ASYMPTOTIC GAUSS QUADRATURE ERRORS AS FOURIER COEFFICIENTS OF THE INTEGRAND [1]

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1. Introduction

The purpose of this paper is to derive asymptotic relations giving the error of a Gauss type quadrature, applied to analytic functions, in terms of certain coefficients in the orthogonal expansion of the integrand. The Fourier expansions of the integrand we consider here are those in terms of the Legendre and the Chebyshev polynomials. In Section 3 we obtain the error of the Gauss-Legendre quadrature expressed in terms of the Legendre-Fourier coefficients of the integrand. In Section 4 the errors of Gauss-Legendre, Lobatto and Radau quadrature formulas are obtained, for large n, expressed in terms of the Chebyshev-Fourier coefficients of the integrand. In deriving these estimates we have used complex variable methods restricting ourselves to the class of analytic integrands; this allows us to obtain simple contour integral representations for the errors of these quadratures for large values of n. However, the form of the estimates obtained indicate that these are applicable to a much wider class of functions.

Examples are given to illustrate the estimates obtained.

Let $P_n^{(\alpha,\beta)}(t)$, $n = 0, 1, 2, \cdots$, be the set of Jacobi polynomials which form an orthogonal system on $[-1, 1]$ with respect to the weight function $(1-t)^\alpha(1+t)^\beta$ $(\alpha > -1, \beta > -1)$ and which have been normalized so that $P_n^{(\alpha,\beta)}(1) = \binom{n+\alpha}{n}$. Let $S = \{0, 1\}$.

Here we are concerned with the error of the n-point Gauss-Legendre, $(n+1)$-point Radau and $(n+2)$-point Lobatto quadrature formulas over the interval $[-1, 1]$:

$$E_n(f) = \int_{-1}^{1} f(t)dt - \sum_{k=1}^{n+\alpha+\beta} \lambda_{n,k} f(t_{n,k}) \tag{1}$$

The abscissas $t_{n,k}$, $k = 1, \cdots, n+\alpha+\beta$ are the zeros of $p(t) = (t-1)^\alpha(t+1)^\beta$. $P_n^{(\alpha,\beta)}(t)$, $\alpha, \beta \in S$; and the corresponding weights are given by

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$$\lambda_{n,k} = (1/p'(t_{n,k}))^{-1} \int_{-1}^{1} (p(t)/(t-t_{n,k}))dt.$$

It is known that $\lambda_{n,k}$ are positive. For a detailed discussion of Gaussian quadrature formulas, see Krylov [1] Chapters 7 and 9.

2. Asymptotic formula for the error

Let $\mathscr{E}_\rho$ $(\rho > 1)$ designate the ellipse $z = \frac{1}{2}(\xi+\xi^{-1})$, $\xi = \rho e^{i\theta}$, $0 \leqq \theta \leqq 2\pi$, with foci at $z = \pm 1$ and semiaxes $a = \frac{1}{2}(\rho+\rho^{-1})$ and $b = \frac{1}{2}(\rho-\rho^{-1})$ so that $\rho = a+b$. Let $A[-1, 1]$ designate the class of functions analytic on the interval $[-1, 1]$. If $f \in A[-1, 1]$, then for some $\rho > 1$, f can be continued analytically so as to be regular in the closed ellipse $\mathscr{E}_\rho$. *We shall designate the class of such functions as* $A(\mathscr{E}_\rho)$.

Let $f \in A(\mathscr{E}_\rho)$, $\rho > 1$, then by combining the results of Theorem 1, p. 161 and Equation (12.2.2), p. 245 of Krylov [1], the error $E_n(f)$ can be obtained as a contour integral:

$$(2) \qquad E_n(f) = \frac{1}{2\pi i}\int_{\mathscr{E}_\rho} \frac{f(z)dz}{(z-1)^\alpha(z+1)^\beta P_n^{(\alpha,\beta)}(z)} \left(\int_{-1}^{1} \frac{(t-1)^\alpha(t+1)^\beta P_n^{(\alpha,\beta)}(t)dt}{z-t}\right)$$

Since

$$(3) \qquad \frac{1}{2}\int_{-1}^{1} \frac{(1-t)^\alpha(1+t)^\beta P_n^{(\alpha,\beta)}(t)dt}{z-t} = (z-1)^\alpha(z+1)^\beta Q_n^{(\alpha,\beta)}(z)$$

where $Q_n^{(\alpha,\beta)}(z)$ is the Jacobi function of the second kind, the error is given by

$$(4) \qquad E_n(f) = \frac{(-1)^\alpha}{\pi i}\int_{\mathscr{E}_\rho} \frac{Q_n^{(\alpha,\beta)}(z)}{P_n^{(\alpha,\beta)}(z)} f(z)dz, \qquad \alpha, \beta \in S$$

See also Davis [2, p. 361].

An asymptotic formula for $Q_n^{(\alpha,\beta)}(z)/P_n^{(\alpha,\beta)}(z)$ has been obtained by Barrett (see [3], Equation (1.6); or see Szegö [4], Equations (8.21.9) and (8.71.19)). For $z \in \mathscr{E}_\rho$ and for large n,

$$(5) \qquad \frac{Q_n^{(\alpha,\beta)}(z)}{P_n^{(\alpha,\beta)}(z)} \simeq \pi\xi^{-(2n+\alpha+\beta+1)}$$

valid in the z-plane with the interval $[-1, 1]$ removed. Combining (4) and (5) we have for large n,

$$(6) \quad E_n(f) \simeq (-1)^{1+\alpha}\frac{i}{2}\int_{C_\rho} f[\tfrac{1}{2}(\xi+\xi^{-1})](1-\xi^{-2})\xi^{-(2n+\alpha+\beta+1)}d\xi \qquad (C_\rho : |\xi| = \rho)$$

3. The Gauss-Legendre quadrature error

For $f \in A(\mathscr{E}_\rho)$, $\rho > 1$, let

$$f(t) = \sum_{n=0}^{\infty} a_n P_n(t) \tag{7}$$

be the Legendre-Fourier expansion of f where $P_n(t)$ is the Legendre polynomial of degree n over $[-1, 1]$ normalized so that

$$\int_{-1}^{1} (P_n(t))^2 dt = \frac{2}{2n+1}. \tag{8}$$

The series (7) converges absolutely and uniformly over $[-1, 1]$. For expansions in terms of orthogonal functions and for results on orthogonal polynomials see Davis [2] Chapters X, XII and Appendix, or see Szegö [4].

If $E_{G_n}(f)$ denotes the error of the n-point Gauss-Legendre quadrature over $[-1, 1]$, then by construction and definition of the rule, $E_{G_n}(f) = 0$ for every polynomial f of degree $\leqq 2n-1$. Moreover, $E_{G_n}(P_m) = 0$ for $m = 2n+1, 2n+3, \cdots$, due to the symmetry of the Legendre polynomials and the quadrature sums. Therefore, from (7) we obtain

$$E_{G_n}(f) = \sum_{m=0}^{\infty} a_{2n+2m} \sigma_{n, 2n+2m} \tag{9}$$

where we have put

$$\sigma_{n, 2n+2m} = E_{G_n}(P_{2n+2m}) \qquad \text{for } m = 0, 1, 2, \cdots. \tag{10}$$

We next evaluate $\sigma_{n, 2n+2m}$ for m fixed and n large. Now, on $\mathscr{E}_\rho$, the Legendre polynomial $P_n(z)$ can be represented [2, Lemma 12.4.1] by

$$P_n(z) = \sum_{k=0}^{n} c_k c_{n-k} \xi^{n-2k} \tag{11}$$

where

$$c_k = \frac{(2k)!}{2^{2k}(k!)^2}.$$

From (10), (6) (with $\alpha = 0$, $\beta = 0$) and (11) we have for large n,

$$\sigma_{n, 2n+2m} \simeq -\frac{i}{2} \sum_{j=0}^{2n+2m} c_j c_{2n+2m-j} \int_{C_\rho} (\xi^{2m-2j-1} - \xi^{2m-2j-3}) d\xi \tag{12}$$

Since

$$\int_{C_\rho} \xi^k d\xi = i\rho^{k+1} \int_0^{2\pi} e^{(k+1)i\theta} d\theta = \begin{cases} 2\pi i & \text{if } k = -1 \\ 0 & \text{if } k \neq -1 \end{cases} \tag{12'}$$

we obtain

$$\sigma_{n, 2n+2m} \simeq \pi(c_{2n+m} c_m - c_{2n+m+1} c_{m-1}) \tag{13}$$

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($c_{-1} = 0$) valid for large n and each fixed $m = 0, 1, 2, \cdots$. In particular

$$\sigma_{n,2n} \simeq \pi \frac{(4n)!}{2^{4n}((2n)!)^2} \tag{14}$$

and from Stirling's formula

$$\sigma_{n,2n} \simeq \sqrt{\frac{\pi}{2n}}. \tag{14'}$$

It should, however, be noted that $\sigma_{n,2n}$ can be obtained exactly:

$$\sigma_{n,2n} = \frac{2}{2n+1} \frac{(4n)!(n!)^4}{((2n)!)^4}. \tag{15}$$

This is most easily derived as follows: Let $P_n(t) = k_n \tilde{P}_n(t)$ where $\tilde{P}_n(t)$ has leading coefficient unity. Then (Krylov [1], Sec. 2.2),

$$\begin{aligned} E_{G_n}(P_{2n}) &= k_{2n} E_{G_n}(\tilde{P}_{2n}) = k_{2n} E_{G_n}(t^{2n}) = \frac{k_{2n}}{k_n^2} E_{G_n}((P_n)^2) \qquad (k_n > 0) \\ &= \frac{k_{2n}}{k_n^2} \int_{-1}^{1} (P_n(t))^2 dt. \end{aligned} \tag{16}$$

Since

$$k_n = \frac{(2n)!}{2^n (n!)^2}$$

(15) now follows from (8) and (16).

For (fixed) $m = 1, 2, \cdots$ and for large n, we have from (13),

$$\sigma_{n,2n+2m} \simeq -\pi \frac{2n+1}{m(2n+m+1)} \frac{(2m-2)!(4n+2m)!}{2^{4n+4m-1}((m-1)!(2n+m)!)^2} \tag{17}$$

and using Stirling's formula and the asymptotic formula $\Gamma(n+a)/\Gamma(n) \sim n^a$ as $n \to \infty$, we obtain

$$\sigma_{n,2n+2m} \simeq -\sqrt{\frac{\pi}{2n}} \frac{(2n+1)(2m-2)!}{2^{2m-1}(2n+m+1)(m-1)!m!}. \tag{18}$$

From (9), (14) and (18) we obtain the following theorem.

THEOREM 1. *For $f \in A(\mathscr{E}_\rho)$, $\rho > 1$, and for large n,*

$$E_{G_n}(f) \simeq \sqrt{\frac{\pi}{2n}} (a_{2n} - \tfrac{1}{2}a_{2n+2} - \tfrac{1}{8}a_{2n+4} - \cdots). \tag{19}$$

Thus, if n is sufficiently large and if the Legendre-Fourier coefficients a_n decrease rapidly, we may take as an estimate:

$$E_{G_n}(f) \simeq \sqrt{\frac{\pi}{2n}} a_{2n}. \tag{20}$$

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But if the coefficients decrease slowly, one or more terms of (19) will have to be taken to obtain a satisfactory estimate for $E_{G_n}(f)$.

REMARK. It should be noted that the coefficients $\sigma_{n,\,2n+2m}$ ($m = 0, 1, 2, \cdots$) in (9) depend only on the Gaussian rule of integration and are independent of the particular function being integrated, and these may be computed for various n once and for all. It should also be noted that Kronrod [5] gives a table of the errors $E_{G_n}(t^{2k})$, $k \geqq n$, for $2 \leqq n \leqq 40$ and various k. Knowing the coefficients of the $P_n(t)$, one could compute the $\sigma_{n,\,2k}$ from Kronrod's table.

Now, from (7) the coefficients a_n are given by

$$a_n = \frac{2n+1}{2}\int_{-1}^{1} f(t)P_n(t)dt. \tag{21}$$

If $f \in A(\mathscr{E}_\rho)$, $\rho > 1$, (21) can be expressed as a contour integral (see Elliott [7], Equation (42) with $\alpha = \beta = 0$):

$$a_n \simeq \frac{2n+1}{2\pi i}\sqrt{\frac{\pi}{2n}}\int_{\mathscr{E}_\rho} \frac{f(z)dz}{(z^2-1)^{\frac{1}{4}}(z\pm\sqrt{z^2-1})^{n+\frac{1}{2}}} \tag{22}$$

where the sign of the square-root is chosen so that $|z\pm\sqrt{z^2-1}| > 1$.

EXAMPLE. To illustrate (20) we consider the function $f(t) = \exp(t)$ for which the corresponding Legendre-Fourier coefficients decrease rapidly. The contour integral for $E_{G_n}(f)$ has been evaluated in [6]; the corresponding contour integral (22) for the coefficients can be evaluated in essentially the same way to obtain a_n's for this function. We find

$$E_{G_n} \simeq \frac{\sqrt{2\pi}(2n+1)\exp(\varphi)}{\sqrt{\varphi}(\varphi+\sqrt{\varphi^2-1})^{2n+1}}$$

where $\varphi = (1+(2n+1)^2)^{\frac{1}{2}}$, and

$$a_n \simeq \left(\frac{n(2n+1)}{2(n+1)}\right)^{\frac{1}{2}} \frac{\exp(\varphi^*)}{(\varphi^*+\sqrt{\varphi^{*2}-1})^{n+\frac{1}{2}}}$$

where $\varphi^* = (1+(n+1)^2)^{\frac{1}{2}}$. Thus for $\exp(t)$,

$$\lim_{n\to\infty} \frac{E_{G_n}}{\sqrt{\frac{\pi}{2n}}\,a_{2n}} = 1.$$

4. Asymptotic errors in terms of Chebyshev-Fourier coefficients of the integrand

Let $f \in A[-1, 1]$, and let

$$f(t) = \sum_{n=0}^{\infty}{}' a_n^* T_n(t) \tag{23}$$

be the Chebyshev-Fourier expansion of f, where the prime on the summation sign indicates that the first term is to be halved. Since $E_n(f) = 0$ whenever f is a polynomial of degree less than N ($N = 2n+\alpha+\beta$, α, $\beta \in S$), from (23) we have

$$E_n(f) = \sum_{k=0}^{\infty} a_{N+k} E_n(T_{N+k}). \tag{24}$$

Since on $\mathscr{E}_\rho$, $T_n(z) = \frac{1}{2}(\xi^n+\xi^{-n})$, from (6) we obtain for large n,

$$E_n(T_{N+k}) \simeq (-1)^{1+\alpha}\frac{i}{4}\int_{C_\rho}(\xi^{k-1}+\xi^{-2N-k-1}-\xi^{k-3}-\xi^{-2N-k-3})d\xi. \tag{25}$$

Evaluating the contour integral in (25) by means of (12′),

$$E_n(T_{N+k}) \simeq \begin{cases} (-1)^\alpha \dfrac{\pi}{2}, & k = 0 \\ -(-1)^\alpha \dfrac{\pi}{2}, & k = 2 \\ 0, & k \neq 0, 2. \end{cases} \tag{26}$$

Substituting (26) into (24) we obtain the error, for large n, expressed in terms of the Chebyshev coefficients of the integrand:

THEOREM 2. *Let $f \in A[-1, 1]$; $N = 2n+\alpha+\beta$, α, $\beta \in S$. Then for large n,*

$$E_n(f) \simeq (-1)^\alpha \frac{\pi}{2}(a_N^* - a_{N+2}^*). \tag{27}$$

We note the following special cases of (27). $\alpha = 0$, $\beta = 0$: Gauss-Legendre:

$$E_{G_n}(f) \simeq \frac{\pi}{2}(a_{2n}^* - a_{2n+2}^*) \tag{27a}$$

$\alpha = 1$, $\beta = 1$: Lobatto (fixed abscissas $t = \pm 1$):

$$E_{L_n}(f) \simeq -\frac{\pi}{2}(a_{2n+2}^* - a_{2n+4}^*) \tag{27b}$$

$\alpha = 0$, $\beta = 1$: Radau (fixed abscissa $t = -1$):

$$E_{R_n^-}(f) \simeq \frac{\pi}{2}(a_{2n+1}^* - a_{2n+3}^*) \tag{27c}$$

$\alpha = 1$, $\beta = 0$: Radau (fixed abscissa $t = +1$):

$$E_{R_n^+}(f) \simeq -\frac{\pi}{2}(a_{2n+1}^* - a_{2n+3}^*). \tag{27d}$$

The Chebyshev coefficients for f are given from (23) by

(28) $$a_n^* = \frac{2}{\pi}\int_{-1}^{1} \frac{f(t)T_n(t)dt}{(1-t^2)^{\frac{1}{2}}}$$

and if $f \in A(\mathscr{E}_\rho)$, $\rho > 1$, then (Elliott [7]) by

(29) $$a_n^* = \frac{1}{\pi i}\int_{\mathscr{E}_\rho} \frac{f(z)dz}{(z^2-1)^{\frac{1}{2}}(z+\sqrt{z^2-1})^n}.$$

Examples. To illustrate the estimate (27a) for the error of the Gauss-Legendre quadrature we consider two functions:

1. $f(t) = (2-t)^{\frac{1}{2}}$. For this function (see [6], Equation (17)),

$$E_{G_n} \simeq -\frac{(3)^{\frac{3}{4}}\sqrt{\pi}}{(2n)^{\frac{3}{2}}(2+\sqrt{3})^{2n+1}}$$

and (see [7], Equation (8)),

$$a_n^* \simeq -\frac{(3)^{\frac{1}{4}}}{\sqrt{\pi}n^{\frac{3}{2}}(2+\sqrt{3})^n}$$

so that

$$\frac{\pi}{2}(a_{2n}^*-a_{2n+2}^*) \simeq -\frac{\sqrt{\pi}(3)^{\frac{3}{4}}}{(2n)^{\frac{3}{2}}(2+\sqrt{3})^{2n+1}}.$$

2. $f(t) = (9t^2+1)^{-1}$. Evaluating the contour integral (29) for this function we obtain

$$a_{2n}^* = (-1)^n \frac{2 \cdot 3^{2n}}{\sqrt{10}(1+\sqrt{10})^{2n}}$$

so that

(30) $$\frac{\pi}{2}(a_{2n}^*-a_{2n+2}^*) = (-1)^n 2\pi \frac{3^{2n}}{(1+\sqrt{10})^{2n+1}}.$$

The values of the estimate (30) are compared with the *actual* error in the Table.

Table 1 [2]

n	Estimate (30)	Actual E_{G_n}
5	−5.718 (−2)	−5.787 (−2)
6	2.968 (−2)	2.891 (−2)
7	−1.542 (−2)	−1.537 (−2)
8	8.008 (−3)	7.904 (−3)
9	−4.160 (−3)	−4.134 (−3)
10	2.161 (−3)	2.143 (−3)
11	−1.123 (−3)	−1.116 (−3)
12	5.832 (−4)	5.794 (−4)
16	4.248 (−5)	4.227 (−5)

[2] Values in the parentheses indicate the power of 10 by which the tabulated values should be multiplied.

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