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Error estimates for Gaussian quadratures of analytic functions

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ABSTRACT

For analytic functions the remainder term of Gaussian quadrature formula and its Kronrod extension can be represented as a contour integral with a complex kernel. We study these kernels on elliptic contours with foci at the points ± 1 and the sum of semi-axes $\varrho > 1$ for the Chebyshev weight functions of the first, second and third kind, and derive representation of their difference. Using this representation and following Kronrod's method of obtaining a practical error estimate in numerical integration, we derive new error estimates for Gaussian quadratures.

1. Introduction

The Gaussian quadrature formula with respect to some positive weight function w on a finite interval which we normalize to be $[-1, 1]$ has the form

$$\int_{-1}^{1} w(t)f(t)\,dt = \sum_{i=1}^{n} \lambda_i f(\tau_i) + R_n^G(f), \tag{1.1}$$

where the nodes τ_i are the zeros of the corresponding orthogonal polynomial $\pi_n(t; w)$ and the weights λ_i are the so-called Christoffel numbers. Formula (1.1) has precise degree of exactness $2n-1$, i.e., $R_n^G(f) = 0$ for all $f \in \mathbb{P}_{2n-1}$.

Let Γ be a simple closed curve in the complex plane surrounding the interval $[-1, 1]$ and $\mathcal{D}$ its interior. If the integrand f is an analytic function in $\mathcal{D}$ and continuous on $\overline{\mathcal{D}}$, then, as is well known, the remainder term $R_n^G(f)$ admits the contour integral representation

$$R_n^G(f) = \frac{1}{2\pi i} \oint_{\Gamma} K_n^G(z; w) f(z)\,dz.$$

The kernel K_n^G can be expressed in the form

$$K_n^G(z) = K_n^G(z; w) = \frac{1}{\pi_n(z; w)} \int_{-1}^{1} \frac{\pi_n(t; w)}{z-t} w(t)\,dt. \tag{1.2}$$

The previous formulae hold for all interpolatory quadrature rules with mutually different nodes.

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Many authors have used them to estimate the error R_n^G in (1.1). In [1] Gautschi and Varga have used estimates of the form

$$|R_n^G(f)| \le C_1 \cdot \max_{z\in\Gamma} |f(z)|, \qquad C_1 = C_1(\Gamma, w) = \frac{l(\Gamma)}{2\pi} \max_{z\in\Gamma} |K_n^G(z; w)|, \tag{1.3}$$

where $l(\Gamma)$ denotes the length of the contour Γ. In [2] Hunter has used estimates of the form

$$|R_n^G(f)| \le C_2 \cdot \max_{z\in\Gamma} |f(z)|, \qquad C_2 = C_2(\Gamma, w) = \frac{1}{2\pi} \oint_\Gamma |K_n^G(z; w)||\mathrm{d}z|. \tag{1.4}$$

The error estimates (1.4) are sharper because of the inequality $C_2 \le C_1$, but it is hard to obtain their explicit expressions in most cases.

A very practical way to estimate the error in numerical integration is to use two quadrature rules: A and B, where the nodes used by rule B form a subset of those used by rule A. Also, rule A should have a higher degree of exactness than B. The difference $|R_m^A(f) - R_n^B(f)|$ $(m > n)$ is usually a rather good error estimate of rule B. If both rules admit the representation (1.2), then it follows that

$$\left|R_m^A(f) - R_n^B(f)\right| = \frac{1}{2\pi} \left| \oint_\Gamma \left(K_m^A(z) - K_n^B(z)\right) f(z)\, \mathrm{d}z \right|,$$

and further, following the same ideas which led to (1.3) and (1.4),

$$\left|R_m^A(f) - R_n^B(f)\right| \le M_i \cdot \max_{z\in\Gamma} |f(z)|, \quad i = 1, 2,$$

where

$$M_1 = M_1(\Gamma, w) = \frac{l(\Gamma)}{2\pi} \max_{z\in\Gamma} \left|K_m^A(z; w) - K_n^B(z; w)\right|$$

and

$$M_2 = M_2(\Gamma, w) = \frac{1}{2\pi} \oint_\Gamma |K_m^A(z; w) - K_n^B(z; w)||\mathrm{d}z|.$$

In this paper we analytically determine the values of M_1 and M_2 when rule B is the Gaussian quadrature formula with respect to one of the three Chebyshev weight functions. The case of Chebyshev weight function of the fourth kind is analogous to the case of Chebyshev weight function of the third kind.

The degree of exactness of the n-point Gauss formula cannot be improved by inserting fewer than $n + 1$ nodes (see [3]). This leads to Gauss–Kronrod quadrature formula

$$\int_{-1}^{1} w(t) f(t) \mathrm{d}t = \sum_{i=1}^{n} \sigma_i f(\tau_i) + \sum_{\nu=1}^{n+1} \sigma_\nu^* f(\tau_\nu^*) + R_{2n+1}^{GK}(f), \tag{1.5}$$

where the new nodes τ_ν^* and all new weights σ_i, σ_ν^* are chosen in such a way that formula (1.5) has maximum degree of exactness at least $3n + 1$. The τ_ν^* are the zeros of a polynomial $\hat{\pi}_{n+1}(t; w)$, called Stieltjes polynomial, which satisfies the orthogonality conditions

$$\int_{-1}^{1} \hat{\pi}_{n+1}(t)\, t^k\, \pi_n(t)\, w(t)\, \mathrm{d}t = 0, \quad k = 0, 1, \ldots, n.$$

The kernel K_{2n+1}^{GK} from the integral representation of the remainder term is given by

$$K_{2n+1}^{GK}(z) = \frac{1}{\pi_n(z)\, \hat{\pi}_{n+1}(z)} \int_{-1}^{1} \frac{\pi_n(t)\, \hat{\pi}_{n+1}(t)}{z - t}\, w(t)\, \mathrm{d}t.$$

Although positive and real Gauss–Kronrod quadrature formulae do not exist in some cases, there are no such problems with Chebyshev weight functions considered in this paper. Moreover, the new nodes τ_ν^* belong to $[-1, 1]$ and interlace with the Gaussian ones τ_i.

For contours Γ we take confocal ellipses

$$\mathcal{E}_\varrho = \left\{ z \in \mathbb{C} : z = \frac{1}{2}\left(u + u^{-1}\right), 0 \le \theta \le 2\pi \right\}, \quad u = \varrho \mathrm{e}^{\mathrm{i}\theta}, \varrho > 1, \tag{1.6}$$

having foci at ± 1 and the sum of semi-axes equal to ϱ. When $\varrho \to 1$, $\mathcal{E}_\varrho$ shrinks to the interval $[-1, 1]$, and, as we can conclude from other papers using this approach, the factors $C_1(\mathcal{E}_\varrho, w)$ and $C_2(\mathcal{E}_\varrho, w)$ usually go to $+\infty$. However, the bounds (1.3) and (1.4) are extremely sharp for large values of ϱ.

2. The weight function $w_1(t) = (1 - t^2)^{-1/2}$

It is well known that $\pi_n(t; w_1) = T_n(t)$ and $\hat{\pi}_{n+1}(t; w_1) = (1-t^2)U_{n-1}(t)$, where T_n and U_n are the nth degree Chebyshev polynomials of the first and second kind, respectively. We use the following representation of K_n^G derived in [1]

$$K_n^G(z; w_1) = \frac{4\pi}{u^n(u - u^{-1})(u^n + u^{-n})},$$

where u is given in (1.6). In the same way we can derive the representation of K_{2n+1}^{GK}

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

Now it is easy to show that

$$K_{2n+1}^{GK}(z) - K_n^G(z) = \frac{-4\pi}{(u - u^{-1})(u^{2n} - u^{-2n})}.$$

In the rest of this section we derive explicit expressions of the factors $M_1(\mathcal{E}_\varrho, w_1)$ and $M_2(\mathcal{E}_\varrho, w_1)$, and compare them with the factors $C_1(\mathcal{E}_\varrho, w_1)$ derived in [1],

$$C_1(\mathcal{E}_\varrho, w_1) = \frac{4(\varrho^2 + 1)}{(\varrho^2 - 1)(\varrho^{2n} + 1)} E\left(\frac{2}{\varrho + \varrho^{-1}}\right),$$

and $C_2(\mathcal{E}_\varrho, w_1)$ derived in [2],

$$C_2(\mathcal{E}_\varrho, w_1) = \frac{4}{(\varrho^{2n} + 1)} \mathcal{K}\left(\frac{2}{\varrho^n + \varrho^{-n}}\right),$$

where $\mathcal{K}$ is the complete elliptic integral of the first kind and E is the complete elliptic integral of the second kind.

Theorem 2.1.

$$M_1(\mathcal{E}_\varrho, w_1) = \frac{4(\varrho^2 + 1)}{(\varrho^2 - 1)(\varrho^{2n} - \varrho^{-2n})} E\left(\frac{2}{\varrho + \varrho^{-1}}\right).$$

Proof. Using equalities $|u^n \pm u^{-n}| = [2(a_{2n} \pm \cos 2n\theta)]^{1/2}$, where

$$a_j = a_j(\varrho) = \frac{1}{2}\left(\varrho^j + \varrho^{-j}\right), \quad j \in \mathbb{N},$$

we get an explicit representation of $|K_{2n+1}^{GK}(z; w_1) - K_n^G(z; w_1)|$ in the form

$$|K_{2n+1}^{GK}(z; w_1) - K_n^G(z; w_1)| = \pi \sqrt{\frac{2}{(a_2 - \cos 2\theta)(a_{2n}^2 - \cos^2 2n\theta)}},$$

which attains its maximum value when $\theta = 0$, i.e., at intersection points of the ellipse $\mathcal{E}_\varrho$ with the real axis. Recalling the well-known fact $l(\mathcal{E}_\varrho) = 2(\varrho + \varrho^{-1})E(2/(\varrho + \varrho^{-1}))$, we complete the proof. □

Theorem 2.2.

$$M_2(\mathcal{E}_\varrho, w_1) = \frac{4}{(\varrho^{2n} + \varrho^{-2n})} \mathcal{K}\left(\frac{2}{\varrho^{2n} + \varrho^{-2n}}\right).$$

Proof. According to (1.6), there hold $|\mathrm{d}z| = \sqrt{(a_2 - \cos 2\theta)/2}\,\mathrm{d}\theta$ and

$$\oint_{\mathcal{E}_\varrho} \left|K_{2n+1}^{GK}(z; w_1) - K_n^G(z; w_1)\right| |\mathrm{d}z| = \pi \int_0^{2\pi} (a_{2n}^2 - \cos^2 2n\theta)^{-1/2} \mathrm{d}\theta$$

$$= 4\pi \int_0^{\pi/2} (a_{2n}^2 - \cos^2\theta)^{-1/2} \mathrm{d}\theta = \frac{4\pi}{a_{2n}} \mathcal{K}\left(\frac{1}{a_{2n}}\right). \quad \square$$

The factors C_i and M_i have very similar explicit expressions, so it is easy to compare them analytically:

$$\frac{M_1(\mathcal{E}_\varrho, w_1)}{C_1(\mathcal{E}_\varrho, w_1)} = \frac{\varrho^{2n} + 1}{\varrho^{2n} - \varrho^{-2n}}, \qquad \frac{M_2(\mathcal{E}_\varrho, w_1)}{C_2(\mathcal{E}_\varrho, w_1)} = \frac{(\varrho^{2n} + 1)\, \mathcal{K}\left(2/(\varrho^{2n} + \varrho^{-2n})\right)}{(\varrho^{2n} + \varrho^{-2n})\, \mathcal{K}\left(2/(\varrho^n + \varrho^{-n})\right)}.$$

When ϱ is fixed and n increases, the complete elliptic integrals of the first and second kind rapidly approach their asymptotic value $\pi/2$. In this way, we get the following asymptotic estimate

$$M_2(\mathcal{E}_\varrho, w_1) = \frac{2\pi}{(\varrho^{2n} + \varrho^{-2n})}\left(1 + O(\varrho^{-4n})\right).$$

3. The weight function $w_2(t) = (1 - t^2)^{1/2}$

It is well known that $\pi_n(t; w_2) = U_n(t)$ and $\hat{\pi}_{n+1}(t; w_2) = T_{n+1}$. We use the following representation of K_n^G derived in [1]

$$K_n^G(z; w_2) = \frac{\pi(u - u^{-1})}{u^{n+1}(u^{n+1} - u^{-(n+1)})},$$

where u is defined in (1.6). In the same way we obtain the representation of K_{2n+1}^{GK}

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

Now it is easy to show that

$$K_{2n+1}^{GK}(z; w_2) - K_n^G(z; w_2) = \frac{-\pi(u - u^{-1})}{(u^{n+1} - u^{-(n+1)})(u^{n+1} + u^{-(n+1)})}.$$

Theorem 3.1.

$$M_1(\mathcal{E}_\varrho, w_2) = \frac{(\varrho + \varrho^{-1})^2}{(\varrho^{2n+2} - \varrho^{-(2n+2)})} E\left(\frac{2}{\varrho + \varrho^{-1}}\right).$$

Proof. Similarly as in the proof of Theorem 2.1, we get an explicit representation of $|K_{2n+1}^{GK}(z; w_2) - K_n^G(z; w_2)|$ in the form

$$|K_{2n+1}^{GK}(z; w_2) - K_n^G(z; w_2)| = \pi\sqrt{\frac{a_2 - \cos 2\theta}{2(a_{2n+2}^2 - \cos^2(2n+2)\theta)}}$$

which attains its maximum value when $\theta = \pi/2$. □

Theorem 3.2.

$$M_2(\mathcal{E}_\varrho, w_2) = \frac{\varrho^2 + \varrho^{-2}}{(\varrho^{2n+2} + \varrho^{-(2n+2)})} \mathcal{K}\left(\frac{2}{\varrho^{2n+2} + \varrho^{-(2n+2)}}\right).$$

Proof. Since $\int_0^\pi \cos 2\theta[1 - k^2\cos^2 m\theta]^{-1/2}\mathrm{d}\theta = 0$, for all integers $m \geq 2$ (see [2, p. 78]), there holds

$$\oint_{\mathcal{E}_\varrho} \left|K_{2n+1}^{GK}(z; w_2) - K_n^G(z; w_2)\right| |\mathrm{d}z| = \frac{\pi}{2}\int_0^{2\pi} \frac{a_2 - \cos 2\theta}{(a_{2n+2}^2 - \cos^2(2n+2)\theta)^{1/2}}\mathrm{d}\theta$$
$$= 2\pi\, a_2 \int_0^{\pi/2} (a_{2n+2}^2 - \cos^2\theta)^{-1/2}\mathrm{d}\theta = 2\pi\, \frac{a_2}{a_{2n+2}}\, \mathcal{K}\left(\frac{1}{a_{2n+2}}\right). \quad \square$$

We are able to compare analytically the factors C_i (from [1,4,2]) and M_i, and obtain

$$\frac{M_1(\mathcal{E}_\varrho, w_2)}{C_1(\mathcal{E}_\varrho, w_2)} = \frac{\varrho^{2n+2} + 1}{\varrho^{2n+2} - \varrho^{-(2n+2)}},$$
$$\frac{M_2(\mathcal{E}_\varrho, w_2)}{C_2(\mathcal{E}_\varrho, w_2)} = \frac{(\varrho^{2n+2} + 1)\,\mathcal{K}\left(2/(\varrho^{2n+2} + \varrho^{-(2n+2)})\right)}{(\varrho^{2n+2} + \varrho^{-(2n+2)})\,\mathcal{K}\left(2/(\varrho^{n+1} + \varrho^{-(n+1)})\right)}.$$

It should be pointed out that it is difficult to determine the factor $C_1(\mathcal{E}_\varrho, w_2)$ when n is even and ϱ is less than some ϱ_n (see [1,4]), because the maximum of $|K_n^G|$ on $\mathcal{E}_\varrho$ is attained slightly off the imaginary axis and depends on n.

When ϱ is fixed and n increases, $M_2(\mathcal{E}_\varrho, w_2)$ can be written in the form

$$M_2(\mathcal{E}_\varrho, w_2) = \frac{\pi(\varrho^2 + \varrho^{-2})}{2(\varrho^{2n+2} + \varrho^{-(2n+2)})}\left(1 + O(\varrho^{-4n-4})\right).$$

4. The weight function $w_3(t) = (1 - t)^{-1/2}(1 + t)^{1/2}$

It is well known that $\pi_n(t; w_3) = V_n(t)$ and $\hat{\pi}_{n+1}(t; w_3) = (1 - t)W_n(t)$, where V_n and W_n denote the nth degree Chebyshev polynomials of the third and fourth kind, respectively. We use the following representation of K_n^G derived in [1]

$$K_n^G(z; w_3) = \frac{2\pi(u + 1)}{u^n(u - 1)(u^{n+1} + u^{-n})},$$

where u is defined in (1.6). In the same way we derive the representation of K^{GK}_{2n+1}

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

Now it is easy to show that

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

Theorem 4.1.

$$M_1(\mathcal{E}_\varrho, w_3) = \frac{2(\varrho+1)(\varrho+\varrho^{-1})}{(\varrho-1)(\varrho^{2n+1}-\varrho^{-(2n+1)})} E\left(\frac{2}{\varrho+\varrho^{-1}}\right).$$

Proof. Similarly as in the proof of Theorem 2.1, we get an explicit representation of $|K^{GK}_{2n+1}(z; w_3) - K^{G}_{n}(z; w_3)|$ in the form

$$|K^{GK}_{2n+1}(z; w_3) - K^{G}_{n}(z; w_3)| = \pi\sqrt{\frac{a_1+\cos\theta}{(a_1-\cos\theta)(a^2_{2n+1}-\cos^2(2n+1)\theta)}}$$

which attains its maximum value when $\theta = 0$. □

Theorem 4.2.

$$M_2(\mathcal{E}_\varrho, w_3) = \frac{2(\varrho+\varrho^{-1})}{(\varrho^{2n+1}+\varrho^{-(2n+1)})} \mathcal{K}\left(\frac{2}{\varrho^{2n+1}+\varrho^{-(2n+1)}}\right).$$

Proof. Since $|\mathrm{d}z| = \sqrt{(a_1-\cos\theta)(a_1+\cos\theta)}\,\mathrm{d}\theta$ and $\int_0^\pi \cos\theta[1-k^2\cos^2 m\theta]^{-1/2}\mathrm{d}\theta = 0$, for all integers $m \geq 2$, there holds

$$\oint_{\mathcal{E}_\varrho} \left|K^{GK}_{2n+1}(z; w_3) - K^{G}_{n}(z; w_3)\right| |\mathrm{d}z| = \pi \int_0^{2\pi} \frac{a_1+\cos\theta}{(a^2_{2n+1}-\cos^2(2n+1)\theta)^{1/2}}\mathrm{d}\theta$$
$$= 4\pi\, a_1 \int_0^{\pi/2} (a^2_{2n+1}-\cos^2\theta)^{-1/2}\mathrm{d}\theta = 4\pi\, \frac{a_1}{a_{2n+1}}\, \mathcal{K}\left(\frac{1}{a_{2n+1}}\right). \quad \square$$

As in the two previous sections we obtain

$$\frac{M_1(\mathcal{E}_\varrho, w_3)}{C_1(\mathcal{E}_\varrho, w_3)} = \frac{\varrho^{2n+1}+1}{\varrho^{2n+1}-\varrho^{-(2n+1)}},$$
$$\frac{M_2(\mathcal{E}_\varrho, w_3)}{C_2(\mathcal{E}_\varrho, w_3)} = \frac{(\varrho^{2n+1}+1)\,\mathcal{K}\left(2/(\varrho^{2n+1}+\varrho^{-(2n+1)})\right)}{(\varrho^{2n+1}+\varrho^{-(2n+1)})\,\mathcal{K}\left(2/(\varrho^{n+1/2}+\varrho^{-(n+1/2)})\right)}.$$

When ϱ is fixed and n increases, $M_2(\mathcal{E}_\varrho, w_3)$ can be written in the form

$$M_2(\mathcal{E}_\varrho, w_3) = \frac{\pi(\varrho+\varrho^{-1})}{\varrho^{2n+1}+\varrho^{-(2n+1)}}\left(1+O(\varrho^{-4n-2})\right).$$

5. Examples

This section contains numerical examples illustrating the quality of the bounds

$$\left|R^{GK}_{2n+1}(f) - R^{G}_{n}(f)\right| \leq M_2(\mathcal{E}_\varrho, w_i)\cdot \max_{z\in\mathcal{E}_\varrho}|f(z)|, \quad i = 1, 2. \tag{5.1}$$

All computations were performed in machine precision of approximately 16 decimal digits, using MATLAB routines for the Gauss and Gauss–Kronrod quadrature rules from [5] to evaluate $|R^{GK}_{2n+1}(f) - R^{G}_{n}(f)|$ and the polynomial approximation to evaluate $\mathcal{K}$. We have optimized these bounds as functions of ϱ.

Example 5.1.

$$\int_{-1}^{1} \frac{\cos(at)}{\sqrt{1-t^2}}\,\mathrm{d}t.$$

The function $f(z) = \cos(az)$ is entire and it is easy to see that

$$|f(z)| \leq \cosh(a(\varrho-\varrho^{-1})/2), \quad z \in \mathcal{E}_\varrho.$$

Our numerical results are summarized in Table 5.1. Numbers in parentheses indicate decimal exponents.

Table 5.1
Optimal bounds (5.1) for Example 5.1.

a	n	ϱ_{opt}	$\lvert R^{GK}_{2n+1}(f) - R^{G}_{n}(f)\rvert$	Bound
1	4	15.9373	5.9202(−7)	2.1132(−6)
	5	19.9499	1.6529(−9)	6.5906(−9)
	7	27.9642	6.2172(−15)	2.0384(−14)
3	5	6.5131	8.1231(−5)	3.1780(−4)
	7	9.2249	1.8097(−8)	8.4441(−8)
	10	13.2579	4.9960(−15)	4.3179(−14)
8	5	2.0000	0.3818	1.2377
	10	4.7913	1.3073(−6)	7.0608(−6)
	15	7.3642	1.1213(−14)	1.9326(−13)
16	5	1.0560	1.2956	5.2747
	10	2.0000	0.1089	0.4876
	15	3.4611	3.4590(−6)	2.1978(−5)

Table 5.2
Optimal bounds (5.1) for Example 5.2.

a	n	ϱ_{opt}	$\lvert R^{GK}_{2n+1}(f) - R^{G}_{n}(f)\rvert$	Bound
1	4	16.0624	1.5560(−7)	1.1248(−6)
	5	20.0499	4.3080(−10)	3.4643(−9)
	7	28.0357	1.3323(−15)	1.0563(−14)
3	5	6.8147	2.9570(−5)	2.4936(−4)
	7	9.4396	5.9949(−9)	5.8235(−8)
	9	12.0829	4.0412(−13)	4.3881(−12)
8	5	2.8638	1.4544	1.6392(1)
	10	5.1939	1.4054(−6)	1.7540(−5)
	14	7.1404	1.4495(−12)	8.6994(−12)

Example 5.2.

$$\int_{-1}^{1} \mathrm{e}^{at}\sqrt{1-t^2}\,\mathrm{d}t.$$

The function $f(z) = \mathrm{e}^{az}$ is entire and $|f(z)|$ for $z \in \mathcal{E}_\varrho$ attains its maximum value when $z = (\varrho + \varrho^{-1})/2$. The corresponding numerical results are summarized in Table 5.2.

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