section we analyze the remainder term of the Gauss–Radau quadrature rule with the end point -1

$$\int_{-1}^{1} f(t)\omega(t)\,dt = \lambda_0^R f(-1) + \sum_{\nu=1}^{n} \lambda_\nu{}^R f(\tau_\nu{}^R) + R_{n+1}^R(f),$$

where τ_ν^R are zeros of $\pi_n(\cdot;\omega^R)$, the orthogonal polynomial on $[-1,1]$ with respect to the Chebyshev weight functions $\omega_2(t)$. The remainder term $R_{n+1}^R(f)$ admits the contour integral representation

$$R_{n+1,r}^R(f) = \frac{1}{2\pi i}\oint_\Gamma K_{n+1,r}^R(z;\omega)f(z)dz.$$

The *kernel* is given by

$$K_{n+1}^R(z;\omega) \equiv K_{n+1}(z,\omega) = \frac{1}{w_{n+1}(z;\omega)}\int_{-1}^{1}\frac{\omega(t)w_{n+1}(z;\omega)}{z-t}\,dt, \quad z \notin [-1,1],$$

where $w_{n+1}(z;\omega) = \prod_{i=1}^{n+1}(z-\tau_i)$. We take $\Gamma = \mathcal{E}_\rho$, where the ellipse $\mathcal{E}_\rho$ is given by (1.3).

In [**3**] Gautschi considered the Gauss–Radau and the Gauss–Lobatto quadrature rules with respect to the Chebyshev weight function ω_2 and presented the conjectures based on numerical considerations. The case $\rho \geqslant \rho_n$ from Gautschi's conjecture has been already proven [**10**]. Here, we consider the case $\rho < \rho_n$ from

Gautschi's conjecture, which supplements earlier work in [**10**]. We also give the strong numerical evidence for the precise values of ρ_n.

2.1. Maximum modulus of the kernel. Gautschi analyzed the maximum modulus of the kernel $K_{n+1}(z;\omega_2)$ and made the conjecture [**3**, p. 224] that the maximum is attained at $\theta=\pi$ if $1<\rho<\rho_n$ and $n\geqslant 4$ where ρ_n is determined for $4\leqslant n\leqslant 10$.

The kernel $K_{n+1}(z;\omega_2)$ is given by

$$K_{n+1}(z;\omega_2)=\frac{\pi}{u^{n+1}}\times\frac{1-u^{-2}+\alpha(u+u^{-1})}{u^{n+2}-u^{-(n+2)}+\alpha[u^{n+1}-u^{-(n+1)}]},$$

where $\alpha=\frac{n+2}{n+1}$, $z=\frac{1}{2}(u+u^{-1})$ and $u=\rho e^{i\theta}$. By introducing some substitutions, we can express the modulus of the kernel in the form

$$|K_{n+1}(z;\omega_2)|=\Big(\frac{\pi^2}{\rho^{2n+2}}\frac{\gamma}{\delta}\Big)^{1/2},$$

where

$$\begin{aligned}\gamma&=|1-u^{-2}+\alpha(u+u^{-1})|^2=\frac{c}{\rho^4},\\ c&=\gamma\cdot\rho^4=\rho^6\cdot\alpha^2+\rho^5\cdot 2\alpha\cos\theta+\rho^4\cdot(1-2\alpha^2\cos 2\theta)\\ &\quad-\rho^3\cdot 2\alpha(\cos\theta+\cos 3\theta)+\rho^2\cdot(\alpha^2-2\cos 2\theta)+\rho\cdot 2\alpha\cos\theta+1.\end{aligned}$$

The terms γ and δ are multiplied by ρ^4 and ρ^{2n+4} respectively

$$\begin{aligned}\delta&=|u^{n+2}-u^{-(n+2)}+\alpha[u^{n+1}-u^{-(n+1)}]|^2=\frac{d}{\rho^{2n+4}},\\ d&=\delta\cdot\rho^{2n+4}=\rho^{4n+8}+\rho^{4n+7}\cdot 2\alpha\cos\theta+\rho^{4n+6}\cdot\alpha^2\\ &\quad-\rho^{2n+5}\cdot 2\alpha\cos(2n+3)\theta-2\rho^{2n+4}\cdot[\cos(2n+4)\theta+\alpha^2\cos(2n+2)\theta]\\ &\quad-\rho^{2n+3}\cdot 2\alpha\cos(2n+3)\theta+\rho^2\cdot\alpha^2+\rho\cdot 2\alpha\cos\theta+1.\end{aligned}$$

We get $|K_{n+1}(z;\omega_2)|^2=\frac{\pi^2}{\rho^2}\frac{c}{d}$. By letting C and D denote the values of c and d at $\theta=\pi$, the square of the modulus of the kernel at $\theta=\pi$ can be expressed as

$$|K_{n+1}(z;\omega_2)|^2=\frac{\pi^2}{\rho^2}\frac{C}{D},$$

with appropriate replacements

$$\begin{aligned}C&=\rho^6\cdot\alpha^2-\rho^5\cdot 2\alpha+\rho^4\cdot(1-2\alpha^2)\\ &\quad+\rho^3\cdot 4\alpha+\rho^2\cdot(\alpha^2-2)-\rho\cdot 2\alpha+1,\\ D&=\rho^{4n+8}-\rho^{4n+7}\cdot 2\alpha+\rho^{4n+6}\cdot\alpha^2+\rho^{2n+5}\cdot 2\alpha\\ &\quad-2\rho^{2n+4}\cdot(1+\alpha^2)+\rho^{2n+3}\cdot 2\alpha+\rho^2\cdot\alpha^2-\rho\cdot 2\alpha+1.\end{aligned}$$

Our task is to show that this is the maximum value of the modulus for all $1<\rho<\rho_n$ if $n\geqslant 4$.

2.2. Gautschi's conjecture. The conjecture suggests that the maximum modulus of the kernel is attained on the negative real axis for all ρ from the interval $(1, \rho_n)$ if $n \geqslant 4$. Whereas that ρ belongs to the bounded interval, it is not possible to conduct any asymptotic analysis.

Referring to the previously introduced notation, we have to show that $\frac{c}{d} \leqslant \frac{C}{D}$ for each $1 < \rho < \rho_n$ and $n \geqslant 4$. The previous inequality can be written as

$$I(\rho) = [cD - Cd] \leqslant 0.$$

The term $I(\rho)$ is a polynomial in ρ whose coefficients depend only on θ

$$\begin{aligned} I(\rho) &= [2\alpha(1+\cos\theta)(1-\alpha^2)] \cdot \rho^{4n+13} + [2\alpha^2(1-\cos 2\theta)] \cdot \rho^{4n+12} \\ &\quad + 2\alpha[\alpha^2 + (3\alpha^2 - 2)\cos\theta + 2\alpha^2 \cos 2\theta - \cos 3\theta - 3] \cdot \rho^{4n+11} \\ &\quad + 4\sin^2\theta[1 + \alpha^4 - 4\alpha^2\cos\theta] \cdot \rho^{4n+10} \\ &\quad - 2\alpha[3\alpha^2 - 2\cos 2\theta + \cos\theta(\alpha^2 + 2\alpha^2\cos 2\theta - 3) - 1] \cdot \rho^{4n+9} \\ &\quad + [4\alpha^2\sin^2\theta] \cdot \rho^{4n+8} + [2\alpha(\alpha^2-1)(1+\cos\theta)] \cdot \rho^{4n+7} + \cdots \end{aligned}$$

i.e., $I(\rho) = \sum_{i=0}^{4n+13} a_i(\theta)\rho^i$, $1 < \rho < \rho_n$. Modeled on the consideration from the previous section, we can write the polynomial $I(\rho)$ as a polynomial in the terms of positive differences $\rho_n - \rho$, and show nonpositivity of its new coefficients.

In order to ensure nonpositivity for $1 < \rho < \rho_n$, first of all, we shift the interval $\rho \in (1, \rho_n)$ iff $-\rho \in (-\rho_n, -1)$ iff $-\rho + \rho_n \in (0, \rho_n - 1)$. The polynomial $I(\rho)$ can be written in the form

$$J(\rho) = \sum_{k=0}^{4n+13} \beta_k(\theta, \rho_n)(\rho_n - \rho)^k.$$

Its nonpositivity on the interval $(0, \rho_n - 1)$ is a sufficient condition for nonpositivity of the initial polynomial $I(\rho)$ on the interval $(1, \rho_n)$. The $\beta_i(\theta, \rho_n)$ coefficients can be expressed by applying the transformation $\rho \mapsto (-1) \cdot \rho + \rho_n$. Some of them are presented

$$\begin{aligned} \beta_{4n+13}(\theta, \rho_n) &= 2\alpha(\cos\theta + 1)(1 - \alpha^2), \\ \beta_{4n+12}(\theta, \rho_n) &= -4\alpha\cos^2\tfrac{\theta}{2}[(\alpha^2-1)(13+4n)\rho_n + 2\alpha\cos\theta - 2\alpha], \\ \beta_{4n+11}(\theta, \rho_n) &= 2\alpha\big[\alpha^2 - 2\cos\theta + 3\alpha^2\cos\theta - 2\alpha^2 - (3+n)(13+4n)(\rho_n)^2 \\ &\qquad \cdot (1+\cos\theta) + 2\alpha^2\cos 2\theta - \cos 3\theta + 8\alpha(3+n)\rho_n\sin^2\theta - 3\big], \\ \beta_{4n+10}(\theta, \rho_n) &= -\tfrac{4}{3}\alpha(11+4n)\rho_n\cos^2\tfrac{\theta}{2}\big[3(5+\alpha^2) + 2(\alpha^2-1)(3+n) \\ &\qquad \cdot (13+4n)(\rho_n)^2 - 12(1+\alpha^2)\cos\theta + 6\cos 2\theta\big] \\ &\quad + 4\sin^2\theta[1 + \alpha^4 + 2\alpha^2(3+n)(11+4n)(\rho_n)^2 - 4\alpha^2\cos\theta], \\ \beta_{4n+9}(\theta, \rho_n) &= -\tfrac{4}{3}\alpha(5+2n)(11+4n)(\rho_n)^2\cos^2\tfrac{\theta}{2}[15 + 3\alpha^2 \\ &\quad + (\alpha^2-1)(3+n)(13+4n)(\rho_n)^2 - 12\cos\theta(1+\alpha^2) + 6\cos 2\theta] \\ &\quad - 2\alpha[3\alpha^2 - 2\cos 2\theta + \cos\theta(\alpha^2 + 2\alpha^2\cos 2\theta - 3) - 1] + \tfrac{8}{3}\rho_n\sin^2\theta \\ &\qquad \cdot (5+2n)\big[3 + 3\alpha^4 + 2\alpha^2(3+n)(11+4n)(\rho_n)^2 - 12\alpha^2\cos\theta\big]. \end{aligned}$$

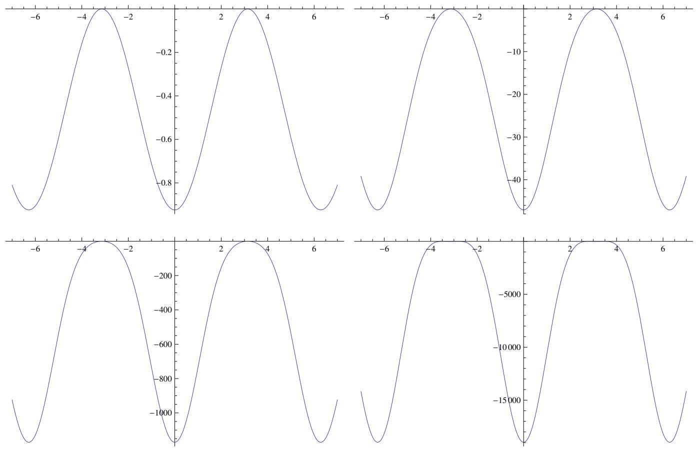

FIGURE 2. The functions $\beta_{49}(\theta,\rho_n),\beta_{48}(\theta,\rho_n),\beta_{47}(\theta,\rho_n),\beta_{46}(\theta,\rho_n)$ in the case $n=9$, $\rho_n=1.0394$

Figure 2 presents the graphs of the previous coefficients in the case $n=9$, $\rho_n=1.0394$.

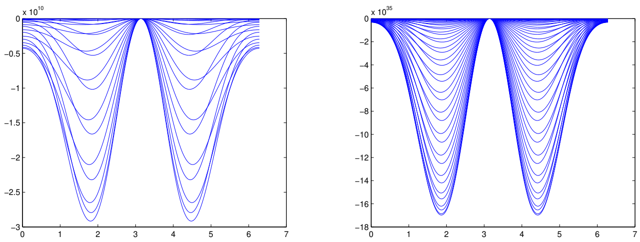

FIGURE 3. The functions $\beta_0(\theta,\rho_n),\dots,\beta_{29}(\theta,\rho_n)$ in the case $n=4$ (left) and the functions $\beta_0(\theta,\rho_n),\dots\beta_{121}(\theta,\rho_n)$ in the case $n=27$ (right)

TABLE 5. The values of ρ_n for $4\leqslant n\leqslant 45$

n	ρ_n	n	ρ_n	n	ρ_n	n	ρ_n	n	ρ_n	n	ρ_n
4	1.2845	9	1.0394	14	1.0156	19	1.0084	24	1.0052	41	1.0017
5	1.1517	10	1.0314	15	1.0136	20	1.0075	25	1.0048	42	1.0017
6	1.0964	11	1.0257	16	1.0119	21	1.0068	26	1.0043	43	1.0016
7	1.0679	12	1.0215	17	1.0105	22	1.0062	⋯	⋯	44	1.0015
8	1.0506	13	1.0182	18	1.0093	23	1.0057	40	1.0018	45	1.0014

The explicit formulae for the coefficients $\beta_i(\theta,\rho_n)$ are complicated trigonometric terms, inappropriate for a further analytical consideration. Numerical calculations show that all coefficients $\beta_i(\theta, \rho_n)$, $i \leqslant 4n+13$ are strictly under the x-axis. We tested the cases $n = 4, 3, \dots, 45$, and some of them are presented (Fig. 3). For fixed $n \geqslant 4$, we treated the terms $J(\rho)$ and tested the largest possible values of ρ_n such that the terms $J(\rho)$ are nonpositive for each $1 < \rho < \rho_n$ (Table 5).

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