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A NOTE ON THE CONTOUR INTEGRAL REPRESENTATION OF THE REMAINDER TERM FOR A GAUSS-CHEBYSHEV QUADRATURE RULE*

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Abstract. It is shown that the kernel $K_n(z)$, $n(\text{even}) \geqq 2$, in the contour integral representation of the remainder term of the n-point Gauss formula for the Chebyshev weight function of the second kind, as z varies on the ellipse $\mathscr{E}_\rho = \{z: z = \rho\, e^{i\vartheta} + \rho^{-1} e^{-i\vartheta}, 0 \leqq \vartheta \leqq 2\pi\}$, $\rho > 1$, assumes its largest modulus on the imaginary axis if $\rho \geqq \rho_{n+1}$, where ρ_{n+1} is the root of a certain algebraic equation. If $1 < \rho < \rho_{n+1}$, the maximum is attained near the imaginary axis within an angular distance less than $\pi/(2n+2)$. The bounds $\{\rho_{n+1}\}$ decrease monotonically to 1.

Key words. Gauss-Chebyshev quadrature, remainder term for analytic functions, kernel of contour integral representation

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1. We are dealing here with the remainder term $R_n(f)$ of the Gaussian quadrature rule for the Chebyshev weight function of the second kind,

$$\int_{-1}^{1} f(t)(1-t^2)^{1/2}\,dt = \sum_{\nu=1}^{n} \lambda_\nu^{(n)} f(\tau_\nu^{(n)}) + R_n(f), \tag{1.1}$$

where $\tau_\nu^{(n)} = \cos(\nu\pi/(n+1))$, $\lambda_\nu^{(n)} = \pi \sin^2(\nu\pi/(n+1))/(n+1)$, $\nu = 1, 2, \cdots, n$. We assume that f is analytic inside of, and continuous on, an ellipse

$$\mathscr{E}_\rho = \{z: z = \tfrac{1}{2}(u + u^{-1}),\ u = \rho\, e^{i\vartheta},\ 0 \leqq \vartheta \leqq 2\pi\} \tag{1.2}$$

with foci at $z = \pm 1$ and with the sum of the semi-axes equal to ρ, $\rho > 1$. The remainder $R_n(f)$ of (1.1) has the form (cf. [1])

$$R_n(f) = \frac{1}{2\pi i} \int_{\mathscr{E}_\rho} K_n(z) f(z)\,dz, \tag{1.3}$$

so that

$$|R_n(f)| \leqq \frac{l(\mathscr{E}_\rho)}{2\pi} \max_{z \in \mathscr{E}_\rho} |f(z)| \cdot \max_{z \in \mathscr{E}_\rho} |K_n(z)|, \tag{1.3'}$$

where $l(\mathscr{E}_\rho)$ denotes the length of $\mathscr{E}_\rho$. Since $f(z)$ and $\mathscr{E}_\rho$ are assumed known, the first two terms on the right side of (1.3′) can be calculated, and our interest then is in determining *where* on $\mathscr{E}_\rho$ the kernel $K_n(z)$ assumes its *maximum modulus.* In view of $K_n(\bar{z}) = \overline{K_n(z)}$ and $K_n(-\bar{z}) = -\overline{K_n(z)}$, the modulus of K_n is symmetric with respect to both coordinate axes:

$$|K_n(\bar{z})| = |K_n(z)|, \qquad |K_n(-\bar{z})| = |K_n(z)|. \tag{1.4}$$

Thus, consideration may be restricted to the first quarter of $\mathscr{E}_\rho$, i.e., to the interval $0 \leqq \vartheta \leqq \pi/2$ in (1.2).

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It is known that, when n is odd, the maximum of $|K_n(z)|$ on $\mathscr{E}_\rho$ is attained on the imaginary axis [1, Thm. 5.2]. It is remarked in [1] that when n is even, the maximum "... is attained slightly off the imaginary axis." The purpose of this note is to amplify this statement and make it more precise. Defining

$$a_j = a_j(\rho) = \tfrac{1}{2}(\rho^j + \rho^{-j}), \quad j = 1, 2, 3, \cdots, \quad \rho > 1, \tag{1.5}$$

we will prove, in fact, the following theorem.

THEOREM 1. *For each positive integer n with $n \geqq 2$, let $\rho_n > 1$ be the unique root of*

$$\frac{a_1(\rho)}{a_n(\rho)} = \frac{1}{n} \qquad (\rho > 1). \tag{1.6}$$

Then, if $n \geqq 2$ is even, we have

$$\max_{z \in \mathscr{E}_\rho} |K_n(z)| = \left| K_n\left(\frac{i}{2}(\rho - \rho^{-1})\right)\right| \quad \textit{if } \rho \geqq \rho_{n+1}, \tag{1.7}$$

i.e., the maximum of $|K_n(z)|$ on $\mathscr{E}_\rho$, when $\rho \geqq \rho_{n+1}$, is attained on the imaginary axis. If $1 < \rho < \rho_{n+1}$, then the maximum in (1.7) is attained at some $z = z^* = \frac{1}{2}(\rho e^{i\vartheta^*} + \rho^{-1} e^{-i\vartheta^*}) \in \mathscr{E}_\rho$ with $(n/(n+1))\pi/2 < \vartheta^* < \pi/2$.

In Table 1 we display ρ_n for $n = 2(1)40$ to 10 decimal places. Since $\rho^{-(n-1)} < a_1(\rho)/a_n(\rho) < 2\rho/\rho^n = 2\rho^{-(n-1)}$ for $\rho > 1$, putting $\rho = \rho_n$ we obtain from (1.6) that

$$n^{1/(n-1)} < \rho_n < (2n)^{1/(n-1)}. \tag{1.8}$$

This shows, in particular, that $\rho_n \to 1$ as $n \to \infty$. The next theorem establishes monotonicity of the ρ_n and sharpens the bounds in (1.8).

THEOREM 2. *The roots $\rho_n > 1$ of* (1.6) *satisfy*

$$\rho_n > \rho_{n+1} \quad \textit{for all } n \geqq 2. \tag{1.9}$$

Moreover, if $\lambda_n := (2n)^{1/n}$, and if μ_n, $n \geqq 2$, is the unique positive root (by Descartes' rule of signs) of

$$M_n(\mu) = 0, \qquad M_n(\mu) := \mu^{n+1} - n(\mu^2 + 1), \tag{1.10}$$

then

$$\lambda_n < \rho_n < \mu_n \quad \textit{for all } n \geqq 2. \tag{1.11}$$

It is easily seen that the bounds in (1.11) are sharper than those in (1.8), except when $n = 2$, in which case the lower bounds are both equal to 2.

TABLE 1
The roots $\rho_n > 1$ of (1.6).

n	ρ_n	n	ρ_n	n	ρ_n	n	ρ_n
		11	1.3290434092	21	1.1956793660	31	1.1427199553
2	2.2966302629	12	1.3068931058	22	1.1884619640	32	1.1390810161
3	1.9318516526	13	1.2878200461	23	1.1818092074	33	1.1356405646
4	1.7390838834	14	1.2712053026	24	1.1756552136	34	1.1323822718
5	1.6180339887	15	1.2565878778	25	1.1699441267	35	1.1292915806
6	1.5341771340	16	1.2436169389	26	1.1646282627	36	1.1263554696
7	1.4722691130	17	1.2320204906	27	1.1596666536	37	1.1235622539
8	1.4244774799	18	1.2215842188	28	1.1550238943	38	1.1209014162
9	1.3863414780	19	1.2121368378	29	1.1506692205	39	1.1183634632
10	1.3551231521	20	1.2035397132	30	1.1465757653	40	1.1159398028

The proofs of Theorems 1 and 2 will be given in §§ 3 and 4, respectively. Section 2 contains some auxiliary results.

2.

LEMMA 1. *For each positive integer n, set*

$$\varphi_n(\sigma) := \frac{\sin \sigma\pi}{\sin((1-\sigma)\pi/(n+1))}, \qquad 0 \leqq \sigma \leqq 1, \tag{2.1}$$

where $\varphi_n(1) := \lim_{\sigma \uparrow 1} \varphi_n(\sigma)$. *Then* $\varphi_n(\sigma)$ *increases monotonically from* $\varphi_n(0) = 0$ *to* $\varphi_n(1) = n+1$ *as* σ *varies from zero to* 1.

Proof. Since $\sin \sigma\pi = \sin[(1-\sigma)\pi]$, we can write $\varphi_n(\sigma)$ as

$$\varphi_n(\sigma) = \frac{\sin[(n+1)u]}{\sin u} \quad \text{where} \quad \frac{(1-\sigma)\pi}{n+1} =: u,$$

so that $0 \leqq u \leqq \pi/(n+1)$. Furthermore,

$$\frac{\sin[(n+1)u]}{\sin u} = U_n(x) \qquad (\cos u =: x),$$

where $U_n(x)$ is the Chebyshev polynomial (of the second kind) of degree n. It is well known that $U_n(x)$ is increasing from $U_n(\cos(\pi/(n+1))) = 0$ to $U_n(1) = n+1$ as x increases from $\cos(\pi/(n+1))$ to 1 (hence σ increases from zero to 1), from which the assertions of Lemma 1 follow. □

LEMMA 2. *Let* φ_n *be as in Lemma* 1, *and set*

$$\psi_n(\sigma) := \cos \sigma\pi + (n+1)\varphi_n(\sigma) \cos\left(\frac{1-\sigma}{n+1}\pi\right), \qquad 0 \leqq \sigma \leqq 1. \tag{2.2}$$

Then $\psi_n(\sigma)$ *increases monotonically from* $\psi_n(0) = 1$ *to* $\psi_n(1) = (n+1)^2 - 1$ *as* σ *varies from zero to* 1.

Proof. The limit values follow directly from the limit values of φ_n in Lemma 1. Differentiating (2.2), we get

$$\begin{aligned} \psi_n'(\sigma) &= -\pi \sin \sigma\pi + \pi\varphi_n(\sigma) \sin\left(\frac{1-\sigma}{n+1}\pi\right) + (n+1)\varphi_n'(\sigma)\cos\left(\frac{1-\sigma}{n+1}\pi\right) \\ &= -\pi \sin \sigma\pi + \pi \sin \sigma\pi + (n+1)\varphi_n'(\sigma) \cos\left(\frac{1-\sigma}{n+1}\pi\right) \\ &= (n+1)\varphi_n'(\sigma)\cos\left(\frac{1-\sigma}{n+1}\pi\right), \end{aligned}$$

which is positive by Lemma 1. □

3.

Proof of Theorem 1. From [1, eq. (5.9)] we have

$$(\pi^{-1}\rho^{n+1}|K_n(z)|)^2 = \frac{a_2(\rho) - \cos 2\vartheta}{a_{2n+2}(\rho) - \cos 2(n+1)\vartheta}, \tag{3.1}$$

$$z = \tfrac{1}{2}(\rho e^{i\vartheta} + \rho^{-1} e^{-i\vartheta}) \in \mathscr{E}_\rho.$$

By (1.4), it suffices to consider $0 \leqq \vartheta \leqq \pi/2$. Denote

$$\kappa_n(\vartheta) = \frac{a_2 - \cos 2\vartheta}{a_{2n+2} - \cos 2(n+1)\vartheta}, \tag{3.2}$$

where a_2, a_{2n+2} are as defined in (1.5). By symmetry,

$$\kappa_n'(0) = \kappa_n'\left(\frac{\pi}{2}\right) = 0. \tag{3.3}$$

Let

$$\vartheta_n := \frac{n}{n+1}\frac{\pi}{2}. \tag{3.4}$$

Since $\cos 2\vartheta \geqq \cos 2\vartheta_n$ for $0 \leqq \vartheta \leqq \vartheta_n$, we have

$$\kappa_n(\vartheta) \leqq \frac{a_2 - \cos 2\vartheta_n}{a_{2n+2} - 1} = \kappa_n(\vartheta_n), \qquad 0 \leqq \vartheta \leqq \vartheta_n, \tag{3.5}$$

where the equality on the right follows from $\cos 2(n+1)\vartheta_n = \cos n\pi = 1$, since n is even. Differentiating (3.2) gives

$$[a_{2n+2} - \cos 2(n+1)\vartheta]\kappa_n'(\vartheta) + \kappa_n(\vartheta)\cdot 2(n+1)\sin 2(n+1)\vartheta = 2\sin 2\vartheta, \tag{3.6}$$

from which it follows that $(a_{2n+2}-1)\kappa_n'(\vartheta_n) = 2\sin 2\vartheta_n$, hence

$$\kappa_n'(\vartheta_n) > 0. \tag{3.7}$$

Letting $\max_{0\leqq\vartheta\leqq\pi/2} \kappa_n(\vartheta) = \kappa_n(\vartheta^*)$, we conclude from (3.5) and (3.7) that

$$\vartheta_n < \vartheta^* \leqq \frac{\pi}{2}. \tag{3.8}$$

Differentiating (3.6) once more, and then setting $\vartheta = \pi/2$, gives

$$\frac{1}{4}(a_{2n+2}+1)\kappa_n''\left(\frac{\pi}{2}\right) = (n+1)^2\frac{a_2+1}{a_{2n+2}+1} - 1 = \left[(n+1)\frac{a_1}{a_{n+1}}\right]^2 - 1, \tag{3.9}$$

since $a_2 + 1 = 2a_1^2$, $a_{2n+2}+1 = 2a_{n+1}^2$. From the definition of ρ_n (cf. (1.6)) and from the fact that $a_1(\rho)/a_{n+1}(\rho)$ for $\rho > 1$ decreases monotonically, we get from (3.9) that

$$\kappa_n''(\pi/2) \gtreqqless 0 \quad \text{iff } \rho \lesseqqgtr \rho_{n+1}. \tag{3.10}$$

If $1 < \rho < \rho_{n+1}$, i.e., $\kappa_n''(\pi/2) > 0$, it is clear from the second relation in (3.3) that $\vartheta^* < \pi/2$ in (3.8), proving the second statement of the theorem.

If $\rho \geqq \rho_{n+1}$, i.e., $\kappa_n''(\pi/2) \leqq 0$, we now show that

$$\kappa_n'(\vartheta) > 0 \quad \text{for } \vartheta_n < \vartheta < \frac{\pi}{2} \qquad (\rho \geqq \rho_{n+1}). \tag{3.11}$$

We introduce the variable σ by

$$\vartheta = \frac{n+\sigma}{n+1}\frac{\pi}{2}, \qquad 0 < \sigma < 1. \tag{3.12}$$

Using $(n+\sigma)/(n+1) = 1 - (1-\sigma)/(n+1)$, we can rewrite (3.6) in the form

$$\frac{[a_{2n+2} - \cos\sigma\pi]^2}{2\sin((1-\sigma)\pi/(n+1))}\kappa_n'(\vartheta) = a_{2n+2} - (n+1)a_2\varphi_n(\sigma) - \psi_n(\sigma), \tag{3.13}$$

with $\varphi_n(\sigma)$ and $\psi_n(\sigma)$ as defined in Lemmas 1 and 2, respectively. By the assumption $\rho \geqq \rho_{n+1}$, which implies $a_{n+1} \geqq (n+1)a_1$, hence

$$a_{2n+2} = 2a_{n+1}^2 - 1 \geqq 2(n+1)^2 a_1^2 - 1 = (n+1)^2(a_2+1) - 1,$$

and using Lemmas 1 and 2, we find that the right-hand side of (3.13) is larger than or equal to

$$(n+1)^2(a_2+1)-1-(n+1)a_2\varphi_n(\sigma)-\psi_n(\sigma)$$
$$>(n+1)^2(a_2+1)-1-(n+1)^2a_2-[(n+1)^2-1]=0, \qquad 0<\sigma<1.$$

Therefore, $\kappa_n'(\vartheta)>0$ for $\vartheta_n<\vartheta<\pi/2$, showing that $\vartheta^*=\pi/2$ in (3.8). □

4. We precede the proof of Theorem 2 with the following lemma.

LEMMA 3. *With λ_n and μ_n as defined in Theorem 2, there holds*

$$\lambda_n>\mu_{n+1} \quad \textit{for all } n\geqq 2. \tag{4.1}$$

Proof. Since $M_n(\mu)$, $n\geqq 2$, in (1.10) has a unique positive zero μ_n, and since $M_n(+\infty)=+\infty$, it is evident that $M_{n+1}(\mu)>0$ implies $\mu>\mu_{n+1}$. It suffices, therefore, to show that

$$M_{n+1}(\lambda_n)>0 \quad \text{for } n\geqq 2. \tag{4.2}$$

This is clearly true when $n=2$, since $\lambda_2=2$ and $M_3(\lambda_2)=1$. We may thus assume that $n\geqq 3$.

We have

$$M_{n+1}(\lambda_n)=\lambda_n^2\cdot\lambda_n^n-(n+1)(\lambda_n^2+1)=\lambda_n^2\cdot 2n-(n+1)(\lambda_n^2+1)=-(n+1)+(n-1)\lambda_n^2.$$

When we write $\lambda_n=e^{l_n}$, $l_n=n^{-1}\log 2n$, there follows

$$M_{n+1}(\lambda_n)=-(n+1)+(n-1)\,e^{2l_n}=-(n+1)+(n-1)[1+2l_n+e^{2l_n}-(1+2l_n)]$$
$$=2[-1+(n-1)l_n]+(n-1)[e^{2l_n}-(1+2l_n)].$$

Here, the expression in the last bracket is clearly positive, and an elementary calculation shows that $-1+(n-1)l_n=-1+(1-n^{-1})\log 2n>0$ if $n\geqq 3$. □

Proof of Theorem 2. To establish (1.9), it suffices to prove the inequalities (1.11), since combining them with the inequality in Lemma 3 immediately gives $\rho_n>\lambda_n>\mu_{n+1}>\rho_{n+1}$ for all $n\geqq 2$.

Now (1.6) is equivalent to

$$L_n(\rho):=\rho^{2n}-n\rho^{n+1}-n\rho^{n-1}+1=0. \tag{4.3}$$

Clearly, L_n (by Descartes' rule of signs) has at most two positive zeros. Since $L_n(0)=1$, $L_n(1)=2-2n<0$, and $L_n(+\infty)=+\infty$, there are exactly two positive zeros, one in $(0,1)$ and the other in $(1,\infty)$. (Because ρ and ρ^{-1} occur symmetrically in (1.6), one zero is the reciprocal of the other.) The larger of the two, as in Theorem 1, is denoted by ρ_n.

We have

$$L_n(\rho)=\rho^{2n}+\rho^{2n-2}-\rho^{2n-2}-n\rho^{n-1}(\rho^2+1)+1$$
$$=\rho^{2n-2}(\rho^2+1)-\rho^{2n-2}-n\rho^{n-1}(\rho^2+1)+1,$$

so that the equation in (4.3), after division by $\rho^{n-1}(\rho^2+1)$, can be written in the form

$$\rho^{n-1}-\frac{\rho^{n-1}}{\rho^2+1}+\frac{1}{\rho^{n-1}(\rho^2+1)}=n. \tag{4.4}$$

Since $L_n(\rho_n)=0$, dropping the third term on the left of (4.4), we arrive at

$$\rho_n^{n-1}-\frac{\rho_n^{n-1}}{\rho_n^2+1}<n \quad \text{or} \quad \rho_n^{n+1}-n(\rho_n^2+1)<0.$$

In terms of the function M_n in (1.10), this says $M_n(\rho_n) < 0$, and hence implies $\rho_n < \mu_n$, the right inequality in (1.11).

To prove the left inequality of (1.11), we will show that

$$L_n(\lambda_n) < 0 \quad \text{for all } n \geqq 2. \tag{4.5}$$

We now express $L_n(\rho)$ from (4.3) as

$$\begin{aligned} L_n(\rho) &= \rho^{2n} - 2n\rho^n + 1 + 2n\rho^n - n\rho^n\left(\rho + \frac{1}{\rho}\right) \\ &= \rho^n(\rho^n - 2n) + 1 + n\rho^n\left[2 - \left(\rho + \frac{1}{\rho}\right)\right]. \end{aligned}$$

Since $\lambda_n = (2n)^{1/n} = e^{l_n}$, $l_n = n^{-1}\log 2n$, this gives

$$L_n(\lambda_n) = 1 + 4n^2(1 - \cosh l_n) = 1 - 2n^2 l_n^2 - 4n^2[\cosh l_n - 1 - \tfrac{1}{2}l_n^2].$$

The expression in brackets, when expanded in Taylor's series, involves only positive terms and hence is positive, while $1 - 2n^2 l_n^2 = 1 - 2(\log 2n)^2 < 0$ for all $n \geqq 2$. This establishes (4.5) and completes the proof of Theorem 2. □

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