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ON THE REMAINDER TERM FOR ANALYTIC FUNCTIONS OF GAUSS-LOBATTO AND GAUSS-RADAU QUADRATURES

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Dedicated to Wolfgang Thron on his 70th birthday

ABSTRACT. We study the kernels in the contour integral representation of the remainder term of Gauss-Lobatto and Gauss-Radau quadratures, in particular the location of their maxima on circular and elliptic contours. Quadrature rules with Chebyshev weight functions of all four kinds receive special attention, but more general weights are also considered.

1. Introduction. Let Γ be a simple closed curve in the complex plane surrounding the interval $[-1,1]$ and $\mathcal{D}$ be its interior. Let f be analytic in $\mathcal{D}$ and continuous on $\overline{\mathcal{D}}$. We consider an interpolatory quadrature rule

$$\int_{-1}^{1} f(t)w(t)\,dt = \sum_{\nu=1}^{N} \lambda_\nu f(\tau_\nu) + R_N(f) \tag{1.1}$$

with

$$-1 \le \tau_N < \tau_{N-1} < \cdots < \tau_1 \le 1 \tag{1.2}$$

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$$\omega_N(z) = \omega_N(z;w) = \prod_{\nu=1}^{N} (z-\tau_\nu), \quad z \in \mathbf{C}, \tag{1.3}$$

denote its node polynomial (which in general depends on w), and define

$$\rho_N(z;w) = \int_{-1}^{1} \frac{\omega_N(t;w)}{z-t} w(t)\,dt, \quad z \in \mathbf{C}\backslash[-1,1], \tag{1.4}$$

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then, as is well known, the remainder term R_N in (1.1) admits the contour integral representation

$$R_N(f) = \frac{1}{2\pi i}\oint_\Gamma K_N(z;w) f(z)\,dz, \tag{1.5}$$

where the "kernel" K_N can be expressed, e.g., in the form

$$K_N(z;w) = \frac{\rho_N(z;w)}{\omega_N(z;w)}, \quad z \in \Gamma. \tag{1.6}$$

This is easily verified by applying the residue theorem to the integral $(2\pi i)^{-1}\oint_\Gamma [f(z)\omega_N(t)/((z-t)\omega_N(z))]\,dz$ and subsequent integration in t, recalling that the weights λ_ν in (1.1) are given by $\lambda_\nu = \int_{-1}^{1}[\omega_N(t)/((t-\tau_\nu)\omega_N'(\tau_\nu))]w(t)\,dt$, since (1.1) is interpolatory. Note that ω_N in (1.3) and (1.4) may be multiplied by any constant $c \neq 0$ without affecting the validity of (1.6). It is also evident from (1.6) that

$$K_N(\bar{z};w) = \overline{K_N(z;w)}. \tag{1.7}$$

In order to estimate the error in (1.1) by means of

$$|R_N(f)| \le (2\pi)^{-1}\ell(\Gamma)\max_{z\in\Gamma}|K_N(z;w)| \cdot \max_{z\in\Gamma}|f(z)|, \tag{1.8}$$

where $\ell(\Gamma)$ is the length of the contour Γ, it becomes necessary to study the magnitude of $|K_N|$ on Γ. This has been done in a number of papers (see [**1**, §4.1.1] for references) for Gauss = type and other quadrature formulae, and for contours Γ that are either concentric circles centered at the origin or confocal ellipses with focal points at ± 1. The thrust of this work has been directed towards upper bounds, or asymptotic estimates, for the maximum of $|K_N|$ in (1.8). In an attempt to remove uncertainties inherent in such estimates, we determined in [**2**] (see also [**3**]), for Gauss formulae, the precise location on Γ where $|K_N|$ attains its maximum, and we suggested simple recursive techniques to evaluate $K_N(z;w)$ for any $z \in \mathbf{C}\backslash[-1,1]$. Here we investigate, in the same spirit, quadrature rules of Gauss-Lobatto and Gauss-Radau type, especially for any of the four Chebyshev weight functions

$$\begin{aligned} &w_1(t) = (1-t^2)^{-\frac{1}{2}}, && w_2(t) = (1-t^2)^{\frac{1}{2}}, \\ &w_3(t) = (1-t)^{-\frac{1}{2}}(1+t)^{\frac{1}{2}}, && w_4(t) = (1-t)^{\frac{1}{2}}(1+t)^{-\frac{1}{2}}. \end{aligned} \tag{1.9}$$

In Section 2 we consider circular contours and general weight functions. In Section 3 explicit formulae are derived for the Lobatto and Radau kernels $K_N(\cdot; w)$ with $w = w_i,\ i = 1, 2, 3, 4$. Their maximum moduli are analyzed in Section 4, both on circular and elliptic contours.

2. Some general results for circular contours. In this section, $\Gamma = C_r$, $C_r = \{z \in \mathbf{C} : |z| = r\}$, where $r > 1$. For positive weight functions w and quadrature rules of Gaussian type, with $N = n$, it is known from [**2**] that

$$\max_{z \in C_r} |K_n(z; w)| = \begin{cases} K_n(r; w) & \text{if } w(t)/w(-t) \text{ is nondecreasing on } (-1, 1), \\ |K_n(-r; w)| & \text{if } w(t)/w(-t) \text{ is nonincreasing on } (-1, 1). \end{cases} \tag{2.1}$$

We now explore the implications of this result to Gauss-Lobatto (Subsection 2.1) and Gauss-Radau formulae (Subsection 2.2).

2.1. *Gauss-Lobatto formulae.* These are the quadrature rules (1.1) with $N = n + 2$, $\tau_N = -1$, $\tau_1 = 1$ and $R_N(f) = 0$ whenever $f \in \mathbf{P}_{2n+1}$ (the class of polynomials of degree $\leq 2n + 1$). They are clearly interpolatory. We denote $w^L(t) = (1 - t^2)w(t)$ and write $\pi_n(\cdot; w^L)$ for the polynomial of degree n (suitably normalized) orthogonal with respect to the weight function w^L. It is well known that

$$\omega_{n+2}(z; w) = (1 - z^2)\pi_n(z; w^L), \tag{2.2}$$

from which there follows

$$\rho_{n+2}(z; w) = \int_{-1}^{1} \frac{(1 - t^2)\pi_n(t; w^L)}{z - t} w(t)\, dt = \int_{-1}^{1} \frac{\pi_n(t; w^L)}{z - t} w^L(t)\, dt = \rho_n(z; w^L)$$

and, therefore, by (1.6),

$$K_{n+2}(z; w) = \frac{K_n(z; w^L)}{1 - z^2}. \tag{2.3}$$

Here, $K_n(\cdot; w^L)$ is the kernel for the n-point Gauss formula relative to the weight function w^L. Since $|1 - z^2|$ attains its minima on C_r at

$z = r$ and $z = -r$, and since $w^L(t)/w^L(-t) = w(t)/w(-t)$, we have as an immediate consequence of (2.1) that

$$\max_{z\in C_r} |K_{n+2}(z;w)| = \begin{cases} \frac{1}{r^2-1} K_n(r;w^L), \\ \frac{1}{r^2-1} |K_n(-r;w^L)|, \end{cases} \tag{2.4}$$

depending on whether $w(t)/w(-t)$ is nondecreasing or nonincreasing, respectively. In particular (cf. [**2**, p. 1172]), for the Jacobi weight function $w(t) = (1-t)^\alpha (1+t)^\beta$, $\alpha > -1$, $\beta > -1$, the first relation in (2.4) holds if $\alpha \le \beta$ and the second if $\alpha > \beta$.

2.2. *Gauss-Radau formulae.* There are pairs of such formulae, namely, (1.1) with $N = n+1$, $\tau_N = -1$, and (1.1) with $N = n+1$, $\tau_1 = 1$, both having $R_n(f) = 0$ for $f \in \mathbf{P}_{2n}$. It suffices to consider one of them, say the former, since the kernels of the two formulae are simply related. If we denote $w(-t) = w^*(t)$ and write $K_N^{(\mp 1)}(\cdot;w)$ for the kernel of the Radau formula with $\tau_N = -1$ and $\tau_1 = 1$, respectively, a simple computation indeed will show that $K_N^{(+1)}(z;w) = -\overline{K_N^{(-1)}(-\bar{z};w^*)}$, where bars indicate complex conjugation. Therefore,

$$|K_N^{(+1)}(z;w)| = |K_N^{(-1)}(-\bar{z};w^*)|, \tag{2.5}$$

i.e., the modulus of $K_N^{(+1)}$ for the weight function w at the point z has the same value as the modulus of $K_N^{(-1)}$ for the weight function w^* at the point $-\bar{z}$, the mirror image of z with respect to the imaginary axis.

For the Radau formula with $\tau_N = -1$, we write $w^R(t) = (1+t)w(t)$ and have, as is well known,

$$\omega_{n+1}(z;w) = (1+z)\pi_n(z;w^R). \tag{2.6}$$

There follows, similar to the case of Lobatto formulae,

$$K_{n+1}(z;w) = \frac{K_n(z;w^R)}{1+z}, \tag{2.7}$$

where $K_n(\cdot;w^R)$ is the kernel for the n-point Gauss formula relative to the weight function w^R. Since $|1+z|$ on C_r attains its minimum at $z = -r$, we can now apply the second result in (2.1), giving

$$\max_{z\in C_r} |K_{n+1}(z;w)| = \frac{|K_n(-r;w^R)|}{r-1}, \tag{2.8}$$

provided $w^R(t)/w^R(-t)$ is nonincreasing on $(-1,1)$. Unfortunately, this condition is not satisfied for the Chebyshev weights w_1, w_2, w_3 (cf. (1.9)). We conjecture, in fact, that the maximum in (2.8) is attained at $z = r$, rather than $z = -r$, when $w = w_3$ (cf. Subsection 4.2).

3. Remainder kernels for Chebyshev weight functions. In this section, after some preliminaries on orthogonal polynomials, we provide explicit formulae, for Lobatto = and Radau = type rules, of $K_N(\cdot; w)$ when $w = w_i$, $i = 1, 2, 3, 4$ (cf. (1.9)).

3.1. *Preliminaries.* We shall need some facts about Jacobi polynomials with half-integer parameters. They are given here in a form general enough to be applicable (if need be) to Lobatto and Radau formulae with multiple fixed points.

Lemma 3.1. *The polynomial of degree n orthogonal on $(-1,1)$ with respect to the weight function $(1-t^2)^{-1/2+k}$, $k \geq 0$ an integer, is given by $T_{n+k}^{(k)}(t)$, where T_m denotes the m^{th} = degree Chebyshev polynomial of the first kind.*

Proof. See Equation (4.21.7) in [**4**] and the paragraph following this equation. □

The following two lemmas are also known, but are stated here in a form more suitable for our purposes. We recall that Chebyshev polynomials U_n, V_n of the second and third kind (orthogonal relative to the weight functions $(1-t^2)^{1/2}$ and $(1-t)^{-1/2}(1+t)^{1/2}$, respectively) are given by

$$U_n(\cos\theta) = \frac{\sin(n+1)\theta}{\sin\theta}, \quad V_n(\cos\theta) = \frac{\cos(n+\frac{1}{2})\theta}{\cos\frac{1}{2}\theta}. \tag{3.1}$$

Lemma 3.2. *Let $U_{n,k}$ be the polynomial of degree n orthogonal on $(-1,1)$ with respect to the weight function $(1-t)^{1/2}(1+t)^{1/2+k}$, $k \geq 0$*

an integer. Then

$$(3.2_0) \qquad U_{n,0}(t) = U_n(t),$$

(3.2_k)

$$U_{n,k}(t) = \frac{1}{1+t}\left\{U_{n+1,k-1}(t) + \frac{(n+k+\frac{1}{2})(n+k+1)}{(n+\frac{1}{2}k+\frac{1}{2})(n+\frac{1}{2}k+1)}U_{n,k-1}(t)\right\},$$

$$k = 1, 2, 3, \ldots .$$

Proof. Define $U_{n,k}(t) = [(n!(n+k+1)!\sqrt{\pi})/(2\Gamma(n+k/2+1)\Gamma(n+k/2+3/2))]P_n^{(1/2,1/2+k)}(t)$, and use the second relation in [**4**, Equation (4.5.4)] with $\alpha = 1/2$, $\beta = -1/2+k$. □

Lemma 3.3. *Let $V_{n,k}$ be the polynomial of degree n orthogonal on $(-1,1)$ with respect to the weight function $(1-t)^{-1/2}(1+t)^{1/2+k}$, $k \geq 0$ an integer. Then*

$$(3.3_0) \qquad V_{n,0}(t) = V_n(t),$$

(3.3_k)

$$V_{n,k}(t) = \frac{1}{1+t}\left\{V_{n+1,k-1}(t) + \frac{(n+k)(n+k+\frac{1}{2})}{(n+\frac{1}{2}k)(n+\frac{1}{2}k+\frac{1}{2})}V_{n,k-1}(t)\right\},$$

$$k = 1, 2, 3, \ldots .$$

Proof. Define $V_{n,k}(t) = [(n!(n+k)!\sqrt{\pi})/(\Gamma(n+k/2+1/2)\Gamma(n+k/2+1))]P_n^{(-1/2,1/2+k)}(t)$, and use the second relation in [**4**, Equation (4.5.4)] with $\alpha = -1/2$, $\beta = -1/2+k$. □

3.2. *Chebyshev-Lobatto formulae.* We begin with the weight function w_1 and consider (1.1) with $w = w_1$, $N = n+2$, $\tau_N = -1$, $\tau_1 = 1$, $R_N(f) = 0$ for $f \in \mathbf{P}_{2n+1}$. Since the nodes τ_ν, $2 \leq \nu \leq N-1$, are the zeros of $\pi_n(\cdot;(1-t^2)w_1) = \pi_n(\cdot; w_2)$, we may take

$$(3.4) \qquad \omega_{n+2}(z; w_1) = (1-z^2)U_n(z),$$

giving

$$(3.5)\quad \rho_{n+2}(z;w_1)=\int_{-1}^{1}\frac{(1-t^2)U_n(t)}{z-t}w_1(t)\,dt=\int_{-1}^{1}\frac{U_n(t)}{z-t}w_2(t)\,dt.$$

Now it is well known (cf. [**2**, p. 1177]) that

$$(3.6)\qquad U_n(z)=\frac{u^{n+1}-u^{-(n+1)}}{u-u^{-1}},\quad \int_{-1}^{1}\frac{U_n(t)}{z-t}w_2(t)\,dt=\frac{\pi}{u^{n+1}},$$

where z and u are related by the familiar conformal map

$$(3.7)\qquad z=\frac{1}{2}(u+u^{-1}),\quad |u|>1,$$

which transforms the exterior of the unit circle, $\{u\in\mathbf{C}:|u|>1\}$, into the whole z-plane cut along $[-1,1]$. Concentric circles $|u|=\rho$, $\rho>1$, thereby are mapped into confocal ellipses

$$(3.8)\qquad \mathcal{E}_\rho=\{z\in\mathbf{C}:z=\frac{1}{2}(\rho e^{i\vartheta}+\rho^{-1}e^{-i\vartheta}),\ 0\le\vartheta\le 2\pi\}$$

with foci at ±1 and sum of semiaxes equal to ρ.

Substituting (3.6) in (3.4) and (3.5), and noting that $z^2-1=(u-u^{-1})^2/4$, one obtains

$$(3.9)\qquad K_{n+2}(z;w_1)=-\frac{4\pi}{u^{n+1}(u-u^{-1})(u^{n+1}-u^{-(n+1)})}.$$

Proceeding to the weight function w_2, we recall that the nodes τ_ν, $2\le\nu\le N-1$, are now the zeros of $\pi_n(\cdot;(1-t^2)w_2)=\pi_n(\cdot;(1-t^2)^{3/2})$, hence, by Lemma 3.1 (with $k=2$), the zeros of T''_{n+2}. Therefore,

$$\omega_{n+2}(z;w_2)=(1-z^2)T''_{n+2}(z),$$

which, by the differential equation satisfied by T_{n+2}, becomes

$$\omega_{n+2}(z;w_2)=zT'_{n+2}(z)-(n+2)^2T_{n+2}(z).$$

With the help of

$$T_{n+2}(z) = \frac{1}{2}[U_{n+2}(z) - U_n(z)], \quad T'_{n+2}(z) = (n+2)U_{n+1}(z)$$

one then gets

$$\omega_{n+2}(z; w_2) = \frac{n+2}{2}\{-(n+2)[U_{n+2}(z) - U_n(z)] + 2zU_{n+1}(z)\},$$

which can be simplified, using the recurrence relation $2zU_{n+1} = U_{n+2} + U_n$, to

$$\omega_{n+2}(z; w_2) = -\frac{(n+1)(n+2)}{2}\left\{U_{n+2}(z) - \frac{n+3}{n+1}U_n(z)\right\}. \tag{3.10}$$

In terms of the variable u, cf. (3.7), using the first relation in (3.6), this can be written as

$$\begin{aligned}\omega_{n+2}(z; w_2) = -\frac{(n+1)(n+2)}{2(u-u^{-1})}\Big\{&u^{n+3} - u^{-(n+3)} \\ &- \frac{n+3}{n+1}\left(u^{n+1} - u^{-(n+1)}\right)\Big\}.\end{aligned}$$

From (3.10) and the second relation in (3.6), we find

$$\begin{aligned}\rho_{n+2}(z; w_2) &= -\frac{(n+1)(n+2)}{2}\Big\{\int_{-1}^{1}\frac{U_{n+2}(t)}{z-t}w_2(t)\,dt \\ &\qquad - \frac{n+3}{n+1}\int_{-1}^{1}\frac{U_n(t)}{z-t}w_2(t)\,dt\Big\} \\ &= -\frac{(n+1)(n+2)\pi}{2u^{n+1}}\left\{u^{-2} - \frac{n+3}{n+1}\right\}.\end{aligned}$$

Therefore, finally,

$$K_{n+2}(z; w_2) = \frac{\pi}{u^{n+1}}\,\frac{u^{-1} - u^{-3} - \frac{n+3}{n+1}(u - u^{-1})}{u^{n+3} - u^{-(n+3)} - \frac{n+3}{n+1}(u^{n+1} - u^{-(n+1)})}. \tag{3.11}$$

In the case $w = w_3$ we have $\omega_{n+2}(t; w_3) = (1-t^2)\pi_n(t; (1-t)^{1/2}(1+t)^{3/2})$; hence, by Lemma 3.2 (with $k = 1$) and (3.2_1),

$$\omega_{n+2}(z; w_3) = (1-z^2)U_{n,1}(z) = (1-z)\left\{U_{n+1}(z) + \frac{n+2}{n+1}U_n(z)\right\}.$$

Using (3.6) together with $1 - z = -(u-1)^2/2u$ yields

$$\omega_{n+2}(z; w_3) = -\frac{1}{2}\frac{u-1}{u+1}\left\{u^{n+2} - u^{-(n+2)} + \frac{n+2}{n+1}\left(u^{n+1} - u^{-(n+1)}\right)\right\}.$$

Furthermore,

$$\begin{aligned}\rho_{n+2}(z; w_3) &= \int_{-1}^{1} \frac{\omega_{n+2}(t; w_3)}{z-t} w_3(t)\, dt \\ &= \int_{-1}^{1} \frac{U_{n+1}(t) + \frac{n+2}{n+1}U_n(t)}{z-t} w_2(t)\, dt \\ &= \frac{\pi}{u^{n+1}}\left(u^{-1} + \frac{n+2}{n+1}\right),\end{aligned}$$

giving

(3.12)

$$K_{n+2}(z; w_3) = -\frac{2\pi}{u^{n+1}}\frac{u+1}{u-1}\frac{u^{-1} + \frac{n+2}{n+1}}{u^{n+2} - u^{-(n+2)} + \frac{n+2}{n+1}(u^{n+1} - u^{-(n+1)})}.$$

The case $w = w_4$ is easily transformed to the previous case, since $w_4(t) = w_3(-t)$ implies $\omega_{n+2}(z; w_4) = (-1)^n \omega_{n+2}(-z; w_3)$ and $\rho_{n+2}(z; w_4) = (-1)^{n+1}\rho_{n+2}(-z; w_3)$. Therefore, $K_{n+2}(z; w_4) = -K_{n+2}(-z; w_3)$ or, equivalently,

$$K_{n+2}(z; w_4) = -\overline{K_{n+2}(-\bar{z}; w_3)}. \tag{3.13}$$

The kernel for $w = w_4$ is thus obtained from that for $w = w_3$ essentially by reflection on the imaginary axis.

3.3. *Chebyshev-Radau formulae.* In analogy to (3.6) one has

$$V_n(z) = \frac{u^{n+1} + u^{-n}}{u+1}, \quad \int_{-1}^{1} \frac{V_n(t)}{z-t} w_3(t)\, dt = \frac{2\pi}{(u-1)u^n}. \tag{3.14}$$

The first relation follows from the second relation in (3.1) by writing all cosines in exponential form, using Euler's formula, and then putting $u = e^{i\theta}$. To prove the second relation, substitute $t = \cos\theta$ to obtain

$$\begin{aligned}\int_{-1}^{1} \frac{V_n(t)}{z-t} w_3(t)\, dt &= 2\int_0^{\pi} \frac{\cos(n+\frac{1}{2})\theta \cos\frac{1}{2}\theta}{z - \cos\theta}\, d\theta \\ &= \int_0^{\pi} \frac{\cos(n+1)\theta + \cos n\theta}{z - \cos\theta}\, d\theta,\end{aligned}$$

and then use Equation (5.3) in [**2**] and the equation immediately following it to evaluate the last integral.

For reasons indicated in Subsection 2.2, we consider only Radau formulae with the fixed point at -1. Thus, $N = n+1$, $\tau_N = -1$ in (1.1), and $R_N(f) = 0$ for $f \in \mathbf{P}_{2n}$. We treat in turn the four weight functions w_i, $i = 1, 2, 3, 4$ (cf. (1.9)).

For $w = w_1$, in view of $\pi_n(\cdot;(1+t)w_1) = \pi_n(\cdot; w_3)$, we can take $\omega_{n+1}(z; w_1) = (1+z)V_n(z)$, which, by the first relation in (3.14) and $1 + z = (u+1)^2/2u$, gives

$$\omega_{n+1}(z; w_1) = \frac{1}{2}(u+1)(u^n + u^{-(n+1)})$$

and, by the second relation in (3.14),

$$\rho_{n+1}(z; w_1) = \frac{2\pi}{(u-1)u^n},$$

hence

$$K_{n+1}(z; w_1) = \frac{4\pi u}{(u^2-1)(u^{2n+1}+1)}. \tag{3.15}$$

In the case $w = w_2$, we are led to $\pi_n(\cdot;(1+t)w_2) = \pi_n(\cdot;(1-t)^{1/2}(1+t)^{3/2})$ and may apply Lemma 3.2 and (3.2_1) to obtain

$$\omega_{n+1}(z; w_2) = (1+z)U_{n,1}(z) = U_{n+1}(z) + \frac{n+2}{n+1}U_n(z).$$

Using (3.6), we find

$$\omega_{n+1}(z; w_2) = \frac{1}{u - u^{-1}}\left\{u^{n+2} - u^{-(n+2)} + \frac{n+2}{n+1}\left(u^{n+1} - u^{-(n+1)}\right)\right\}$$

and

$$\rho_{n+1}(z; w_2) = \frac{\pi}{u^{n+1}}\left(u^{-1} + \frac{n+2}{n+1}\right),$$

giving

$$K_{n+1}(z; w_2) = \frac{\pi}{u^{n+1}} \frac{1 - u^{-2} + \frac{n+2}{n+1}\left(u - u^{-1}\right)}{u^{n+2} - u^{-(n+2)} + \frac{n+2}{n+1}\left(u^{n+1} - u^{-(n+1)}\right)}. \tag{3.16}$$

For $w = w_3$, since $\pi_n(\cdot; (1+t)w_3) = \pi_n(\cdot; (1-t)^{-1/2}(1+t)^{3/2})$, we can appeal to Lemma 3.3 (with $k = 1$) and (3.3_1) and obtain, similarly as above, using (3.14), that

(3.17)
$$K_{n+1}(z; w_3) = \frac{2\pi}{u^n} \frac{u+1}{u-1} \frac{u^{-1} + \frac{2n+3}{2n+1}}{u^{n+2} + u^{-(n+1)} + \frac{2n+3}{2n+1}\left(u^{n+1} + u^{-n}\right)}.$$

Finally, when $w = w_4$, we have $(1+t)w_4 = w_2$, so that $\omega_{n+1}(z; w_4) = (1+z)U_n(z)$, and we find, using (3.6), that

$$K_{n+1}(z; w_4) = \frac{2\pi}{u^{n+1}} \frac{u-1}{(u+1)(u^{n+1} - u^{-(n+1)})}. \tag{3.18}$$

4. The maximum of the kernel for Chebyshev weight functions. In this section we present results, in part theoretical, in part empirical, concerning the location of the maximum of $|K_N(z; w)|$ as z varies on the circle C_r or the ellipse $\mathcal{E}_\rho$, both for Lobatto and Radau type formulae, and for the Chebyshev weight functions $w = w_i$, $i = 1, 2, 3, 4$ (cf. (1.9)).

4.1. *Lobatto formulae.* For circular contours, the question of interest is already settled by the discussion in Subsection 2.1, for any of the four Chebyshev weight functions (in fact, for arbitrary Jacobi weights). For elliptic contours $\mathcal{E}_\rho$ (cf. (3.8)) we must insert $u = \rho e^{i\vartheta}$ in the respective formulae for $K_{n+2}(\cdot; w_i)$ and study the behavior of $|K_{n+2}(\cdot; w_i)|$ as a function of ϑ. Because of (1.7), it suffices to consider $0 \le \vartheta \le \pi$, and for the weight functions w_1 and w_2 to consider $0 \le \vartheta \le \pi/2$, because of the additional symmetry $|K_{n+2}(-\bar{z}; w_i)| = |K_{n+2}(z; w_i)|$, $i = 1, 2$.

The analysis is simplest in the case of $w = w_1$. We have

$$|u^m - u^{-m}|^2 = \rho^{2m} + \rho^{-2m} - 2\cos 2m\vartheta, \quad u = \rho e^{i\vartheta},$$

which, for any natural number m, attains its minimum $(\rho^m - \rho^{-m})^2$ at $\vartheta = 0$. Therefore, from (3.9), one immediately obtains

$$\begin{aligned} \max_{z \in \mathcal{E}_\rho} |K_{n+2}(z; w_1)| &= K_{n+2}\left(\frac{1}{2}\left(\rho + \rho^{-1}\right); w_1\right) \\ &= \frac{4\pi}{(\rho - \rho^{-1})(\rho^{2n+2} - 1)}. \end{aligned} \tag{4.1}$$

Thus, we have

Theorem 4.1. *The kernel of the* $(n+2)$*-point Lobatto formula for the Chebyshev weight function* w_1 *attains its maximum on the ellipse* $\mathcal{E}_\rho$ *on the real axis; the value of the maximum is given by* (4.1).

For $w = w_2$ and $w = w_3$ we have only empirical and asymptotic results. In the case $w = w_2$, computation shows that $|K_{n+2}(z; w_2)|$, $z \in \mathcal{E}_\rho$, attains its maximum on the real axis if $n = 1$ or $n = 2$. If n is odd and ≥ 3, the maximum is attained on the real axis if $1 < \rho < \rho_n$, and on the imaginary axis if $\rho_n < \rho$ (at either place if $\rho = \rho_n$). If $n \geq 4$ is even, the behavior is more complicated: we have a maximum on the real axis if $1 < \rho < \rho_n'$, on the imaginary axis if $\rho_n < \rho$, and in between if $\rho_n' < \rho < \rho_n$, where ρ_n', ρ_n are certain numbers satisfying $1 < \rho_n' < \rho_n$. Numerical values for $n = 3(1)20$ have been determined by a bisection procedure and are shown in Table 4.1.

TABLE 4.1. The bounds ρ_n', ρ_n, $n = 3(1)20$, for Lobatto formulae with Chebyshev weight w_2.

n	ρ_n'	ρ_n	n	ρ_n'	ρ_n	n	ρ_n'	ρ_n
3		1.4142	9		1.0350	15		1.0127
4	1.2093	1.5955	10	1.0287	1.3138	16	1.0113	1.2237
5		1.1170	11		1.0235	17		1.0099
6	1.0822	1.4483	12	1.0199	1.2756	18	1.0089	1.2051
7		1.0580	13		1.0169	19		1.0080
8	1.0451	1.3671	14	1.0147	1.2466	20	1.0073	1.1896

The empirical observations above can be verified asymptotically as $\rho \downarrow 1$, or as $\rho \to \infty$, for any fixed n. In the first case, a lengthy calculation reveals that when $\vartheta = 0$ (i.e., $z = (\rho + \rho^{-1})/2$),

(4.2)
$$\left| K_{n+2}\left(\frac{1}{2}(\rho + \rho^{-1}; w_2\right)\right| \sim \frac{3\pi}{(n+1)(n+2)(n+3)}(\rho - 1)^{-2}, \quad \rho \downarrow 1,$$

whereas, for other values of ϑ, including $\vartheta = \pi/2$, K_{n+2} is either $O(1)$ or $O((\rho - 1)^{-1})$ as $\rho \downarrow 1$. Interestingly, for example, there

are local peaks of $O((\rho-1)^{-1})$ for values $\vartheta \in (0,\pi/2)$ satisfying $(n+1)\sin(n+3)\vartheta-(n+3)\sin(n+1)\vartheta=0$. When $\rho\to\infty$, one finds
(4.3)

$$|K_{n+2}(z;w_2)| \sim \frac{(n+3)\pi}{(n+1)\rho^{2n+3}}\left\{1-2\frac{n^2-5}{(n+1)(n+3)}\rho^{-2}\cos 2\vartheta\right\}^{1/2}, \quad \rho\to\infty.$$

For $n=1$ and 2, the coefficient multiplying $\cos 2\vartheta$ in (4.3) is positive, while for $n\geq 3$ it is negative, which explains the behavior observed, at least when ρ is large.

In the case $w=w_3$, there is numerical evidence that the maximum of $|K_{n+2}(\cdot;w_3)|$ on $\mathcal{E}_\rho$ is attained consistently on the positive real axis. This can be verified asymptotically, both for $\rho\downarrow 1$ and $\rho\to\infty$. In the first case,

$$\text{(4.4)} \qquad \left|K_{n+2}\left(\frac{1}{2}(\rho+\rho^{-1});w_3\right)\right| \sim \frac{(2n+3)\pi}{(n+1)(n+2)}(\rho-1)^{-2}, \quad \rho\downarrow 1,$$

the value at $z=-(\rho+\rho^{-1})/2$ being of the same order, but with smaller coefficient $3\pi/((n+1)(n+2)(2n+3))$. Again, there are sharp peaks of $O((\rho-1)^{-1})$ at values of $\vartheta\in(0,\pi)$ satisfying, this time, $(n+1)\sin(n+2)\vartheta+(n+2)\sin(n+1)\vartheta=0$. In the second case,
(4.5)

$$|K_{n+2}(z;w_3)| \sim \frac{2(n+2)\pi}{(n+1)\rho^{2n+3}}\left\{1+2\frac{2n^2+4n+1}{(n+1)(n+2)}\rho^{-1}\cos\vartheta\right\}^{1/2}, \quad \rho\to\infty.$$

The same behavior, modulo reflection at the imaginary axis, holds for $w=w_4$, by virtue of (3.13).

4.2. *Radau formulae; circular contours.* The case w_1, again, is amenable to analytic treatment. We now have $z=re^{i\theta}$, $r>1$, and, by (3.7),

$$\text{(4.6)} \qquad u=z+\sqrt{z^2-1}=e^{i\theta}\left(r+\sqrt{r^2-e^{-2i\theta}}\right),$$

where the branch of the square root is taken that assigns positive values to positive arguments. There follows

$$\frac{u}{u^2-1}=\frac{1}{u-u^{-1}}=\left(2e^{i\theta}\sqrt{r^2-e^{-2i\theta}}\right)^{-1},$$

hence

$$\left|\frac{u}{u^2-1}\right| \le \frac{1}{2\sqrt{r^2-1}},$$

the bound being attained for $\theta = 0$ and $\theta = \pi$. Furthermore,

$$\begin{aligned}\left|u^{2n+1}+1\right| &= \left|\left(r+\sqrt{r^2-e^{-2i\theta}}\right)^{2n+1} + e^{-(2n+1)i\theta}\right| \\ &\ge \left|r+\sqrt{r^2-e^{-2i\theta}}\right|^{2n+1} - 1 \ge \left(r+\sqrt{r^2-1}\right)^{2n+1} - 1,\end{aligned}$$

with equality holding for $\theta = \pi$. Consequently, by (3.15),

$$\max_{z\in C_r} |K_{n+1}(z;w_1)| = |K_{n+1}(-r;w_1)| = \frac{4\pi}{R-R^{-1}}\frac{1}{R^{2n+1}-1}, \tag{4.7}$$

where

$$R = r + \sqrt{r^2-1}. \tag{4.8}$$

We have shown

Theorem 4.2. *The kernel of the* $(n+1)$*-point Radau formula* (*with fixed node at* -1) *for the Chebyshev weight function* w_1 *attains its maximum modulus on* C_r *on the negative real axis; the maximum is given by* (4.7), (4.8).

For $w = w_2$, we conjecture

$$\begin{aligned}\max_{z\in C_r} |K_{n+1}(z;w_2)| &= |K_{n+1}(-r;w_2)| \\ &= \frac{\pi}{R^{n+2}}\frac{\left(R-R^{-1}\right)\left(R-\frac{n+1}{n+2}\right)}{\frac{n+1}{n+2}\left(R^{n+2}-R^{-(n+2)}\right)-\left(R^{n+1}-R^{-(n+1)}\right)}\end{aligned}$$

(where the denominator is easily shown to be positive for $R > 1$), and, for $w = w_3$,

$$\begin{aligned}\max_{z\in C_r} |K_{n+1}(z;w_3)| &= K_{n+1}(r;w_3) \\ &= \frac{2\pi}{R^{n+1}}\frac{R+1}{R-1}\frac{R+\frac{2n+1}{2n+3}}{\frac{2n+1}{2n+3}\left(R^{n+2}+R^{-(n+1)}\right)+\left(R^{n+1}+R^{-n}\right)},\end{aligned}$$

where R is given by (4.8). When $w = w_4$, the kernel (3.18) is sufficiently simple to be treated analytically. Note, first of all, that by (4.6) we have $|u| \geq R$ (with equality for $\theta = \pi$), hence

$$|u^{n+1} - u^{-(n+1)}| \geq |u|^{n+1} - \frac{1}{|u|^{n+1}} \geq R^{n+1} - \frac{1}{R^{n+1}},$$

again with equality holding for $\theta = \pi$. Next, from the relation (3.7) between z and u, there follows $(z-1)/(z+1) = [(u-1)/(u+1)]^2$, so that

$$\left|\frac{u-1}{u+1}\right|^4 = \left|\frac{z-1}{z+1}\right|^2 = \frac{r^2 - 2r\cos\theta + 1}{r^2 + 2r\cos\theta + 1} \leq \left(\frac{r+1}{r-1}\right)^2 = \left(\frac{R+1}{R-1}\right)^4.$$

Here again, the bound is attained for $\theta = \pi$. Consequently, by (3.18),

$$\text{(4.9)} \qquad \max_{z \in C_r} |K_{n+1}(z; w_4)| = |K_{n+1}(-r; w_4)| = 2\pi \frac{R+1}{R-1} \frac{1}{R^{2n+2} - 1}.$$

This proves

Theorem 4.3. *The kernel of the* $(n+1)$*-point Radau formula* (*with fixed node at* -1) *for the Chebyshev weight function* w_4 *attains its maximum modulus on* C_r *on the negative real axis; the maximum is given by* (4.9), (4.8).

4.3. *Radau formulae; elliptic contours.* Putting $u = \rho e^{i\vartheta}$ in (3.15), one obtains, for $w = w_1$,

$$|K_{n+1}(z; w_1)| = \frac{4\pi\rho}{[(\rho^4 - 2\rho^2\cos 2\vartheta + 1)(\rho^{4n+2} + 2\rho^{2n+1}\cos(2n+1)\vartheta + 1)]^{1/2}},$$

which clearly takes on its maximum at $\vartheta = \pi$. Thus,

$$\text{(4.10)} \qquad \max_{z \in \mathcal{E}_\rho} |K_{n+1}(z; w_1)| = \left|K_{n+1}\left(-\frac{1}{2}\left(\rho + \rho^{-1}\right)\right)\right| = \frac{4\pi\rho}{(\rho^2 - 1)(\rho^{2n+1} - 1)},$$

and we have

Theorem 4.4. *The kernel of the* $(n+1)$*-point Radau formula* (*with fixed node at* -1) *for the Chebyshev weight function* w_1 *attains its* *maximum modulus on $\mathcal{E}_\rho$ on the negative real axis; the maximum is given by* (4.10).

For $w = w_2$ and $w = w_3$, the kernel is found by computation to behave more curiously. In the former case, we have a situation similar to the Lobatto formula for the same weight function, namely, the maximum is attained on the negative real axis, when $n = 1, 2, 3$, and also when $n \geq 4$, but then only if $1 < \rho < \rho_n'$ or $\rho_n < \rho$, where ρ_n', ρ_n are shown in Table 4.2; otherwise, the maximum point moves on the ellipse $\mathcal{E}_\rho$ from somewhere close to the imaginary axis to the negative real axis as ρ increases.

TABLE 4.2. The bounds ρ_n', ρ_n, $n = 4(1)10$, for Radau formulae with Chebyshev weight w_2.

n	ρ_n'	ρ_n	n	ρ_n'	ρ_n
			7	1.0681	12.267
4	1.2845	4.7385	8	1.0506	14.385
5	1.1518	7.7651	9	1.0394	16.470
6	1.0965	10.087	10	1.0317	18.533

Asymptotically one finds, consistent with the above, that

(4.11)
$$|K_{n+1}(z; w_2)| \sim \frac{(n+2)\pi}{(n+1)\rho^{2n+2}} \left\{1 - 2\frac{2n+3}{(n+1)(n+2)}\rho^{-1}\cos\vartheta\right\}^{\frac{1}{2}}, \quad \rho \to \infty,$$

and

(4.12)
$$\left|K_{n+1}\left(-\frac{1}{2}(\rho+\rho^{-1}); w_2\right)\right| \sim \frac{6\pi}{(n+1)(n+2)(2n+3)}(\rho-1)^{-2}, \quad \rho \downarrow 1,$$

the value at the other end approaching the finite limit $(2n+3)\pi/(2(n+1)(n+2))$ when $\rho \downarrow 1$, and there being the familiar peaks of $O((\rho-1)^{-1})$ when $(n+1)\sin(n+2)\vartheta + (n+2)\sin(n+1)\vartheta = 0$, $0 < \vartheta < \pi$.

For $w = w_3$, there is numerical evidence to suggest that the maximum is attained on the negative real axis for $1 < \rho < \rho_n$ and on the positive real axis for $\rho > \rho_n$, where ρ_n is as shown in Table 4.3.

TABLE 4.3. The values ρ_n, $n = 1(1)10$, for Radau formulae with Chebyshev weight w_3.

n	ρ_n	n	ρ_n
1	1.1339	6	1.0022
2	1.0318	7	1.0015
3	1.0126	8	1.0010
4	1.0063	9	1.0008
5	1.0036	10	1.0006

There is, again, asymptotic corroboration:

(4.13)
$$|K_{n+1}(z; w_3)| \sim \frac{2(2n+3)\pi}{(2n+1)\rho^{2n+2}} \left\{1 + 4\frac{4n^2+4n-1}{(2n+1)(2n+3)}\rho^{-1}\cos\vartheta\right\}, \quad \rho \to \infty,$$

and

(4.14)
$$\left|K_{n+1}\left(-\frac{1}{2}(\rho+\rho^{-1}); w_3\right)\right| \sim \frac{6\pi}{(n+1)(2n+1)(2n+3)}(\rho-1)^{-2}, \quad \rho \downarrow 1.$$

There are secondary peaks, as $\rho \downarrow 1$, of order $O((\rho-1)^{-1})$ at $\vartheta = 0$ and at values of $\vartheta \in (0, \pi)$ satisfying $(2n+1)\cos(n+3/2)\vartheta + (2n+3)\cos(n+1/2)\vartheta = 0$.

The values ρ_n in Table 4.3 are conjectured to be solutions of the equation

$$\frac{\rho^{2n+3} + 1 + \frac{2n+3}{2n+1}\rho\left(\rho^{2n+1}+1\right)}{\rho^{2n+3} - 1 - \frac{2n+3}{2n+1}\rho\left(\rho^{2n+1}-1\right)} = \left(\frac{\rho+1}{\rho-1}\right)^2 \frac{\rho + \frac{2n+1}{2n+3}}{\rho - \frac{2n+1}{2n+3}} \tag{4.15}$$

expressing equality of the values of $|K_{n+1}(\cdot; w_3)|$ at both real vertices of the ellipse $\mathcal{E}_\rho$.

Finally, when $w = w_4$, Equation (3.18) for $u = \rho e^{i\vartheta}$ implies

$$|K_{n+1}(z; w_4)| = \frac{2\pi}{\rho^{n+1}} \left\{\frac{\rho^2 - 2\rho\cos\vartheta + 1}{(\rho^2+2\rho\cos\vartheta+1)(\rho^{2n+2}+\rho^{-(2n+2)} - 2\cos(2n+2)\vartheta)}\right\}^{\frac{1}{2}},$$

which is largest when $\vartheta = \pi$, giving

$$\max_{z\in\mathcal{E}_\rho}|K_{n+1}(z;w_4)| = \left|K_{n+1}\left(-\frac{1}{2}\left(\rho+\rho^{-1}\right);w_4\right)\right|$$

$$= 2\pi\frac{\rho+1}{\rho-1}\frac{1}{\rho^{2n+2}-1}. \tag{4.16}$$

Thus, we have

Theorem 4.5. *The kernel of the* $(n+1)$*-point Radau formula* (*with fixed node at* -1) *for the Chebyshev weight function* w_4 *attains its maximum modulus on* $\mathcal{E}_\rho$ *on the negative real axis; the maximum is given by* (4.16).

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