Comm. Korean Math. Soc. 8 (1993), No. 3, pp. 545–554

ERROR BOUND FOR THE GAUSSIAN QUADRATURE ON THE ELLIPSE CONTOUR

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1. Introduction

Gaussian quadrature formula for special functions, especially of the Chebyshev type, has been studied for a long time. The following classical representation for the remainder term $R_n(f)$ can be found in [2]:

$$R_n(f) = f^{(2n)}(\xi)[(2n)!]^{-1}k_n^{-2}, \tag{1.1}$$

where $-1 < \xi < 1$ and k_n is the leading coefficient of the orthogonal polynomial $\pi_n(\cdot)$ of degree n corresponding to the weight function $w(x)$ on $[-1,1]$. The above representation (1.1) for $R_n(f)$ is of little practical value, since the derivative $f^{(2n)}$ are usually too difficult to obtain. Davis and Rabinowitz [4] give a more convenient method for obtaining an upper bound for the error in the quadrature of analytic functions. McNamee [7] has discussed complex-variable methods for obtaining upper bounds for the errors of the Gaussian quadrature applied to analytic functions, and Barrett [1] has discussed their convergence. In [2], Chawla and Jain have shown derivative–free asymptotic error estimate for the Gauss–Legendre rule.

Let f be single-valued analytic in a domain D which contains $[-1,1]$, and Γ is a closed contour in D surrounding $[-1,1]$. Let the nonnegative weight function $w(x)$ be defined on the interval $[-1,1]$ such that the moments $\int_{-1}^{1} x^k w(x)\,dx$ exist for $k = 0,1,2,\ldots$. Denoting the zeros of the orthogonal polynomial $\pi_n(x)$ with respect to the weight function

Received March 2, 1993.

*This paper was partially supported by the Basic Science Research Institute Program, Ministry of Education, 1991.

$w(x)$ on $[-1,1]$ by $(\tau_k)_1^n$, applying the residue theorem to the contour integral

$$\frac{1}{2\pi i}\int_\Gamma \frac{f(z)}{(z-x)\pi_n(z)}\,dz, \tag{1.2}$$

we get

$$f(x)=\sum_{k=1}^{n}\frac{\pi_n(x)}{(x-\tau_k)\pi_n'(\tau_k)}f(\tau_k)+\frac{1}{2\pi i}\int_\Gamma \frac{f(z)\pi_n(x)}{(z-x)\pi_n(z)}\,dz. \tag{1.3}$$

Integrating both sides with respect to $w(x)$ on $[-1,1]$, we get

$$\int_{-1}^{1} f(t)w(t)\,dt=\sum_{k=1}^{n}\lambda_k f(\tau_k)+R_n(f), \tag{1.4}$$

where τ_k are the zeros of the nth degree orthogonal polynomial $\pi_n(\cdot\,;w)$ on $[-1,1]$ and the weights λ_k are defined by

$$\lambda_k=\int_{-1}^{1} w(t)\frac{\pi_n(t)}{(t-\tau_k)\pi_n'(\tau_k)}\,dt. \tag{1.5}$$

The remainder term $R_n(\cdot)$ can be represented as a contour integral

$$R_n(f)=\frac{1}{2\pi i}\int_\Gamma K_n(z)f(z)\,dz, \tag{1.6}$$

where the kernel K_n is given by

$$K_n(z)=\frac{\rho_n(z)}{\pi_n(z)}. \tag{1.7}$$

Here, $\pi_n(z)$ is the orthogonal polynomial $\pi_n(\cdot\,;w)$ evaluated at z, while $\rho_n(z)$ is defined by

$$\rho_n(z)=\int_{-1}^{1}\frac{\pi_n(t)}{z-t}w(t)\,dt. \tag{1.8}$$

Basically, from (1.6) the estimate takes the form

$$|R_n(f)| \leqslant \frac{l(\Gamma)}{2\pi} \cdot \max_{z\in\Gamma} |K_n(z)| \cdot \max_{z\in\Gamma} |f(z)|, \tag{1.9}$$

where $l(\Gamma)$ denotes the length of Γ. In [5], [6], Gautschi has given an explicit representation of the kernel K_n on Γ, where Γ is an elliptic contour

$$\Gamma = \{z : z = \frac{1}{2}(\rho e^{i\theta} + \rho^{-1}e^{-i\theta}), \quad 0 \leqslant \theta \leqslant 2\pi, \quad \rho > 1\},$$

for a Jacobi measure $w(t) = (1-t)^{\alpha}(1+t)^{\beta}$, where α and β assume such pair of values $\alpha = \frac{1}{2}, \beta = \frac{1}{2}$, and $\alpha = -\frac{1}{2}, \beta = -\frac{1}{2}$, and $\alpha = -\frac{1}{2}, \beta = \frac{1}{2}$ and also has determined the maximum points on the ellipse.

2. Main Results

Consider the contour is given by an ellipse

$$\Lambda_p = \{z : z = \frac{1}{2}(u + u^{-1}); \quad u = \rho e^{i\theta}, \quad 0 \leqslant \theta \leqslant 2\pi, \quad \rho > 1\}.$$

If Jacobi measure with $\alpha = \frac{1}{2}, \beta = -\frac{1}{2}$, that is, $w(t) = (1-t)^{\frac{1}{2}}(1+t)^{-\frac{1}{2}}$, then the orthogonal polynomials in this case with respect to $d\lambda(t) = \sqrt{(1-t)/(1+t)}dt$ given by

$$A_n(z) = U_{2n}\left(\sqrt{\frac{1}{2}(z+1)}\right), \tag{2.1}$$

where U_{2n} is the Chebyshev polynomial of the second kind. With $z = \frac{1}{2}(u+u^{-1})$, so that $\sqrt{\frac{1}{2}(z+1)} = \dfrac{u+1}{2\sqrt{u}}$ and

$$U_n(z) = \frac{1}{2\sqrt{z^2-1}}[(z+\sqrt{z^2-1})^{n+1} - (z-\sqrt{z^2-1})^{n+1}],$$

we find by elementary calculation,

$$A_n(z) = \frac{u^{n+1} - u^{-n}}{u-1}, \qquad z = \frac{1}{2}(u+u^{-1}). \tag{2.2}$$

Furthermore we have

$$\int_{-1}^{1} \frac{A_n(t)}{z-t}\sqrt{\frac{1-t}{1+t}}\,dt = \int_0^{\pi} \frac{2\sin(2n+1)\frac{\theta}{2}\sin\frac{\theta}{2}}{z-\cos\theta}\,d\theta$$
$$= \int_0^{\pi} \frac{\cos n\theta - \cos(n+1)\theta}{z-\cos\theta}\,d\theta.$$

Using

$$\int_0^{\pi} \frac{\cos n\theta}{z-\cos\theta}\,d\theta = \frac{1}{2}\int_0^{2\pi} \frac{\cos n\theta + i\sin n\theta}{z-\cos\theta}\,d\theta$$

and setting $t = e^{i\theta}$, we see that

$$\int_0^{\pi} \frac{\cos n\theta}{z-\cos\theta}\,d\theta = -\frac{1}{i}\int_C \frac{t^n}{(t^2-2zt+1)}\,dt,$$

where C is unit circle.

Applying the residue theorem, we get

$$\int_0^{\pi} \frac{\cos n\theta}{z-\cos\theta}\,d\theta = \frac{\pi}{\sqrt{z^2-1}}(z-\sqrt{z^2-1})^n \tag{2.3}$$

hence

$$\int_{-1}^{1} \frac{A_n(t)}{z-t}\sqrt{\frac{1-t}{1+t}}\,dt = \frac{2\pi(1-u^{-1})}{u^n\cdot(u-u^{-1})}, \qquad z = \frac{1}{2}(u+u^{-1}). \tag{2.4}$$

There follows

$$K_n(z) = \frac{\rho_n(z)}{\pi_n(z)} = \frac{2\pi(u^{\frac{1}{2}}-u^{-\frac{1}{2}})^2}{(u-u^{-1})\cdot u^n\cdot(u^{n+1}-u^{-n})}. \tag{2.5}$$

By an elementary computation,

$$|K_n(z)| = 2\pi\left|\frac{u^{-\frac{1}{2}}(u^{\frac{1}{2}}-u^{-\frac{1}{2}})^2}{(u-u^{-1})\cdot u^n\cdot(u^{n+\frac{1}{2}}-u^{-(n+\frac{1}{2})})}\right|$$
$$= \frac{2\pi}{\rho^{n+\frac{1}{2}}}\,\frac{\frac{1}{2}|u^{\frac{1}{2}}-u^{-\frac{1}{2}}|^2}{\sqrt{\frac{1}{2}|u-u^{-1}|^2}\cdot\sqrt{\frac{1}{2}|u^{n+\frac{1}{2}}-u^{-(n+\frac{1}{2})}|^2}}.$$

and hence

$$(2.6)\quad |K_n(z)| = \frac{2\pi}{\rho^{n+\frac{1}{2}}} \frac{a_1(\rho) - \cos\theta}{[(a_2(\rho) - \cos 2\theta)\cdot(a_{2n+1}(\rho) - \cos(2n+1)\theta)]^{\frac{1}{2}}},$$

where

$$z = \frac{1}{2}(\rho e^{i\theta} + \rho^{-1}e^{-i\theta}) \in \Lambda_p,$$

$$(2.7)\qquad a_j(\rho) = \frac{1}{2}(\rho^j + \rho^{-j}), \qquad j = 1,2,3,\ldots \text{and} \quad \rho > 1.$$

LEMMA 2.1. *There holds , $a_j(\rho)$ is defined by* (2.7).

$$(2.8)\qquad \frac{a_1(\rho)a_{2n+1}(\rho) - 1}{a_2(\rho) - 1} > (n + \frac{1}{2})^2, \qquad n = 1,2,3,\ldots,\ \rho > 1.$$

Proof. By definition (2.7) of $a_j(\rho)$, we have

$$\frac{a_1(\rho)a_{2n+1}(\rho) - 1}{a_2(\rho) - 1} = \frac{1}{2}\left\{\frac{\rho^{2n+2} - 1}{\rho^n(\rho^2 - 1)}\right\}^2 + \frac{1}{2}\left\{\frac{\rho^{2n} - 1}{\rho^{n-1}(\rho^2 - 1)}\right\}^2.$$

Since

$$\frac{\rho^{2n} - 1}{\rho^{n-1}(\rho^2 - 1)} = \rho^{n-1} + \rho^{n-3} + \cdots + \rho^{-(n-3)} + \rho^{-(n-1)},$$

the sum on the right is larger than $2\left(\frac{n}{2}\right) = n$ if n is even, and larger than $2[\frac{(n-1)}{2}] + 1 = n$ if $n \geqslant 2$ is odd, and equal to 1 if $n = 1$, so that $\left\{\frac{\rho^{2n} - 1}{\rho^{n-1}(\rho^2 - 1)}\right\}^2 \geqslant n^2$, which produces the lower bound

$$\frac{1}{2}[(n+1)^2 + n^2] = n^2 + n + \frac{1}{2} > n^2 + n + \frac{1}{4} = (n + \frac{1}{2})^2.$$

For the detail, we refer to [6].

LEMMA 2.2. *There holds*

$$\left|\frac{\cos(2n+1)\theta}{\cos\theta}\right| \leqslant 2n+1 \qquad (n=0,1,2,\dots). \tag{2.9}$$

Proof. True for $n=0$, by induction

$$\begin{aligned}\left|\frac{\cos(2n+1)\theta}{\cos\theta}\right| &= \left|\frac{2\cos\theta\cos 2n\theta-\cos(2n-1)\theta}{\cos\theta}\right| \\ &\leqslant 2|\cos 2n\theta| + \left|\frac{\cos(2n-1)\theta}{\cos\theta}\right| \\ &\leqslant 2+(2n-1) = 2n+1.\end{aligned}$$

THEOREM 2.3. *If* $d\lambda(t)=\sqrt{\dfrac{(1-t)}{(1+t)}}\,dt$ *on* $(-1,1)$, *then*

$$\max_{z\in\Lambda_p}|K_n(z)| = K_n\left(-\frac{1}{2}(\rho+\rho^{-1})\right) \qquad (\rho > \frac{3+\sqrt{5}}{2}) \tag{2.10}$$

i.e., the maximum of $|K_n(z)|$ *on* Λ_p *is attained on the negative real axis.*

Proof. We will show that (2.6) considered as a function of θ on $[0,\pi]$ and attains its maximum only at $\theta=\pi$. Using $a_2(\rho)=2[a_1(\rho)]^2-1$, we can write this assertion in the form

$$\frac{a_1-\cos\theta}{(a_1+\cos\theta)(a_{2n+1}-\cos(2n+1)\theta)} < \frac{a_1+1}{(a_1-1)(a_{2n+1}+1)}, \tag{2.11}$$

since $(a_2-\cos\theta)=2(a_1-\cos\theta)(a_1+\cos\theta)$ and if $\rho>\frac{3+\sqrt{5}}{2}$, then $(a_2-\cos\theta)>(a_1+\cos\theta)$. Clearing the denominators, and multiplying out everything, produces that the equivalent inequality

$$\begin{aligned} a_1a_{2n+1} &+ a_1\frac{\sin^2(2n+1)\frac{\theta}{2}}{4} \\ &-\frac{1}{2}(a_1-1)(a_1+1)\frac{\cos^2(2n+1)\frac{\theta}{2}}{\cos^2\frac{\theta}{2}} - \cos^2(2n+1)\frac{\theta}{2} > 0.\end{aligned} \tag{2.12}$$

By Lemma 2.2, the left- hand side of (2.12) is larger than

$$a_1 a_{2n+1} - 1 - \frac{1}{2}(a_1 - 1)(a_1 + 1)(2n + 1)^2, \tag{2.13}$$

and using $2(a_1(\rho) - 1)(a_1(\rho) + 1) = 2[a_1(\rho)]^2 - 2 = a_2(\rho) - 1$, then (2.13) is

$$(a_2 - 1)\left\{\frac{a_1 a_{2n+1} - 1}{a_2 - 1} - (n + \frac{1}{2})^2\right\} \tag{2.14}$$

which is positive, by Lemma 2.1.

3. Error Bound

Since the ellipse Λ_p has length,

$$l(\Lambda_p) = 4\varepsilon^{-1}E(\varepsilon), \quad \varepsilon = \frac{2}{\rho + \rho^{-1}}, \quad E(\varepsilon) = \int_0^{\pi/2} \sqrt{1 - \varepsilon^2 \sin^2\theta}\, d\theta.$$

According to theorem 2.3, we obtain the error bound in the final form from (1.9)

$$|R_n(f)| \leqslant \frac{2}{\pi}\varepsilon^{-1}E(\varepsilon)K_n(-\varepsilon^{-1}) \max_{z\in\Lambda_p} |f(z)|, \qquad \varepsilon = \frac{2}{\rho + \rho^{-1}}. \tag{3.1}$$

In section 4, we show that it is possible to optimize the bound on the right of (3.1) as a function of ρ.

4. Example

For the given

$$\int_{-1}^{1} \frac{\sin[w(t+1)]}{\sqrt{4+t}}\sqrt{\frac{1-t}{1+t}}\, dt, \qquad w > 0,$$

we consider $d\lambda$ as the Jacobi measure $d\lambda(t) = \sqrt{\frac{1-t}{1+t}}\, dt$, and $f(z) = \frac{\sin[w(z+1)]}{\sqrt{4+z}}$.

To bound f on the ellipse contour Λ_p, using

$$|\sin[w(z+1)]| \leqslant \frac{1}{2}\left(e^{-\frac{1}{2}w(\rho-\rho^{-1})\sin\theta} + e^{\frac{1}{2}w(\rho-\rho^{-1})\sin\theta}\right), \quad z \in \Lambda_p$$

and

$$|\sqrt{4+z}| \geqslant \sqrt{4-|z|}, \quad z \in \Lambda_p,$$

we obtain

$$|f(z)| \leqslant \frac{\cosh\left(\frac{1}{2}w(\rho-\rho^{-1})\right)}{\sqrt{4-\frac{1}{2}(\rho+\rho^{-1})}}, \quad z \in \Lambda_p.$$

Theorem 2.3 tell us that the maximum of $|K_n(z)|$ on Λ_p is attained on the negative real axis. i.e., $\theta = \pi$. So

$$\begin{aligned}\max_{z\in\Lambda_p} |K_n(z)| &= \frac{2\pi}{\rho^{n+\frac{1}{2}}} \frac{\left[\frac{1}{2}(\rho+\rho^{-1})+1\right]}{\left[\left(\frac{1}{2}(\rho^2+\rho^{-2})-1\right)\left(\frac{1}{2}(\rho^{2n+1}+\rho^{-(2n+1)})+1\right)\right]^{1/2}} \\ &= 2\pi\frac{\rho+1}{(\rho-1)(\rho^{2n+1}+1)}.\end{aligned}$$

From (3.1), we can get the error bound in the final form

$$(4.1) \qquad |R_n(f)| \leqslant \frac{2}{\pi}\varepsilon^{-1}E(\varepsilon)\frac{2\pi(\rho+1)}{(\rho-1)(\rho^{2n+1}+1)}\frac{\cosh\left(\frac{1}{2}w(\rho-\rho^{-1})\right)}{\sqrt{4-\frac{1}{2}(\rho+\rho^{-1})}},$$

where

$$\varepsilon = \frac{2}{\rho+\rho^{-1}}, \quad \frac{3+\sqrt{5}}{2} < \rho < 4+\sqrt{15}, \quad E(\varepsilon) = \int_0^{\pi/2}\sqrt{1-\varepsilon^2\sin^2\theta}\,d\theta.$$

We have optimized this bound as a function of ρ. Numbers in parentheses indicates decimal exponents below table 4.1. Several interesting features are worth noting. The optimal $\rho_{opt}(n)$, approaching $\rho = 4+\sqrt{15}$, when w is small. This is so, because of the "weak" nature of the singularity. Increasing w, on the other hand, we have the effect of reducing $\rho_{opt}(n)$.

Table 4.1.
Optimal error bound

w	n	$\rho_{opt}(n)$	bound	w	n	$\rho_{opt}(n)$	bound
1	5	7.316	3.263(-7)	10	10	3.762	2.332(-4)
	10	7.640	5.623(-16)		15	5.645	4.535(-11)
	15	7.726	7.777(-25)		20	7.055	3.893(-19)
	20	7.766	9.972(-34)		25	7.554	8.340(-28)
	25	7.789	1.230(-42)		30	7.691	1.240(-36)
	30	7.804	1.482(-51)		35	7.748	1.643(-45)
5	5	3.787	2.118(-2)	15	15	3.752	2.567(-6)
	10	6.761	1.089(-9)		20	5.072	9.405(-12)
	15	7.534	2.669(-18)		25	6.288	2.680(-20)
	20	7.688	4.015(-27)		30	7.194	1.311(-28)
	25	7.746	5.336(-36)		35	7.576	2.600(-37)
	30	7.777	6.713(-45)		40	7.695	3.827(-46)

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