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ERRORS OF GAUSS-RADAU AND GAUSS-LOBATTO QUADRATURES WITH DOUBLE END POINT

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Starting from the explicit expression of the corresponding kernels, derived by Gautschi and Li (W. Gautschi, S. Li: *The remainder term for analytic functions of Gauss-Lobatto and Gauss-Radau quadrature rules with multiple end points*, J. Comput. Appl. Math. 33 (1990) 315–329), we determine the exact dimensions of the minimal ellipses on which the modulus of the kernel starts to behave in the described way. The effective error bounds for Gauss-Radau and Gauss-Lobatto quadrature formulas with double end point(s) are derived. The comparisons are made with the actual errors.

1. INTRODUCTION

We analyze the remainder term of Gauss-Radau quadrature rule with the end point -1 of multiplicity r,

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

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

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

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In the case of Gauss-Lobatto quadrature rule with the end points ∓ 1 of multiplicity r (r is even), we have

$$(2)\quad \int_{-1}^{1} f(t)\omega(t)\,dt = \sum_{\rho=0}^{r-1} \kappa_\rho{}^L f^{(\rho)}(-1) + \sum_{\rho=0}^{r-1} \mu_\rho{}^L f^{(\rho)}(1) + \sum_{\nu=1}^{n} \lambda_\nu{}^L f(\tau_\nu{}^L) + R^L_{n,r}(f),$$

where $\tau_\nu{}^L$ are zeros of $\pi_n(\cdot;\omega^L)$, orthogonal polynomial on $[-1,1]$, with respect to the weight function

$$\omega^L(t) = (t^2-1)^r\omega(t).$$

Also, $R^R_{n,r}(f) = 0$ for all $f \in P_{2n+r-1}$ and $R^L_{n,r}(f) = 0$ for all $f \in \mathbb{P}_{2n+2r-1}$. Let Γ be a simple closed curve in the complex plane surrounding the interval $[-1,1]$ and let $\mathcal{D} = \text{int}\Gamma$ be its interior. If the integrand f is analytic function in a domain $\mathcal{D}$ containing $[-1,1]$, then the remainder terms $R^{R,L}_{n,r}(f)$ admit the contour integral representation

$$(3)\qquad R^{R,L}_{n,r}(f) = \frac{1}{2\pi i}\oint_\Gamma K^{R,L}_{n,r}(z;w)f(z)dz.$$

The *kernel* $K^R_{n,r}$ is given by

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

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

The *kernel* $K^L_{n,r}$ is given by

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

where $(z^2-1)^r\pi_n(z;\omega^L) = \omega^L_{n,r}(z;\omega)$, and $\varrho^L_{n,r}(z;\omega) \equiv \varrho_{n,r}(z,\omega) = \int_{-1}^{1} \frac{\omega^L_{n,r}(z;\omega)}{z-t}\,\omega(t)dt$

The integral representation (3) leads to the error estimate

$$|R^{R,L}_{n,r}(f)| \le \frac{\ell(\Gamma)}{2\pi}\left(\max_{z\in\Gamma}|K^{R,L}_{n,r}(z;\omega)|\right)\left(\max_{z\in\Gamma}|f(z)|\right),$$

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

$$(4)\qquad \mathcal{E}_\rho = \left\{ z \in \mathbb{C} \mid \; z = \frac{1}{2}\left(u+u^{-1}\right),\; 0 \le \theta \le 2\pi \right\}, \quad u = \rho\, e^{i\theta}.$$

Furthermore, we take $r = 2$, meaning we are dealing with endpoints of multiplicity 2. The goal is to determine where precisely the kernel attains its maximum modulus along the contour of integration. When $\rho \longrightarrow 1$, the ellipse (4) shrinks to the interval $[-1, 1]$, while with increasing ρ it becomes more and more circle-like. The advantage of elliptical contours over circular ones is that such a choice requires the analyticity of f in a smaller region of the complex plane.

In [**3**] Gautschi and Li considered Gauss-Radau and Gauss-Lobatto quadrature rules with multiple end points with respect to the four Chebyshev weight functions

$$\omega_1(t) = \frac{1}{\sqrt{1-t^2}}, \quad \omega_2(t) = \sqrt{1-t^2}, \quad \omega_3(t) = \sqrt{\frac{1+t}{1-t}}, \quad \omega_4(t) = \sqrt{\frac{1-t}{1+t}},$$

and derived explicit expressions of the corresponding kernels $K(z; \omega_j),\ j = 1, 2, 3, 4,$ in terms of the variable $u = \rho e^{i\theta}$.

Gautschi and Lis conjectures on Gauss-Lobatto quadratures with Chebyshev weight functions of the third and the fourth kind were already proved in [**6**]. Those cases required a simpler analysis compared to the cases addressed here. In order to obtain the corresponding effective error bounds of Gauss-Radau quadrature with $\omega = \omega_3$ and Gauss-Lobatto quadrature with $\omega = \omega_2$, which is the main aim of the paper, we follow the approach of Gautschi et al. [**4**], and T. Schira [**9**] based on a determination of the intervals $[\rho^*, +\infty)$, $\rho^* > 1$, on which $|K_{n,r}(z; \omega)|$ attains its maximum on the real or on the imaginary axis. For additional details see [**5**], [**11**]. For error bounds of quadrature rules for analytic functions see the recent survey paper by Notaris [**8**].

2. GAUSS-RADAU QUADRATURE WITH CHEBYSHEV WEIGHT FUNCTION OF THE THIRD KIND

2.1 Preliminary

In [**3**] Gautschi and Li analyzed the maximum modulus of the kernel with $K^R_{n,r}(z; \omega_3)$. Based on numerical computations, they *stated* ([**3**, pg. 326]) that the maximum is attained at:

1) $\theta = \pi$ if $\rho > 1$ and $n = 1$;

2) $\theta = 0$ if $\rho \geq \rho_n$ and $n \geq 2$.

Here, ρ_n is some number greater than 1. Gautschi and Li proved the asymptotic results and determined the conjectured values of ρ_n for $2 \leq n \leq 20$. Let $f(\theta) := |K^R_{n,2}(z; \omega_3)|$ (below) be function implemented in arithmetic with higher precision in `Matlab`.

Gautschi and Li [**3**, Eqn. (2.8)] derived the explicit representations of the kernels on $\mathcal{E}_\rho$,

$$K_{n,2}^R(z;\omega_3) = \frac{2\pi(u+1)}{(u-1)u^{n+2}} \times \frac{u^2+\alpha u+\beta}{\beta[u^{n+3}+u^{-(n+2)}]+\alpha[u^{n+2}+u^{-(n+1)}]+[u^{n+1}+u^{-n}]},$$

where $\alpha = \dfrac{2n+1}{n+2}$, $\beta = \dfrac{(n+1)(2n+1)}{(n+2)(2n+5)}$, $z=(u+u^{-1})/2$ 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 $\theta=0$ and $\theta=\pi$ because of the corresponding *statements*.

By introducing some substitutions, we can easily express the modulus of the kernel in the following form

$$|K_{n,2}^R(z;\omega_3)| = \sqrt{4\pi^2\frac{ac}{bd}},$$

where

$$\begin{aligned} a &= |u+1|^2 = \rho^2+2\rho\cos\theta+1, \qquad b=|u-1|^2=\rho^2-2\rho\cos\theta+1,\\ c &= |u^2+\alpha u+\beta|^2\\ &= \rho^4+2\alpha\cos\theta\rho^3+(\alpha^2+2\beta\cos2\theta)\rho^2+2\alpha\beta\cos\theta\rho+\beta^2,\\ d &= \rho^{2n+4}\left|\beta[u^{n+3}+u^{-(n+2)}]+\alpha[u^{n+2}+u^{-(n+1)}]+[u^{n+1}+u^{-n}]\right|^2. \end{aligned}$$

We get

$$\left|K_{n,2}^R(z;\omega_3)\right|^2 = 4\pi^2\frac{ac}{bd}.$$

By letting A_0, B_0, C_0, D_0 denote the values of a,b,c,d at $\theta=0$, the square of the modulus of the kernel at $\theta=0$ can be expressed as

$$\left|K_{n,2}^R(z;\omega_3)\right|^2 = 4\pi^2\frac{A_0C_0}{B_0D_0},$$

where

$$\begin{aligned} A_0 &= \rho^2+2\rho+1, \qquad B_0=\rho^2-2\rho+1,\\ C_0 &= \rho^4+2\alpha\cdot\rho^3+(\alpha^2+2\beta)\cdot\rho^2+2\alpha\beta\cdot\rho+\beta^2,\\ D_0 = \beta^2 &\cdot\rho^{4n+10}+2\alpha\beta\cdot\rho^{4n+9}+(\alpha^2+2\beta)\cdot\rho^{4n+8}+2\alpha\cdot\rho^{4n+7}+\rho^{4n+6}\\ &+ 2\beta\cdot\rho^{2n+7}+(2\alpha+2\alpha\beta)\cdot\rho^{2n+6}+(2+2\beta^2+2\alpha^2)\cdot\rho^{2n+5}\\ &+ (2\alpha\beta+2\alpha)\cdot\rho^{2n+4}+2\beta\cdot\rho^{2n+3}+\rho^4\\ &+ 2\alpha\cdot\rho^3+(\alpha^2+2\beta)\cdot\rho^2+2\alpha\beta\cdot\rho+\beta^2. \end{aligned}$$

Our aim is to show that, if $n \geq 2$, this is the maximum value of the modulus for all $\rho \geq \rho_n$ and $\theta \in [0, 2\pi]$. Similarly, by letting $A_\pi, B_\pi, C_\pi, D_\pi$ denote the values of a, b, c, d at $\theta = \pi$, the square of the modulus of the kernel at $\theta = \pi$ can be expressed as

$$\left|K_{n,2}^R(z;\omega_3)\right|^2 = 4\pi^2 \frac{A_\pi C_\pi}{B_\pi D_\pi},$$

with appropriate replacements given bellow

$$\begin{aligned}
A_\pi &= \rho^2 - 2\rho + 1, \quad B_\pi = \rho^2 + 2\rho + 1, \\
C_\pi &= \rho^4 - 2\alpha \cdot \rho^3 + (\alpha^2 + 2\beta) \cdot \rho^2 - 2\alpha\beta \cdot \rho + \beta^2, \\
D_\pi = \beta^2 & \cdot \rho^{14} - 2\alpha\beta \cdot \rho^{13} + (\alpha^2 + 2\beta) \cdot \rho^{12} - 2\alpha \cdot \rho^{11} + \rho^{10} \\
- & 2\beta \cdot \rho^9 + (2\alpha + 2\alpha\beta) \cdot \rho^8 + (-2 - 2\beta^2 - 2\alpha^2) \cdot \rho^7 \\
+ & (2\alpha\beta + 2\alpha) \cdot \rho^6 - 2\beta \cdot \rho^5 + \rho^4 \\
- & 2\alpha \cdot \rho^3 + (\alpha^2 + 2\beta) \cdot \rho^2 - 2\alpha\beta \cdot \rho + \beta^2.
\end{aligned}$$

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

2.2 The main results

Theorem 2.1. *For the Gauss-Radau quadrature formula with double end point -1 with the Chebyshev weight function of the third kind, it holds that the modulus of the kernel $\left|K_{n,2}^R(z;\omega_3)\right|$ attains its maximum value*

1) *on the negative real axis ($\theta = \pi$) for all $\rho \geq \rho_n = 1$, and $n = 1$;*

2) *on the positive real axis ($\theta = 0$) for all $\rho \geq \rho_n$, and $n \geq 2$,*
*where the values ρ_1, $\rho_n \in (1, \infty)$, given in the Table 1 (extended version of [**3**, Table 3.2]) are calculated at least on the 4 significant decimal digits i.e.*
1) $\rho \geq \rho_n$, $n = 1$

$$\max_{z \in \mathcal{E}_\rho} \left|K_{n,2}^R(z;\omega_3)\right| = \left|K_{n,2}^R\left(-\frac{1}{2}(\rho + \rho^{-1}), \omega_3\right)\right|,$$

2) $\rho \geq \rho_n$, $n \geq 2$

$$\max_{z \in \mathcal{E}_\rho} \left|K_{n,2}^R(z;\omega_3)\right| = \left|K_{n,2}^R\left(\frac{1}{2}(\rho + \rho^{-1}), \omega_3\right)\right|.$$

Proof. 1) Referring to the previously introduced notation, we have to show that

$$\frac{ac}{bd} \leq \frac{A_\pi C_\pi}{B_\pi D_\pi}$$

for each ρ greater than some ρ_n and $n = 1$.
The previous inequality can be written as $I_\pi(\rho) = acB_\pi D_\pi - A_\pi C_\pi bd \leq 0$.

We can easily see that I_π is a polynomial in ρ, of degree equal to 21, whose coefficients depend only on θ, i.e. $I_\pi = I_\pi(\rho) = \sum_{i=0}^{21} a_i(\theta)\rho^i$.

2) In this case we have to show that

$$\frac{ac}{bd} \le \frac{A_0C_0}{B_0D_0}$$

for each $\rho \ge \rho_n$ and $n \ge 2$. i.e. $I_0(\rho) = acB_0D_0 - A_0C_0bd \le 0$.
$I_0(\rho)$ is also a polynomial in ρ whose coefficients also depend only on θ.

In order to ensure the non-positivity of polynomial $I(\rho)$ for each $\rho \ge \rho_n$, we wrote the initial polynomial as a polynomial in the terms of positive differences $\rho - \rho_n$, and show the non-positivity of its new coefficients (in the hope that it holds, since it is obviously not a necessary condition for the non-positivity of the corresponding polynomial). We have

$$I_0(\rho) = J_0(\rho - \rho_n) = \sum_{i=0}^{4n+17} b_i(\theta, \rho_n)(\rho - \rho_n)^i. \tag{5}$$

Explicit formulae for coefficients $b_i(\theta, \rho_n)$ are also complicated trigonometric functions given in the terms of the coefficients $a_j(\theta)$

$$b_k(\theta, \rho_n) = \sum_{i=0}^{4n+17-k} (-1)^i \binom{k+i}{i} a_{k+i}(\theta)\rho_n^i. \tag{6}$$

The coefficients $b_0(\theta, \rho_n), b_1(\theta, \rho_n), \ldots, b_{4n+17}(\theta, \rho_n)$ are inappropriate for further analytical consideration. In the same way, the numerical calculations for all the other values of n show that all the functions $b_i(\theta, \rho_n)$, $i = 0, 1, \ldots, 4n + 17$ are non-positive for all θ on the interval $[0, 2\pi]$ (Fig.1). The method has been tested for all the values of n from 2 to 100 and it gives the optimal results. In general, the non-positivity of the coefficients $b_i(\theta, \rho_n)$ is not a necessary condition for non-positivity of a polynomial for each $\rho \ge \rho_n$, but in this case, it is obviously a sufficient condition. Numerical computations show that if $n = 1$, the coefficients

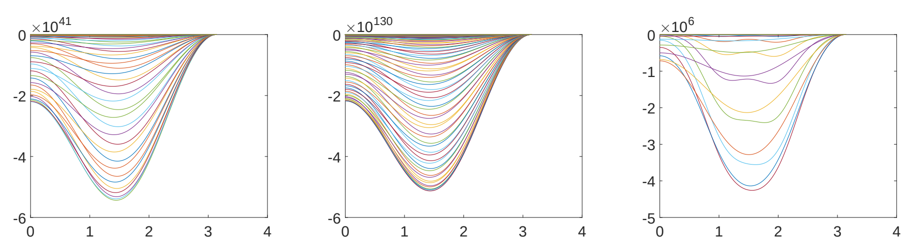


Figure 1: The functions $b_0(\theta, \rho_n), ..., b_{137}(\theta, \rho_n)$ in the case $n = 30$ (left); the functions $b_0(\theta, \rho_n), ..., b_{417}(\theta, \rho_n)$ in the case $n = 100$ (middle); the functions $b_0(\theta, \rho_n), ..., b_{21}(\theta, \rho_n)$ in the case $n = 1$, $\rho_n = 1$ (right).

of the corresponding polynomial $J_\pi(\rho - \rho_1, \theta)$ are non-positive (Fig.1, right). □

For each fixed $n \geq 2$, we have considered the term $J_0(\rho,\theta)$ and tested (using the bisection procedure) the smallest possible values of ρ_n such that the terms $J_0(\rho,\theta)$ are non-positive for each $\rho \geq \rho_n$. Exactly those values were the input for the calculating the corresponding coefficients $b_i(\theta,\rho_n)$. In this sense we mean that the described method gives the optimal results. The values ρ_n for $n \geq 21$ are presented in Table 1.

Table 1: The values of ρ_n for $21 \leq n \leq 56$

n	ρ_n	n	ρ_n	n	ρ_n	n	ρ_n	n	ρ_n	n	ρ_n
21	1.0141	27	1.0098	33	1.0081	39	1.0077	45	1.0070	51	1.0066
22	1.0131	28	1.0093	34	1.0079	40	1.0077	46	1.0069	52	1.0065
23	1.0122	29	1.0090	35	1.0078	41	1.0076	47	1.0069	53	1.0065
24	1.0114	30	1.0086	36	1.0077	42	1.0075	48	1.0068	54	1.0063
25	1.0108	31	1.0084	37	1.0075	43	1.0074	49	1.0069	55	1.0064
26	1.0102	32	1.0083	38	1.0074	44	1.0073	50	1.0066	56	1.0062

2.3 Numerical examples

From a practical point of view, our aim was to precisely determine the minimal value of ρ_n suggested in the paper [**3**] and defined by Theorem 2.1.

Let us consider the numerical calculation of the following integral by (2) with $\omega = \omega_2$,

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

According to the previously introduced notation, under the assumption that f is analytic inside $\mathcal{E}_{\rho_{\max}}$, the error bound of the corresponding quadrature formula can be optimized by

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

where

$$r_n(f) = \inf_{\rho_n<\rho<\rho_{\max}} \left[\frac{\ell(\mathcal{E}_\rho)}{2\pi}\Big(\max_{z\in\mathcal{E}_\rho}|K_{n,2}^R(z,\omega_3)|\Big)\Big(\max_{z\in\mathcal{E}_\rho}|f(z)|\Big)\right].$$

Here, $\ell(\mathcal{E}_\rho)$ represents the length of the ellipse $\mathcal{E}_\rho$, and can be estimated by (see [**9**])

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

where $a_1 = (\rho+\rho^{-1})/2$. Depending on n, the kernel attains its maximum value at $\theta = 0$ or $\theta = \pi$, i. e.

$$\max_{z\in\mathcal{E}_\rho}|K_{n,2}^R(z,\omega_3)| = 2\pi\sqrt{\frac{AC}{BD}}.$$

Error bound $r_n(f)$ reduces to
(7)
$$r_n(f,\omega_3) = \inf_{\rho}\left[a_1\left(1-\frac{1}{4}a_1^{-2}-\frac{1}{64}a_1^{-4}-\frac{5}{256}a_1^{-6}\right)\max_{z\in\mathcal{E}_\rho}|K^R_{n,2}(z,\omega_3)|\Big(\max_{z\in\mathcal{E}_\rho}|f(z)|\Big)\right].$$

In order to check the proposed error bounds we made several tests and compared them with respect to the exact (actual) errors. Examples are made for some special functions, appearing in the literature. "*Error*" denotes the actual error bound of the corresponding formula. Authors are thankful to prof. Miodrag Spalević for helping with computation of actual errors of Gauss-Lobatto and Gauss-Radau quadratures.

Example 1. Let $f_1(z) = \dfrac{\cos(z)}{z^2+w^2}$, $w > 0$. Table 2 displays the error bounds and actual errors which correspond to the quadrature rules (2) with the *Chebyshev* weight functions of the third kind.

Table 2: Error bounds $r_n(f_1,\omega_3), (r_n)$ and actual errors ($Error$)

n	$r_n,\ \omega=2$	$Error$	$r_n,\ \omega=5$	$Error$	$r_n,\ \omega=50$	$Error$
1	1.892(-1)	2.545(-2)	5.601(-3)	1.549(-3)	3.071(-5)	1.080(-5)
2	9.201(-3)	1.051(-3)	7.839(-5)	1.671(-5)	2.048(-7)	6.366(-8)
3	6.221(-4)	4.858(-5)	1.088(-6)	1.572(-7)	8.917(-10)	2.374(-10)
4	4.090(-5)	2.395(-6)	1.371(-8)	1.416(-9)	2.495(-12)	5.933(-13)
5	2.627(-6)	1.225(-7)	1.635(-10)	1.285(-11)	4.846(-15)	1.053(-15)
8	6.354(-10)	1.821(-11)	2.339(-16)	1.045(-17)	6.449(-24)	1.150(-24)
20	1.219(-24)	1.354(-26)	4.286(-40)	6.899(-42)	5.521(-66)	5.967(-67)

Example 2. Let $f_2(z) = e^{e^{\cos(\omega z)}}$, $\omega > 0$. The Table 3 displays some error bounds and actual errors.

Table 3: Error bounds $r_n(f_2,\omega_3)$, r_n and actual errors ($Error$)

n	$r_n,\ \omega=1$	$Error$	$r_n,\ \omega=0.2$	$Error$	$r_n,\ \omega=0.02$	$Error$
1	6.930(+1)	4.017(+0)	1.149(-1)	2.155(-2)	1.113(-5)	2.293(-6)
2	5.843(+0)	5.426(-1)	7.932(-4)	1.234(-4)	8.083(-10)	1.315(-10)
3	9.309(-1)	6.968(-2)	5.812(-6)	7.391(-7)	5.819(-14)	4.828(-15)
4	1.368(-1)	8.698(-3)	3.974(-8)	4.342(-9)	3.955(-18)	4.687(-19)
7	3.031(-4)	1.390(-5)	8.888(-15)	7.117(-16)	8.887(-31)	7.845(-32)
12	5.196(-9)	1.738(-10)	3.185(-26)	1.866(-27)	3.266(-52)	2.124(-53)
20	3.714(-17)	9.271(-19)	4.257(-45)	1.843(-46)	4.567(-87)	2.197(-88)
30	7.200(-28)	1.429(-29)	2.904(-69)	9.863(-71)	3.290(-131)	1.240(-132)

3. GAUSS-LOBATTO QUADRATURES WITH CHEBYSHEV WEIGHT FUNCTION OF THE SECOND KIND

3.1 Preliminary

Gautschi and Li [**3**, Section 4.2] analyzed the maximum modulus of the kernel $K^L_{n,2}(z;\omega_2)$ [**3**, Eqn. 2.13] . For $\omega = \omega_2$ they presented some numerical evidence and proved the asymptotic results. Based on numerical calculations, they *stated* that the maximum is attained:

1) on the positive real axis if $\rho > 1$ and $1 \le n \le 9$;

2) on the imaginary axis if $\rho \ge \rho_n$ and $n \ge 10$;

3) on the positive real axis if $1 < \rho < \rho_n$ and $n \ge 10$.

Here, ρ_n is some number greater than 1. Gautschi and Li determined the conjectured values ρ_n for $10 \le n \le 20$ by means of a bisection procedure.

Let $f(\theta) := |K^L_{n,2}(z;\omega_2)|$. The *statements* 2) and 3) claim that the function $f(\theta)$ attains its maximum either at $\theta = 0$ or $\theta = \pi/2$, when $n \ge 10$. When we take, for instance, $n = 20$ and $\rho = 1.13 > 1.1244$ (see [**3**, Table 4.1]), a simple calculation gives as follows:

$$f(0) = 0.022769... \ ; \ f(\pi/2) = 0.023550... \ ; \ f(1.5094) = 0.023680... \ .$$

The function $f(\theta)$ is implemented by using symbolic computation in `Matlab`. From here the phenomenon grows more and more. For example, if we take $n = 30$, then for $\rho = 1.1368$ or any number from the interval $[1.1368, \infty)$, the maximum occurs at $\theta = \pi/2$ (as the *statement* 2) claims); for $\rho = 1.0629$, or any number from the interval $(1, 1.0629]$, the maximum occurs at $\theta = 0$. On the other side, if we take $n = 30$ and any number from the interval $(1.0629, 1.1368)$, for instance specialized on $\rho = 1.090$, then we have

$$f(0) = 0.01457367... \ ; \ f(\pi/2) = 0.02162440... \ ; \ f(1.6157) = 0.02175132... \ .$$

It seems that there is a small range of the parameter ρ where the function $f(\theta)$ does not attain its maximum neither at $\theta = 0$ or $\theta = \pi/2$. In fact, these examples imply that the *statement* 3) holds on the restricted interval $(1, \rho'_n]$ where $\rho'_n \le \rho_n$. In this part of the paper we confirm (again with the proof in the best sense it is possible to be done here) the precise values of ρ_n and then present the effective error bounds for Gauss-Lobatto quadrature rule with $\omega = \omega_2$.

3.2 The main results

We get the following Theorem:

Theorem 3.2. *For the Gauss-Lobatto quadrature formula with double end points* ∓ 1 $(r = 2)$ *with the Chebyshev weight function of the second kind, it holds that the modulus of the kernel* $\left|K^L_{n,2}(z;\omega_2)\right|$ *attains its maximum value*

i) on the real axis $(\theta = 0)$ *for* ρ *greater than* ρ_n *and* $1 \le n \le 9$,

ii) on the imaginary axis $(\theta = \frac{\pi}{2})$ *for* $n \ge 10$ *and* ρ *greater than or equal to* ρ_n. *i.e.*
i) for $\rho \ge \rho_n$, $1 \le n \le 9$,

$$\max_{z\in\mathcal{E}_\rho}\left|K^L_{n,2}(z;\omega_2)\right| = \left|K^L_{n,2}\left(\frac{1}{2}(\rho+\rho^{-1}),\omega_2\right)\right|;$$

ii) for $\rho \ge \rho_n$, $n \ge 10$,

$$\max_{z\in\mathcal{E}_\rho}\left|K^L_{n,2}(z;\omega_2)\right| = \left|K^L_{n,2}\left(\frac{i}{2}(\rho-\rho^{-1}),\omega_2\right)\right|.$$

The values ρ_n, given in the Table 4 and [**3**, Table 4.1], are the minimal possible calculated to four decimal places. The values from the Table 4 that differ from the corresponding values from [**3**, Table 4.1] are bolded. The values ρ_n are delivered in the same way as previously described. Here, we confirm them in the cases when n is odd and compute some additional cases for $n \le 64$ (Table 4).

Table 4: The values of ρ_n.

n	ρ_n	n	ρ_n	n	ρ_n	n	ρ_n	n	ρ_n
10	**1.7531**	21	1.1141	32	1.1303	43	1.0359	54	1.0869
11	1.4925	22	1.1725	33	1.0541	44	1.1020	55	1.0248
12	**1.3733**	23	1.0975	34	1.1244	45	1.0335	56	1.0845
13	1.3013	24	1.1617	35	1.0493	46	1.0985	57	1.0235
14	**1.2530**	25	1.0847	36	1.1191	47	1.0314	58	1.0822
15	1.2170	26	1.1523	37	1.0452	48	1.0953	59	1.0223
16	**1.2179**	27	1.0746	38	1.1142	49	1.0295	60	1.0800
17	1.1683	28	1.1443	39	1.0417	50	1.0923	61	1.0212
18	**1.2000**	29	1.0664	40	1.1098	51	1.0277	62	1.0779
19	1.1365	30	1.1368	41	1.0386	52	1.0895	63	1.0203
20	**1.1851**	31	1.0597	42	1.1057	53	1.0262	64	1.0760

3.3 Modified Gautschi and Li's statement 3)

The *statement* 3) suggests that the maximum modulus of the kernel is attained on the positive real axis for all ρ from the interval $(1, \rho_n)$, if $n \ge 10$. Here, we apply similar method which has been used in thorough the study of the *statements* 1) and 2). The interval $1 < \rho < \rho'_n$ requires a bit different approach because the differences $\rho - \rho'_n$ are not positive. In order to show the non-positivity of polynomial $I_0(\rho)$ given by the term

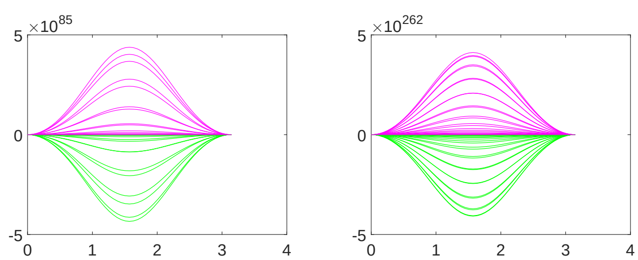
$$I_0(\rho) = \sum_{i=0}^{4n+30} a_i(\theta)\rho^i,\ 1 < \rho < \rho'_n,$$

first of all, we shift the argument, which leads to a polynomial

$$I_0(\rho) = M(\rho - 1 - \rho'_n) = \sum_{i=0}^{4n+30} c_i(\theta, \rho'_n)(\rho - 1 - \rho'_n)^i, \quad -\rho'_n < \rho - 1 - \rho'_n < -1.$$

Non-positivity of this polynomial is a sufficient condition for the non-positivity of the initial polynomial $I_0(\rho)$ on the interval $(1, \rho'_n)$. The term $\rho' = \rho - 1 - \rho'_n$ is negative, so the terms $(\rho')^i$ are positive if degree i is an even number and they are negative if it is an odd number. All numerical calculations (with steps $\dfrac{\pi}{k}$ where $k = 100, 1000...$) show that for the noted values ρ'_n all the coefficients $c_i(\theta, \rho'_n)$ are strictly non-positive when i is an even number, while all the coefficients $c_i(\theta, \rho'_n)$ are strictly non-negative when i is an even number. Conversely, for odd degrees i, negative terms $(\rho')^i$ are multiplied by all positive coefficients $c_i(\theta, \rho'_n)$. Therefore, the sum of all products $c_i(\theta, \rho'_n)(\rho - 1 - \rho'_n)^i,\ i = 0, 1, \ldots, 4n + 30$, i.e. the term $I_0(\rho)$, is non-positive. Fig.2 shows all the coefficients (positive and negative) drawn together in the same graph for selected values of n.

Figure 2: The function $c_0(\theta, \rho'_n), ..., c_{102}(\theta, \rho'_n)$, in the case $n = 18$, $\rho'_n = 1.1512$ (left) and the function $c_0(\theta, \rho'_n), ..., c_{290}(\theta, \rho'_n)$, in the case $n = 65$, $\rho'_n = 1.0193$ (right.) Even coefficients are under the x-axis (green), while the odd ones are above x-axis (violet).
.



The value ρ'_n can be numerically determined treating the terms $I_0(\rho, \theta)$ for $n \geq 10$ and again, the method works when we take exactly those values for input arguments of the functions $c_i(\theta, \rho'_n)$. The results derived using `Matlab` show that if n is odd, then $\rho'_n = \rho_n$. Otherwise, if n is even, starting from $n = 16$, there exists a difference between the values ρ'_n and ρ_n, as the Table 5 shows.

Table 5: The values of ρ'_n and ρ_n when n is even.

n	ρ'_n	ρ_n	n	ρ'_n	ρ_n	n	ρ'_n	ρ_n
16	1.1903	1.2179	30	1.0629	1.1368	44	1.0346	1.1020
18	1.1512	1.2000	32	1.0567	1.1303	46	1.0323	1.0985
20	1.1246	1.1851	34	1.0515	1.1244	48	1.0303	1.0953
22	1.1053	1.1725	36	1.0471	1.1191	50	1.0285	1.0923
24	1.0907	1.1617	38	1.0433	1.1142	52	1.0269	1.0895
26	1.0794	1.1523	40	1.0400	1.1098	54	1.0254	1.0869
28	1.0703	1.1443	42	1.0371	1.1057	56	1.0240	1.0845

3.4 Numerical examples

The error bound $r_n(f)$ is computed similarly to the previous chapter. In order to check the proposed error bounds, we made several tests and compared them with respect to the exact (actual) errors, '*Error*'. In order to compute the actual error we have modified Gautschi's `Matlab` code `globatto.m` (cf. [**1**], [**2**]) to a high precision arithmetic.

Example 1. Let $f_1(z) = \dfrac{e^{e^z}}{(a+z)^k(b+z)^l(c+z)^m}$, with the value of parameters a, b, c often used in literature: $a = -1.408333333333333$; $b = -1.892857142857143$; $c = -2.408695652173913$; $k = 1$; $l = 5$; $m = 10$. The corresponding error bounds and actual errors are displayed in Table 6.

Table 6: Error bounds $r_n(f_1)$ (r_n) and actual errors ($Error$)

n	r_n	$Error$	n	r_n	$Error$
4	3.736 (-1)	1.592(-2)	16	4.295(-9)	7.115(-11)
5	9.290 (-2)	3.916(-3)	18	1.582(-10)	2.153(-12)
6	2.271(-3)	9.279(-4)	20	5.639(-12)	6.404(-14)
7	5.401 (-3)	2.101(-4)	25	1.234(-15)	9.596(-18)
8	1.201 (-3)	4.547(-5)	30	2.488(-19)	1.447(-21)
9	2.735(-4)	9.432(-6)	40	8.886(-27)	3.390(-29)
10	5.987 (-5)	1.884(-6)	50	2.867(-34)	8.123(-37)
12	2.710 (-6)	6.853(-8)	64	8.560(-45)	1.775(-47)

Example 2. Let $f_2(z) = e^{e^{\cos(\omega z)}}$, $\omega > 0$. Table 7 displays error bounds and actual errors.

Example 3. Let $f_3(z) = \dfrac{\cos(z)}{z^2+\omega^2}$, $\omega > 0$. The corresponding error bounds and actual errors are displayed in Table 8. Finally, in the Table 9 we display the values of $r_n(f_3)$, and $\rho_{\text{opt}} \in (\rho_n, \rho_{\max})$, for the same values n and ω from Table 8, in which the expression in brackets under the sign of inf in (7) attains its minimum.

Table 7: Error bounds $r_n(f_2)$ (r_n) and actual errors ($Error$)

n	$r_n,\ \omega = 3$	$Error$	$r_n,\ \omega = 1$	$Error$	$r_n,\ \omega = 0.5$	$Error$
3	7.178(+1)	1.447(+0)	8.100(-2)	7.546(-3)	2.056(-4)	2.308(-5)
6	3.777 (+0)	1.678(-1)	1.275(-4)	1.103(-5)	8.127(-9)	7.218(-10)
9	2.769 (-1)	1.701(-2)	1.679(-7)	1.287(-8)	2.435(-13)	1.808(-14)
15	2.101 (-3)	1.217(-4)	1.757(-13)	1.019(-14)	1.140(-22)	6.420(-24)
20	3.077(-5)	1.514(-6)	1.129(-18)	5.547(-20)	1.155(-30)	5.526(-32)
25	3.612(-7)	1.564(-8)	5.293(-24)	2.280(-25)	8.397(-39)	3.527(-40)
35	3.078(-11)	1.094(-12)	5.803(-35)	2.044(-36)	2.129(-55)	7.334(-57)
50	1.037(-17)	2.978(-19)	6.212(-52)	1.763(-53)	7.492(-81)	2.085(-82)
70	8.339(-27)	1.935(-28)	3.174(-75)	7.341(-77)	1.719(-115)	3.905(-117)

Table 8: Error bounds $r_n(f_3)$ (r_n) and actual errors ($Error$)

n	$r_n,\ \omega = 0.5$	$Error$	$r_n,\ \omega = 1$	$Error$	$r_n,\ \omega = 5$	$Error$
4	9.305(-1)	2.775(-2)	2.201(-3)	1.114(-4)	1.093(-10)	9.763(-12)
6	1.068 (-1)	3.707(-3)	6.208(-5)	2.847(-6)	1.266(-14)	7.720(-16)
9	5.201 (-3)	1.914(-4)	3.333(-7)	1.274(-8)	1.493(-20)	6.150(-22)
12	3.087 (-4)	1.091(-5)	1.971(-9)	5.987(-11)	1.695(-26)	5.247(-28)
15	2.013(-5)	5.511(-7)	1.152(-11)	2.883(-13)	1.868(-32)	4.629(-34)
20	2.035(-7)	4.337(-9)	2.105(-15)	4.071(-17)	2.101(-42)	3.905(-44)
25	1.977(-9)	3.453(-11)	3.715(-19)	5.855(-21)	2.273(-52)	3.380(-54)
30	1.871(-11)	2.767(-13)	6.394(-23)	8.507(-25)	2.394(-62)	2.966(-64)
50	1.278(-19)	1.173(-21)	4.830(-38)	3.959(-40)	2.515(-102)	1.870(-104)
70	7.597(-28)	5.054(-30)	3.196(-53)	1.893(-55)	2.303(-142)	1.223(-144)

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Table 9: Error bounds $r_n(f_3)$ (r_n) and values ρ_{opt} for some values of n, ω

n	$r_n,\ \omega = 0.5$	ρ_{opt}	$r_n,\ \omega = 1$	ρ_{opt}	$r_n,\ \omega = 5$	ρ_{opt}
4	9.305(-1)	1.5200	2.201(-3)	2.2320	1.093(-10)	8.9710
6	1.068 (-1)	1.5350	6.208(-5)	2.2720	1.266(-14)	9.3090
9	5.201 (-3)	1.5520	3.333(-7)	2.3080	1.493(-20)	9.5580
12	3.087 (-4)	1.5643	1.971(-9)	2.3303	1.695(-26)	9.6883
15	2.013(-5)	1.5730	1.152(-11)	2.3450	1.868(-32)	9.7690
20	2.035(-7)	1.5830	2.105(-15)	2.3600	2.101(-42)	9.8500
25	1.977(-9)	1.5890	3.715(-19)	2.3700	2.273(-52)	9.8990
30	1.871(-11)	1.5940	6.394(-23)	2.3770	2.394(-62)	9.9320
50	1.278(-19)	1.6030	4.830(-38)	2.3910	2.515(-102)	9.9980
70	7.597(-28)	1.6070	3.196(-53)	2.3980	2.303(-142)	10.0270

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